FROM IDEA TO MARKET

10TH INTERNATIONAL CONFERENCE : ADVANCED MATERIALS AND TECHNOLOGIES

BOOK OF ABSTRACTS

24–26 OCT, 2018
NINGHAI · CHINA

CONFERENCE INTRODUCTION

10-th International Conference **“ADVANCED MATERIALS AND TECHNOLOGIES: FROM IDEA TO MARKET”,** sponsored by National Academy of Sciences of Ukraine (NASU), Chinese Academy of Sciences (CAS), and NingboMunicipal Government, will be organized byFrantsevich Institute for Problems of Materials Science of National Academy of Sciences of Ukraine (IPMS NASU)and Ningbo Institute of Materials Technology and Engineering of Chinese Academy of Sciences (CNITECHCAS) and Ninghai County Government under the support of Ningbo Frantsevich Material Research Institute and Chinese Science and Technology Center of IPMS NASU.

Ningbo is a unique city that takes new materials industry as the first pillar industry. It has planned the largest new material science and technology campus in China, occupying an area of 55 square kilometers. The CNITECH of CAS is a leading research institute in transforming R&D achievements of new materials into industrial applications.

The idea of this conference is based on traditions of two previous big International Materials Science Forums: “Materials and coatings for extreme environments” and “International conference on hydrogen materials science and chemistry of carbon nanomaterials”, which were organized in Crimea (Ukraine) since 2000 and 1987 respectively.

This international conference will accelerate the international cooperation of China and Central and Eastern Europe in the fields of science and technology, materials science innovations, personnel training and transfer of scientific and technological achievements in the field of new advanced materials. One of the peculiarities of this conference is the organization of joint applied scientific sessions with the representatives of Chinese industrial sector with the possibility of discussions of the main points of technical requirements from industry and the way of their achievements from scientific community. Such joint cooperation is the base of innovative development in domestic and international scale.

THE MAIN CONFERENCE TOPICS (title of sessions):

A. Metal-based materials and composites.
B. Magnetic materials.
C. Ceramic-based materials and composites.
D. Polymer-based materials and composites.
E. Advanced technologies for recycling of industrial wastes.
F. Materials and technologies for extreme environments including coatings.
G. Biomaterials and biotechnologies.
H. Materials for hydrogen technologies and fuel cells.
I. Materials for energy applications
J. Nanomaterials and nanotechnologies.
K. Technical needs and requirements for new materials from industrial representatives of China.
L. Scientific, organization and information problems of cooperation between scientists in the field of materials science.

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ADDITIVE METALLURGICAL TECHNOLOGIES IN THE REPUBLIC OF BELARUS: POWDER PRODUCTION AND MANUFACTURE OF PARTS

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The first experience in the field of selective laser melting of spherical titanium powders in Belarus was obtained in 2001 in conjunction with the Powder Metallurgy Institute of the National Academy of Sciences of Belarus (Minsk) and the Institute of Technical Acoustics of the National Academy of Sciences of Belarus (Vitebsk). A feature of this technology was the defocusing of the laser beam and the movement of the platform with powder only along the Z axis. By 2005, the Powder Metallurgy Institute and the Institute of Physics of the National Academy of Sciences of Belarus produced a unit for selective laser sintering of metallic powders, which to a greater extent comes close to modern machines: the process takes place on a vertically moving technological platform with powder placed in a working chamber with a protective argon atmosphere; the optical system allows scanning with a laser beam in a horizontal plane along a specified path; monitoring of the sintering zone is carried out with a video camera; temperature control in the laser impingement point is carried out by means of a computer that also controls the operation of the unit in real-time mode. The Scientific Center for Special Powders and 3D Printing was founded at the Powder Metallurgy Institute in 2017. A plant of vacuum induction melting and atomization with inert gas JT-QWH-25KG was mounted and commissioned at the Institute to develop and study the processes of producing powders for 3D printing. The metallurgical 3D printer ProX DMP 300 was mounted and put into operation for the development of manufacturing technologies and production of parts for aerospace and special equipment. The Institute has research equipment for studying the processes of powder production by spraying and MASHS method: mixers, activator devices, attritors; planetary, jet and vibrating mills; SHS-reactors, pneumatic classifiers of various capacities for separation of powders of a narrow fraction. There are also a high-temperature vacuum furnace T-22X24-GG-2900-VM-G and hot isostatic pressing equipment AIP6-30 HOT AMERICAN ISOSTATIC PRESSES to study the post-processing processes of samples moulded by selective laser melting.

SYNTHESIS, PROPERTIES AND APPLICATION OF NANOSTRUCTURED FERROMAGNETIC MATERIALS

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This study is devoted to the synthesis, investigation of properties and analysis of the possibility to use of three types of materials based on: M-type barium hexaferrite, ferrites with the spinel structure and lanthanum-strontium manganites with the perovskite structure. Nanostructured ferromagnetic materials are the weakly agglomerated nanoparticles, films, multilayer and periodical structures as well as polycrystalline materials based on nanoparticles, which have unique properties.

Single-domain, weakly agglomerated nanoparticles of *Ba-hexaferrite* were synthesized via sol-gel method and by precipitation from solutions. It was studied the effect of fractal structure in the amorphous precipitate on the phase composition and physical-chemical properties of crystalline nanoparticles. It was established the conditions, at which amorphous nanoparticles forms the complex tree-level fractal structure that allow obtaining the weakly agglomerated, monodispersed crystalline nanoparticles.

Ferrites nanoparticles AFe_2O_4 (A = Mn, Fe, Co, Ni, Zn) and core/shell structures based on them were synthesized by different methods (precipitation in diethylene glycol solution and in microemulsions, criochemical method). Weakly agglomerated nanoparticles with average sizes 3 – 15 nm and superparamagnetic properties were obtained. It was shown the possibility to effect on the properties of nanoparticles by development of the core/shell structures based on them.

Weakly agglomerated crystalline nanoparticles of *lanthanum-strontium manganites* $La_{1-x}Sr_xMnO_3$ with narrow sizes distribution and an average diameter of 30 – 40 nm were synthesized via sol-gel method.

It was shown that *magnetic fluids* developed on the basis of magnetic nanoparticles with the spinel and perovskite structures heat up effectively under the action of an alternating magnetic field. It was established that obtained fluids are biocompatible and promising for their possible application in medicine as the inducers of magnetic hyperthermia treatment.

Based on the synthesized nanostructured ferrites it was developed the left-handed medias, resonant UHF elements as well as multilayer systems, in which properties of developed materials may be controlled by the action of electromagnetic field and which can find application in the modern connection systems.

SYNTHESIS, STRUCTURE, PROPERTIES ANDAPPLICATIONS OF CERAMIC 1-D MICRO-AND NANOSTRUCTURES

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The studies of synthesis and properties of nanowires and nanotubes of various materials, including ceramics, suggest their use in microelectronics, in optoelectronics, in medicine and in technology to create new composite materials with improved characteristics.

Due to the high values of thermal and chemical resistance, hardness, of such ceramics as carbides, nitrides, borides, etc. are particularly attractive nanowire of these materials. For example, the strength of the SiC nanofibers having diameter 17.6 nm, is equal to 32.9 GPa, and decreases to 10.8 nm in diameter, it increases to 57.0 GPa (J. Am. Chem. Soc. – 2002. – Vol. 124, No. 10. – P. 14464–14471).

During the last 10 years in the Frantsevich Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine (IPMS) the investigations on the study of synthesis processes, properties and the use of 1-d ceramic structures also are carried out.This presentation describes synthesis, structure, properties and applications of 1-d micro-and nanostructures BN, SiC, TiC, Si_3N_4 etc. Nanostructures of these materials were deposited by CVD method with the use such catalysts as Fe, Co, Ni, the nature of which affects both the kinetics of deposition and the morphology of the synthesis products. Researches on the use of nano fibers as reinforcing elements, as well as to create a fine water filters are carried out.

1-d ceramic structures have been used for the reaction of a new composite materials based on PTFE and dental plastics reinforced with SiC nanofibres. Such materials were developed for tribotechnical and medical application and have been patented in Ukraine.

STRUCTURE FORMATION AND PROPERTIES OF THE INTERMETALLICS OF THE TIAL SYSTEM OBTAINED DIRECTIONAL SOLIDIFICATION

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The report presents the results of investigation of the processes of structure formation and mechanical properties at directional solidification of β-stabilized intermetallic alloy Ti–44Al–5Nb–3Cr–1.5Zr (at.%).

It is shown that directional solidification at crucibleless induction zone melting produces a specific microstructure of alloy Ti–44Al–5Nb–3Cr–1.5Zr (at.%). The impact of high temperature gradient on controlling the structure, phase composition and physico-mechanical properties was studied. Solidification and post-solidification annealing of the alloy at such a gradient lead to ordering and orientation of the secondary phase microstructure of the material, and to improvement of its physico-mechanical properties. It was found that at meting rate of 150 mm/h the temperature gradient is equal to 300 $°C\cdot cm^{-1}$ that provides a uniform optimum structure of the ingot during melting. Regulation of the microstructure allows an essential improvement of the high-temperature mechanical properties, namely ultimate strength, Young’s modulus, and creep resistance.

Investigation results showed that the temperature limit of structural applicability of this type of alloys can be expanded from 750–800 °C up to 900–950 °C.

DESIGN OF Ti-ALLOY BY INTEGRATING HIGH THROUGHPUT EXPERIMENTS AND CALCULATIONS

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The speed for development of new materials is too slow has been emerging as the bottleneck for the innovation of the manufacturing technology. However, on the one hand, application of the computer and information technology to the materials science and engineering has made it possible for us to estimate the properties for single phases, model the microstructure evolutions, and predict the material properties. On the other hand, in order to verify the calculation results, we should develop and use the high throughput methods. In this talk, we introduce some new progress in materials calculation and high throughput experiments, especially the high throughput determination of the phase diagram, diffusion coefficients, and thermal-physical properties; and the high throughput verification of the response of the materials microstructure and properties to the compositions and heat treatment temperatures. Some preliminary results on the attempt of development of high strength and high toughness Ti alloy has been introduced.

EFFECT OF LIQUID MELT TREATMENT BY BRIQUETTED MODIFIERS ON STRUCTURE AND PROPERTIES OF ROLL-FOUNDRY STEEL

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The results of investigation for influence of melt processing by powder briquetted modifiers in the casting of steel for manufacturing of supporting rolls with ∅530 mm on the features of the structure and basic mechanical properties of the latter are presented. As the basic composition in the experiment, steel was used, containing: 1.5% C; 1.1% Cr; 0.50% Mo; 1.20% Ni; 0.9 % Mn; 0.4 % Si; 0.05 % P; 0.03% S; 0.06% Cu.

The treatment of the melt was carried out by the method of ladle modification with briquetted modifiers consolidated from a mixture consisting of rare-earth metals alloy with silicon, magnesium, copper and iron powders. The total amount of the modifier was 1.5 ÷ 2.0% with respect to the melt mass. The casting temperature of the melt was 1550 °C.

As a result of the structure studying of the modified alloy, it was shown that use of the proposed composition of the powder modifier in steel casting for the production of support rolls provided a noticeable reduction in the grain size of the dendritic structure of the steel compared to the same steel obtained by casting without the use of modification process. In particular, a decrease in the dimensions of the carbide eutectic is observed with an increase in the number of axes of the dendrites branches of the 1 st, 2 nd and 3 rd order.

The increase in the dispersion of the alloy steel structure provided the corresponding increase in the basic mechanical properties, in particular, the impact strength (up to 4.2÷4.65 J/cm^2) compared to the steel without the use of the briquetted powder modification (2.95÷3.0 J/cm^2)). In addition, the rolls obtained from the modified steel exhibited a more even hardness distribution (HSD 55÷56) over the length (up to 7000 mm) of the roll.

The mentioned effects are explained both by the influence of the modifying and microalloying action on the melt of the modifier as well as by its inoculating effect due to the infusion into the metallic melt of dispersed particles performing the functions of microchiller, which upon solidification of the metal become the additional centers of crystallization.

EFFECT OF HOT FORGING ON ELASTIC PROPERTIES OF TI-BASED METAL-MATRIX COMPOSITES

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The results of investigations of the structure and the elastic characteristics of the Ti-based metal-matrix composites, obtained by hot forging with use of various technological schemes are presented. It is shown that the material obtained by hot forging differ with appreciable anisotropy, which is characterized by the elongation of the particles of the matrix phase in the normal direction to forging force. Hereupon the resulting value of both normal elasticity modulus and shear modulus in the plane normal to the direction of the deforming force during hot forging, are of 12–15% higher than the corresponding characteristics in the direction of deformation. For all of the above manufacturing process the elastic characteristics of the investigated Ti-based metal-matrix composites exceeds by 40–70% (depending on the direction of sounding) the Young modulus of titanium, and the respective characteristics of the shear modulus are higher by 8–15%.

FABRICATION OF LOW COST AND HIGH PERFORMANCE TITANIUM AND TITANIUM ALLOY STRUCTURAL MEMBERS AND COMPONENTS BY THERMOMECHANICALPOWDER CONSOLIDATION

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Thermomechanical processing can be used in consolidating metallic and metal matrix composite powders to produce near-net shaped components and structural members. This route of powder metallurgy has the advantages of high relative density, fine and uniform microstructures, excellent mechanical properties and high production rate. The process entails fast heating powder compacts to an elevated temperature and holding at the temperature for a short time (in the order of 5-10minutes), and then subjecting the hot and partially sintered powder compacts to thermomechanical processing such as forging, extrusion or extrusion-forging to shape the powder compacts and complete the consolidation. The process relies on fast densification of the powder compacts and diffusion bonding between powder particles through applying pressure and plastically deforming the powder particles. We have applied this process to consolidate titanium, titanium alloy, titanium hydride and hydrogenated titanium alloy powders to produce near-net shaped components and structural members with excellent mechanical properties. This talk will present and discuss the major findings of our work in this area, and comment on the potential of commercializing this powder consolidation technology in titanium industry.

THE PROCESS OF MANUFACTURE OF BIMETALLIC TUBE ELEMENTS FROM DIFFERENT METALS BY DRAWING WITH THINNING

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Various metals and alloys with high relative strength indexes, as well as specific functional properties, such as aluminum and titanium alloys and steels, are widely used in the design of engineering products to ensure efficient operation. The connection of pipeline elements from different metals is efficiently performed using bimetallic tubular elements (BTE), for example Al + Ti systems; Al + steel and others. Such tubular joints are produced in metallurgical mass production, usually by rolling. In the experimental engineering industry, in a number of cases it is necessary to produce BTE with single specimens – 2–3 pieces.

The authors proposed a method for manufacturing bimetallic tubular elements in machine-building production by means of a joint drawing with thinning of dissimilar sheet metals and alloys. The drawing with a thinning is made in the heated state, which provides the conditions for obtaining the joining of the layers.

A mathematical model of the process of joint deformation of two dissimilar metals during stretching with thinning in a heated state is constructed. A correlation is established in the form of analytical dependences of the kinematics of the flow of layers, the degree of their deformation and the parameters of the stress-strain state on the boundary surface with the initial geometric parameters of the workpiece, the mechanical properties of the individual layers, and the geometry of the working surface of the matrix.

Based on numerical modeling in CAD / CAE ANSYS and DEFORM-3D, the main analytical results are confirmed with a cone angle of 4º ... 10º. It is shown that the maximum compressive stresses and shear deformations occur near the surface at the exit from the deformation center on the boundary surface of the composite workpiece, with the difference in the axial strain rates reaching zero, which facilitates the interaction of the layers. To increase the contact stresses and contact time of layers under load, it is suggested to use an additional angle of 1º ... 2º on the conical surface of the matrix.

The experimental study was performed for various combinations of alloys. Comparison of calculated results and experimental data showed that the maximum error in calculating the energy-strength parameters does not exceed 7 ... 10%. The deformation of the layer thickness after stretching with thinning does not exceed 10 ... 14% for different coefficients of mechanical heterogeneity of metals. Metallographic analysis showed that when deformation of wall thinning 40 ... 50% between the layers, metal bonds form which join the layers.

Technological recommendations on the implementation of the process of joint drawing of two dissimilar metals have been developed. An algorithm is proposed for calculating the technological parameters of the process of drawing a two-layer billet with thinning, which are necessary for the production of BTE. New promising technical solutions have been obtained that ensure the efficiency of joint extraction with thinning of dissimilar metals.

The technological process of manufacturing has been worked out and prototypes of BTE have been obtained.

NUMERICAL MODELING OF PROCESS OF MANUFACTURING OF BIMETALLIC TUBULAR ELEMENTS DRAWING OUT WITH THINNING OF DISSIMILAR METALS

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In mechanical engineering at the present stage, widely used laminated metal compositions of tubular form (bimetal tubular elements - BTE). BTE, as a rule, is used to connect pipelines from heterogeneous metals in responsible structures of aerospace engineering. The processes of plastic molding of two-layer materials are currently under investigation.

Traditional technologies for manufacturing bimetallic parts of cylindrical shape are aimed at large-scale production (metallurgical technologies) or they have a high complexity and specifics of implementation (technology using explosive energy). But at the same time, these technologies are not economically expedient to use for the production of single or small BTE series in machine-building industries.

Thus, the development of the theory of plastic molding of two-layer materials is of particular relevance in machine-building production.

In this paper, the authors performed a numerical simulation of the process of joint extraction with the thawing of two heterogeneous metals in the heated state in the specialized CAD / CAE ANSYS and DEFORM-2D software complexes. An analysis of the stress-strain state in CAD / CAE ANSYS showed that there is a rupture of normal stresses σ_y and equivalent stresses σ_{ekv}. On the boundary surface of the layers, while the radial stresses σ_x perpendicular to the boundary surface are continuous and have a negative sign. The maximum error when comparing numerical calculations with the theoretical for an ideal plastic material does not exceed 12.5%. It is also shown that taking friction forces into account reduces the error of the theoretical calculation with respect to numerical calculation to 8 ... 9%.

The calculations performed in the CAD / CAE DEFORM-2D system are in line with the main results obtained numerically in CAD / CAE ANSYS. The calculation error in these systems according to accepted models does not exceed 5% and allowed to perform a numerical calculation of the stress-strain state of the bimetallic billet depending on the geometrical parameters of the instrument. Therefore, taking into account the higher calculation speed, the system – CAD / CAE DEFORM-2D was chosen for further research.

It was found that on the boundary surface there are significant radial stresses, the distribution of which showed that their gradual increase is proportional to the change in the degree of compression. The maximum radial stress σ_x of the compression corresponds to the zone close to the exit from the matrix, with their magnitude increasing with a decrease in the angle α and a decrease in the coefficient of friction. The analysis of the distribution of axial velocities of deformations and the difference in axial velocity of displacement during pull-out with thinning showed that the increase of the angle of the cone of the matrix leads to a significant increase in the axial velocities of the deformations and the maximum values of the difference in axial velocity of movement in the deformation cell, which determines more elongation of the layer with a lower yield strength relative to to a layer with a higher yield strength, depending on the degree of compression. At the output of the matrix, the difference in axial velocity of displacement is zero. This kind of deformation facilitates the interaction of layers.

The analysis of the stress-strain state and the kinematics of the interaction of the layers has shown that in the deformation cell conditions are created which contribute to the diffusion bonding of the layers:

- maximum compressive stresses on the boundary surface of the layers, the magnitude of which is close to the boundary of the fluidity of the metal with a lower yielding boundary;
- the difference between the axial velocities of deformation and deformation of the layers, as well as the presence of shear deformations in the interaction of layers on the boundary surface, which ensure the destruction of the oxide films of materials and the formation of juvenile surfaces, which facilitates the interaction of layers;
- reduction of the difference of the displacement of layers to zero in the zone close to the exit from the matrix;
- the presence of heating of the layers to the activation temperatures of their interaction.

The use of an additional angle β for controlling power and kinematic parameters, as well as a stress-strain state of a two-layer billet in the case of pulling with thinning with different values of the coefficient of friction, is proposed. The analysis showed that the correction of the profile of the western part of the cone matrix enables to increase the range of contact stresses on the boundary surface of heterogeneous materials in the deformation cell while maintaining them in size and allows to increase the contact time under the load of the layers, which provides activation of the interaction of dissimilar metals on the boundary surface.

INVESTIGATIONON FORMABILITY ENHANCEMENT OF5A06 ALUMINIUM SHEET BY IMPACT HYDROFORMING

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High strain rate (HSR) forming has been found to be able to enhance the formability of sheet metals like electro-magnetic forming. Impact hydroforming (IHF) is proposed, in which the sheet is formed with high-pressure pulse combining hydroforming and HSR forming. An IHF bulge test setup was designed, 5A06 aluminium sheet was tested with strain rate of $2\times10^3 s^{-1}$ showing remarkable thickness strain improvement compared to quasi-static condition. A new IHF equipment is designed, the IHF process was verified effective with the equipment, aluminium aircraft sheet part with very small fillets was formed that cannot be formed with quasi-static hydroforming.

STUDY ON ADVANCED ZINC ALLOYS

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Study on advanced zinc alloys. Zinc based alloys have been widely used in industry for instead of cast iron, a part of copper-based alloys and aluminium-based alloys, for their excellent mechanical properties, low melting point, low mass density, and low cost. In this work, by adjusting the alloy elements, forming process and heat treatment process, the phase structure and the properties of Zn alloys were modified. Deformation were applied on zinc alloy for improve the ductile property by refining the grains. The influence of alloy elements on the mechanical properties, degradation behavior, biocompatible behavior were investigated.

NEW MHD-EQUIPMENT AND CONCOMITANT TECHNOLOGIES AT PRODUCTION OF ALUMINIUM ALLOYS AND CASTINGS FOR HI-TECH INDUSTRIES

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It was developed the original multifunctional electrotechnological casting MHD-equipment, namely magnetodynamic mixers-batchers. Application of physical actions in such equipment and new technologies for processing of liquid aluminium alloys provides: – to intensify the dissolution of components in melt and to achieve high homogeneity of chemical composition and temperature; – to promote the destruction of microinhomogeneities and reducing of sizes of clusters in melt; – at degassing of aluminium melts by argon blowing to decrease hydrogen content to 0.05 cm^3/100 g; – at synchronous multiple filtering of current-carrying melt through foam ceramic filters, it is possible to remove up to 80% of nonmetallics.

The realization of rational modes of thermal & forced melt processing have provided the effect of physical modifying of different types of aluminium alloys, in particular, hypoeutectic silumins (A356, AK7), hypereutectic silumin (A390), high-strength Al–Cu alloy similar to VAL10, and master alloy Al-5% Zr for production of Al-Cu alloys. So, there is allowed to transform of branched dendritic structure into compact one, substantial reducing of sizes of grains, and increasing of elongation of samples of the alloys from castings up to 3–5 times in comparison with the requirements of standards and parameters of traditional technologies.

The high quality of aluminium alloys prepared in the developed MHD-equipment by indicated technologies was confirmed by their subsequent thermomechanical treatment. In this case, the power inputs for deformation were reduced significantly, and the deformed metal takes superplasticity.

ULTRAFINE W-Cu PSEUDO ALLOYS: PRODUCTION, PROPERTIES, APPLICATION

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The unique complex of W-Cu pseudo alloys consisting from the metals which do not interact each other is ensured by extreme properties of W and Cu and also by the new properties of hetero phase structure of composite materials. Such hetero phase structure helps maintain the highly disperse state of the substance.

Highly disperse state of the powder mixture allows to produce high density materials by the most simple way: one time pressing and sintering.

Initial ultra fine W-Cu powder mixtures had been produced by three ways:

by mechanical mixing of initial powders of W with grain sizes of 0,05–0,3 μm and of Cu with grain sizes of 0, 5–3 μm

by the reduction of WO_3 and CuO oxide mixture in hydrogen atmosphere

by the reduction of $CuWO_4$

Unlike metal powders W and Cu, their oxides are similar in properties; they are brittle and are not prone to agglomeration during mixing-grinding. The degree of mixing of components in this case is higher. However, the maximum degree of mixing of W and Cu takes place in the chemical compound $CuWO_4$. The problem consists in the greatest possible preservation of the initial homogeneity of the distribution of the components during the transfer of the oxide charge to the metallic charge during the reduction process.

Using of highly dispersed metal powders W and Cu allowed to determine optimal mixing-grinding technological modes, which made it possible to obtain homogeneous mixtures that actively compacted during sintering. The optimal sintering regimes which make it possible to obtain a sufficiently dense (97-98%) material were determined.

Using of WO_3 and CuO powders allowed to produce ultrafine-grained pseudo alloys containing from 5 to 30% Cu with homogeneous structure. Optimum modes of mixing for oxide powders and optimal recovery regimes were determined, which make it possible to obtain homogeneous highly disperse powder mixtures of W and Cu. Such mixtures are characterized by high activity during sintering, which makes it possible to obtain a dense material at low temperatures. The highly disperse structure of such pseudo alloys ensures high hardness and erosion resistance of corresponding materials. Charges obtained by CuWO4 reduction are characterized by unique values of compacting rate during sintering. The pseudo alloys produced from such charges have more homogeneous structure and greater degree of dispersion.

The developed ultrafine-grained W-Cu pseudo alloys showed high efficiency when using as an electrode tool material for dimensional electro erosion processing, contact welding electrodes, temperature compensators-radiators for high-power semiconductor devices, electric contacts for city electric transport.

REVERSING THE STRENGTH-DUCTILITY TRADE OFF IN HIGH-PERFORMANCE METALLIC MATERIALS

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Although metallic materials have been utilized by human being for thousands of years, recent social and economic development require novelsuperior alloys for lightweight design strategies and advanced energy applications. However, most conventional metallurgical approaches for increasingstrength usually reduce ductility, an effect referred to as the strength-ductility trade-off.In this talk, our recent research efforts onreversing such tradeoff and developing noveladvanced metallic materials with much enhanced propertieswill be summarized:

1) A counterintuitive strategy for the design of ultra-high strength alloys by massive and highly dispersed second-phase nanoprecipitation with minimal lattice misfit will be presented. Fully coherent precipitates, showing very low lattice misfit with the matrix and high anti-phase boundary energy, effectively strengthen alloys without sacrificing ductility. The minimized elastic misfit strain around the particles does not contribute much to the dislocation interaction which is typically needed for strength increase. Instead the chemical ordering effect which creates backstress when precipitates are cut by dislocationswas exploited as the new strengthening mechanism. With this approach, a class of steelswith a strength up to 2.2 GPa and good ductility (~8.2 %) were created.
2) An anomalous interstitial strengthening effect of oxygen in a family of single-phase refractory high-entropy alloys (HEAs) at ambient temperature will be discussed. In contrast to conventional interstitial strengthening, strength and ductility are both substantially improved (tensile strength by 48.5±1.8 % and ductility by 95.2±8.1 %) when doping a model TiZrHfNb HEA with 2.0 at.% oxygen, breaking the paradigm of the strength-ductility trade-off with an inexpensive and ubiquitous element. Alloying with oxygen leads to the formation of ordered oxygen complexes (OOCs) which pin dislocations and subsequently promote their cross slip and multiplication. This novel strain hardening mechanism improves work-hardening capability and thus ductility.

HIGH ENTROPY SHAPE MEMORY ALLOYS - NOVEL FUNCTIONAL MATERIALS

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The development of conventional shape memory alloys almost came to a halt and the main market is still nitinol for medical applications. The reason why industrial leaders became disenchanted with shape memory alloys is related to functional degradation upon thermal cycling and structural fatigue phenomena. These effects appear due to plastic deformation and/or diffusion processes. To cope with these, the so-called high entropy approach was employed with some success on as-cast multicomponent TiZrHfCoNiCu alloys using binary TiNi as a prototype. Exceptional stability of the shape memory behavior has given some hope to renew industrial interest in shape memory alloy applications. Specifically, these novel high entropy shape memory alloys performed in a much wider temperature range than nitinol and even demonstrated a two-fold increase in yield strength and elastic modulus.

The present study is dedicated to the discussion of the key elements of high entropy shape memory alloys design including not just the common parameters like valence electron concentration, atomic size difference, enthalpy and entropy of mixing but also considers structural stability through the analysis of crystal and electronic structure, and interatomic interaction. The formation of different types of high entropy shape memory alloys will be analyzed, namely, multicomponent intermetallic compounds and solid solutions, and directions required for the successful development of high entropy shape memory alloys will be discussed.

NANO-PHASE STRENGTHENED MAGNESIUM ALLOYS AND GRAIN REFINING

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A series high strength magnesium alloys aredeveloped with the second nano-phase precipitation through multiple alloyingand uniqueaging treatment. The nano-phases precipitate parallel to the c-axis which effectivelypin dislocations during plastic deformation so as the strength of the magnesium alloys is greatly enhanced. Several casting alloy and wroughtmagnesium alloys with nano-phase precipitation strengthenare introduced as examples in the presentation.Furthermore, a process for solidification grain refinement with an external pulsed magnetic field is introduced. By this method, As-cast grains aresignificantly refined and the deformability of magnesium alloys is enhanced observably.

DEEP CRYOGENIC TREATMENT OF STEELS: PHYSICAL BACKGROUND AND OPTIMAL TECHNOLOGY

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Available experimental data on the effect of deep cryogenic treatment, DCT, on the mechanical and tribological properties of carbon steels and proposed hypotheses about the operating mechanisms are analyzed.

By means ofMössbauer spectroscopy, transmission electron microscopy, X-ray diffraction and mechanical spectroscopy, the low temperature isothermalmartensitic transformation and crystal structure of precipitated carbides are studiedon the example of tool steels.

It is shown that, in contrast to the conventional shallow cryogenic treatment, the main feature of DCT is the low temperature isothermal martensitic transformation below –100 °C causing plastic deformation. Theobtained virgin martensite formedis soft because the carbon diffusiondoes not occur at these temperaturesand dislocations are not blocked.The immobile carbon atoms are capturedand transferred by gliding dislocations creatingcarbon clouds around them. Depending on chemical composition of steels, the isothermal martensitic transformation takes place in temperature range between –100 °C and –196 °C, partly proceeds in the course of cooling down tofrom RT to –196 °C and does not occur during holding in liquid nitrogen.

Carbon atoms captured by dislocations do not take part in formation of the low temperatureε-carbide during subsequent tempering if DCT was performed in the temperature range of intensive isothermal martensitic transformation. A reason is the higher enthalpy of binding between carbon atoms and dislocations, ~0.8 eV, in comparison with the solution enthalpy of ε-carbide.

Moreover, the capture of carbon atoms by dislocations shift precipitation of carbides towards higher temperatures of tempering. No special carbides precipitate at 500 ºC in tool steels containing Cr and V, if DCT is performed at optimal temperatures of isothermal martensitic transformation, whereas atomic complexes of these elements with carbon are retained in the solid solution.

Such a special structural state reserves a significant potential for further strain- and temperature-induced precipitation during the usage of tools.

DESIGN AND FABRICATION OF DISCONTINUOUSLY REINFORCED TITANIUM MATRIX COMPOSITES

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In order to remarkably enhance the mechanical properties of titanium alloys, titanium matrix composites (TMCs) with special reinforcement distribution were designed and fabricated. The fabricated network structured TiBw/Ti composites exhibited a superior combination of mechanical properties, such as, the tensile strength and the tensile elongation can be controlled in the ranges of 1100-1500MPa and 3-13%, respectively. In addition, the high temperature tensile strength can be reached 980MPa and 780MPa at 600^{o}C and 700^{o}C, respectively. Recently, in order to further enhance their properties, (Ti_5Si_3+TiBw)/Ti6Al4V composites with two-scale network architecture were designed and successfully fabricated by reaction hot pressing. TiB whiskers (TiBw) were synthesized in situ around the Ti6Al4V matrix particles and formed the first-scale network structure. Ti_5Si_3 needles (Ti_5Si_3) were precipitated in the β phase around the exquiaxed α phase and formed the secondary-scale network structure. The results showed that the two-scale network structured composites exhibited more superior performances, such as, strength and ductility at room and high temperatures, high temperature oxidation resistance, high temperature creep resistance, and so on. The high compressive strength can be increased to 2300MPa after heat treatment. The tensile strength can be increased to 1050MPa and nearly 900MPa at 550^{o}C and 600^{o}C for Ti6Al4V matrix composites (Ti6Al4V alloys just service at 400^{o}C). In addition, the creep rate of the composites remarkably reduced by an order of magnitude compared with Ti6Al4V alloys. Moreover, the rupture time of the composites increased by 20 times, compared with Ti6Al4V alloys at 550 ^{o}C/300 MPa.

INCREASING PHYSICOMECHANICAL PROPERTIES OF SINTERED IRON-COPPER COMPOSITES BY ALLOYING WITH MOLYBDENUM

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The structure and physicomechanical properties of composites Fe-30%Cu (hereinafter FeCu) and Fe–(29.4-27)%Cu–(2–10)%Mo (hereinafter FeCuMo) after solid-phase and liquid-phase sintering have been studied. Powder mixtures of FeCuMo and FeCu were prepared by mechanical alloying during co-milling of commercial powders of the initial metals. The mean mixture particle size did not exceed 0.5 µm. Compressed samples from the mixtures with a porosity of 27 % were sintered at 1000 and 1130 °C in hydrogen. The relative density of FeCuMo samples after solid-state sintering was 98.8 %, and it was 99.3 % after liquid-state sintering.

It was established that alloying of FeCu composites with molybdenum simultaneously affects both strength and plasticity. With increasing molybdenum content in the composites, the solubility of iron in copper decreases, which increases their plasticity, whereas the formation of copper and molybdenum solid solutions in iron improves their strength characteristics.

In the Fe-Cu system, the solubility of iron in copper sharply decreases with reducing temperature. That is why FeCuMo composites were subjected to diffusion hardening (quenching and annealing) after sintering. The samples were quenched from 1000°C into water and annealing at 450 °C. After diffusion hardening, FeCuMo composites obtained by liquid-phase sintering exhibited an ultimate tensile strength of $\sigma_в$ = 741-752 MPa, extension elongation of δ = 8.2-9.4% and narrowing of ψ = 12.5-19.7 %. After solid-phase sintering and diffusion hardening, FeCuMo composites had the following characteristics: $\sigma_в$ = 683-694 MPa, δ = 12.1-12.4 %, and ψ = 24.0-25.9 %. Under the same conditions, FeCu composites after solid-phase sintering and diffusion hardening possessed higher strength along with very low plasticity: $\sigma_в$ = 832 MPa, δ = 2.5 %, and ψ = 2.5 %.

The FeCu and FeCuMo alloys are widely used in various industries as construction materials for parts subjected to shock loads, for example components of friction units, as well as for the manufacture of materials with high damping properties. They are also used in the manufacture of valve seats for internal combustion engines, gears, brackets, and parts of turbine rotors. In addition, FeCu alloys are applied as electrical contacts characterized by high plasticity, heat resistance, and workability.

THE STRUCTURE AND PROPERTIES OF POWDER COPPER HARDENED BY NANOSIZED TUNGSTEN PARTICLES

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Copper alloys hardened with fine oxide particles are known to show increased mechanical properties, but the oxide phase substantially decreases their conductivity. However, when copper is hardened by fine conducting tungsten particles, the conductivity of such pseudoalloys decreases to a smaller extent and depends on the refractory phase content only, since copper and tungsten are mutually insoluble. The contradictory requirements for simultaneously improving the mechanical properties of pseudoalloys and retaining their conductivity at the level of that of copper can be overcome through using Cu–W pseudoalloys with a small volume content of fine tungsten particles.

This work is devoted to examination of a possibility to improve mechanical properties of Cu–W pseudoalloys and to retain their high conductivity through directional microstructure formation by introducing small volumes of nanosized tungsten particles (2, 5, and 10 vol%) into a copper matrix. Bulk samples of hardened Cu–W pseudoalloys with a relative density of up to 99.1–99.6% were fabricated by shock compaction. Introduction of nanosized tungsten particles (30–40 nm) into Cu-W pseudoalloys increased their strength under tension and compression along with insignificant reduction in plasticity ($\delta = 13\%$ and $\psi=16\%$ for pseudoalloy containing 10 vol% W).

The obtained Cu–W pseudoalloys are characterized by high electrical conductivity ($\lambda\rho=0.875\%$ IACS) and increased hardness (to $2.7H_{Cu}$ for 10 vol% W).
The microstructures of the Cu–W pseudoalloys are analyzed.

SUPERIOR MECHANICAL PROPERTIES OF TITANIUM MATRIX COMPOSITES WITH NETWORK MICROSTRUCTURE

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In order to remarkably enhance the mechanical properties of titanium alloys, titanium matrix composites (TMCs) with special reinforcement distribution were designed and fabricated. Firstly, the TiBw/Ti composites with single network microstructure were achieved by powder metallurgy (PM) process including low energy ball milling and reactive hot-pressing sintering. The fabricated network structured TiBw/Ti composites exhibited superior mechanical properties, such as, the tensile strength and the tensile elongation can be controlled in the ranges of 1100-1500 MPa and 3-13%, respectively. Especially, the service temperature of TMCs can be increased to 600-800°C compared with that of titanium alloys. For example, the high temperature tensile strength can be reached 980 MPa and 780 MPa at 600°C and 700°C, respectively. Recently, (Ti_5Si_3+TiBw)/Ti composites with two-scale network microstructure were successfully fabricated by PM process. The two-scale network structured composites exhibited more superior performances. The tensile strength can be increased to 1050 MPa and nearly 900 MPa at 550°C and 600°C for Ti6Al4V matrix composites. Moreover, the rupture time of the composites increased by 20 times, compared with Ti6Al4V alloys at 550 °C/300 MPa.

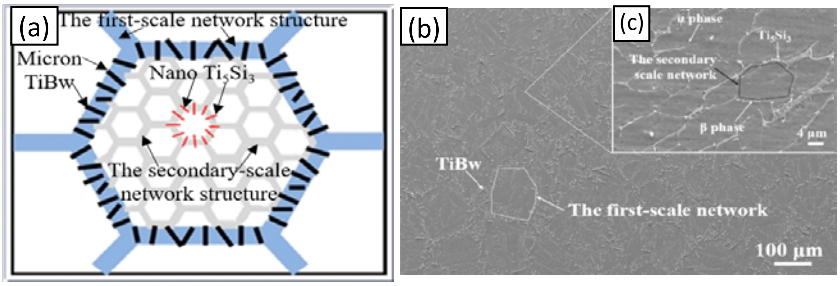

Fig. 1 Schematic illustration of (Ti_5Si_3+TiBw)/Ti6Al4V composites with two-scale network mictrostructure

IN SITU TI-SI-X COMPOSITES BASED ON INTERMETALLIC COMPOUNDS α_2Ti_3X (X–Al, Ga, Sn): STRUCTURE AND PROPERTIES

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The interest in natural (*in situ*) Ti–Si–X composites being obtained at eutectic solidification is associated primarily with their enhanced high-temperature properties. A number of strengthening mechanisms such as compositional (eutectic), dispersion, solid solution, and structural may be realized in alloys of Ti-Si-X systems where titanium is alloyed with p–(Si, Al, Ga, Sn) elements in a wide concentration range in accordance with their phase diagrams of ternary Ti–Si–Al, Ti–Si–Ga and Ti–Si–Sn systems to form eutectics between the Ti_5Si_3 silicide and βTi or intermetallic phase α_2-Ti_3X. As results, materials based on titanium intermetallics have advantages over alloys with metal matrix composites such as lower specific density, greater rigidity, higher operating temperature, higher high temperature strength and heat resistance etc.

The aim of this work was to study relationships between composition, structure and properties of three systems of eutectic Ti–Si–X alloys based on intermetallics of α_2Ti_3X (X–Al, Ga, Sn). Such intermetallic titanium *in situ* composites might attract a special attention due to their unique combinations of various properties, which might allow using them in new high technologies.

Even though intermetallic compounds Ti_3Al, Ti_3Ga, and Ti_3Sn have the same DO_{19} crystal structure, and practically the same parameter c/a ~0.80 of crystal lattice, their crystallization conditions and intervals of homogeneity existence are different significantly. Authors have showed that the features of their fine structure as matrixes of Ti-Si-X eutectic alloys like domain structure size, nature of antiphase boundaries, formation of twins are quite different too.

Mechanical properties of Ti–Si–(Al, Ga, Sn) eutectic alloys have been analyzed in the 20–800 ^{o}C temperature range. It was found that these alloys are as perspective basis for elaboration of high-temperature materials of new generation. At the same time, Ti-Si-Ga alloys, which have high elasticity modulus and Vickers hardness at RT, demonstrate lower long-term hot hardness in comparison with their Ti–Si–Al counterparts.

In situ composites of Ti-Si-Sn system containing 15–22-at. % Sn have exhibited unusual mechanical behavior where a decrease of elastic module by almost 1.5–2.3 times (for example, from 60 GPa to 26 GPa for alloy with 10-at. % Si) have taken place as result of plastic deformation of the Ti_3Sn intermetallic phase in the temperature range of thermoelastic martensitic transformation.

PHASE - STRUCTURE FORMATION AND FEATURES OF THE BEHAVIOR OF IRON – HIGH-CARBON FERROCHROMIUM - NICKEL BORIDE POWDER MATERIALS UNDER ABRASIVE WEAR CONDITIONS

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The influence of nickel borides additives on phase - structure formation, physical and mechanical properties and stability of iron - high - carbon ferrochrome powder to abrasive wear was studied. It is shown that nickel boride additives provide the formation of a multiphase, microheterogeneous structure of a matrix-filled type consisting of chromium steel and solid inclusions of complex chromium-iron carbides such as Me_7C_3 and $Me_{23}C_6$ and borides FeB, Fe_2B, which significantly increase the microhardness of solid phases from 8.4 to 11.5–11.8 GPa. Also, it has been studied that the increase in the content of a doping additive from 3.5 to 8.7 wt. % increases the density from 7.38 g / cm^3 to 7.5 g / cm^3 and a little bit decreases the hardness and bending strength from 75 to 74.2 HRA and from 1560 to 1340 MPa respectively. Also, alloying with Ni_3B increases the stability of the base material against abrasion wear from 5.0 to 12.2 km / mm.

The method of optical profilometry was used to study the topographical features of the morphology of worn surfaces, to estimate the depth and local development of wear on the sample surface through standardized roughness parameters calculated from 2D or 3D profiles. The roughness parameters (R_p, R_v, R_a) for each composition were found: R_p = 2.195 μm, R_v = 6.3 μm, R_a = 1.86 μm for the base material, and R_p = 1.4 μm, R_v = 0.64, R_a = 0.4 μm for materials of doped with Ni_3B 6.7 – 8.7 wt.%. It was determined that the perspective compositions, which combine acceptable physical and mechanical properties and improved resistance to abrasive wear on fixed particles of a diamond circle are materials based on the Fe - 35% FH800 system containing 6.7–8.7 wt.% of Ni_3B.

THE RELATIONSHIP OF HARDENING WITH THE ENERGY OF INTERACTION OF ATOMIC PLANES IN*HIGH-ENTROPY ALLOYS* (HEAS)

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A family of equiatomic binary, ternary and quaternary alloys based on Fe, Ni, Co, Cr, and Mn elements with fcc crystal structure was considered to study the physical properties of a new class of HEAs.

Using the pseudopotential method, the parameters of the crystal lattices, the distortions (relative, absolute, mean square, etc.) and elastic moduli were computed for both pure metals and alloys with 2-, 3-, 4-, and 5 -th elements with fcc structure on the basis of Co, Cr, Fe, Mn with the obligatory presence of Ni. In the course of the study, it was found that an increase in distortion does not necessarily lead to hardening.

The considered nickel-base alloys having fcc structure can be represented in hexagonal axes. Then, in calculating the physical characteristics, one can use not the total energy of the electron-ion system averaged over the volume of the unit cell, but a somewhat more local,the parameter of interaction energy of parallel close-packed atomic planes. For different nickel-based alloys, the interaction energies of close-packed atomic planes were calculated. It is found that the close-packed atomic planes in Ni are related to each other a little weaker than the atomic planes populated by other atoms besides Ni. The strongest connection between close-packed atomic planes is observed in the NiCoCr alloy, which has the maximum modulus of elasticity. As a result, it was found that the value of the elastic modulus is proportional to the strength of the coupling acting between close-packed atomic planes, i.e. in a HEA with anfcc structure, the hardening is primarily related to the energy of interaction of atomic planes.

INTENSIFICATION OF THE PROCESS OF DEEP DRAWING OF RECTANGULAR BOXES

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In the course of the study, done computer simulation of deep drawing of rectangular boxes from traditional blanks. Defects of finished products are established. To avoid this defects, created a new technology for calculation form's and dimensions for workpiece deep drawing of rectangular boxes.

A new installation was designed for modeling deep drawing of rectangular boxes. We can use this new installation for reverse drawing of rectangular boxes. Also the computer simulation of the process in the DEFORM 3D software was performed.

The resulting blanks were used for direct drawing. After comparing the results, a useful height of rectangular boxes of different shapes was obtained.

Computer simulation has shown that when using the proposed blanks, rectangular boxes are obtained of highest. Consequently, from the same area of blanks we obtain box-shaped products of optimal height. For rectangular box-shaped products of optimum height, perimeter cutting isn't required. The rectangular boxes obtained from the propose blanks, don't need pruning the excess metal. Thus, the waste of metal is reduced to zero.

Therefore, the topic of the study is relevant. This is one of the directions of intensification of the process of deep drawing of rectangular boxes. This study will improve the technology of manufacturing thin-walled hollow box-shaped parts in different shapes in accordance with modern requirements.

As the production practice shows, the initial form of blanks to reduce of the number of operations. Also the method we proposed influences to ensure quality products. In addition, it reduces the amount of metal to be cut.

In most cases, such forms can be found by trial and error. This method of searching is very expensive. It takes a long time. It also requires a lot of work and costs of metal. For its implementation it is necessary expensive equipment and instruments.

Therefore, one of the directions for improving the drawing of box-shaped sheet metal parts is the creation of scientific bases for determining the optimal shape of blanks. The implementation of the new method became possible with the use of computer modeling. For example, you can use the software package DEFORM 3D.

RECENT RESEARCH AND DEVELOPMENT OF NEW TYPE HIGH PERFORMANCE TITANIUM ALLOYS FOR AVIATION APPLICATION IN CHINA

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Titanium alloys have been widely used in aviation and aerospace industry, ordnance industry, marine industry and chemical industry, and so on. The output capacity of titanium sponge and mill products in China has ranked the first in the world. Compared with the developed countries, the aviation application level and amount of high performance titanium alloys in China still far lags behind that of developed countries. By synthetically strengthening and toughening processes, so there is a pressing need of developing new type titanium alloy series with low cost and better processing properties, such as a good match of super-high strength, anti-fatigue properties, and wear and shock resistance, etc. to enlarge the amount of application of titanium alloys in premium application areas, key load-bearing parts and extreme environments, continually uplifting the application level and catching up with and even surpassing the international advanced level. Besides, the technology maturity promotion approaches of new type and key titanium alloys is also given by means of the optimization of synthetical properties, the variety and complete specifications, the expansion of the application scales, the sophistication of standard and specifications, the sufficiency of testing and verification, etc. And it is also very necessary to establish an aviation-oriented titanium alloys system with Chinese characteristics, to meet the design requirements of high performance, low cost, and a raised amount of consumption and application level of titanium alloys

INFLUENCE OF CARBON CONCENTRATION ON STRUCTURE AND MECHANICAL PROPERTIES OF $CrFe_2MnNiV_{0.25}C_x$ HIGH ENTROPY ALLOYS

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Significant increase of strength characteristics of the CoCrFeMnNi high-entropy alloy by doping carbon was established earlier. A similar result was obtained for CrFeMnNiV alloy, which has no expensive cobalt and contains a strong carbide-forming element - vanadium. The goal of this work is to study the effect of carbon concentration increasing on the microstructure and mechanical properties of $CrFe_2MnNiV_{0.25}C_x$ (x = 0.175, 0.5, 1) alloys.

Alloys were melted in argon arc furnace; the purity of the initial metals was more than 99.9%. To ensure the composition and structure homogeneity ingots were melted 5 times with turning over after each remelting. As a result of the work, it was found that the microstructure of the $CrFe_2MnNiV_{0.25}C_{0.175}$ alloy consists of dendrites and dispersed interdendritic eutectic. The volume fraction of dendrites is around 40%. The dendrite body and the matrix of the eutectic have fcc lattice with parameter a = 3.619±0.002Å. The secondary phase in the interdendritic eutectic is Cr_7C_3-type carbide, in which part of the chromium is replaced by other elements. Annealing of samples at 1050°C for 24 hours did not lead to noticeable changes in the microstructure. The eutectic structural component part increases with increasing carbon concentration and primary carbide crystals appear. The hardness of the $CrFe_2MnNiV_{0.25}C_{0.175}$ alloy in annealed state is 2400 MPa, the yield point is 600 MPa. This alloy is ductile and does not collapse upon compression by more than 60%, has high ability to hardening under deformation. Further increasing of carbon concentration significantly increases hardness and yield strength (hardness of the $CrFe_2MnNiV_{0.25}C_{0.5}$ alloy is 3500MPa and $\sigma_{0.2}$ – 900 MPa). During compression tests of the $CrFe_2MnNiV_{0.25}C_{0.5}$ alloy it was not possible to go beyond the elastic zone - the yield strength of the alloy is more than 2000 MPa, the hardness is 5150 MPa.

The formation processes of the structural state of the studied alloys, hardening mechanisms and possible areas of their application are discussed.

NEW HIGH-STRENGTH CASTING ALUMINUM ALLOY POTENTIALLY DEFORMABLE

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Today aluminum alloys occupy second place for production amount after ferrous metals. Casting aluminum alloys occupy a very special place in all this diversity. The most common in modern industry are aluminum alloys that are based on the binary Al–Si system. Despite quite average level of mechanical properties of these alloys compared to alloys from other systems, more than 90 % of all shaped castings are made from them because of its high casting properties.

The main requirement for modern casting alloys is a combination of high mechanical and casting properties. One of the essential difficultly removable drawbacks of modern casting alloys concerns their chemical and phase composition. The matter is in that the increase in the number and amount of alloying elements is inevitably accompanied by a decrease in the melting temperature of alloys and expansion of the interval of their melting. As the result the technological properties are deteriorated. It is no longer possible to achieve considerable increase of traditional casting aluminum alloy characteristics only by modifying its composition and processing regimes. At present the resources of such classical approach are almost exhausted.

To develop new Al-based alloys our team has advanced own approach:

- usageof ternary and more complicated phase diagrams, containing quasi-binary eutectics of aluminum with intermetallic phases;
- alloying system of the eutectic alloys is developed taking into account the coordinates of eutectic transformation in multicomponent system;
- realization of dispersion strengthening by creation of nano-size particles, which differ from the chemical composition of the phases that form eutectic;
- these particles do not interact with eutectic colonies and are formed in solid solution matrix after thermal treatment.

Above mentioned principles were realized at creating unique casting&deformable high-strength aluminum alloys based on the eutectic (□□Al+Mg_2Si) of the ternary Al-Mg-Si system by the experimental laboratory procedure.

Next there are comparative data of mechanical properties before and after extrusion

<table>
<tr><th>UltimateStrength, MPa</th><th>YieldStrength, MPa</th><th>Elongation %</th></tr>
<tr><td colspan="3">Mechanical properties of alloys in short-term tests under tension after thermal treatment</td></tr>
<tr><td>460-575</td><td>360-520</td><td>3.0-1.00</td></tr>
<tr><td colspan="3">Alloys allow deformation by extrusion: mechanical properties after thermal treatment of rods with a diameter of 8 mm which were received by extrusion of ingots with a diameter of 25 mm</td></tr>
<tr><td>556-575</td><td>460-520</td><td>8.4-6.3</td></tr>
</table>

So, such unique characteristics of alloys have to in demand at industrial application.

QUANTITATIVE CHARACTERIZATION OF THE STRUCTURE OF METALLIC FILMS FROM THEIR ELECTRON-PHOTOGRAPHIC IMAGES

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The general idea that the structure of the material determines its properties is not in doubt. However, strictly defined quantitative value, characterizing such structures and adopted by materials science community, has not yet been introduced into the materials science. Good chances for such a rigorous mathematical definition are given by methods of fractal geometry, which began to develop intensively in the last years of the last century.

Therefore, in this paper we consider a model of multifractal formalism applied to two-dimensional images of material science. Based on the model, an algorithm for determining the multifractal characteristics of two-dimensional images obtained by electron microscopy is developed and implemented in the form of a computer program.

As model images were used the results of electron microscopy of chromium and titanium films deposited under different conditions. As a result of the processing of these photographs, multifractal characteristics of the structures of these films were obtained, both when considering grain boundaries as fractal structures and grains as a whole.

On the basis of the obtained data and data of studies of the mechanical characteristics of films, the correlation between the multifractal characteristics of the images and the mechanical characteristics of the films depicted on them was shown.

FORMATION OF HIGH-STRENGTH CONDITIONS IN TITANIUM ALLOYS USING SPECIAL RAPID HEAT TREATMENT

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Employment of titanium alloys in design of new aerospace structures requires more and more increased strengths well-balanced with others important mechanical and service properties. This complicated task can be solved using developed in the G.V. Kurdyumov Institute for Metal Physic special rapid heat treatment (RHT), which is based on continuous heating up to different temperatures in top part of $\alpha+\beta$ field or single-phase β-field without exposures at peak temperature, followed by controlled cooling and tailored regimes of final aging. Such a treatment ensures formation of a unique not achievable by conventional heat treatments microstructures that unite fine β-grains (providing high ductility) with high-disperse intragrain $\alpha+\beta$ mixture (forming high-strength). This technological approach, being tested on a wide range of alloys and responsible application products, on the one hand, presents special requirements to the quality of the initial microstructure of titanium alloys, and on the other hand, when optimizing all processing parameters, it ensures in the real products the strength at a level above 1500 MPa with plasticity not less than 8%. In the present paper a number of practical applications for a wide range of well-known alloys are described. Particular attention is paid to the feasibility of applying this technology to the new TC18 alloy that was carried out within the framework of research cooperation between Ukraine and China.

INVESTMENT CASTING AND POWDER METALLURGY FORMING OF TI AND NI ALLOYS

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Components made of titanium or nickel based alloys are frequently difficult or expensive to form through conventional wrought approach. Under such circumstances near net-shape processes such as precision casting and powder metallurgy forming are of particular interest. In this talk examples will be given of the manufacture of near net-shape components using two approaches. Efforts to tack problems such as coarse grain size in thick sections and avoiding prior particle boundaries will be highlighted. It will be shown that the mechanical properties of samples taken from the components prepared using optimized processing parameters meet the requirements of application.

FORMATION OF HIGH ENTROPY CARBIDES IN EQUIATOMIC ALLOYS OF THE SYSTEM OF Ti–Cr–Fe–Ni–Cu–C

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Recently, for the design of alloys with high physical and mechanical properties, the idea of a thermodynamic approach is used, the essence of which is to reduce the Gibbs free energy by creating a maximum entropy of mixing elements in the alloy. These alloys were called high entropy (HEAs) and are characterized by high strength, hardness and thermal stability. But the term " high entropy alloys" refers mainly to metal alloys, so in the literature there are few works relating to the synthesis of these alloys with the addition of non-metallic elements. The aim of this work is to study the processes of formation of carbides in situ formation of the microstructure during the synthesis of the alloy system Ti–Cr–Fe–Ni–Cu–C.

For carrying out synthesis did sample powders of the above system in equiatomic ratio, and 16.67 at.% each. The initial powder mixtures were mixed in a drum mixer for 2 hours by wet mixing. The resulting charge was pressed into cylindrical samples with a diameter of 20 mm and 40 mm at a pressure of 700 MPa. Alloys were produced by two methods of powder metallurgy – vacuum sintering and hot stamping with subsequent annealing. Sintering and annealing of samples was carried out in a vacuum furnace at a temperature of 1200 °C. The time of isothermal aging during sintering and annealing was 2 hours.

The result was obtained equiatomic alloy TiCrFeNiCuC. Local micro-x-ray spectral analysis showed the presence of two main phases in alloys – FCC and BCC and carbides of titanium and chromium. During sintering Cr and Ti, as the most active elements, interact with the carbon, forming carbides Cr_3C_2 and TiC, as evidenced by difractometric and spectral research. Iron carbide Fe_3C is not detected.

Analysis of the processes of structure formation of high entropy phases formed in alloys of TiCrFeNiCuC composition, inclusions of various compounds showed a significant increase in the defectiveness of crystal structures and, accordingly, an increase in the microhardness of both individual structural components and hardness of the alloy as a whole, using preliminary hot stamping of porous compounds. In the sintered alloy, the hardness is 30 HRC, in the alloy with the preliminary hot stamping, the hardness increased to 42 HRC.

Thus, preliminary hot stamping during the formation of a highly entropy alloy intensifies the processes of structure formation, causes redistribution of carbon, and also provides processes that lead to a significant distortion of the crystal lattice of the emerging phases, which contributes to the increase in the strength of alloys.

INFLUENCE OF WEAR-RESISTANT COATINGS ON DURABILITY OR SERVICE LIFE OF TITANIUM ALLOYS AT ALTERNATING LOADS

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Structures of modern aircrafts contain parts and units which simultaneously carry out two functions –they operate as a couple of friction and their working surfaces are exposed to wear, as well as they are used as load-bearing structural element and are exposedto external alternating loads and vibrations, i.e. they operatein fatigue conditions. These parts and units are the following: landing gear shock-absorbers, hydraulic cylinders, flap operating mechanisms, etc. As the resultthe wear-resistant coatings without which titanium alloys in friction units cannot be used, have to possess not only high wear-resistant properties, but should not reduce fatigue properties of structural material of the parts - titanium alloys.

In this work galvanic coatings, which are traditional for aircraft industry and new types of wear-resistance coatings (plasma, ion-plasma, diffusion, electric spark) were investigated, their tribotechnical properties and their influence on fatigue properties of titanium alloys were established. The optimum coatings combining high tribotechnical properties and resistance to alternating loads were determined. Technology approaches for creating the friction units which have the high resistance to alternating loads were established. Two kinds of coatings - diffusion (vacuum nitriding) and electric spark alloying with molybdenum in the combination of the subsequent diamond burnishing which provides high fatigue properties of a composite consisted oftitanium basis and anti friction coating were offered.

ELECTROCHEMICAL METHOD OF FATIGUE CRACK GROWTH ARREST IN STRUCTURAL STEELS: FROM IDEA TO TECHNOLOGY

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Novel method of fatigue crack growth arrest in structural steels based on artificial creation of crack closure effect is proposed. Special technological solution is used which, falling into a crack cavity, forms due the electrochemical interaction with metal solid products there. These products practically totally fill up a crack cavity and serve as a wedge which prevents crack closure during semi-cycle of unloading and, respectively, cyclic deformation in a crack tip. It was experimentally confirmed by a registration of the diagrams force F – crack displacement δ (see figure). They indicate a sharp increase of crack closure in a case when the crack treated with solution. It leads, in its turn, to a sharp decrease of effective range of stress intensity factor ΔK_{eff}, which causes crack retardation up to its arrest.

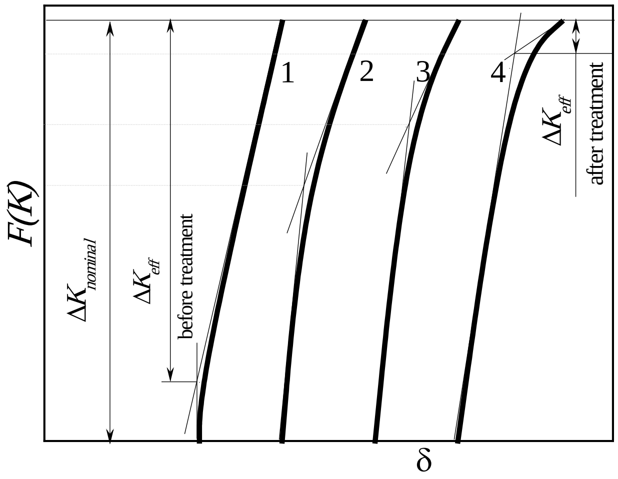

Figure. Diagrams F – δ for an evaluation of fatigue crack closure effect: step by step during cycling loading an increase of crack closure effect from curve 1 to curve 4

Fatigue crack growth curves are built for low alloyed steel without and with crack treatment which demonstrate crack arrest in a wide range of stress intensity factor (SIF) ΔK, from the threshold level up to almost fatigue fracture toughness K_{fc}. i.e. for the whole actual range of ΔK.

The peculiarity of artificial crack closure is accentuated: a decrease of effective ΔK is accompanied by an increase of a middle level of SIF therefore a risk of stress corrosion cracking and corrosion fatigue rises. This factor is especially important for long-term operated steels which lost their initial brittle fracture resistance.

This method can be extended also for an increase of fatigue strength of structural elements without preliminary formed fatigue crack growth since a stage of crack propagation exists in this case too.

The interaction of active components of the technological environment with a metal at the crack surface which provides formation of solid products in a crack cavity is analyzed. Some technological aspects for practical application of the proposed method are discussed.

The possibilities of a spread the proposed method for aluminum, titanium and copper alloys are considered.

Conclusions:

The electrochemical method of fatigue crack growth arrest in steels by artificial crack closure creation due a crack treatment by the special liquid solution, what leads to a filling of crack cavity by solid products of the active solution components with crack surfaces metal interaction.

The proposed method of fatigue crack arrest is effective in all actual range of stress intensity factor ΔK range.

Implementation of the proposed method for long term operated steels could lead to of practically constant static stresses in the crack tip during cyclic loading, which should be taken into account in a view of the hazard of stress corrosion cracking and hydrogen embrittlement.

DEFINITIONS OF MECHANICAL PROPERTIES OF STEELS UNDER CONDITIONS OF ACTION DIFFERENTIATED COUNTER PRESSURE

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Development designs of installations for testing specimens for tension with torsion under conditions of action of differential pressure of the liquid on the side of the surface of samples, and also using the finite element method in the DEFORM 3D software package, to determine by calculation, the possibility of constructing a plasticity diagram for low-plastic steels.

Design/methodology/approach. To carry out experimental studies, we proposed two designs of installations for the implementation of the tensile and tension with torsion tests under hydrostatic pressure conditions. A study was conducted to determine the plasticity diagrams by calculation using the FEM. Calculated data make it possible to determine the parameters of cold forming in the simulation of FEM without destroying the blanks from low-plastic steels. To construct the plasticity diagrams, a number of numerical experiments were performed inthe DEFORM-3D software complex

Findings. The work presents the installations which ensure the possibility of experimentally performing tests of specimens for tension test and tension with torsion alunder conditions of action of differentiated hydrostatic pressure on samples, the value of which also depends on the tensile force. The possibility of constructing plasticity diagrams by calculation, using the finite element method and the DEFORM 3D soft ware complex. Computer simulation has established the effect of the hydrostatic pressure on the increase in plasticity in these tests. Ananalys is of the stress-strain state during tensile test and tensile with torsion under hydrostatic pressure of different value. Using the values of the calculation results, plasticity diagrams were constructed for steels SHX-15 (analogue 100Cr6) and 12XH3A.

Originality/value. These results of the work make it possible to obtain a methodic for constructing plasticity diagrams for low-plasticity steels without carrying out experimental work.

FORMING OF THE STRUCTURE AND MECHANICAL PROPERTIES OF THIN-WALLED ELEMENTS BY ISOTHERMAL PRESSING WITH USING THIXOTROPIC PROPERTIES OF ALUMINUM ALLOYS AL-CU-MG AND AL-ZN-CU-MG

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The effect of heat-power action in the liquid state on the formation of a non-dendritic structure in cast billets of high-strength aluminum alloys Al–Cu–Mg and Al–Zn–Cu–Mg and their thixotropic properties during subsequent isothermal deformation by pressing s investigated.

General patterns of structure formation of castings from alloys of systems Al–Cu–Mg and Al–Zn–Cu–Mg are the same. Molded samples were obtained with additional rotor treatment of the melt and its subsequent high-speed cooling. This treatment leads to a decrease in the size of the crystals of the α-solid solution of sink morphology up to 50–100 μm, the volume fraction of which is also 96%, with a content of dendrites of 2.3%. Pre-heating of the workpiece from an aluminum alloy Al–Zn–Cu–Mg to temperature of 600 ^{o}Cwith followed by cooling in air leads to a change in its microstructure, morphology α-solid aluminum solution. Rosaceous crystals of the α-phase are transformed into substantially equilateral, globular, crystals of 100–400 μm in size, with a form factor of ~ 0.95. This structural changes in the workpiece contribute to the increase of the efficiency of the thixoforming process.

Cast billets was obtained using a rotary melt treatment in a bucket and pouredinto three-layerformsof aluminum foil with subsequent quenching in water.Prepared workpieceswere subjected to isothermal firmingfor the purpose of manufacturing a thin-walled element. The heating temperature of the billet was 550 ^{o}C, the temperature of the matrix was 500 ^{o}C.The microstructure of the resulting component with a thin-walled element is represented by grains of the α-solid solution, stretched in the direction of the metal flow during deformation. Their intermetallic phases are forming part of eutectic colonies having a width of 5–10 microns, a length up to 20 microns, as well as intermetallics in the free state. Most likely, this is the eutecticα-Al–$CuAl_2$–S(Al_2CuMg) of the intermetallic compounds S(Al_2CuMg) of complex structure, Mg_2Al_3, $CuAl_2$emited from a solid aluminum solution when the preform is heated prior to isothermal forming, as well as by stresses occurring during plastic deformation .

In the process of isothermal pressing, the metal flows quite well, filling the cavity of the mold, including the narrowest part of it with a size of up to 0.6 mm.

Thus, in the structure of cast samples of high-strength aluminum alloys of Al–Cu–Mg and Al–Zn–Cu–Mg systems obtained under thermal-force conditions, an α-solid solution of rosette morphology of various dispersity is formed. In the process of heating the billet before pressing, the rosette crystals transform into globular crystals. This positively affects its thixotropic properties in the process of deformation, in particular, for products made of aluminum alloys of Al–Cu–Mg systems.

EXPERIMENTAL INVESTIGATION OF ADHESIVE STRENGTH CHARACTERISTICS FOR TITANIUM-COMPOSITE JOINT

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The competitive aircraft industry imposes more severe improving of the efficiency and safety of the aircrafts which entails their operational characteristics enhancement, in order to capitalize the market. One of the most efficient methods of such improving is the decreasing the aircraft weight through considerable usage of composite materials in primary aircraft structures, as a fuselage and the wing structures. Therefore, one of the crucial tasks is the development of the titanium -composite adhesive joint for aviation production. In this study, the titanium - composite adhesive joint specimens were tested to determine their strength properties for the possible usage in the aircraft structures. Two batches of specimens were produced without preliminary processing of the adhesive - bonded surfaces (batch No 1) and with the preliminary processing (batch No 2). The analysis of the data obtained from the experimental investigations of the adhesive strength of the titanium - composite adhesive joints shows that the mean value of the maximum stresses for the specimens of batch No 2 is 6.712 MPa, while for batch No 1 – 5.037 MPa, and the distribution of the adhesive mixture over the adhered surfaces has a nonuniform character. Also, for the specimens of batch No 1, after fracture, the large portion of the adhesive mixture remained on the titanium plates, while for batch No 2, which have higher strength characteristics, the adhesive mixture with some portion of the composite material was transferred to the titanium plate. Thus, the preliminary processing of the surfaces of the adhered plates leads to the enhancement of adhesion and increase of the maximum stress level to fracture by 30%.

TITANIUM HYDRIDE POWDER METALLURGY AND ITS APPLICATION FOR MEDICAL TYPE ALLOYS

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Hydrogen is unique alloying element which can be temporary entered in the metals and alloys to controllably affect their phase composition, physical and mechanical characteristics. Hydrogen is also used in powder metallurgy techniques to activate powder sintering and to reduce impurity content in the materials. Earlier, blended elemental powder metallurgy (BEPM) approach using hydrogenated titanium (or titanium hydride) powders instead of conventional metal powders was used to produce titanium alloys with improved characteristics. Upon vacuum heating of powder compacts, atomic hydrogen emits from titanium crystal lattice to safe final concentrations, at the same time ensures powder refinement from impurities (O, Cl, C), increases sintered density and, hence, improves mechanical properties of final alloys. Ti–6Al–4V, high-strength Ti–5Al–5V–5Mo–3Cr, Ti–10V–2Fe–3Al and some other compositions were successfully produced, which mechanical properties met standard requirements for corresponding alloys. In present study, this approach was applied to produce low-modulus biocompatible Ti-Zr-Nb and Ti–Zr–Nb–Ta–Si alloys for medical application. Titanium hydride, as well as zirconium hydride and master alloy powders were used as starting materials in BEPM press-and-sinter processing.

The influence of various starting powders on sintering behaviour and final microstructure of alloys was shown. Similarities and differences between TiH_2 and ZrH_2 hydride powders and peculiarities of hydrogen emission from titanium and zirconium crystal lattices were established. The influence of post-sintering hot deformation on microstructure and mechanical properties was also studied. Optimization of processing parameters resulted in desired microstructure, chemical uniformity and mechanical properties of alloys sufficient for practice application.

DETERMINATION OF ATOMIC DIFFUSION COEFFICIENT AND DEPENDENTDENSIFICATION MECHANISM DURING SPARK PLASMA SINTERING

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Powder sintering is a technique of consolidating powder particles together into a coherent bulk solid structure by the reduction of interface energy. In general, powder shrinkage and densification mechanism are affected by various physical parameters, such as average particle size (L), surface energy (γ), and viscosity (η), especially during the early stage of powder shrinkage, which is typically characterized byneck formation between powder particles. As for powder sintering during spark plasma sintering (SPS), it is particularly interesting of the corresponding powder shrinkage and densification mechanism in view of its specificphysicochemical mechanism:sparkgenerationandsputteringeffects between powder particles. Specifically, for a given alloy composition, powder particles with varied L would likely have varied grain morphology, varied γ and η. Spontaneously, this would affect powder shrinkage and thus underlying densification mechanism during SPS. Analytically, densification mechanism during SPS can be embodied by specific physical quantities determined by the aforementionedphysical parameters. Inessence, powder shrinkage and densification behavior during SPS are associated to reducing total interface area and forming coherent metallurgical bondingbetween powder particles induced by atomic and mass transfer. Unfortunately, as a direct physical quantity that can represent the ability of mass transfer governing densification mechanism of powder particles, a densification-related atomic diffusioncoefficient (D) during SPS has heretofore never been attempted analytically and derived quantitatively.

In light of the above questions, based on Stokes-Einstein, Arrhenius equation and Frenkel model, the objective of this study is to establish a framework that can be used to derive the value of a coefficient$D$, which can clarify the underlying densification mechanism during SPS of $Ti_{40.6}Zr_{9.4}Cu_{37.5}Ni_{9.4}Sn_{3.1}$ metallic glass powders. Interestingly, as will be discussedbelow,thevalueof the as-derived$D$ for the atomized metallic glass powder is alwayslower than that of the milledcounterpart.Our work substantiatesthe viewpointthat the coefficient$D$ can represent the ability of mass transfer governing densification mechanism of powder particles during powder sintering.

DEVELOPMENT OF FENICRBSIC-MEB$_2$ COMPOSITE MATERIALS FOR WEAR-RESISTANT COATINGS

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Self-fluxing alloys are widely used in a variety of industrial fields as protective coatings for machine parts, whose surfaces are subjected to severe tribological conditions. The performance of FeNiCrBSiC plasma sprayed coatings can be substantially improved by reinforcement with hard borides such as CrB_2, TiB_2, ZrB_2. The goal of this study is to develop the composite powder materials of the FeNiCrBSiC-MeB_2 system for the plasma-spraying wear-resistant coatings.

The wetting behaviour and the interfacial reactions between refractory borides and self-fluxing alloys were investigated. The FeNiCrBSiC-TiB_2 system was found to be attractive candidate for the development of wear-resistant composite materials for coatings deposition due to the good wetting and formation of additional hard boride phases.

The FeNiCrSiB-based composite powder with 20 wt.% TiB_2 particles content was produced. The initial powders of FeNiCrSiB and TiB_2 were mixed and than sintered in vacuum at 1200 ^oC for 30 min. It has been found that sintering process induces chemical reactions between components of FeNiCrSiB-20wt.%TiB_2 system that leads to the active formation of complex boride phases. The sintered composite material of FeNiCrSiB-TiB_2 system was crushed and classified into a powder of size range 60−100 μm. The composite powder was deposited on steel substrates by plasma spraying. The FeNiCrSiB-TiB_2 coating has heterogeneous structure, that comprises metallic matrix and grains of reinforcing phases.

The sliding ball-on-disk friction and wear tests were performed using CETR UMT Multi-Specimen Test System. In this study Al_2O_3 ball was used as countrebody that slides against the coated flat disc. It was determined that the FeNiCrSiB-TiB_2 coating demonstrates in 2–3 times lower wear rate as compared to the NiCrSiB coating. Besides, the wear rate value of the developed FeNiCrBSiC-TiB_2 coating decrease with the increasing temperature from the 20 to 400 ^oC.

THE EFFECT OF CARBIDE BORON AMOUNT ON STRUCTURE AND PROPERTIES FORMATION OF A MULTI-COMPONENT TITANIUM-MATRIX COMPOSITE

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In recent years use multi-component alloying for expanding the application of titanium alloys, improve their heat resistance and durability while maintaining sufficient ductility, which provide a fundamentally new material with a wide range of properties. Introduction small additives of modifiers (B, Fe, Si, Mn, Mo, C) replaces the main parameters of the crystallization process in the melt, which leads to a changes in the structure and properties of titanium.

The purpose of this work is to study the effect of boron carbide amount on structure and phase formation after reaction synthesis of a multi-component titanium matrix composite which contain iron, silicon, manganese and boron carbide.

Commercial titanium hydride (TiH_2), ferromanganese silicon (FMS) and boron carbide powders were used as starting materials. Synthesis and condensation powders were conducted in accordance with the following procedure. The starting powders were mixed, in a planetary mill within 12 minutes. Formation of the compacts was carried out in a steel collapsible mold under the pressure of 800 MPa. The reaction synthesis was performed in vacuum furnace in two successive stages: heating to 600 °C within 30 min and further heating to 1250 °C within1 h.

During the work it was shown that in the process of the thermal synthesis actively interacts with the FMS. This process is accompanied by the dissociation of the FMS and the formation of a compound multiphase system whose main phases are TiC, TiB, Ti_5Si_3, Mn_5Ti and a certain amount of the ternary Ti_3SiC_2 phase.

It was established that the main phase of the alloy with a content of 2% boron carbide was a hexagonal titanium silicide Ti_5Si_3. Increasing the amount of boron carbide to 4% leads to the increase of independent lines of orthorhombic titanium monoboride and changes in stoichiometry of cubic titanium.

Further increase of B_4C leads to a change in the phase pattern, in which the TiB becomes the leading phase, together with the TiC. Addition to the initial charge of 4%–5% B_4C leads to the appearance on the X-ray patterns of the ternary carbosilicide phase, as a result of the introduction of carbon into the intermetallic system: Ti-Si.

It was shown that titanium reacts with boron carbide to form titanium monoboride and boron carbide.

THE NEW TOOL STEEL FOR WARM DIE FORGING OF Al AND Cu ALLOYS

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The results of work on the die steel development with adjustable austenitic transformation which have an increase in the values of physical and mechanical properties are compared with the grades of steels H-10 and H-13. The urgency of the work is that the developed steel can be applied in the field of mechanical engineering for hot die forging of copper-nickel alloy of grades C70400 and C71500 with the increased exploitation life in compare with steel H-10. The work is carried out in complex temperature-force conditions in the operating temperature range of 860–960 ºC. In addition, developed die steel can be used for warm deformation of copper at operating temperatures of 550–620 ºC with an increased operating life, compared with steel H-13. The investigation of the phase-structural state of steel, depending on the optimal thermal treatment regimes, is presented. Optimized thermal treatment (annealing) of steel with partial recrystallization, made it possible to mechanically handle ingots for making matrixes of a die tool. A special role in improving the service properties of a stamping steel tool with adjustable austenitic transformation has the effect of doping components (nitrogen, vanadium) on the Cr–Mo–Ni system. The increase of the tempering temperature by 60–70 ºC, taking into account the lack of the recrystallization process, allows dissolving a considerable number of carbide phases M_7C_3 and $M_{23}C_6$ in homogeneous austenite. The given phases actively influence on the steel hardening during the process of release. Thus, during the quenching of steel, conditions were created for the dissolution of the carbide phases, where overpressure of the alloying components of the martensitic structure occurred. This made it possible to obtain other carbide phases that less coagulate and stabilize the steel during the release process. The obtaining of the carbonyl phases of the test steel played a key role in the working zone of the matrix of the stamping tool, which provides high wear resistance in the initial period of operation at a temperature of 860 ºC and, under the force of effort, there is an additional deformation strengthening of the thin surface working layer, which leads to an increase in thermal stability.

THE FEATURES OF DESIGN AND IMPLEMENTATION PROCESSES OF PLASTIC FORMING PRODUCTS OF EUTECTIC COMPOSITE MATERIALS OF THE SYSTEM, $Ti–TiB_2$

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An effective way to increase the strength of structures engineering is the use of high strength structurally inhomogeneous evtektika-hardened materials, including eutectic hardened, for example, titanium alloys of system $Ti–TiB_2$.

The presence of hard ceramic TiB_2.eutectic provides improved strength of the alloy by 10–15%, and also stability of mechanical properties at high temperatures of operation.The main disadvantage quasi-composite structurally inhomogeneous material is the reduction of plastic properties to 2–3%. The reason is the colonial structure of the reinforcing component eutectic TiB_2, which blocks all slip systems during plastic deformation.

To improve plastic properties quasi-composite of the material system $Ti–TiB_2$ developed an approach that includes two-stage of plastic deformation of the material of the source structure.

In the first stage, the material is plastic worked under conditions of large shear strain, such as the method of intensive plastic deformation.In the works of the authors proposed a method of processing a spiral widening extrusion (Patent of Ukraine No. 64346 from 10.11.11) and developed modes of plastic working for quasi-composite eutectic material based on titanium alloy BT8 (Ti-6.8Al-3.5Mo-0.32Si).

To justify the modes of plastic working were performed theoretical and experimental researches. They showed that as a result of plastic deformation there is a grinding of the solid phase of the eutectic TiB_2.The size of the particles decreases in proportion to the increase in shear strain in the processing. At the boundaries of the fracture of the solid phase TiB_2, damage is healed by creating a comprehensive pressure under conditions of hot plastic deformation.The plasticity of the metal during standard tests is increased to 12–15%.

At the second stage the billet with modified structure is processed by plastic deformation to shape the product.

Worked in a production environment, the process of extrusion billet compressor blades of a gas turbine engine from the eutectic material system $Ti-TiB_2$-based titanium alloy BT8 (Ti-6.8Al-3.5Mo-0.32Si). It is shown that the implementation process provides increased mechanical properties compared to cast structure on 10-16% in the castle part of the pen blades, and in the body of the pen blades – 12–17%.

HIGH ENTROPY ALLOYS –KEY FINDINGS AND PROSPECTS FOR APPLICATIONS

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The field of high entropy alloys has stimulated new ideas and has inspired the exploration of the vast composition space offered by multi-principal element alloys. Here we present a critical review of this field, with the intent of summarizing key findings, uncovering major trends and providing guidance for future research and practical application efforts. Major themes in this review include thermodynamic analysis of complex; taxonomy of current alloy families; microstructures; mechanical properties; and potential applications. The field is shown to include both structural and functional materials applications. A number of future efforts are recommended, with an emphasis on developing high-throughput experiments and computations for structural materials. The field has a growing potential and continues to rise new questions and offer new possibilities. The vast range of complex compositions and microstructures remains the most compelling motivation for future studies and applications.

MODELING ELASTIC MODULI OF POROUS MATERIALS WITH IMPERFECT INTER-PARTICLE CONTACTS FOR VARIOUS MODES OF DEFORMATION

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One of the most intriguing problem in up-to-date materials engineering is the macroscopic description of the mechanical behavior of composites, powder materials and multi-material systems that are inhomogeneous, nonlinear, and disordered on a ‘‘mesoscopic’’ scale. From the viewpoint of quality maintenance, it is important to monitor the powder materials during each operation of manufacturing processes.

The classic acoustic techniques, based on the generalized Hook’s law, assume independence of the elastic properties on the loading path, however numerous experimental results demonstrate essential nonlinear elastic behavior of granular materials under modest quasistatic and dynamic loading. Therefore, it is possible to elicit additional information about materials structure from acoustic measurements taking into account the elastic nonlinearity. A continuum description of powder materials is generally needed in field applications and non-destructive testing. It demands to find micro-based macroscopic constitutive relations for acoustically nonlinear elastic materials.

The effective elastic characteristics of materials containing pores and imperfect contacts were studied in this work with the method of direct computer simulation on a unit cell. Modelings based on new assumption about specific elastic energy of the materials allowed describe the effect of sensitivity of their elastic behavior to direction of deformation and connect the degree of imperfection of inter-particle contacts with parameters of non-linear elastic behavior of materials.

The results of the simulation may be use for interpretation of experimental data, including resonant ultrasound measurement, and for development of new techniques of non-destructive testing and monitoring of materials manufacture and degradation during operation.

INFLUENCE OF SIZE OF DISPARITY AT THE ASYMMETRIC ROLLING OF POWDERS ON THE EPURE OF TOTAL NORMAL CONTACT TENSION

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The purpose is a study of the influence of disparity on the normal contact stress distribution diagrams at the asymmetric rolling of metal powders.

Now the economical and competitive technique for production of sheet products is under development in a metallurgy, which consists in rolling of powders followed by sintering and end densification rolling. As a rule, the powder materials are subjected to rolling in symmetric deformation zone. However, such approach is connected with great difficulties caused mainly by impossibility to ensure both the back and front tension of rolled strip. The shortcomings in making rolled products are especially prominent in case of rolling the strips having density more than 0.80–0.85 of relative density of cast material.

Now the researchers began to pay attention to asymmetric rolling of powder materials. .The asymmetric rolling of powder materials makes it possible to activate considerably the shear deformation of powder material. In this case, the effects from lengthwise tensile stress that causes fracture of rolled product decreases essentially.

During the study of energy-power parameters of the process of asymmetric rolling of powders, rollers were used as equipped with specifically designed point pressure capsules allowing measuring the contact stress and angular parameters in the deformation site on the both rollers simultaneously. The study of power parameters of the process of asymmetric rolling of powders revealed a difference both in configuration of the deformation site while measuring the normal contact tensions on each of the rollers and the values of the normal contact tensions themselves on the greater and the smaller roller. To obtain the same density of tapes, maximal contact normal tensions at the traditional (symmetric) rolling was always higher than at the asymmetric rolling, both on the greater and the smaller roller. Thus, there was diminishing of general effort of rolling at the asymmetric rolling

Diminishing of the general effort at the asymmetric rolling must be determined by decreasing of the total normal contact tensions. To conduct an analysis and achieve a summing up of normal contact tensions distribution diagrams, data were used relative to the asymmetric rolling of ferrous powder at the different values of disparity. The study of the tape rolling to obtain tapes of similar densities was due to the desire to provide the similarity of conditions for forming powdered tapes.

As a result of the research carried out on the asymmetric rolling of metallic powders, a considerable effect of the disparity values on the length of intermediate area between neutral corners can be observed as compared to rolling of compact metals. Analysis of the diagram of normal contact stress diagrams for rolling with a misalignment of 1.32 and 1.42 shows that with an increase in the error value, the contact arc increases (17 and 22 degrees, respectively) and the extent of the intermediate zone (2.8 and 8 degrees), in which tangential components of the direction towards. The increase in the intermediate zone leads to the appearance of dips on the total diagram of the normal contact stress, which leads to a decrease in the total rolling pressure. Depending on the chosen conditions of the asymmetric rolling (in particular, values of disparity), one can see both variation of the intermediate area dimension between the neutral angles and change of the direction of tangential forces of friction. The resulting normal contact tensions distribution diagrams show the presence of intermediate areas in which tangential constituents are directed to meet each other, that lead to appearance of dips and accordingly to diminishing of general effort of rolling.

EFFECT OF SINTERING AND HOT FORGING ON STRUCTURE AND MECHANICAL PROPERTIES OF Ti-BASED METAL MATRIX COMPOSITES MANUFACTURED WITH USE OF TiH_2 POWDER

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The results of investigations are presented for influence of the type of armoring additions (TiC, TiB_2, B and B_4C) and application of hot forging of powder preforms on structure formation and mechanical properties of Ti-based sintered metal matrix composites. It was shown that microstructure of sintered composites considerably depends on the type of armoring additions. Spherical particles of TiC are not interacted with metal matrix upon sintering. At the same time addition of TiB_2 powder resulted in formation of needle-shaped TiB particles having 1–5 microns wideness and 10–25 microns in length. Microstructure of composites produced by sintering of TiH_2 and B_4C powder blend contains 20–50 μm conglomerates of disperse needle titanium boride phases and low amount of globular TiC particles.

The highest values of the composite hardness (HV 466) was achieved using the mixture of titanium hydride and TiB_2 powder as a reinforcing additive, whereas when using a mixture of TiH_2 with TiC or B_4C the composite hardness was significantly lower (HV 410 and HV 330 correspondingly).

The values of tensile strength, hardness and elastic modulus, despite some porosity growth of the sintered alloy, increase with the addition of 5 % of TiB_2 powder, while increasing the content of the high modulus component in the mixture to 10 % leads to decrease in the level of these characteristics. At compression tests, the yield point and the compressive strength increase monotonically with increase in TiB_2 content, despite the increase in porosity of the latter, due to a significantly lower effect of porosity on the value of the resistance to deformation in compression compared with the stretching.

When using the hot forging of sintered preforms for the composites produced from the same powder mixtures, the main mechanical properties significantly increase. While the sintered at 1350 °C specimens, produced from power mixtures of TiH_2 with 5 and 10 % TiB_2, had the values of compression elastic limit at of 800 and 1030 MPa, whereas the same composites after hot forging – 875 and 1260 MPa correspondingly.

RESOURCE TESTS OF Nb-BASED ALLOY SAMPLES UNDER RADIATION AND CONVECTIVE TYPES OF HEATING

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The purpose of the study was to establish the possibility of using a Nb-based alloy for metallic thermal protection working up to 100 twenty-minute cycles. Samples for testing were manufactured using production technology developed by prof. V.Solncev

In the conditions of furnace (bulk) heating at 1200 ^{o}C temperature, it was found that this alloy lost 11% of its mass within 100 twenty-minute heating cycles.

At radiation heating on a solar power plant with a parabolic mirror diameter of 2 m, an attempt was made to determine the possibility of a further temperature increasing. However, after 40 cycles of heating at 1300 ^{o}C, the sample was broken. Therefore, it was decided to limit the operating temperature for Nb-based alloys by 1200 ^{o}C.

However, the closest conditions to operational ones are realized with one-way convective heating on a universal thermojet gas-dynamic test stend (UTS) in the supersonic jet of combustion products "air kerosene". In this case, the greatest increase in the weight of the sample occurs in the first 40 minutes of heating (49.4 mg), when the oxide film forms and grows, then during two hours there is an equally intense loss of mass, after which the process of mass change is gradually stabilized. Weight loss for the total heating time of 23,400 s was equal 16.7 mg, which corresponds to a loss of 61 g/m^{2}. So for the sheet of 0.5 mm thick it is less than 2.3% of the initial weight.

X-ray diffraction analysis of the samples before and after the tests under conditions of radiation and convection heating showed that the high efficiency of the developed alloys is due to the formation of protective films on their surface.

Thus, testing samples of Nb-based alloys at a temperature of 1200 ^{o}C in conditions of convective heating by combustion products at the UTS stand showed that heat resistance is sufficient for the use of these alloys in metal thermal protection systems for reusable space vehicles.

FLUX-COREDFILLERWIRE FOR TIG WELDING OF HIGH-STRENGTH TITANIUM ALLOY VT22

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Nowadays, a high-strength thermally hardened titanium alloy VT22 (Ti-5Al-5Mo-5V-1Fe-1Cr system) is used in welded units of power elements of AN type aircraft. It is used mainly in the annealed state, because during the heat treatment it is not possible to achieve an even strength of the seam and the base metal (1100 MPa). This is due to the composition of the applied filler wires, which, while heat-treated, do not allow the seam to be reinforced for the required value.

A possible way to solve this problem is to reduce the degree of alloying of the welded joint.

The work presents the results of studies on the effect of weld metal alloying degree reduction on its strength characteristics during the subsequent hardening of the heat treatment.

A fundamentally new filler material for titanium welding is a flux-cored titanium filler wire consisting of a VT1-00 titaniums heat hand a core containing a metal (VT22 alloy) and flux components. A controlling magnetic field was used to control the process of formation of the welded seam.

It has been established that the use of a flux-cored titanium filler wire in combination with a control magnetic field has a positive effect on the properties of the welded joint with the selected standard annealing mode. Despite the reduction in the degree of alloying of the weld metal, its strength (1121.5 MPa) is slightly higher than the strength of the base metal (1057.5 MPa), and its toughness is 70 – 75% of the toughness of the base metal.

INVESTIGATION OF THE MORPHOLOGY OF THE STRUCTURE AND GRANULOMETRIC CHARACTERISTICS OF THE NON-SPHERICAL POWDERS OF TITANIUM ALLOY OF THE BRAND VT6

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In such areas as mechanical engineering and the aerospace industry, metal powders are the main material for the manufacture of products by the methods of additive technologies. The most promising are powders of titanium alloys. Existing equipment for additive technologies such as laser 3D printers usually uses spherical powders. However, obtaining spherical powders is a complex and expensive process. The cost of such powders will fluctuate in the range of 300–700 dollars/kg, which significantly increases the cost of manufacturing the finished product. Therefore, the actual task is to develop alternative types of raw materials for additive technology.

The purpose of the work was to study the morphology of the structure and granulometric characteristics of the non-spherical powders of the titanium alloy of the brand VT6 obtained by the method of HDH.

Metallographic studies were performed on EVO 40XVP scanning electron microscope. Granulometric analysis was carried out using the specialized material analysis complex ImageJ.

Investigation of the morphology of the surface structure of the powders of the brand VT6 showed that the outer surface of the powder particles is characterized by a non-spherical developed porous structure. At the same time, the presence of particles of cup-shaped and lamellar form is caused by insufficient saturation of hydrogen titanium sponge during hydrogenation.

According to the histogram of the distribution of particles of the powder of the alloy VT6 and the Gauss curve constructed on its basis, it has been established that the degree of heterogeneity of the investigated powder size is 12–16%. Thus, the non-spherical powder obtained by the HDH method cannot compete with the characteristics of spherical powders. However, given the low cost (about 50-100 USD / kg) of receipt, such a powder can be used for the manufacture of low-level parts, mock-ups or shapes that do not require high levels of specific strength.

WEAR-AND HEAT RESISTANT COATINGS OBTAINED USING TITATIUM HYDRIDE

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Recently, there is a need to qualitatively new materials intended for use in an air atmosphere at high temperatures as well as materials that have not only good mechanical properties and heat resistance, but also a number of special physical properties and utilities.

The coatings sprayed from a powder with an average size of 40.3 microns. Coatings were deposited onto a substrate of a titanium alloy VT-16 by setting Dnipro-5MA and plasma spraying installation UPU-3D.

Tribological tests were carried out in the process of front edge friction of the cylindrical sample by ring counterbody. As counterbody used titanium alloy OT-4 and stainless steel 07X16H6. The slipping speed was 0.5 m/s. In all cases, the tests were performed without lubricant at a load P = 3.12 MPa for 20 minutes.

The following conclude can be done during the process of analysis of the behavior of materials under friction that in the case of steel it is significantly different for different materials. In a pair of steel with hard coating based on titanium aluminide, and chemical-resistant titanium nitride inclusions ($H\mu$ = 20.5 GPa) and aluminum nitride ($H\mu$ = 12.5 GPa) are not predisposed to interact with the adhesive coating. This corresponds to the minimum mass loss of these objects that are in contact during friction. Moreover, the wear of friction pairs in these largely relates generally less solid steel counterbody. The surface of the track friction friction pair steel counterbody - coatings after running have a stable profile without scratching, galling and pitting. Thus the surface of the less hard counterbody naturally has a higher roughness.

The effect of the presence in the structure of nitrides can be considered natural, as titanium nitride coatings are known as wear-resistant, which are widely used to reduce the coefficient of friction on the working surfaces, for example, cutting tools, particularly in the processing of steel. This is because the titanium nitride coatings have high resistance to diffusion and chemical reaction with the iron.

For maximum heat resistance of the materials in the system Ti-Al phase formation issue at high temperatures, despite the large amount of research remains the key to achieving the maximum level of heat resistance of the materials of the system. At the thermodynamic calculations the problem is difficult to accurately account for all the factors that influence the formation of oxides (temperature, partial pressure of oxygen and nitrogen, corrosive environment, dissolved oxygen).

The test was performed in an electric furnace grade SNOL 2.3.1.3 / 11I2 at 900 °C. The furnace is used for different types of heat treatment of materials under steady state conditions. Total oxidation time in air for all the samples was 28 hours. Experimental tests on samples of titanium alloy BT-16 (10 mm in diameter and 25 mm in height), for which plasma and detonation methods were obtained using sputtered titanium hydride coating, showed that the coating stable in air up to 900 °C. On the surface of the solid layer is obtained from alumina, which protects the surface from oxidation in the air next.

NEW HIGH-STRENGTH (α + β) - TITANIUM ALLOY WITH UTS ≥ 1200 MPa

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Currently, there is a steady tendency throughout the world to increase the share of high-strength titanium materials, whose welded joints provide a high level of mechanical and operational properties. At the same time, there are no known titanium alloys with tensile strength ≥ 1200 MPa, good ductility and weldability in annealed condition. Development of a new high-strength (α + β) -titanium alloy with such characteristics will significantly expand the nomenclature of critical parts for the military, aviation, space and other industries.

The most promising direction of improving the structural strength in the development of high-strength titanium alloys is a method called complex alloying. In this work, based on the results of calculations and carried out experiment, a new high-strength (α + β) -titanium alloy T120 based on the eight-component alloying system of Ti-Al-Mo-V-Nb-Cr-Fe-Zr is proposed, with strength limit not less than 1200 MPa.

Also presented results of experiments on obtaining welding joints from new high-strength titanium alloy T120. The welded joints of high-strength titanium alloys, produced using arc welding, have unsatisfactory values of mechanical properties compared to base metal. The influence of welding thermal cycle results in change of structures of weld and HAZ metal and in decline of mechanical characteristics of the joint. By analyzing the effect of welding thermal cycle, type of filler metal and the post-weld heat treatment on the structure and properties of welded joints of the new two-phase high-strength titanium alloy T120 allowed to obtain welded joints with mechanical properties on level of 90–95% of base metal.

This newly developed alloyand its welding joints considered for use in the military and aerospace industries.

THREE PRINCIPLES FOR PREPARING AL WIRE WITH HIGH STRENGTH AND HIGH ELECTRICAL CONDUCTIVITY

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The trade-off relation between the strength and the electrical conductivity has been a long-standing dilemma in metallic materials. In the study, three key principles, i.e., elongated grains, hard texture and nano-scale precipitates, were presented for preparing Al wire with high strength and high electrical conductivity based on the specially designed experiments for breaking the mutually exclusive relation between the strength and the electrical conductivity. The results show that the elongated grains could lead to a higher electrical conductivity in Al wire without sacrificing the strength; while, the <111> hard texture can efficiently strengthen the Al wire without influencing the electrical conductivity. Furthermore, nano-scale precipitates with proper size can simultaneously improve the strength and electrical conductivity of Al alloy wire. Under the guidance of the above three key principles, Al wires with high strength and high conductivity were prepared.

"ANTONOV - FUTEC. GOALS AND FUTURE TRENDS IN COOPERATION"

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The aircraft industry belongs to industries which development was always defined and continues to be defined and followed by use of constructional and functional materials of new generation with high requirements to their properties and operational reliability. The same tendency belongs to technological processes for treating such materials and manufacturing structures of aviation appointment from them.

Among a big variety of the materials applied in a design of the modern plane titanium alloys took the special place and that complex of properties which these alloys possess are the reason for that. Modern achievements, first of all, in the field of technologies of processing and methods of regulation and control of parameters of processing and production of semi-finished products from titanium alloys give the chance to receive on them levels of properties, especially on specific values, not below, and in many cases even above, than at widespread and applied high-strength steels. These technological decisions in combination with known provisions for a complex alloying gave the chance to develop a series of titanium alloys of new generation, including for special application.

The offered presentation does the review of collaborations of "ANTONOV" and the "NINGBO FUTEC" company in the field of development of a series of new titanium alloys, including in relation to requirements of aviation appointment. For implementation of the tasks between "ANTONOV" and the NINGBO FUTEC company the Protocol is signed, Programs of collaborations in various subjects which are actual for the solution of tasks in aircraft industry and, in particular, on "ANTONOV" for today were made up.

The direction concerning tubes made of a high-strength titanium alloy of FT-01:

- the specifications for delivery were approved;
- the industrial techniques for manufacturing the tubes made of the high-strength alloy was developed which includes methods of extrusion and rolling;
- the modes of heat treatment for achieving various levels of properties were perfected;
- the EBW technology and heat treatment of welded joints were perfected;
- the technology for applying wear-proof coatings was perfected with using method of chemical nickel plating;
- for "ANTONOV" the pilot lot of tubes for carrying out qualification tests is made.

The direction concerning welded chains from a high-strength titanium alloy of FT-01:

- ANU (technical requirements)for production, test and delivery wereapproved;
- the technological sequence formanufacturing the chains was developed;
- the modes of heat treatment for achieving various levels of properties were perfected;
- the technology for bending, welding and heat treatment is performed for welded joints and chains.

The direction concerningarmored protected elements made of a high-strength titanium alloy of FT-01:

- the specifications for delivery were approved;
- the industrial techniques for manufacturing the sheet blanks made of the high-strength alloy was developed which includes methods of package rolling;
- the modes of heat treatment for achieving various levels of properties were perfected;
- for "ANTONOV" the pilot lot of sheets for carrying out qualification tests is made.

The direction concerningupset forged fastenersmade of a high-strength titanium alloy of FT-01:

- the specifications for delivery were approved;
- the industrial techniques for manufacturing upset forged fasteners at high temperature were developed;
- the robotized complex for upsetting the blanks was designed and launchedfor trial operation;
- the modes of heat treatment for achieving various levels of properties were perfected;
- for GP "ANTONOV" the pilot batch for carrying out qualification tests is made.
- for "ANTONOV" the pilot lot of sheets for carrying out qualification tests is made.

The expected effect from realization of the works:

- the weight reduction of structural elements will be about 20-30% in comparison with the traditional ones in which the high-strength steels applied;
- the corrosion resistance of structural elements will be increased;
- the service life termsof structures will be ensuredduring operation terms.

Conclusions:

Modern level of metallurgical productions, and also laboratory base and scientific researches of FUTEC company and other enterprises, including the development and ensuring technological processes, functioning and compliance of them to the international standards for monitoring the quality system of production, can provide the performance of tasks for achieving high requirements of properties and quality which are imposed to the materials applied for designing and manufacturing modern aircrafts today.

ELECTRONIC GLASS AND CRYSTALS IN THE MANGANITE THIN FILMS

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Constituent atoms and electrons determine matter properties together and they can form ordering and disordering phases respectively. For atoms, the ordering phase is called as crystal and its disordering one forms glassy phase. For electrons, which are parasitic within the lattice crystal house, their disordering and ordering phases has more complicated relationships. Moreover, distinguishing and isolating the electronic phases out from the lattice crystal is a crucial issue in contemporary materials science. However, the intrinsic structure/behavior of an electronic ordering/disordering is difficult to observe because it can be easily affected by many external factors. In this report, we present the observation of electronic glass and electronic multiple ordering and their dynamics at the micrometer scale in a manganite thin film. For instance, the strong internal couplings among multiple electronic degrees of freedom in the electronic ordering phases make its morphology robust against external factors, and visible via well-defined boundaries along specific axes and cleavage planes, which behaves like a multiply ordered electronic crystal. A strong magnetic field up to 17.6 T is needed to completely melt such EMO at 7 K, and the corresponding formation, motion and annihilation dynamics are imaged utilizing a home-built high field magnetic force microscope. These observations may provide a microscopic foundation for the understanding and control of the electronic ordering and the designs of the corresponding devices.

AMORPHOUS AND NANOCRYSTALLINE ALLOYS FOR INDUSTRIAL APPLICATIONS

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The examples of Research and Development efforts of the Institute for Metal Physics of NAS of Ukraine related to design of amorphous and nanocrystalline iron, cobalt, copper based magnetic alloys and their industrial application at its academic startup enterprise MELTA Ltd. established for this purpose and that has been successfully operating more than 25 years are considered.

The basic direction is the development of production technologies for magnetic cores made of soft magnetic alloys. High temperature-time stability of initial magnetic permeability of cores made of the developed alloys is ensured by new methods of their final treatment and minimization of their packing process (use of liquid impregnating heat-resistant materials and new polymeric coatings) influence on a level of properties.

Physical principles for amorphous and nanocrystalline magnetic material production will be presented. Perspectives of the development for industrial application of MELTA$^{\square}$ magnetic cores in the field current measuring transformers (converters), power medium frequency, broadband and pulse small- size transformers, filter chokes, reactors, storage transformers, induction sensors and ferroprobes will be discussed.

3D PRINTING OF BULK METALLIC GLASSES —AN APPROACH TO BREAK THROUGH THE BOTTLENECK OF MANUFACTURING OF BMGS

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Bulk Metallic glasses have received continuous attentions in last decades due to their unique atomic disordering structures and outstanding properties, including high strength and elasticity, good corrosion and well resistance, and excellent magnetic properties, etc. However, the applications of BMGs are restricted by size limitation and difficulty in manufacturing of the materials. 3D printing (also called as additive manufacture) based on laser systems provides an alternative opportunity for the fabrication of bulk metallic glasses with complex geometries. In this talk, we present the recent progress in 3D printing of Fe-based and Zr-based BMGs and composites using selective laser melting (SLM) technique in the author’s group, including 3D printing processing, microstructures and mechanical properties of the BMGs prepared. In addition, functional properties of 3D-printed Zr-based BMGs are also investigated. As example, using the 3-dimentional porous framework pre-prepared by 3D printing, micro/nano-hierarchical porous structures were fabricated by chemical dealloying, which exhibited excellent catalytic properties towards waste-water treatments. At last, several challenges in 3D printing of BMGs, such as selection of amorphous systems, defects and crystallization which have great influences on the fabrication and properties of BMGs, are also addressed.

NEW APPROACH FOR OBTAINING NANOSTRUCTURED ANISOTROPIC SINTERED RARE EARTH – TRANSITION METALS MAGNETS

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The high-performance permanent magnets are constituents of wind turbines, electric cars and vehicles, robotics and automation, household electrical appliances, and power and consumer electronics. Anisotropic nanocomposites will be magnets of future. A few methods are developed for nanostructuring of ferromagnetic materials. However the nanostructured magnets have $(BH)_{\max}$ lower than the theoretically predicted limit due to magnet isotropy.

The researchers of Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine have developed the methodology for obtaining the nanostructured anisotropic sintered rare earth-based magnets based on hydrogen-induced phase transformations - hydrogenation, disproportionation, desorption, recombination (HDDR).

The approach includes:

1) the modified HDDR rout when materials microstructures are fined up to nanosized level;
2) an assumption on the texture mechanism after HDDR which is experimentally verified;
3) the low-temperature sintering (LTS) of magnets by hydrogen treatment.

Ferromagnetic material microstructures are grinded up to nanoscale by the combined hydrogen treatment: the initial grinding of the microstructure up to the grain size of several microns and the next HDDR process. Grain size of the $SmCo_5$-based powder particles equals 35-100 nm. Hysteresis loops of such type powder are magnetically single phase with a coercivity of 40 kOe.

The $Nd_2Fe_{14}B$-based powder particles include grains of 50-100 nm and the $Sm_2(Co,Fe,Zr,Cu)_{17}$-based ones of 70-140 nm.

It was shown, by an X-ray diffraction technique, the ferromagnetic materials are magneto anisotropic if after disproportionation they contain the remaining ferromagnetic phase. These ones are the crystallization centers for directional grain growing of the recombined phase. The possibility of the LTS of ferromagnetic powders up to 950 °C by hydrogen induced-phase transformations was confirmed. This is possible due to the powder particle low size and an increasing alloy components diffusion speed caused by hydrogen presence and phase transformations. The sintered materials have a porosity of 0.1-5%. Grain size of the ferromagnetic phase in sintered materials is 90-100 nm for $SmCo_5$-based alloys; 110-140 nm for $Nd_2Fe_{14}B$-based alloys and 90-180 nm for $Sm_2(Co,Fe,Zr,Cu)_{17}$–based alloys.

ATOMISTIC INSIGHTS FOR THE Β RELAXATION IN METALLIC GLASSES

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Atomic rearrangements are an essential property of glassy materials,they are critical in controlling resistance to flow and are central to the evolution of many properties of glasses, such as their stability and mechanical and magentic performance. The Johari-Goldstein secondary (JG) relaxations are an intrinsic feature of supercooled liquids and glasses. They are crucial to many properties of glassy materials, but the underlying mechanisms are still not established. In a model metallic glass, we study the atomic rearrangements by molecular dynamics simulations at time scales of up to microseconds. We demonstrate that a kind of string-like cooperative atomic motions are fundementally are fundamently related to the JG relaxation in metallic glasses. Structurally, they are promoted by the higher tendency of cage-breaking events of their neighbors. Our results provide atomistic insights for different signatures of the β relaxation that could be helpful for understanding the low-temperature dynamics and properties of metallic glasses.

DEVELOPMENT AND APPLICATION OF WIDE RIBBON OF IRON-BASED SOFT MAGNETIC AMORPHOUS ALLOYS

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The scientific and technological issues concerning the wide ribbon of iron-based soft magnetic amorphous alloys have been investigated in this article. The composition of the alloys has been developed based on simulation of first neighboring relation between iron and nonmetallic elements at different temperatures. Recycle over-heating treatment of the alloy melt was used for full alloying of the iron and nonmetallic elements. Newly developed quenching equipments mainly consist of the pre-stressed mechanical cylindrical roller with a symmetrical capability of cooling and a melt container which has the large volume and electrical heater that can fast heat the melts automatically once the detected temperature of the melts below the designed value. The alloy melts continuously flowing out of the container at the bottom to the cooling roller were accurately controlled during continuous casting and the resulted iron-based alloy ribbons are completely flatted and uniform in quality. The iron-based amorphous ribbons have been applied to production of various motor cores made by the specially developed configuration cutting and shaping techniques.

BARKHAUSEN EFFECT AND ITS APPLICATION TO THE TECHNICAL DIAGNOSTICS

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To determine the object condition the standard acoustic emission (AE) procedure provides the step increase of the loading by 25%. Sometimes it is impossible for degraded material of the working engineering constructions. That is why we propose a new approach for diagnostics the state of ferromagnetic elements of engineering objects. This approach combines two well-known physical phenomena: the acoustic emission and Barkhausen effect.

The proposed methodology of technical diagnostics consists in scanning the ferromagnetic constructional element by a quasi-static magnetic field. According to well-known phenomenological model the structural changes of ferromagnetic material make alterations of the domain structure. In particular, some new barriers for the domain walls movement may appear. It means that magnetization reversal of the ferromagnetic by an external quasi-static magnetic field will accompany by movement of the domain walls. Such movement is different for undamaged and damaged material on the assumption of invariability the magnetizing force. We decide to estimate the acoustic manifestation of material damaging under the influence of different factors – plastic deformation, structural changes, local hydrogenation.

First we obtain a good agreement between the calculated and measured amplitude of AE signal for two different materials: commercially pure nickel and steel 15. After solution of the corresponding boundary value problem of the elasticity theory and calculating the displacement vector we take into account that the radial component of this vector is proportional to the amplitude of AE signal. The measured value of such amplitude we obtain using the accepted AE instruments designed in our Institute.

We studied the influence of some physical factors on the sum of AE signal amplitudes. We established that the sum of AE signal amplitudes decreases in the plastic deformed samples in comparison with the initial ones. The magnitude of plastic deformation and damage rate of ferromagnetic have a similar influence. We observed an opposite effect for the hydrogenated samples: the higher hydrogen concentration in ferromagnetic the greater sum of AE signal amplitudes which was registered during magnetization of this material. Also we established that carbon depresses the activity of generation of the magnetic AE similarly to the plastic deformation. However the hydrogenation of ferromagnetic material raises the magnetic AE activity independently on temper.

We obtain different structures of ferromagnetic owing to thermal treatment of the carbonated steel 65Г. Low, medium and high tempering of this steel was executed after the samples harden (their carbon saturation). As a result we observed that activity of the magnetic AE generation grow with increase of the residual ferrite in the structure. Also we establish that the threshold of sensitivity of the magnetic AE method as applied to material damage (formation of a plastic deformation zone) comes to 0,5–0,8% for low-carbon and 0,07–0,11% for high-carbon steels.

Thus, the main steps of new methodology for finding a ferromagnetic local damage using Barkhausen effect consist in the following. We plot the calibration curve for the AE signals damping using the samples of stock material. Passing on to the acting object we obtain the similar plot but with some lower values of AE signals due to the degradation of the worked material. Scanning the object surface by quasi-static magnetic field we can detect the peculiar parts on the curve depending on the type of material damage. In the areas of higher hydrogen concentration the curve has part of increased activity of magnetic AE generation and quite the contrary in the places of plastic deformation of ferromagnetic.

ENERGY-EFFICIENT ELASTOCALORIC COOLING BASED ON MAGNETIC SHAPE MEMORY ALLOYS

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In the past decade, there has been an increased surge in the research on elastocaloric materials for solid-state refrigerators. The strong coupling between structure and magnetism inspires the discovery of new multi-field driven elastocaloric alloys. Novel characteristics appear in magnetostructural transition materials other than conventional shape memory alloys. In this talk, I will take typical magnetic elastocaloric materials to illustrate some general strategies of the maximization of elastocaloric temperature change, the increase of performance reversibility and the enhancement of magnetoelastic interaction coupling.We have verified that the enhancement of the strength of magnetoelastic coupling between lattice and magnetic freedoms results in the increased caloric response. The strengthened coupling of the magnetoelastic effect can be considered as an effective way to improve the caloric performance for these alloys having the same sign of magnetic and elastic entropy changes contributed to the total caloric effect.

RECENT DEVELOPMENT AND CHALLENGES FOR SPINTRONIC DEVICES

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The recent development together with challenges for spintronic devices will be firstly introduced. The spin dependent tunneling properties in perpendicular magnetic multilayers will be presented, mainly in perpendicular MgO-based magnetic tunnel junctions and Hall balance. Finally, up-dated progress about the topological magnetism such as skyrmions will be provided in various magnetic systems, together with a brief introduction about the photoemission electron microscopy (PEEM) excited by a DUV-DPL laser.

DEVELOPMENT OF POWDER IRON-BASED THERMOMAGNETIC MATERIALS FOR SWITCHING DEVICES

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Precision alloys are widely used in electrical and radio engineering, aerospace and nuclear, electronic and instrument-making industries, as well as in industries that create communication and automation systems, computers and microprocessors. Precision alloys also include thermomagnetic materials, the feature of which is the strong dependence of magnetic induction on temperature in a certain range (in most cases, from – 60 to +150 °C).

It was performed investigations on the conditions of formation of a mixed crystal structure and the influence of structural transformations on the saturation magnetization and Curie temperature of powder metallurgy thermomagnetic materials. The influence of the heat treatment conditions on the character of thermomagnetic curves was studied with the aim to provide an abrupt decrease in the magnetization as the Curie temperature is approached. A steep drop in magnetization in the range of operating temperatures of 120-180 ºC is reached due to high-precision doping with alloying additions in powder form, a deviation from the structure of an ideal solid solution and artificially created heterogeneity in the composition.

The materials will be used as heat-sensitive elements in relay-action switching devices. The principle of operation of these devices is based on the interaction of elements of a powder metallurgy heat-sensitive material with a permanent magnet. The actuation moment of such a device is determined by the temperature near the Curie point of this material and kinematic connections of the permanent magnet with a contacting block. This makes possible to control the displacement of the working point of the material and the actuation moment of the device.

ELECTRIC-FIELD CONTROL OF MAGNETIC ORDER: FROM FERH TO TOPOLOGICAL ANTIFERROMAGNETIC SPINTRONICS

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Using an electric field to tailor the electronic properties of magnetic materials is promising for realizing ultralow energy-consuming memory devices. In this talk, I wouldpresent recent results on the giant magnetization and resistivity modulation in a metamagnetic intermetallic alloy – FeRh, which is achieved by electric-field-controlled magnetic phase transitions in multiferroic heterostructures. Furthermore, this approach is extended to topological antiferromagnetic spintronics, and the antiferromagnetic order parameter can be switched back and forth by a small electric field as well.

INFLUENCE OF CHEMICAL-THERMAL PROCESSING AND TYPE OF PROFESSIONALS ON ABRASIVE LOADING OF POWDERED SOFT MAGNETIC DETAILS

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The effect of chemical-thermal treatment on the wear resistance of layered samples is investigated. It is established that the use of gas-phase boronization makes it possible to increase the wear resistance of ferromagnetic plates 3–4 times. It is shown that the wear resistance largely depends on the composition and thickness of the interlayers. The obtained results can be effectively used in the manufacture of magnetic plates for flat grinding machines.

ROBUST MANIPULATION OF MAGNETIC PROPERTIES IN MAGNETIC SEMICONDUCTOR (Ga, Mn)As

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Magnetic semiconductor is an ideal material system for manipulating the spin degree of freedom of charge carriers in semiconductors to merge functionalities ofinformation storage, computation logic and optical communications into one chip. III-V group (Ga,Mn)As with a well-accepted intrinsic ferromagnetism is apresentative material in the family of magnetic semiconductors. Through modulation of the hole density, electrical gating has been shown to alter the magnetic properties of (Ga,Mn)As films, but with limited electric-field effects on the Curie temperature ~10K and coercive force of ~10Oe [1-3]. HereI present our recent work on modulation of magnetism in (Ga,Mn)As. We have realized a giant manipulation of the magnetism in (Ga,Mn)As ultra-thin films viaelectric field with the assistance of a special dielectric, ionic liquid or solid state ionic gel. The maximum modulation of the Curie temperature is up to 100K.

POWDER LAYERED SOFT MAGNETIC MATERIAL

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The effect of the thickness of the magnetic circuit and the number of insulating layers on the magnetic properties of a powdered soft magnetic material based on iron in an alternating magnetic field is studied. It is established that an increase in the thickness of the magnetic circuit and the frequency of the alternating current leads to a deterioration of its magnetic characteristics. The creation of a layered structure in which the ferromagnetic layers alternate with the electrical insulating layers leads to a decrease in the specific magnetic losses.

STRAIN-MEDIATEDMAGNETOELECTRIC COUPLING EFFECTS IN MULTIFERROICHETEROSTRUCTURES

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A great deal of experimental results have demonstrated that multiferroicheterostructures composed of ferromagnetic (FM) thin films grown on ferroelectric single crystals (e.g. Pb(Mg1/3Nb2/3)O3-PbTiO3 (PMN-PT) exhibit strain-mediated magnetoelectric coupling effects, which can be achieved by applying an electric field across the ferroelectric (FE) single crystals. Using the La0.5Ca0.5MnO3/PMN-PT, SnO2:Co/PMN-PT, and Cr:Bi2Se3/PMN-PT as model systems, we demonstrate that the relative importance of the lattice strain and interfacial charge on the magnetoelectric effect depends on the charge carrier density of the FM films. For the La0.5Ca0.5MnO3/PMN-PT structure, the 71o and 109o FE domain switching has strong impact on the electrical resistance, magnetization, charge-ordering phase transition temperature, and magnetoresistance of the La0.5Ca0.5MnO3 film. However, the 180o FE domain switching has little effects on the electrical resistance of the film, implying that the effects of domain switching-induced interfacial electric charge on the properties of the La0.5Ca0.5MnO3 film is minor and could be neglected. While for the SnO2:Co/PMN-PT and Cr:Bi2Se3/PMN-PT heterostructures, both the 71o/109o and 180o FE domain switching induced interfacial electric charge has dramatic effects on the electronic transport properties of the SnO2:Co and Cr:Bi2Se3 films whose charge carrier densities are in the order of 1019/cm3. For the latter two heterostructures, the domain switching-induced strain has little effects on the electronic transport properties of the films. All these results demonstrate that the relative importance of the strain effect and charge effect in PMN-PT-based multiferroicheterostructures could be tuned by appropriately adjusting the charge carrier density of the films.

INFLUENCE OF THE BORON ON STRUCTURE AND MAGNETIC CHARACTERISTICS POWDERED Fe–Co–P MATERIALS

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In recent years, in order to solve the problem of using powder soft magnetic materials in a-c fields, new technologies of manufacture of special composite materials (SMC), in which particles of initial powders are coated with a film (interlayer) from an alloying component, have been developed; as an alloying component, metals, non-metals, organic and inorganic materials can be used. Works on the encapsulation of powder particles of initial materials are promising and are being increasingly developed in the research and production practice of leading companies of the world.

For the preparation of clad iron powders, the method of thermal deposition from solutions of corresponding salts with additives of required reducers and complexing agents was used.

An investigation of the influence of the sintering technology on properties of materials made from iron powder in the initial state and from iron powder clad with a Co - P film was performed. In order to form a liquid phase in the material, commercially pure boron powder in amounts of 0.25–1.0 mass % was introduced. Sintering was performed in air in containers with a fusible seal and in vacuum at a temperature of 1200°C with an exposure for 2 h.

The results of a metallographic examination and of density determination show that, at a sintering temperature of 1200°C, in the presence of boron, the active formation of fusible eutectics ($\alpha + Fe_2B$, $\alpha + Co_2B$), accompanied by a decrease in the porosity and by the formation of a liquid phase, which spreads in the form of a thin film along grain boundaries, occurs (fig. 1).

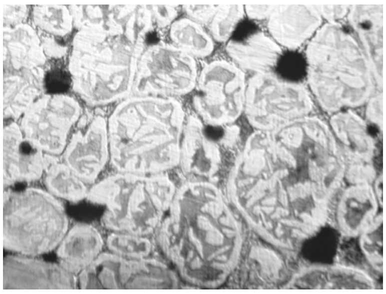

Fig. 1 Structure alloy Fe-Co-P with 0,75 mass % B after sintering at 1200 ^{0}C

The influence of the sintering regimes on the magnetic properties in d-c and a-c fields depending on the boron content was investigated. The results of measurements of the magnetic properties showed their dependence on the porosity and chemical composition and the substantial influence of the sintering medium.

From the presented plots (fig. 2 a, b) it is seen that the maximum values of the induction and magnetic permeability are observed in specimens containing 0.5—0.7 mass % of boron. After cladding of iron powder with cobalt, the magnetic loss decrease, which is connected both with the structural state of the material and with a nearly twofold increase in the electric resistance.

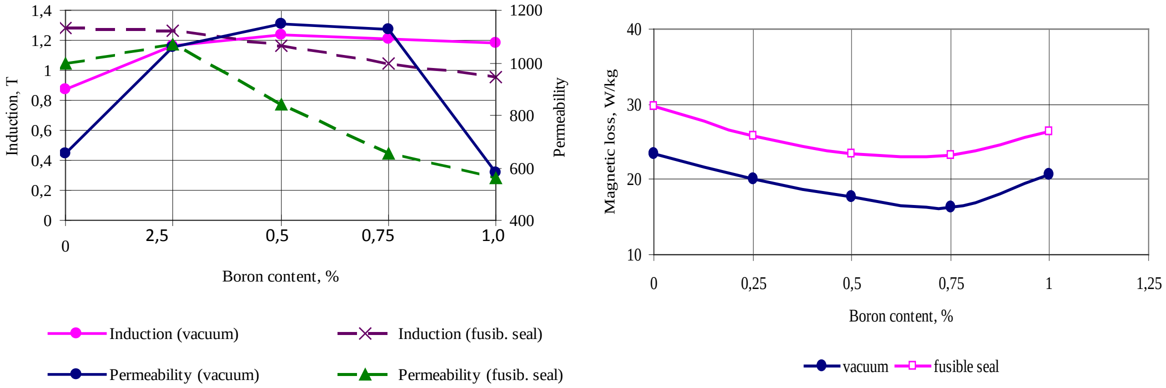

Fig. 2 The dependency of magnetic characteristic for alloy Fe-Co-P from contents of the boron in constant (a) and variable (b) fields.

THE DESIGN AND FABRICATION OF SPIN VALVE DEVICES

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Our study focuses on the design and fabrication of spin valve devices with novel electrodes and transport spacer materials using both experimental and theoretical methods. Recently, exchange magnetic coupling interactions between *L*10-MnGa and ultrathin Co (Fe) films were studied by firstprinciplescalculations. An unexpected oscillation of magnetic coupling was observed by varying the thicknessCo or Fe layer. Moreover, the coupling types are different for Co and Fe with *L*10-MnGa. The magneticcoupling maintains the ferromagnetic interaction for *L*10-MnGa/Fe, even if the thickness of Fe layer varies.Interestingly, a change from ferromagnetic to antiferromagnetic couplings appears alternately for *L*10-MnGa/Cotill Co thickness is up to 11 atomic layers. The coupling oscillations were attributed to the quantum well statesformed in the Co (Fe) films. The orbital characters of the quantum well states were analyzed. Our results are useful to further understand the magnetic coupling interactions and design new magnetic nanostructures.

STUDY OF CRYSTALLOGRAPHIC FEATURES OF THE STRUCTURE OF COMPOSITES BASED ON CARBIDES OF TITANIUM

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The creation of new refractory composites of the Ti–C–Fe–Ni system by the self-propagating high-temperature synthesis of initial powders is one of the effective technologies for obtaining materials based on refractory compounds. The method allows simultaneously synthesizing a metal matrix composite in which titanium carbide forms a high-strength refractory skeleton in a ductile iron-nickel matrix.

The purpose of this study is to study the structural features of synthesized titanium carbides of eutectic composition embedded in a ductile metal matrix based on transition metals and the effect of a ductile iron-nickel matrix on the structure and properties of the carbide framework by X-ray diffraction analysis.

For the Ti–C–Fe–Ni system, the titanium and carbon content for all alloys is the same, the composition of the plastic matrix is varied in order to select the optimum concentrations for producing a composite with an ultrahard carbide framework in a plastic matrix. The content of nickel and iron varies from 0% to 20%.

Titanium monocarbide in the synthesis process for a carbon system crystallizes into a cubic face-centered lattice with syngony (Fm3m) of the NaCl type, forming interstitial phases in the homogeneity region with different lattice periods, depending on the atomic ratio of carbon to titanium (C/Ti). For the Ti–C–Fe–Ni system, the maximum lattice period of 4.322 A is observed when the nickel content in the matrix is up to 5% and iron 15%, which corresponds to titanium carbide with $TiC_{0.72}$ stoichiometry.

According to the X-ray diffraction analysis, the presence of free carbon for all studied composites is recorded on radiographs. With a nickel content of 5%, free carbon is practically absent, the stoichiometry of the obtained titanium carbide is optimal. The largest amount of free carbon was detected in a sample with a nickel content of 20%. The carbon content of titanium carbide is the smallest among all synthesized composites, and the number of vacancies in the carbon sublattice is the largest. The period of the titanium monocarbide lattice decreases and is equal to 4.315A, which corresponds to titanium carbide with $TiC_{0.63}$ stoichiometry.

The presence of iron and nickel in the initial charge leads to the formation of iron and nickel carbides fixed on the radiographs, reducing the amount of free carbon in the synthesized composite. For the entire series of studied composites of the Ti–C–Fe–Ni system, the change in the crystallographic lattice period, depending on the atomic ratio of the carbon atoms to the titanium atoms, is practically linear in character with a small break. The smallest number of vacancies in carbon is observed when the content of nickel in the plastic matrix is 5%.

The size of the coherent scattering blocks for titanium carbide in the synthesized samples varies from 200A to 260A, and for solid iron-based solutions, the coherent scattering blocks have a larger size from 350A to 400A.

THE MODEL OF FORMATION OF EUTECTIC COMPOSITES BY DIRECTED SOLIDIFICATION METHOD

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A continual model of formation of ceramic two-component eutectic composites in the process of directional solidification is proposed. The problem of modeling of composite formation is formulated as a modified one-dimensional Stefan problem. The essential difference of the modified Stefan problem from the classical one is that the boundary condition at the crystallization front takes into account, along with the conventional specific (latent) heat of crystallization, the energy contributions associated with the formation of composite micro-structure, such as surface energy of inter-phase boundaries. Thus, the model employs the energy conservation law and does not consider the specific kinetic mechanisms of structure formation, which enables one to draw rather general conclusions. The solutions of the modified Stefan problem were used to establish general relations between the parameters of the composite structure (like fiber diameter) and those determining the solidification process (like pulling velocity and front position). The preliminary examination of these latter reveals a qualitative agreement with the known experimental data. In particular, simple initial-boundary value problems are formulated and first estimates provided for the eutectic composites formed from hexaborides of rare earth metals and diborides of transition metals (e.g., LaB_6–ZrB_2).

SURFACE COATING OF ADVANCED CERAMIC POWDERS FOR ENHANCED MECHANICAL OR FUNCTIONAL PERFORMANCE

Zhang Jianfeng

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Surface modification of fine ceramic powders is important for many promising applications. This talk will focus on the modification techniques, such as sol-gel and impregnation, rotary CVD (RCVD) and successful applications with Ni or Cu as an example catalyst, which were dispersed on ceramic powders, and exhibited superior catalytic performance. The challenges were also presented for further applications.

COMPUTER DESIGN OF ADVANCED CERAMIC MATERIALS FOR THE WORK IN EXTREME CONDITIONS

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Development of the techniques on the modern stage requires drastically elevation of level of service properties of responsible articles and mechanisms working in extreme conditions (hypervelocity impact, superhigh and super low temperatures, chemical corrosion, etc.) Computer design of material has a task to predict composition, microstructure and macrostructure of a material which could provide required for this article level of properties and thus the technology of production of this material exists. It brings to a necessity to coordinate computer modeling of both behavior of material at its exploitation and the technology of is production. This computer modeling requires building of mathematical models of the specified processes, their investigations and algorithmic realization into software packages to carry out numerical experiment which would be responsible for questions put by a designer. Extreme conditions of materials service bring to the models with essential non-linearities band other mathematical complications that require new non-traditional approaches to resolve appearing problems. This report is targeted on analysis peculiarities of computer designing of ceramic materials and is based on more than 40 years' experience of the author in this field.

THERMOELECTRIC: RESEARCH AND APPLICATION

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Thermoelectric materials can realize directly and reversibly converting between heat and electricity, and have thus drawn increasing attention over the past several decades. The key of promoting this promising power generation technology into massive application is to increase the low conversion efficiency and to develop more distinctive and irreplaceable applications. In this report, we reviewed the progress about Bi_2Te_3-based thermoelectric cooling from the view of new product. To meet the current market requirement and industrialization technology, there are still many technical and cost problems should be resolved for mass produce, controllable, and cost-effective Bi_2Te_3-based product. We then shared our study of another layered thermoelectric materials SnSe from the view of new material. By component design and modified preparation, the mechanical and thermoelectric properties of SnSe-based materials have been continuously improved.

COMPOSITE CERMET POWDERS OF (Ti,Cr)B_2–NiAl SYSTEMS FOR GAS-THERMAL DEPOSITION OF COATINGS

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The main kinds of materials for gas-thermal spraying are powders of metals, alloys, refractory compounds, composite materials and mechanical mixtures of different materials. For the deposition of coatings with various special properties used of refractory compounds, which have excellent mechanical and service properties: hardness, abrasive capability, wear-, heat-, and corrosion resistance. High brittleness substantially restricts the application of pure refractory compounds. As far as deposition coatings subjected to intensive wear, corrosion, and shock loads is concerned, refractory compounds should be used as a composite material, where they is the basic component and a metallic binder is the plastic component.

A promising refractory component of cermet materials is titanium-chromium diboride $TiCrB_2$, which is characterized by high hardness (H_μ=33–43 GPa), heat-resistance up to 1200 ^oC, low density (5 g/cm^3). To produce the composite powders, the starting compositions were mixed in a vibratory mill and then sintered in vacuum. The sinters were ground and sieved to separate 40–60 μm powder particles. The particles of the obtained powders have an oval shape with a heterophase microstructure in which a metal alloy and a refractory compound are fairly uniformly distributed. Technological characteristics of the developed composite powders with different content of refractory and metallic components: fluidity – 45–12 sec, the apparent density – 1.488–2.652 g/cm^3, the average granulometric composition – 33–47 µm). Detonation coatings from the conglomerated powders of the $(Ti,CrB)_2$-NiAlCr system have a strength of adhesion to the substrate – 130–175 MPa, hardness – HV5000–10500 MPa, density – 90–99%. The developed powders can be used for detonation and plasma deposition of work surfaces of parts working under dry friction conditions at speeds up to 15 m/s and loads up to 7 MPa.

COMPOSITE POWDERS OF THE SI_3N_4 – ZRN SYSTEM

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The silicon nitride thanks to combination a high hardness, high-resistant durability, thermostability, and resistance to oxidation is the most perspective ceramic materials. Introduction such electrical conductivity tungsten compounds such as nitride (TiN, ZrN), boride (TiB_2, ZrB_2), and carbide (TiC) with the specific resistance $(1,4 – 5,3)\times10^{-5}$ Om·cm allows to give an electrical conduction as well as increasing its behaviors and condensing under sintering.In order to creation of composite materials with homogeneouss and uniformdistribution of components it is suitable to use the precursors in which all the needed elements entrance.

The behaviorof Si_3N_4 + Z rreaction mixtures has beenin vestigatedin vacuumin the temperature range (700 – 1450) °C. According to obtained data in the presence of zirconium Si_3N_4began to interact with zirconium at the temperature 750 ^oC with formation solid solution nitrogen in zirconium (α-$ZrN_{0,28}$). The product of the solid-state interaction at a temperature of 1000 $^oC$is dispersing powder, which, during its subsequent nitrating, enables us to obtain a Si_3N_4 – ZrN composite material. Theprocessofpreparation oftheSi$_3$N$_4$ – ZrN nitride ceramics in the wide concentration range (11 – 33 vol. % ZrN) hasbeenstudied. At the temperature 1450 $^oC$$Si_3N_4$ reflexdid not detected thatsayto about who legoinginteraction between siliconnitride and zirconium.

The spark plasma sintering has made it possible to obtain specimenswithadensityof above 95 % of the theoretical density at a temperature of 1750 ^oC. Thisis connected with the formation of acontinuousconductive three-dimensional network consisting of ZrN particles.

MATERIAL INFORMATICS ACCELERATES INNOVATIVE DESIGN OF MULTIFUNCTIONAL THERMAL ENVIRONMENTAL BARRIER COATING MATERIALS

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SiCf/SiC ceramic matrix composites (CMCs) are the key high temperature structural materials in next generation gas turbines. Multifunctional thermal environmental barrier coating (TEBC) is critically requested to protect CMC-components from severe high temperature oxidation and corrosion in extreme combustion environments. There are crucial challenges for the optimal choices of TEBC candidates due to their complex and tunable crystal chemistry and performances. Highly efficient screening of advanced TEBC materials would be promoted based on material informatics of diverse candidates. Strategic material-genome initiative would also prevail to disclose mechanisms of property diversity and to further adopt novel concepts for the design of robust TEBC for advanced SiCf/SiC CMCs.

NANOSIZED POWDERS OF SOLID SOLUTIONS BASED ON MOLYBDENUM DISILICIDE

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Our previous investigations about peculiarity formation of disilicide of transitional metal under mechanical synthesis showed that in depending on energy state of their formation interaction were going through two mechanism, namely, solid diffusion (SD) and mechanical stimulated reactions (MSR). The evidentiary standardof mechanism reactions under mechanical synthesis is as large as the adiabatic temperatures which at MSR will be exceed 1800 К.

The influence of the energy state of reaction mixtures on the features of the mechanical synthesis of $Mo_{0.9}Cr_{0.1}Si_2$, $Mo_{0.9}Nb_{0.1}Si_2$ and $Mo_{0.9}W_{0.1}Si_2$ solid solutions has been investigated. It has been shown that the increase in the energy intensity of the mechanotreatment process due to using an “AIR-0,015” high-energy planetary mill has made it possible to reduce substantially the induction period of mechanical synthesis of the solid solutions. Nanosized powders with an average particle size of at most 150 nm have been obtained. A technological regime for the manufacture of targets from the nanosized powders of the solid solutions has been developed. The use of the nanosized powders has enabled us to reduce the sintering temperature by (400 – 450) ^{o}C.

The synthesis of powders of solid solutions disilicide(SD) by the method of low-temperature vacuum synthesis with preliminary mechanotreatment has been investigated too. Products in the form of nanosized powders have been obtained at a temperature lower by 300–400 ^{o}C than the temperature of synthesis without mechanotreatment. Such powders of solid solutions are promising for the manufacture of resistive materials by the methods of ion-plasma and magnetron sputtering of targets.

SYNTHESIS OF HIGH-DENSITY BORON CARBIDE-BASED CERAMICS USING INTENSIVE RECRYSTALLIZATION CONDITIONS

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Boron carbide is an important high-strength non-metallic material with high melting temperature, chemical resistance, wear resistance and low density. The combination of these properties leads to the widespread use of boron carbide: military industry, mechanical engineering, electronics, energy, and others. Traditionally, for the fabrication of boron carbide-based ceramics various methods of sintering are used: hot pressing, sparkling plasma, traditional sintering, infiltration, etc. Recently, the method of infiltration of porous boron carbide sample by the liquid silicon has become increasingly popular. However, residual silicon, which is formed in the process of infiltration, significantly reduces the mechanical properties of the ceramics. In order to reduce the content of residual silicon, it is proposed to apply a zone melting method that allows melting only one component (silicon). Moreover, the presence of a temperature gradient field should provide for the recrystallization of boron carbide through a silicon melt and as a result ceramics with almost monolithic structure could be obtained. The purpose of this work was to establish the possibility of obtaining high-density boron carbide-based ceramics by zone melting of the fusible component (silicon) using porous press. In order to determine the influence of the sample velocity in the field of the temperature gradient samples were obtained with the speed of the inductor moving 0.5 – 2 mm / min. Studies of the microstructure of specimens with different silicon content showed that 10% by volume of silicon is sufficient to form a zone of its melt and recrystallize boron carbide through a melt. It is shown that depending on the velocity of the field of the temperature gradient, the microstructure of the resulting ceramics is changed. As a result using intense recrystallization of boron carbide through a liquid silicon leads to the remaining silicon content of less than 2 wt.%.

INFILTRATION OF BORON CARBIDE WITH DIFFERENT CONTENT OF CARBON FIBERS

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Boron carbide is a representative of refractory compounds. Due to the combination of such properties as: low density, high hardness, high melting point, unique heat and electrical conductivity, materials from boron carbide have been used as materials of a cutting tool, armor protection, wear-resistant materials, materials for absorption of electrons, etc. The main drawback and obstacle to the wide application of ceramic materials is their low fracture toughness. The reinforcement is the most effective method for improving mechanical characteristics. Because of it in the work the influence of the amount of reinforcing carbon fibers on the structure, phase composition and mechanical properties of boron carbide based ceramics has been established. The choice of carbon fibers as a reinforcing component is due to their high strength and elastic modulus, 2 ... 3.5 GPa and 220 ... 700 GPa, respectively. Moreover, as a result of the reaction between silicon and carbon fibers, the secondary silicon carbide was formed, which also has high mechanical characteristics. A preformed mixture of B_4C powder and various amounts of carbon fibers (0, 5, 10, 15, 20 wt%) was infiltrated in a vacuum by liquid silicon.

As a result of mechanical tests on three point bending test, it was found that increasing the concentration of carbon fibers up to 10 wt% leads to an increase in ceramic strength from 350 MPa to 510 MPa. A further increase leads to a decrease in strength. This behavior can be explained by the formation of coils (agglomerates) of fibers during the preparation of the mixture, which in the process of impregnation form large areas (up to 100 mμ) of silicon and carbon carbides that were detected during microstructure studies. It was found that the number of fibers determines the phase composition of the boron carbide-based ceramics.

FUNCTIONAL MATERIALS PROCESSED BY NON-CONVENTIONAL SPARK PLASMA SINTERING

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This work is focusing on the fabrication of thermoelectric bulk materials processed by the unconventional sintering technique called Spark Plasma Sintering (SPS). SPS is a promising rapid consolidation method that results in a better control of the sintering kinetics than other techniques. Three main steps will be reported.

•The basic description of the Spark Plasma Sintering. What is SPS? The principle and the sintering mechanism

•Preparation of textured lamellar $Ca_3Co_4O_9$, Bi_2Te_3 compounds using a modified SPS process called “Spark Plasma Texturing” (SPT). During SPT, the bulk material can freely deform itself. As a result, inter-grain preferential crystallographic orientation is favoured. The SPS versus SPT properties will be analysed with the highlighting of the anisotropy of the thermoelectric properties.

•In addition, the SPS allows to obtain MgB_2-based ceramics with tailored microstructures. The obtained material is denser (98 % relative density of the theoretical value) than the samples obtained by Hot-Pressing (HP) and/or Conventional Sintering-CS. Superconducting properties were measured and the influence of the processing conditions on the properties was evidenced. Herein, the trapped field up to 3.9 T has been measured at 20 K in a magnetized stack of two disc-shaped bulk MgB_2 superconductors of 20 mm diameter and 10 mm thick. On the other hand, the feasibility to use the MgB_2 in Maglev vehicle has been investigated between 17 to 35 K. The levitation forces up to 45 N were performed at 20K. The results show that, the bulk MgB_2 superconductors could be a viable variant for magnetic levitation applications and/or as cryo-magnets.

THE FABRICATION OF HIGH-STRENGTH (LAB_6-TIB_2) -CU COMPOSITE WITH REINFORCED GRAIN BOUNDARY

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The metal-ceramic composites, due to the combination of properties of ceramic and metal materials, have high performance characteristics: hardness, wear resistance, durability, electrical conductivity, etc. However, the presence of a partition boundary between the ceramic and metal components of composite, which is characterized by a high degree of defect, is quite often caused by a dramatically decrease in the physical and mechanical characteristics of metal ceramics. One of the most effective methods of improving the strength of the material is reinforcement. Usually reinforcement provides the strength of the material by placing the reinforcing component in its volume of another component. The paper proposes a mechanism for increasing the mechanical properties of (LaB_6-TiB_2)-Cu composite by reinforcing of the boundary between the particles of the eutectic composition LaB_6-TiB_2 and copper.

In order to obtain high-density composites of the system (LaB_6-TiB_2)-Cu, the method of spark plasma sintering of powder mixtures was used. The densification were carried out at temperatures of 850–1050 °C. In order to save the initial structure of the surface of the LaB_6–TiB_2 particles and to ensure the reinforcement of the interface between the phases, a high heating rate of 200 °C/min. Microstructure and phase composition of the sintered samples were investigated.

The increase in the temperature of sintering is accompanied by a decrease in the initial porosity and the formation of strong contacts between the phases. Microstructure studies of the grain boundary of a composite sintered at a temperature of 1050 °C indicate the formation of a reinforced grain boundary during densificarion of the powder mixture of the eutectic composition of LaB_6–TiB_2 and copper. Measuring the compressive strength showed that the composites with reinforced grain boundaries have a strength of about 500 MPa. It should be noted that the strength of the composite with reinforced sections of the section is 25–30% higher compared with non-reinforced grain boundaries.

THE MECHANISM OF UHTCS STRUCTURE AND PROPERTIES FORMATION

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Ultra-high-temperature ceramics (UHTC) has an increasing popularity in the world and, particularly, in Ukraine, for the problems of machines and units reliability in power engineering, aviation and space machinery used in the temperature range of 1600–2500 °C. The present work is devoted to the investigation of activated sintering processes and analysis of the structural state and structural sensitivity of the mechanical properties of ultra-high-temperature ceramics based on zirconium boride. The processes of phase interactions in the grain boundary zones with the determination of the grain-boundary strength characteristic and the relationship between grain-boundary strength and the mechanical properties of composites have been studied. The eutectic systems where, at solid-state sintering, the activation of sintering takes place have been considered. The activation is connected with the diffusion zones formation, phase interactions and transformations with an increased diffusion characteristics in the region of phase boundaries. The study of the structural sensitivity of the strength of the ceramics under investigation is carried out by measuring a wide range of mechanical characteristics, including grain-boundary strength. Indentation methods at high loads on the indenter, when contact fracture processes are developed in the penetration area have been used. Correlation dependences between the ceramics basic mechanical characteristics, first of all connecting grain-boundary strength with fracture toughness, compressive strength, flow stress, etc., have been found. It is the ground of the analysis of the brittle materials structural sensitivity of the mechanical properties, which determines the prospects for obtaining ceramics with the predetermined properties.

ZrB_2 ULTRA-HIGH-TEMPERATURE CERAMIC COATINGS ON CARBON-CARBON COMPOSITE SUBSTRATES

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The composition and structure of plasma coating on C / C- SiC composite obtained by $60ZrB_2 + 20SiC + 20AlN$ composition powder (mass%) deposition have been studied. The coating of 320 ... 370 µm thickness is characterized by a heterophase structure, a tight adjustment the substrate without pores and cracks. The coating phase composition corresponds to the sprayed powder one. After high-temperature coating oxidation in supersonic C_2H_2-O_2 flows in the thermal cycling regime (~2000 °C, 2 min; 30 cycles), the main phases of the coating are zirconium dioxide m-ZrO_{2n}, mullite solid solution Al_2SiO_5 and zircon $ZrSiO_4$; the oxidation rate was < 7 µm / min. Based on the analysis of the microstructure and elemental chemical analysis of both the initial and oxidized coating cross section, a mechanism for its high-temperature oxidation has been established. The results obtained testify to the resistance of the coating to high-temperature corrosion up to temperatures of ~ 2000 °C.

POROUS SIC CERAMICS PREPARED VIA AN IN-SUIT REACTION-BONDING PROCESSING

Yu-Ping Zeng

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For Example: Nature and marine always give us inspirations for fabricating functional materials by mimicking the structure design or stimuli-responsive capability of biomaterials. However, the strict preparation conditions, multi-step processes and high cost of the methods to create biomimetic systems at interface and in bulk, limited their practical applications. Therefore, developing simple, cheap but effective method becomes the focus of our research in this feld. The amazing properties of biomaterials are the result of evolution for billions of years. Generally, biomaterials are assembled with limited supply of constitutes available to living organism under mild conditions. The surprising properties of biomaterials are largely resulted from the sophisticated hierarchical structures.

Following the design principles of nature to prepare manmade materials has drawn great research interests in materials science and engineering. In the past decades, a large number of papers in this feld have been published. In this report, the recent progress in the preparation of bio-inspired materials focused on the structure mimicking is summarized. Selected examples from low to high dimension are described with emphasis on the relationship between the structure and the corresponding functions.

HIGH-PERFORMANCE PRECISION PROCESSING OF CERAMIC BALLS

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There are many ways of precision processing of ceramic balls. However, the methods known today have some of disadvantages that do not allow processing balls of modern high-hard ceramics with the high accuracy and productivity, such as boron carbide (CB4) and silicon carbide (SiC). Such ceramics has several of distinctive properties, such as record high hardness and strength, high chemical and temperature resistance, low density. This allows the use of CB_4 and SiC balls in extreme conditions, with high loads, temperature, in chemically-aggressive environments. Such balls are necessary for ball bearings, pump valves and other mechanisms that are in demand in the aviation, space industry, chemical industry, etc. Currently, very few manufacturers make precision ceramic balls from SiC, and almost no one makes them from CB_4, due to the high complexity of processing such materials.

For highly efficient processing of precision ceramic balls in the ISM developed a new method of processing in the V-grooves with variable radius. This method allows for high performance and quality processing balls of different ceramics, including CB4 and SiC. The developed method is based on standard equipment, which simplifies its implementation.

When processing in V-grooves with variable radius the position of the balls rotation axis is constantly changing according to a certain law. As a result, the entire surface of the balls is quickly covered by uniform tool traces grid. This ensures high quality of processing. Continuous change in the position of the balls in the radial direction ensures the processing of the batch of balls without any difference in their size. It is possible to make such a tool, when the balls will move at the same speed and damage due to the contact of ceramic balls during processing will be excluded.

A significant increase in productivity is achieved by increasing the sliding speeds in the processing areas. This is provided by the mismatch of the motion direction the contacting surfaces of the balls and plate.

The new method allows regardless control the formation of the tool traces grid on the surface of the ball and processing productivity. To calculate the necessary parameters of the V-groove for performance and precision machining, a mathematical model was built. It takes into account the pressure distribution in the areas of contact, wear plates and material of the balls.

RESEARCH AND INDUSTRIALIZATION OF CE:GGAG CERAMIC SCINTILLATORS

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Scintillator, which can convert the high energy rays into visible light, is the critical component in many detectors for radiation detection and nuclear medical diagnostics. $(Y,Gd)_2O_3$:Eu, Gemstone and Gd_2O_2S:Pr are three ceramic scintillators that are used in the commercial medical CT detectors at present, but only Gd_2O_2S:Pr is available on the market. Recently, there is a strong demand for a new ceramic scintillator that can meet the requirement of high-end CT detectors. Among many scintillator candidates, cerium doped gadolinium gallium aluminum garnet (Ce:GGAG) ceramics have shown great promising application in medical CT system, becasue of its excellent performances, such as high light yield and extremely low afterglow. During the last few years, we have been focusing on the fabrication, performances tuning and the array processing of Ce:GGAG ceramics. The main scintillation properties have exceeded the similar commercial products. This product has already realized industrialization. Moreover, we have also worked on how to raisethe transparency of GGAG ceramic aiming at extending its application in high power LED/LD lighting. Results show that the transmittance of the sample can reach 81% at the emissionpeak wavelengthby means of partial Ysubstitution at the Gd site.

GRINDING WITH SUPERABRASIVE WHEELS WITH ORDERED WORKING LAYER

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Traditional superabrasive wheels contain diamond grains that arranged randomly. Each of the diamond grains is processing the surface of the workpiece in different ways. Grain differently oriented and the material is cut with different cutting depth. Therefore, they have different loads and wearing out. As a result, the efficiency of the use of grains of superhard material is low. According to various estimates, less than half of the cutting grains efficient to make processing of the workpiece.

Method to significantly increase the efficiency of the grinding tool is a using tools with a structured working layer. This allows you to make a tool in which diamond grains will have the best for treatment of the condition and can show much more efficient processing.

When structuring the working layer also becomes possible to control the microprofile on the surface of the machined part. For example, it can be typical for grinding chaotic profile or regular (periodic) profile, which is typical for cutting. Form of microprofile surface in many cases is of great importance for exploitation processed detail.

The presentation describes several manufacturing methods and ways controlling the structural orientation of the elements in the working layer of superabrasive wheels. Regularities of formation of surface roughness and microprofile when machining with these wheels are analyzed. When machining by superabrasive grinding wheel with the ordered working layer the roughness and profile of the workpiece changes regularly according to wear out each of ordered layers and there is a change to the next ordered layer.

Described one of variants of manufacturing structured tool through the use of additives. As additive is proposed to use grains of shredding kiborit. This significantly improves the efficiency of grinding. Grains of shredding kiborit perform multiple functions at once:

- abrasive substance that grinds the workpiece together with the diamond grains wheel
- the material of the reinforcing main material of superabrasive grinding wheel and increases tool life
- forms on the working surface of the grinding wheel developed surface with the formation of pockets for sludge.

To determine the range of performance grinding the method of evaluation of the working surface using an acoustic emission sensor is proposed.

MECHANOSYNTHESIS OF CERAMICS COMPOSITE TiC–2TiB$_2$

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Ceramic-matrix composites based on TiC–TiB$_2$ have attracted enormous interest during recent years because, in comparison to single-phase ceramics, they exhibit superior properties including high hardness, good wear resistance and high fracture toughness. The application of TiC–TiB$_2$ composites has been limited due to the fact that they have been difficult to synthesize and fabricate.That is why these processes have got a lot of attention among researchers. Much of the attention has been given to the TiC–TiB$_2$fabrication that is based primarily on self-propagating high-temperature synthesis. However, macrocrystalline composite obtained during this method, is difficult to process at the next consolidation. In order to achieve consolidation, it is important to receive powders in nanocrystalline form that can be done by decreasing the temperature. At the low temperature, this can be achieves by millingboron carbide and titanium in a planetary mill (as born carbide is unstable in the presence of titanium at low temperatures).

The aim of this work was to study the peculiarities of TiC-TiB$_2$ nanocomposite formation during milling powder mixture titanium and boron carbide in a planetary mill. Milling was carried out under argon atmosphere. The rotational speed of the carrier was 735 rev/min, and roller speed -1840 rev/min. The ratio of steel balls and milled powder was 20:1. X-ray analysis was carried out on the installation DRON3 in copper Ka radiation.

X-ray diffraction show only lines correspond to the phases TiB$_2$ and TiC after 25 min milling of powder mixtures Ti+B$_4$C. Electron-microscope examination show that the TiC–2TiB$_2$ composite consists of nanograins sizing less than 30 nm. The mechanism formation of theTiC–2TiB$_2$ compositeafter milling powder mixture of titanium and boron carbide is similar to the mechanism formation of TiB$_2$ and TiC after milling powder mixture of titanium with boron(orcarbon) and runs by the mechanically-induced reaction of self-propagating synthesis.

HIGH THROUGHPUT FABRICATION AND PROPERTIES INVESTIGATION OF Si-B-(C, N) BASED MATERIALS

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Si-B-(C, N) based materials possess low density, excellent mechanical properties and high temperature resistance, making them potential candidates using as hot structures for aero engines, which attract a great attention from all over the world. The development of Si-B-(C, N) based materials by conventional approach have the disadvantages of high R&D cost, long experiment period and high consumption of raw materials. Based on the idea of material genetic engineering, the new approach of high throughput preparation and characterization of the materials has become the focus of international research in this field. In this work, a multi-channel temperature gradient chemical vapor deposition (CVD) system is developed. Through temperature gradient design in the reaction chamber as well as the flow rate control of reactive gas mixtures in different reaction channels, high throughput fabrication and investigation of Si-B-(C, N) with varied chemical compositions is realized. Furthermore, coupling characterization of Si-B-(C, N) based- composite is realized by combined utilization of acoustic emission, mechanical properties and fatigue test, etc. It provides a novel way for properties optimization of the materials.

cBN-BASED MATERALS WITH SILICIDE BINDERS

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Polycrystalline cubic boron nitride (cBN) materials are well-known in industry. cBNis second hardest to diamond, yet providesbetterthermal stability and lower chemical reactivity with metals under aggressive cutting conditions.

Currentstudy is dedicatedto the development and investigation of novel HPHT sintered materials with refractory silicide compounds as a binder phase –$MoSi_2$, CrSi, VSi. Aluminum was alsointroduced to the mixture as an oxygen getter.

Sintering wasdone in HPHT toroid type apparatus under pressure of 7.7 GPa and temperature range of 1600–2450 °C for 45s. Phase composition and microstructure of sintered samples were investigated by X-ray analysis and SEM respectively. Elastic properties of the materials were studied by ultrasonic pulse-echo technique. Indentation technique wasused for microhardness and fracture toughness measurements. Performance testing wasdone underconditions of high speed longitudinal turningof austenitic stainless steel SS-EU1.4404 (AISI 316L).

Microhardness of the sintered samples was found to be strongly dependenton the sintering temperature in all investigated systems, with a local maximum in the middle of the temperature range. Similarly, the lowest tool wear was also found for thesamples sintered at temperature range of 2000-2150 °C.

Acknowledgements: This research was supported by European Union’s Horizon 2020 Research and Innovation Programme under Flintstone2020 project (grant agreement No 689279) and Visby Scholarship by the Swedish Institute (grant number02757/2016).

TEMPERATURE DEPENDENCE OF THE MODULUS OF ELASTICITY OF MATERIALS

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In studying the physical properties of materials at high temperatures, the determining factor is the energy of the interatomic bond and the melting point temperature. To calculate the mechanical characteristics at high temperatures, the quasi-harmonic approximation model developed by the authors is used.

Strength characteristics were calculated for borides, carbides and LaB_6–MeB_2eutectic system under extreme conditions (high temperature and deformation) using the a priori pseudopotential method. In the case of composites, when calculating the modulus of elasticity, the "modified rule of mixtures" developed by the authors is used to evaluate the effect of the interface.

As a result, an analytical formula is obtained describing the temperature dependence of the relative modulus of elasticity for borides, carbides, composites, and also for metals (both simple and transient). For metals, also there is an experimental confirmation of the temperature dependence of the elastic moduli.

With the help of the obtained universal relation, it becomes possible to estimate the modulus of elasticity of crystals at any temperature, if its value at zero temperature and melting temperature is known.

THE CERAMIC WASTE FORM DEVELOPMENT FOR IMMOBILIZATION OF FISSION (CS, SR)-FRACTION WASTE STREAMS

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The decommissioning and waste-management activities at the Unit 4 (Shelter) of ChNPP will generate significant amounts of radioactive waste with a wide range of characteristics that will need to be safely managed. In developing of HLW processing technologies much attention has been focused on the possibility of fractionation, i.e., the separation of cesium-strontium and rare-earth fractions of actinide isotopes to immobilise in the matrices of the optimal composition. At present using of borosilicate and alumino-phosphate glasses for immobilization of long-lived radionuclides can not guarantee the safe management of HLW. To solve the problems of new matrices HLW synthesis, from both practical and theoretical points of view, it is important to take into account the existence of crystal chemistry criteria of existence of various phases of a given structure type. Ceramic incorporation of waste elements is based on the isomorphism of mineralogy. Most actinides and fission products can be incorporated into polycrystalline phases, such as zirconolite, perovskite, garnet and hollandites, etc. The SI IEG performing research to identify compositions that promote hollandite formation and Cs incorporation across a wide range of RedOx conditions resulting in a flexible Cs immobilization host material

Direct incorporation of HLW into ceramic hosts has been the topic of extensive study over many years and a number of reviews are available. Since 1997 the Department of Nuclear Geochemistry of the SI IEG has developed several different types of crystalline host-phases acceptable for the economically feasible perform research to and environmentally safe immobilization of high level wastes. Hollandites matrix is a good candidate because of its high cesium incorporation ability and its excellent chemical stability. The works have been done in Institute in recent years is devoted to the synthesis and micro structure ceramic matrices characterization.

CERAMIC COATINGS FOR PROTECTING CARBON/CARBON COMPOSITES AGAINST OXIDATION

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Carbon/carbon (C/C) composites are the leading candidates for high temperature structural components in aerospace fields. One key drawback of these composites for such an application is oxidation during their exposure to an oxygen-containing atmosphere and the resulting rapid recession. Therefore, the applications of C/C composites as the high-temperature structural materials depend on the development of protection technique against oxidation. Currently, multi-layer and multi-phase ceramic coatings are the most promising approach. From the late 1990s, silicon-based ceramic coatings had been investigated widely for anti-oxidation of C/C composites by forming a slow-growing and dense silica glass. After the discovery of cracking from the mismatch of thermal expansion between silicon-based ceramic coatings and C/C composites substrate, the focus of anti-oxidation coating research has been shifted towards the elimination of cracks in the ceramic coatings. Subsequently, some novel coating systems were developed, such as the multi-phase inlay ceramics, whisker-toughed ceramics and gradient ceramic coatings. Simultaneity, pre-oxidation was applied to obtain a transition layer to improve the thermal stress resistance of the coatings. This report will give a brief introduction of the history and the current status of oxidation resistant ceramic coatings for C/C composites in our university, and the protection and failure reasons of some coatings at high temperature will also be provided.

NOVEL THEORY OF PLASTICS WELDING AND ITS APPLICATION

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Creation of novel technologies first of all needs novel knowledge. Earlier in 1988 an idea that conventional views about mechanisms of welding of polymers, on which the most widely-distributed theories, namely diffusion, rheological and diffusion-rheological theories, are based, consist numerous assumptions. That encourages scientists to conduct new and new investigations and, basing on their results, form novel theory of plastics welding.

Previously it was shown that during short-term contact and thermal impact at boundary area of two polymers transitional layer, in which only segments of macromolecules interact and its thickness is not more than length of these segments, is formed. Just on this effect a novel theory of welding is based, since welding is mostly short-term process. With time confirmation of this point of view became possible due to appearance of new, more powerful and precise methods and approaches of scientific investigations, tests and calculations. It was found that the thickness of this transitional layer, structure and properties of which differs from structure and properties of both polymers, is not more than 8 nm. A hypothesis is made that orientation of macromolecules at surfaces of both polymers occurs during welding and, due to impact of thermal energy, rotational movement of their segments with changing of conformation of macromolecules in volume of the transitional layer and forming of mixed structure of segments of both polymers, takes place. Because of that a novel theory has the title “Conformation theory of welding (of polymers)”. It doesn’t contradict the possibility of interdiffusion of macromolecules of polymers during long-term thermal impact, but it limits that for short-term welding process. Confirmation of that was found during researches in the field of additive technologies, mainly 3D printing, and basing on it an innovative technology of welding of plastic pipelines was developed.

DEVELOPMENT OF CARBON FIBER COMPOSITES IN CNITECH

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Carbon fiber composites have been widely used in aerospace, automotive, civil engineering and other fields due to their excellent properties. CNITECH has established a first-class Advanced Composites Innovation Center. Our current research interests are focused on polymer chemistry, composite design and simulation, processing, manufacturing equipment, joining, testing and evaluation. Recently, we have specially made a breakthrough in the lightweight carbon fiber compositesfor vehicles with the cooperation of OEMs.

The presentation will show the following progress we have made:

(1) Colored carbon fiber and interface modification of carbon fiber composites

(2) Structure design and process simulation

(3) Self-developed automatic equipment and facilities

(4) Application examples of carbon fiber composites.

EXTRA HIGH TEMPERATURE RESISTANT POLYMERS AND COMPOSITES FROM MONOMERS POSSESSING C≡N FUNCTION

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Two types of polymer materials have been developed on the base of cyanate ester resins (CER) and bisphthalonitriles (BPN), correspondingly, possessing C≡Nfunction in their structure.At polycyclotrimerization of CER, densely crosslinked polymer networks with high temperature resistant triazine cycles in the network junctions are formed, and polymerization of BPN monomers leads to formation of crosslinked polymers having such thermally stable heterocyclic fragments as isoindoline, triazine and phthalocyanine. Additionally, the glass transition temperature and elastic modulus for both the polymer systems were increased by incorporation of ultra-low amounts (0.01–1.00 wt.%) of specifically functionalized inorganic nanofillers such as epoxy-POSS, amino-POSS, amino-montmorillonite(amino-MMT), amino-SiO_2, etc. It was found that in all the polymer compositions the separate nanoparticles of reactive inorganic nanofiller were incorporated covalently into the polymer network structure ensuring impossibility of their agglomeration and thus providing their very effective dispersing and significant improvement of thermal and mechanical characteristics for the nanocomposites obtained. The structure-properties relationships of the novel nanocomposites developed were characterized using FTIR and far-infrared spectroscopy (FIRS), scanning transmission electron microscopy (STEM), energy dispersive X-ray spectroscopy (EDXS), DMA, DSC, TGA techniques.

For CER based systems increasing T_g by ~50^0, modulus by ~60% at room temperature and its multifold rise at high temperatures were observed.For BPN based nanocomposites the $T_g$values reached 460-560^0C and after heating in N_2 up to 570 °C, at next scanning total disappearance of glass transition and constant modulus value (~ 3 GPa) over the 20–600 °C temperature rangewere observed. The best nanocomposite samples in nitrogen lost some mass but maintained integrity up to 900 °C.

The polymer matrixes as well as their organic-inorganic hybrid nanocomposites were used for development of carbon plastics. The samples of carbon plastics tested have shown high mechanical performance with high percentage of strength(flexural, tensile, compression) retention at temperatures up to 300 °C.The composites developed are promising for using in aerospace, microelectronics, etc.

IONIC SKIN

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Skin-like materials have received increasing research interests for their broad applications in artificial intelligence, wearable devices, and soft robotics. However, profound challenges remain in terms of imitating human skin because of its unique combination of mechanical and sensory properties. In this work, a bioinspired mineral hydrogel is developed to fabricate a novel type of mechanically adaptable ionic skin sensor. Due to its unique viscoelastic properties, the hydrogel-based capacitive sensor is compliant, self-healable, and can sense subtle pressure changes, such as a gentle finger touch, human motion, or even small water droplets. It might not only show great potential in applications such as artificial intelligence, human/machine interactions, personal healthcare, and wearable devices, but also promote the development of next-generation mechanically adaptable intelligent ski-like devices.

DEVELOPMENT OF MODIFIED EPOXY-POLYESTER MATERIALS FOR FRICTION UNITS OF TRANSPORT VEHICLES

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Every year, polymer composite materials (CM) are widely used in all branches of industry. The constant development of industry puts high demands on the structure and functionality of composites. The combination of different nature of the binders, the structural and volume modification of composites, the introduction of various dispersion of fillers, allow to get composite materials with increased operational characteristics in the complex. The development of transport technologies is important today, which is impossible without the use of modern developments in the field of material science. Therefore, the development of materials with increased physico-mechanical, tribological and thermophysical properties is a topical issue for the modern field of transport and materials science.

In this work two-component bidispersed epoxy-polyester composite materials were developed and investigated. On the first stage of the research, was studied of adhesion and physical and mechanical properties of epoxy-polyester composites. It was found, that the introduction of a polyester resin into an epoxy binder results in the improvement of these properties. Then studied the effect of fillers of different nature on the performance properties of epoxy-polyester composite. At the same time, it was argued that from an economic point of view it is inappropriate to carry out a large number of experimental studies. Proceeding from the above, the mathematical planning of the experiment was carried out to determine the optimum content of the components in a two-component bidispersed epoxy-polyester matrix. On the second stage, the influence of the methylene diphenyl diisocyanate modifier was studied and the regularities of improving the adhesion and cohesive properties of the developed materials was found. It was determined, that the introduction of this modifier influences the processes of structure formation in an epoxy-polyester binder.

The developed epoxy-polyester composite materials were kept during 30 days in aggressive environments: petrol, sea and river water, oil environment and alkaline environments (NaOH (50%)). It was found that the aggressive environments do not significantly affect the ability of polymeric materials to resist shock loads. It was found that the decrease in the properties of the material was observed in the specimen which was kept in petrol environment.

At the next stage, the study of tribological properties of epoxy-polyester CM was carried out. It has been determined that the contact temperature index of the specimen in the area of mechanical interaction of surfaces increases significantly to $T = 366–369$ K during the dry friction. The coefficient of friction in this case is $f = 0.33–0.35$. It is proved that the material that was tested in a seawater environment are characterized by improved tribological properties. The contact temperature in the friction area is – $T = 295–298$ K. At the same time, the coefficient of friction is $f = 0.08–0.09$, which is 3–4 times lower in comparison with specimen, which was tested at dry friction. It is determined that the material, tested in lubrication differs with the low indexes of wear rate and friction coefficient: $I_m = 0.25–0.30$ mg/km, f = 0.03–0.04. The running-in distance under these conditions is L = 1500–2000 m. In our opinion, this is due to the fact that the introduction of disperse fillers increases the strength of composite materials, which, in turn, helps decrease the friction coefficient and increase wear resistance. It is confirmed that the wear rate at dry friction is higher than with the lubricant. It was analyzed that the filler particles are evenly located on the friction surface, and it can be asserted that they are directly involved in the friction contact.

Also, a study of the specimen surfaces after the test in different environments was carried out by optical microscopy. Using the method of scanning electron microscopy, an analysis of the microstructure of surface of friction was conducted and the elemental composition was determined. It is confirmed that the system is heterogeneous, dispersed fillers are evenly distributed in the volume of the matrix. The obtained results of the analysis of optical and electronic scanning microscopy are confirmed by the results of experimental studies of tribological properties. The experiment data is also confirmed by surface studies in phase contrast mode.

The use of developed epoxy-polyester composite materials will significantly improve the life of friction units of transport vehicles.

HIGH PERFORMANCES OF PLANT FIBER REINFORCED COMPOSITES AND THEIR APPLICATIONS

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Plant fiber reinforced composites have raised great attentions among materials scientists and engineers in the recent decades due to their light weight, environmental friendly, interesting mechanical and physical properties, et. al. Realizing high performances of plant fiber reinforced composites are the necessity for expanding their application potentials

Compared to man-made fibers, plant fibers possess unique multi-scaled structures. On the basis of the shear-lag model, a double interface model was proposed and successfully calculated the interfacial behaviors of plant fiber reinforced composites so that the multi-scaled interfaces could be designedTherefore, improving the mechanical properties of plant fiber reinforced composites were attempted by hybridizing with glass and carbon fibers and by incorporating carbon nanotubes. Multi-scaled failure modes were obtained and the mechanical properties were remarkably improved.

The acoustic properties of plant fiber reinforced composites were also investigated both theoretically and experimentally based on the above multi-scaled methodology. It was found that both plant fibers and their composites had superior capability for noise reduction. The sound absorption mechanisms of plant fibers were proposed and the multi-scaled and hollow lumen structures provided major contributions.

Demonstration parts made by plant fiber reinforced composites used for aircraft interiors, car roof and other transportation vehicles were manufactured and applied in the national key projects.

DEVELOPMENT OF MODIFIED EPOXY NANOCOMPOSITE COATINGS FOR RESTORING OF TRANSPORT VEHICLES

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Recently, in order to increase economic independence of the leading countries of the world, it is important to use the latest technologies in the import and export of manufactured products. In this context, the leading economic point of view is the use of not only new technologies, but also the use of composite materials with increased performance characteristics. An actual for today is the development of transport technologies, which involves the use of environmentally-green materials of low cost with improved properties. In this context, there is a need to use polymer composites in the form of protective coatings for restoring and repair of means of transport.

Proceeding from the above, it is necessary to state the expediency of developing new polymer composites, which in the complex would be marked by increased performance characteristics. This is achieved by the introduction of modifiers, nano-and micro-dispersed fillers of various nature. In this case, the use of particles that are industrial waste to achieve high indexes of performance characteristics of the coating is relevant both in terms of economic costs for the formation of composites, and for increasing the reliability of operation and decreasing the volume of repair work of equipment. Such an approach, in our opinion, will allow to get protective coatings that need be used for restoring parts of vehicles and machinery of means of transport, especially river and marine.

The work shows the technological regimes of the formation of compositions, methods of their application on the means of transport in natural conditions, as well as analysis of the main directions of increasing the performance of epoxy composites. At the same time, the relevant for increasing the reliability of the work of the parts of transport with polymeric coatings, the adhesion strength of the adhesive to the base and the cohesive properties of the coating. The latter can be improved by the introduction of ingredients that are active prior to the interaction with the polymer. This will allow to get materials with improved anti-corrosion properties and wear resistance.

The influence of the paraminoazobenzene modifier on the processes of the formation of an epoxy binder has been studied for the first time. The regularities of improving the adhesion, physico-mechanical and thermophysical properties of a modified polymer matrix have been established by introducing an additive of the optimum content due to the formation of a material with a uniformly distributed structure characterized by a significant number of chemical bonds per volume.

The influence of the powder in the form of a mixture of nanodispersed compounds (d = 30–90 nm) on the properties of composites was studied and its optimal content in the epoxy binder was determined. It is proved that the introduction of nanoparticles for optimal content causes a change in the topological structure of the composite and a conformational set of macromolecules, which improves the cohesive, including the thermophysical properties of the material.

The regularities of the influence of microdisperse particles (d = 8–12 microns), and also the iron scale (d = 60–63 microns) on the processes of structuring of materials are established. It allows to receive composites with increased indexes of mechanical and thermophysical characteristics by introducing microparticles into the binder for insignificant content due to the interaction of active C-O and OH-groups on the surface of particles with macromolecules and segments of the epoxy binder. This will significantly increase the lifetime of the coatings of parts of vehicles.

New polymer composites and technology of their formation are introduced at the enterprises of Ukraine. As a result of tests of developed protective coatings, it was found, that an increase in the corrosion resistance of parts of vehicles is 2.3–2.8 times, and resistance to hydroabrasive in alkaline aggressive environments is 1.6–1.8 times in compare with traditional protective coatings.

PREPARATION, STRUCTURE AND PROPERTIES OF POLYMER-BASED NANOCOMPOSITES

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The nanocomposites are materials, which involve fillers in the nanometer scale, yielding substantial improvements. Polymer based nanocomposites have received much attention during the past decades and have great interest both in the academic field and in industry, since they often give more attractive improvement to material properties than both micro- and macrocomposite materials.

These studies devoted to the preparing and investigating of different types of novel polymer nanocomposites. In the first part, epoxy-ZnO/CdS (EP-ZC) nanocomposites capable of shielding both UV and blue radiation were developed. The ZnO/CdS nanoparticles were synthesized through the growth of CdS on prefabricated ZnO quantum dots (ZnO QDs). The ZnO/CdS nanoparticles exhibited strong absorption over the wavelength region extending from UV light to blue light. In situ polymerization was employed to prepare the EP-ZC nanocomposites, which were highly transparent at wavelengths greater than 500 nm. It was found that the EP-ZC nanocomposites could almost completely block UV light between 200–400 nm as well as more than 80% of the blue light between 400–450 nm with addition of 0.3 wt% ZnO/CdS nanoparticles. Their optical transparency to visible light beyond blue light was the same as that of pure epoxy. In the second part, reactive antioxidant and UV-absorbent groups were successfully immobilized onto the surface of nanosilica particles through aminosilane coupling agents which acted as cross-linkers. Two kinds of novel anti-ageing nanosilica particles were synthesized and their structures were characterized. The anti-aging behaviours of the nanosilica-immobilized antioxidant and the UV-absorbent in polyethlylene (PE) and polypropylene (PP) were investigated by thermogravimetric analyses, oxidation induction time tests and accelerated thermal ageing and UV light ageing tests. The results indicated that the novel anti-ageing nanosilica particles can significantly improve the thermal oxidant stability and photostability of PE and PP composites. It was found that there existed clear synergistic effects of the thermal oxidation resistance behaviours between the two kinds of functional nanosilica.

COMPOSITE MEMBRANES BASED ON INERT MACROPOROS POLYMERS MODIFIED WITH INORGANIC NANOPARTICLES FOR PROCESSING OF WASTES AND FEEDSTOCK OF FOOD INDUSTRY

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Hydrophilization of inert polymer membranes is an important practical task, This approach allows us to reach higher liquid flux, to improve rejection ability and to prevent fouling with organics. The membranes based on inert macroporous polyacrylonitrile were modified with nanoparticles of hydrated zirconium dioxide or zirconium hydrophosphate. The membranes were studied using SEM, their active layer was researched with TEM (after its grinding). A theoretical approach was applied to precipitation of inorganic particles inside pores of the polymer. In accordance with Ostwald-Freundlich equation, the particles of zirconium hydrophosphate are larger comparing with oxide evidently due to bigger molar volume. Therefore, the particles of zirconium hydrophosphate occupy only the support of the membrane due to steric limitations, whereas the oxide particles are deposited both inside the support and active layer. The nanoparticles of hydrated zirconium dioxide has been found to form aggregates, pores between nanoparticles are responsible for secondary porosity that provides rejection of colloidal species. In fact, inorganic particles form so called intraporous active layer, which is located inside pores of polymers.

The membranes were calibrated by filtration of the solutions of bovine serum albumin (BSA. 69 kDa) and polyethylene glycols (PGE, 40 kDa). Regarding the membranes containing oxide, the rejection of PGE and BSA is 10 and 90 %% respectively. It means, the size of secondary pores are within the interval of 14-18 nm. In the case of pristine membranes and materials containing zirconium hydrophosphate, no rejection has been found. The membranes obey Darcy law up to 4 bar. The thickness of intraporous active layer has been estimated based on Kozeny-Carman equation. This characteristic is about 40 μm for the membrane containing zirconium oxide, it is comparable with the thickness of an active layer attached to the polymer substrate. In the case of the membrane modified with phosphate, the thickness is several hundreds of microns. This corresponds to thickness of a substrate. The oxide-containing membranes were applied to processing of milky whey and sugar beet juice. Fouling of the oxide-containing membranes is due to cake formation on their outer surface. This precipitate can be removed easy without aggressive reagents.

CATALYZING CARBONIZATION OF POLYMER ITSELF BY COMBINED CATALYSIS: IMPROVING FIRE RETARDANCY

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Polymers (such as polypropylene (PP) and polyethylene (PE)) are a kind of the largely consumed materials. They exhibit desirable physical, mechanical, and processing properties that make them a versatile material. However, polymers have some deficiencies that hinder their wide usage in various fields, such as their flammability. Consequently, the improvement of flame retardancy of polymers has been an urgent topic. Among various environmentally friendly methods for the flame retardancy of polymers, forming carbonaceous protection layers during combustion has been proven to be an effective way, as carbonaceous materials have the properties of less flammability, being able to reflect energy and generating a barrier between the degradation products of the polymer and the flame. Unfortunately, many polymers (such as PP and PE) are a type of thermally degradable materials (non-charring materials), so their degradation products are volatile fragments that combust easily without any residual char. To improve the flame retardancy of these polymers, a general way is to add various intumescent flame retardants (IFRs) to form the protective layer, but the IFR system is often moisture sensitive and capable of migrating to the surface of the composites, leading to decreased flame retardancy efficiency.

In contrast, forming a carbonaceous protection layer via catalyzing the carbonization of the polymer itself during combustion is another more attractivestrategy [1-4], due to its advantages, including highly efficient flame retardancy, long-term stability with no deterioration, no damage to the mechanical and processing performances of polymer matrix, etc. In this report, we have demonstrated that some of the combined catalysts are effective in promoting carbonization of common polymers such as PP and PE [2, 4]. As a result, fire retardancy of these polymers could be improved. Subsequently, we found that a novel combined catalyst of nanosized carbon black with Ni_2O_3 could promote the carbonization of PP [5], which results in the improvements of fire retardancy of PP. Also the above phenomena have been observed in other polymers, such as PE, polystyrene [5] and even polylactide (PLA) [6]. Very recently, we found that some inorganic binders could be used as synergists to further enhance fire retardancy of polymers in different test standard, including LOI and UL94 testing. The mechanism about the effect of synergists on the combined catalysis was investigated.

THE SYNTHESIS AND EVOLUTION OF STRUCTURE-PROPERTY RELATIONSHIPS OF CORE-SHELL NANOCOMPOSITES OF INTRINSICALLY CONDUCTING POLYMERS

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Duringlastdecadeinterests in studies and applications of intrinsically conducting polymers (ICPs) significantly shifted to their multifunctional composite materials for using in high-tech and socially importantareas e.g. in photovoltaic, electrochromic and sensory devices, biomedical systems, supercapacitors, in electromagnetic interference shieldingcoatings, etc. An essential factor that affects properties of these composites is specific interactions between their components. We demonstrate that this effect isvery noticeable in the nanocompositeswithacore-shell morphology, in which the core is of organic or inorganic nature, and the shell is ICPnanolayer deposited on the surface of the coredue to polymerization a monomer. Control of such interactions opens significant perspectives in creating the new composite materials with specified properties.However, effectiveness of the control depends not only on the choice of the core/shell nature and understanding the interactions at the interfaces in the nanocomposite, but also on our knowledge of changes in the polymer of the shell in comparison with the pure one. Such issues of ICPs composite materials are studied enough yet.

In fact, our report is an attempt to partially disclose theseissues on the basis of the results of studies of the regularities of synthesis, morphology, structure, molecular, electrical and other properties of ICPs (polyaniline, polytrimethylthiophene, polypyrrole) contained in the shells of their nanocomposites with metaloxidesandchalcogenides, carbon nanotubes, dielectric polymers. This allowed us to discoverthat ICPs in shells compared with the pure polymers, differ greatly in the degree of crystallinity, crystallite sizes, molecular weight, oxidation and conjugationdegree, electrical conductivity, thermal stability, sensing propertiesetc. These results can be used to develop methods to manufacture the multifunctional ICP composite materials with high operational properties.

RESEARCH PROGRESS ON BIO-BASED POLYMERIC MATERIALS

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Bio-based polymers are a class of polymers which were derived from renewable resources. Great attention has been paid from both academic and industrial society since they are sustainable and renewable materials. Some progress was made at Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences. This talk will review our research progress on synthesis of 2,5-furandicarboxylic acid and its polyesters, and natural fiber reinforced polymer composites with high load. The results indicate that the furan based polyester (PEF) showedbetter properties of heat resistance and gas barrier than benzene based counterparts (PET) (Table 1). The natural fiber reinforced polymer composites exhibit higher mechanical properties and water resistance than conventional wood-plastic composites which are mainly composed of wood powder and polymer.

Table 1: Property comparison between PEF and PET

Properties	PET	PEF	Note
Tg (°C)	70	88	Increase 18°C
Tm (°C)	260	217	Decrease 43°C
CO_2 Barrier (10^{-10} cm^3•cm/cm^2•s•cmHg)	0.11	0.0078	14 times of PET
O_2 Barrier (10^{-10} cm^3•cm/cm^2•s•cmHg)	0.044	0.0074	6.8 times of PET
Stress (MPa)	60	85	Increase 40%
Modulus (GPa)	1.9	2.8	Increase 47%
Elongation (%)	>110	5.4	Decrease

ELASTIC-PLASTIC CHARACTERISTICS OF POLYVINYL CHLORIDE PLASTISOL-THERMALLY EXPANDED GRAPHITE NANOCOMPOSITES

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The influence of thermally expanded graphite (TEG) on the structure and elastic-plastic characteristics of nanocomposite materials (NCM)on the base of polyvinyl chloride plastisol (PVCP) is considered in this study. The processing criteria for composite components have been specified to achieve the uniform distribution of TEG particles in the sample and to optimize the practically important characteristics of such nanocomposites.

It was shown that the concentration of the filler effects the formation of the layered structure and elastic characteristics of the material. It was found that, stability of NCM samples in response to shock wave loading varies depending on the concentration of TEG filler. There was less material's resistance atconcentrations close to the percolation threshold and > 15 vol.% and higher resistance for the concentration of 12 vol.%.

It was shown that at TEG concentrations up to 4 vol.%, the matrix, cohesive filler bonds and the filler-matrix bonds strengths determine the strength of NCM samples. The character of fracture is plastic. When filling> 4 vol. %, there is a transfer from elastic to viscoelastic deformation and the cohesive strength between TEG particles increases. At high graphite concentrations, the plasticity of the composite material decreases, and the elastic limit increases. The elasticity modulus of the NCM increases with increasing in filler concentration. For unfilled PVCP, the modulus of elasticity is 9.6 MPa, and for NCM with a content of 50 vol. %TEG it increases to 730 MPa.

INVESTIGATION OF ADHESIVE STRENGTH OF PROTECTIVE EPOXY COMPOSITE COATINGS

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Epoxy composite coatings are the most common type of protective coatings used in engineering, construction and chemical industries. The dissemination of these coatings is facilitated by their low cost, easy method of obtaining, the possibility of material modification and long service life.

For increasing the mechanical and performance characteristics of epoxy resins, fillers of various functional applications are introduced into their composition. Since the coating has to work under abrasive wear and aggressive environment, the following finely divided fillers are selected: chromium oxide, aluminum oxide and titanium oxide.

Determination of the optimum content of fillers in the epoxy matrix is carried out by the nature of the effect on the composite material adhesion strength. It has been experimentally determined that the maximum content of fillers, in which the growth of adhesion strength increases, is 45...55 mass fraction, which can be explained by the formation of additional chemical bonds. The highest adhesive strength values were obtained for epoxy composites filled with aluminum oxide powder at a content of 50 mass fraction. (45,5 MPa). For composites filled with chromium oxide and titanium oxide, the lower adhesion strength values are obtained. Content of fillers over 70 mass fraction led to a decrease in this characteristic due to defect structure.

The surface of the adhesive seam of the epoxy composite with aluminum oxide occupies a larger area than the incomplete polymer, indicating an increase in the adhesion strength of the material with a metal surface. Chromium oxide powder has the lowest adhesive ability to form strong bonds with the epoxy matrix and metal surface, which is confirmed by the presence of a small number of areas covered with the developed material. The introduction of titanium oxide into the composition enhances adhesion strength in a manner similar to that of an alumina oxide powder due to the high surface energy of the filler.

Taking into account the high values of adhesion strength, it is recommended to use alumina oxide powders and titanium oxide powders in the amount of 40-60 mass fraction to study the mechanical and operational characteristics of the epoxy composites.

FLUORESCENT AND COLORIMETRIC SENSOR SYSTEMS FOR FOOD TOXINS AND ENDOCRINE DISRUPTORS DETECTION BASED ON MOLECULARLY IMPRINTED POLYMER MEMBRANES

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Easy-to-use fluorescent and colorimetric sensor systems based on rationally-designed molecularly-imprinted polymer (MIP) membranes for efficient detection of trace levels food toxins and endocrine disruptors have been developed. The MIP membranes were synthesized according to the principle of semi-interpenetrating polymer networks (semi-IPN) formation. The composition of the MIP membranes having synthetic toxin-selective receptor sites was optimized using the method of computational modelling. The affinity MIP membranes for the selective recognition of a broad range of analytes (food toxins i.e. aflatoxin B1, zearalenone and endocrine disruptors i.e. phenol, bisphenol A, and sulfamethoxazole) were synthesized *in situ* and used as a basis for the optical sensor systems. The sensor systems function according to the following principle: 1) the analytes are to be selectively adsorbed by synthetic receptor systems; 2) the further UV-irradiation of the latter initiates native fluorescence of the small organic molecules (aflatoxin B1, zearalenone) with the intensity proportional to their concentration in the analyzed sample. Alternatively, colorimetric sensor systems for the molecules capable of colour complexes' formation (phenol, bisphenol A and sulfamethoxazole) were developed. Intensity of staining of the polymeric membranes with the selectively adsorbed small organic molecules was proportional to their concentration in the analyzed samples. High adsorbtion capability and affinity of the synthesized MIP membranes resulted in high sensitivity of sensor systems on their basis as well as wide linear dynamic range (1-1000.0 ppb). High selectivity of the sensor systems was confirmed in experiments with close structural analogues of the analytes. The proposed MIP membranes are capable of not only selective recognition of the analytes but also for the generation of the sensor response, which can be easily registered. Practical application of the described sensor systems does not require expensive equipment. Their application in food and environmental monitoring would increase safety of environment, drinking water, and foodstuffs.

ACKNOWLEDGEMENT. Financial support from National Academy of Sciences of Ukraine and Ministry of Science and Education of Ukraine is gratefully acknowledged.

SYNTHESIS, STRUCTURE AND PROPERTIES OF POLYOLEFIN THERMOPLASTIC ELASTOMERS

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Polyolefin elastomers are widely applied in the past decades, among which ethylene-propylene-diene terpolymers (EPDM) have been produced since 1970's, and ethylene-α-olefin copolymers (POE and OBC) have been developed in 1990's. The last two decades witnessed rapid growth of POE and OBC materials for their wide applications as thermoplastic elastomers. However, there are still strong needs for new types of polyolefin thermoplastic elastomers (TPO) that show unique properties and can be produced at low costs.

In this presentation, we will introduce our recent studies on synthesis, characterization and properties of three types of polyolefin thermoplastic elastomers.[1-4] TPO based on ethylene-propylene copolymerization with metallocene catalysts has been synthesized. By using bis(2,4,7-trimethylindenyl)zirconium dichloride as catalyst and BHT-treated MAO (BMAO) as cocatalyst, ethylene-propylene copolymer with broad composition distribution was synthesized. The material showed no obvious yielding point during tensile test and high recovery from 100% strain, which indicate properties of a thermoplastic elastomer. By ethylene polymerization with novel α-diimine Ni(II) complexes activated by $AlEt_2Cl$, highly branched polyethylene (HBPE) with different branch density and molecular weight were synthesized. The new catalysts showed evidently improved thermal stability and strong chain-walking ability at high temperature and high ethylene pressure. HBPE synthesized with the new catalysts showed excellent elastic recovery properties, exhibiting potential applications as a new type of thermoplastic elastomer. A novel type of TPO based on polyethylene/poly(ethylene-*co*- propylene) in-reactor alloy was also synthesized by periodic switching polymerization process (PSPP) using supported Ziegler-Natta catalyst. Mechanical properties of the products are similar to those of TPO. Mechanical blends of PP with the PE/EPR alloy showed much better toughness than PP/EPDM blends of the same composition, meaning that the novel PE/EPR reactor alloys may be used as highly efficient toughnening agent for PP and other comodity resins.

CARBON FIBROUS FILLER OF KNITTED STRUCTURE FOR MULTIFUNCTIONAL POLYMERIC COMPOSITE MATERIALS

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Carbon fibers (CF) have a complex of high physical and mechanical properties such as, low specific gravity, electrical and thermal conductivity, thermal and chemical resistance, which provide advanced characteristics of composite materials based on them in the aerospace, mechanical engineering, wind power engineering, electrical engineering, etc. For better realization of the properties of both carbon fibers and corresponding multifunctional composites reinforcing filler based on knitted structure produced from high-strength and high modulus carbon fibers had been developed. The high fragility of carbon fibers, especially high-strength carbon fibers from Polyacrylonitrile (PAN) precursor, complicates their textile processing because of necessity of multiple bending. To avoid multiple bendingthe special structure of a weft knitted fabric had been developed where high-strength CF from PAN-precursors are laid in a knitted fabric with a straight thread, i.e. they are not bent by the needles of a knitting machine to form loops.

Samples with different filler packing patterns - unidirectional (1D) and two-dimensionally reinforced (2D) polymer composites had been produced from carbon fibers Tenax-J/E HTA 40F13 and UKN 5000. The obtained level of mechanical properties for 1D and 2D composites, taking into account the location of high-strength carbon fibers, makes it possible to choose the most rational variant of the reinforcement scheme, where the most part of the high-strength fibers are located in the direction of the action of mechanical loads under service conditions.

The electrical conductivity of knitted fabrics had been investigated depending on the direction of high-strength carbon fibers. The anisotropy of the electrical conductivity along the high-strength fibers had been revealed in comparison with the loop rows. The development of combined carbon-glass canvases makes it possible to use them as a heating element.

The results of screening properties tests for polymer based composites reinforced by carbon weft-knitted cloths have shown the possibility of their using as shielding materials with the ability to absorb electromagnetic radiation.

UTILISATION OF SLUDGE WASTE PRODUCTS OF BEARING STEEL FOR MANUFACTURING OF WEARPROOF MATERIALS

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Among the secondary metal-containing waste products generated during the processing of structural alloy steels, one of the most technologically advanced is bearing steel SHK-15 cutting chip and sludge. A significant part of the bearing steel waste is a non-abrasive sludge - waste of surface generation operations, which is a powdery chip moistened with organic based lubricating coolant.

In the Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine was developed a technology for obtaining blanks and products from wear-resistant material based on these wastes using powder metallurgy methods.

When choosing the alloying scheme of the developed material it was taken into account that new possibilities for obtaining high-efficiency economically-alloyed steels opens up the use of boron as an alloying element. As basic boron-containing alloying admixture the boron carbide was used.

The technological process for manufacturing of billets from the material includes reduction annealing of the initial powderlike sludge, its mixing with 0.5-1.5% of boron carbide, consolidation of porous preforms, their sintering in a reducing atmosphere and subsequent hot forging in the closed or semi-open die.

It is shown that at the sintering of iron-carbon alloys with boron carbide, the effect of the formation of specific framework structure is revealed, which is exhibited in the fact that carbides enter predominantly in perlite, and borides are localized mainly along the grain boundaries.

After hot forging and subsequent heat treatment, the obtained materials have a strength of 920÷1130 MPa and a hardness of about 25÷35 HRC with a substantially heterogeneous structure containing significant amount of solid carbide and boride phases.

The results of tribotechnical tests of hot-forged blanks on the basis of slurry wastes with 0.5 ÷ 1.5 % of boron carbide and 0.6 % graphite, which were carried out without lubrication at a sliding speed of 1 m /s and loads of 1÷8 MPa with counterbody of hardened steel 45 (HRC 45-48) showed high wear resistance of the resulting materials.

DEVELOPMENT OF H_2O_2-MEDIATED PATHWAY MODEL FOR ELUCIDATING THE OXYGEN REDUCTION MECHANISM IN WASTEWATER TREATMENT AND RECYCLING SYSTEM

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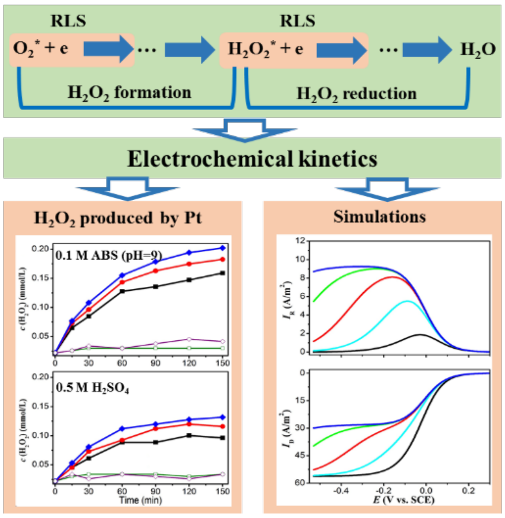
Oxygen reduction reaction (ORR) on an electrode is a vital process for energyconversion, wastewater purification and recycling, and chemical production as well. This process is a multi-stepone that most likely involves H_2O_2 as a stable product, and the mechanism of this reaction focusing on the productionsof H_2O and H_2O_2 has not to be elucidated yet. In this study, simplifying the multi-stepprocess of ORR by means of rate-limiting step (RLS)-based unit reaction led to a H_2O_2-mediated pathway model. The model is comprised of two unit reactions from O_2 to H_2O_2, then further to H_2O. A parameter called the tending degree (R_{H2O2}) was proposed to quantify the reaction tendency towardH_2O or H_2O_2 production. Thereafter, electrochemical kinetic equations were established to describe the sub-processes of ORR, and enabled this model to relate the elementary RLS. By using the established equations, the ORR behaviors in rotating ring-disk electrode (RRDE) system were simulated. The simulation results indicated that thereaction tendency in terms of R_{H2O2} value between 1 and 0 unified all ORR observations, validating the H_2O_2-mediated pathway model. Furthermore, the state-of-the-art direct 4e catalyst of Pt was shown to follow this model by the RRDE tests and the electro-generation experiments of H_2O_2. The developed H_2O_2-mediated pathway model was demonstrated to be widely applicable and provided a new insight into the ORR mechanism.



TECHNOLOGY FOR MANUFACTURING OF FERROSILICON ALLOY BY UTILIZATION OF HEAT POWER PLANT ASH WASTES

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When burning coal in heat power plants the mineral components are converted to ash and slag, which are stored as waste of energy production in ash dumps. Characteristics of ash are different in different heat power plants, because they depend on the composition of the mineral components of the coal, the method of preparing fuel for combustion, combustion technology, and the flue gas cleaning system from ash.

In the present work, the material from the ash dump of the Trypillia thermal power plant (Ukraine) was investigated by methods of emission spectral, solution chemical and electron-probe analysis and a technology for their processing with the production of silicon-containing ferroalloy as a final product was proposed. It is established that the analyzed slags are heterogeneous in composition and represent a fractional mixture, the main components of which are iron and silicon (mainly in oxide form). In some fractions there is also a lot of aluminum, calcium and magnesium (in similar coal). Some fractions contain titanium of the order of one percent, and in one of the fractions - manganese, vanadium and nickel (about 0.1%).

The technology for utilization of the waste was carried out by melting them in a protective medium with the addition of sodium tetraborate to the initial charge. The composition of the resulting alloy is: Fe–86.4%, Si-10.6 % (wt.), containing also Ti, V, Mn, Cr, P, S in the amount of 0.15–1.26 %. The phase composition of this ingot is: iron silicide Fe_3Si – 85.14 %, cementite Fe_3C – 14.86 (wt.) %. Part of silicon impurities and the bulk of aluminum and calcium impurities have passed (in the oxides form) to the slag, whose composition in this case is close to the marl - raw material for the production of cement. The ingot obtained from the slurry has a high hardness ranging from 40 to 51 HRC.

The results of the research indicate the possibility of using the ash dump in the production of ferroalloys for their further use in metallurgical production, and also for the development of wear-resistant steel based on this material.

POLYMERIC JANUS MEMBRANES FOR DESALINATION

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Janus membrane with asymmetric wettability has been widely explored in oil/water separation, distillation, fog-collecting, directional fluid transportation, bubbling etc. The current fabrication methods include floating, electro-spinning, surface coating, surface grafting etc., which limit the scaling up due to the complicated process. In addition, the facile tuning of wettability of top and bottom surfaces is still challenging. We proposed a chemical phase inversion strategy to achieve porous Janus membrane with opposite wettability. We control the directional segregation of hydrophilic polymer via an inside-out or outside-in route to enrich on the top surface of the membrane, and then form a robust network via hydrothermal crosslinking reaction. The contact angle difference can be ~140° . Based on Janus membrane, we further immobilize plasmonic nanoparticles on the hydrophilic side to produce a Janus membrane for photo-thermal conversion. It assembles light adsorption, thermal confinement, water drawing, vapor transpiration and self-floating in one thin-film membrane to realize the seawater desalination via only solar input. In addition, the Janus membrane shows unprecedented forward osmosis performance with ultra-high water permeability and ultra-low reverse salt flux. The hydrophilic side can transport water unidirectionally, while the hydrophobic side and repel the reverse salt flux via the trapping air cushion.

COMPOSITES BASED OF HYDRATED ZIRCONIUM DIOXIDE MODIFIED WITH ADVANCED CARBON NANOMATERIALS

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The subject of this work is to develop multifunctional adsorbents for water decontamination: the materials give the possibility to remove both inorganic ions and organic pesticides from diluted aqueous solutions. The composites included hydrated zirconium dioxide and graphene oxide (GO, ≈2 mass %). The carbon nanomaterials were obtained using both classical chemical method and electrochemical techniques. The composites were synthesized by deposition from sol of insoluble zirconium hydroxocomplexes, in which the nanosized GO particles were dispersed. The adsorbent as well as its constituents were investigated with XRD and XPS analysis, FTIR spectroscopy, TEM and SEM. It has been found that GO nanoparticles cover the particles of inorganic oxide. On the other hand, the composites involve agglomerated GO sheets. Several groups, which are characteristic for GO, were found: vibration spectroscopy indicated C–OH (attributed both to hydroxyl and carboxyl groups), C=O (related to carboxyl groups) and C–O–C bonds (epoxy groups). Among them, carboxyl and phenol groups are responsible for ion exchange. At the same time, hydrophobic regions of GO provide adsorption of organics. Main regularities of adsorption of toxic species (Pb^{2+} cations and $HCrO_4^-$ anions) were studied. Adsorption of such pesticides as epoxiconazole, quizalofop-ethyl, tebuconazole, acetamiprid, carboxyn, thiamethoxam from the mixed solutions was also researched. For instance, the solution contained initially 0.85-170 mg dm^{-3} of carboxyn and 0.35–70 mg dm^{-3} of epoxiconazole. As found, GO improves adsorption of Pb^{2+} ions. Since anion exchange ability of GO is weakly expressed, the modifiers depress $HCrO_4^-$ adsorption. Depending on initial content of pesticides in a solution, adsorption capacity of the composites reaches, for example, up to 79 mg g^{-1} (towards carboxyn) and up to 7 mg g^{-1} (epoxiconazole). When the most diluted solution is used, the pesticide content in water is lower than maximal allowable concentration. The advantages of the composites over known carbon materials is mechanical strength and large granules. This gives a possibility to use them in adsorption columns. Comparing with inorganic adsorbents, the composites are multifunctional: they are able to remove both ions and molecular substances from water.

HEREDITARY MODIFICATION OF STEEL WITH THE USE OF SECONDARY METAL WITH A PREPARED STRUCTURE

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In the world foundry industry the volume of alloy steels secondary metal use has been increased in recent years. This opens new technological opportunities for improving the quality and properties of cast products through the use of structural heredity. Industrial waste in the form of waste parts, charge blanks, as well as ligature and modifying additives with a nonequilibrium prepared structure has useful hereditary information. Hereditary bond in the system "solid-liquid-solid" metal can be effectively used to improve the characteristics of the structure and properties of cast products.

On the basis of systematic studies the dominant role of the temperature and time conditions of crystallization on the formation of the cast structure and elements of heredity in the components of the charge and modifying additives were established.

It was shown that introduction into the melt of dispersion-structured additives of steels of similar chemical composition (15–20%), which is dispersed by accelerated crystallization, creates the prerequisites for the formation of a considerable amount of nuclei of crystallization, an increase the strength of steel by 15–20%, plasticity by a factor of 1.5-2 and impact strength by 30–40%. The perspectives of using as modifiers of the hereditary modification of granular and powdered metals that got at rapid cooling (Osprey process) during the crystallization as well as steels after hardening and deformation-thermal treatment are show. All the proposed modification improves characteristics of dendrite structure, grind grain, reduce liquation and increase the level of mechanical properties of steels to the level of details from deformed and thermally strengthened metal.

The established regularities of the effect of the prepared highly disperse structures of the charge components and modifying additives open new way to control cast structure and improve the properties of steel castings, the creation of new foundry technologies and materials.

MOLECULAR SIEVE MEMBRANES

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Gas separation with membranes is energy efficient and environmentally friendly alternative to cryogenic, adsorptive or absorptive gas separation processes. It is well known that conventional polymeric membranes are suffering from the so-called Robeson's upper-bound, i.e., a trade-off relationship between permeability and selectivity. Molecular sieve membranes are expected to overcome this limitation relying on their size exclusive separation ability. Zeolite is a representative as inorganic molecular sieve. Unlike amorphous carbonaceous or oxide molecular sieves, crystalline zeolites contain uniformly sized pores of molecular dimensions, which makes them ideal candidates for molecular sieve membranes.MOFs are novel crystalline hybrid materials consisting of metal ions or clusters interconnected by a variety of organic linkers. Their unique properties, such as highly diversified structures, high surface areasand specific adsorption affinities, makes them excellent candidates for usage in the construction of molecular sieving membranes with superior performances. Moreover, many layered MOFs materials with abundant porous structure and functional surface groups has been reported in recent years. They could serve as a diverse source of MOF-based 2D nanosheet membranes. In this presentation, I would like to highlight our research achievements on the synthesis and application of zeolite membranes as well as MOF membranes, including our latest breakthroughs in the preparation of2D MOF nanosheetsmembranes. In addition, I also would like to talk about the successful implementation of zeolite membranes in pervaporation and vapor permeation processes in industrial dewatering applications.

THE MANUFACTURE OF DIE-CASTING TOOL FOR MOLD CASTING OF COPPER AND COPPER ALLOYS

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The results of work on the stamping steel development with adjustable austenitic transformation, which have an increase in the values of physical and mechanical properties, are compared with the grades of steels H-10 and H-13. The urgency of the work is that the developed steel can be applied in the field of mechanical engineering for hot pressing of the copper-nickel alloy of grades C70400 and C71500 with the increased exploitation life, in compare with steel H-10. The work is carried out in complex temperature-force conditions in the operating temperature range of 860–960 ºC. In addition, developed stamped steel with adjustable austenitic transformation can be used for warm deformation of copper at operating temperatures of 550–620 ºC with an increased operating life, compared with steel H-13. The investigation of the phase-structural state of steel, depending on the optimal thermal treatment regimes, is presented. Optimized thermal treatment (annealing) of steel with partial recrystallization, made it possible to mechanically handle ingots for making matrixes of a die tool. A special role in improving the service properties of a stamping steel tool with adjustable austenitic transformation has the effect of doping components (nitrogen, vanadium) on the Cr-Mo-Ni system. The increase of the tempering temperature by 60–70 ºC, taking into account the lack of the recrystallization process, allows dissolving a considerable number of carbide phases M_7C_3 and $M_{23}C_6$ in homogeneous austenite. The given phases actively influence on the steel hardening during the process of release. Thus, during the quenching of steel, conditions were created for the dissolution of the carbide phases, where overpressure of the alloying components of the martensitic structure occurred. This made it possible to obtain other carbide phases that less coagulate and stabilize the steel during the release process. The obtaining of the carbonyl phases of the test steel played a key role in the working zone of the matrix of the stamping tool, which provides high wear resistance in the initial period of operation at a temperature of 860 ºC and, under the force of effort, there is an additional deformation strengthening of the thin surface working layer, which leads to an increase in thermal stability.

NON-PRECIOUS METAL-CARBON CATALYSTS FOR SUSTAINABLE PRODUCTION OF CARBON-NEUTRAL PRODUCTS AND ENGINEERING CATALYTIC MATERIALS FOR INDUSTRIAL USE

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The increasing concentration of CO_2 in the atmosphere threatens the world's sustainability with the global warming. Electrochemical CO_2 reduction reaction (CO_2RR) to produce CO combined with hydrogen evolution reaction (HER) can realize sustainable production of syngas with tunable H_2/CO ratio, in addition to the coal, biomass or natural gas-derived syngas, for Fischer-Tropsch synthesis (FTS) to produce carbon-neutral fuels and fine chemicals, which results in negative CO_2 emission or net CO_2 removal from the atmosphere. Although noble catalysts show good activities for catalyzing these processes, their expense and scarcity are prohibitive to large-scale commercialization. Hence, there is a need to develop precious-metal-free catalysts with comparable or even better CO_2RR, HER and FTS performances.

In this presentation, the well-designedZnO/CNTs, MNx/carbon and Ni/NiO@C catalysts were developed for the CO_2RR and/or HER to produce CO and/or H_2. The catalyst structure-performance relationships are established by combining DFT calculations with multiple techniques such as the aberration corrected HAADF-STEM and the synchrotron radiation-based X-ray absorption spectroscopy (XAS). Then, on theχ-Fe_5C_2 Fischer-Tropsch catalyst, activation and subsequent conversion of CO and H_2 were further investigated via FTS to produce fuels and fine chemicals. Compared to monometallic FTS catalysts, the χ-Fe_5C_2 catalyst exhibits unique structural and electronic properties. Interestingly, the charge of the involved surface Fe atoms for the CO activation is discriminated as a good descriptor for the facet-dependent CO activation, and the surface C atoms are found to be involved in the FTO reaction, which always locate at the end of the carbon chain of the products. It is not expected that this catalyst shows not only the unfavorable formation of lower olefins, but also rapid deactivation due to the formation of the encapsulating carbon. Furthermore, the introduction of promoters can significantly improve the selectivity to lower olefins as well as the catalyst stability.The insights revealed here could shed new light on the rational design of non-precious metal-carbon nanocatalysts for the production of carbon-neutral products.

PROCESSING OF CARBON-CONTAINING WASTE CONTAMINATED WITH HAZARDOUS OR RADIOACTIVE IMPURITIES

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The report is devoted to the problem of energy recycling from carbon-containing wastes that are hazardous or radioactive. The most known among the hazardous wastes are chlorinated. In accordance with the Directive 2000/76/EC the temperature should be maintained at the level of 1100 °C in case of incinerations containing more than 1% wt. of halogenous organic substances in terms of chlorides, and each local volume of gas produced in the processing has to be kept at this temperature over time ≥ 2 s.

The savage sludge of the aeration stations is one more well-known group of hazardous wastes, in which accumulated heavy metals.

A full-scale pilot sample of the technological line for the energy-efficient processing of hazardous wastes is presented, meeting the highest ecological requirements. In the current version, it is oriented to the processing of chlorine-containing waste and savage sludge of the aeration stations containing heavy metals. In the case of chlorinated wastes, they are gasified at a temperature of not less than 1100 °C. After rapid cooling, the gasification products are washed through a filtering liquid in which the chlorine passes into neutral compounds. Purified gasification products can be used for the production of electrical and / or thermal energy or as valuable chemical raw materials. In the case of processing of savage sludge, the line is supplemented with equipment for their granulation and vitrification of the resulting slags. The latter includes liquid slag removal at temperatures above 1400 °C. Heavy metals remain incorporated in the obtained melt of the ash residue, and the resulting lava-like mass after its cooling is not leached and is safe for the environment. Steam-water plasma is used for additional blasting in the gasifier to ensure maximum reliability and safety of the process.

The expediency of extending the same technology to the processing of radioactive contaminated biofuels is discussed.In Ukraine it may be the radioactive wood from the Red Forest of the Chernobyl zone. In this case, both the ash residue and the filtrate of the gas cleaning system are to be immobilized.

NEW TRENDS IN DEVELOPMENT OF METALLURGICAL SLAGS RECYCLING TECHNOLOGIES

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The analysis of the state of ecological and economic efficiency of metallurgical slags processing is carried out. A modern principle in metallurgy is proposed, according to which slags should be considered not as waste, but as a material, the production of blast-furnace production, which requires the development of complex of new technological processes for processing slag melt and solid (granulated) slag, ensuring the production of valuable materials. The thematic focus of research and technological developments for the implementation of the proposed modern principle in metallurgy is determined.

Considering the metallurgical slags as products of blast-furnace production, research has been carried out, the main directions for development have been determined and a number of new technological processes have been developed for complete and non-waste processing and recycling of slag melts and granulated slag, i.e.:

- determination of the heat content of fiery-liquid slags (melts) and calculation of the power capacity of the installation using recycled heat of slag melts;
- development of technology and devices for the production of PCs (Portland cement) from slag melt, methods for granulation and enrichment of slag, as well as heat recovery;
- development of technology for semi-dry and wet granulation of slag melt, as well as equipment for granulation of metallurgical slags;
- investigation of the effect of fineness of grinding on the hydraulic activity of blast-furnace slags and selective activation of slag-slag;
- development of technological scheme and technological line for obtaining besklinkernogo cement from blast furnace slags;
- investigation of the effect of PC clinker additives on the hydraulic activity of thin-grained granules and the development of a technological scheme and technological line for obtaining binders from blast-furnace slag;
- development of technological scheme and a technological line for the processing of waste slag and a production line for the production of PC clinker;
- development of the technology of foaming slag melt and installation of the production of slag pumice - a valuable material for the construction of a "warm house";

- use of granulated hydrogen sulphide slag water for medicinal purposes (in balneology); research of properties, chemical composition and development of a scheme for the production and use of slag water;
- development of a comprehensive scheme for processing metallurgical slags.

NON-PRECIOUS METAL-CARBON CATALYSTS FOR SUSTAINABLE PRODUCTION OF CARBON-NEUTRAL PRODUCTS

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The increasing concentration of CO_2 in the atmosphere threatens the world's sustainability with the global warming. Electrochemical CO_2 reduction reaction (CO_2RR) to produce CO combined with hydrogen evolution reaction (HER) can realize sustainable production of syngas with tunable H_2/CO ratio, in addition to the coal, biomass or natural gas-derived syngas, for Fischer-Tropsch synthesis (FTS) to produce carbon-neutral fuels and fine chemicals, which results in negative CO_2 emission or net CO_2 removal from the atmosphere. Although noble catalysts show good activities for catalyzing these processes, their expense and scarcity are prohibitive to large-scale commercialization. Hence, there is a need to develop precious-metal-free catalysts with comparable or even better CO_2RR, HER and FTS performances.

In this presentation, the well-designedZnO/CNTs, MNx/carbon and Ni/NiO@C catalysts were developed for the CO_2RR and/or HER to produce CO and/or H_2. The catalyst structure-performance relationships are established by combining DFT calculations with multiple techniques such as the aberration corrected HAADF-STEM and the synchrotron radiation-based X-ray absorption spectroscopy (XAS). Then, on theχ-Fe_5C_2 Fischer-Tropsch catalyst, activation and subsequent conversion of CO and H_2 were further investigated via FTS to produce fuels and fine chemicals. Compared to monometallic FTS catalysts, the χ-Fe_5C_2 catalyst exhibits unique structural and electronic properties. Interestingly, the charge of the involved surface Fe atoms for the CO activation is discriminated as a good descriptor for the facet-dependent CO activation, and the surface C atoms are found to be involved in the FTO reaction, which always locate at the end of the carbon chain of the products. It is not expected that this catalyst shows not only the unfavorable formation of lower olefins, but also rapid deactivation due to the formation of the encapsulating carbon. Furthermore, the introduction of promoters can significantly improve the selectivity to lower olefins as well as the catalyst stability.The insights revealed here could shed new light on the rational design of non-precious metal-carbon nanocatalysts for the production of carbon-neutral products.

ADVANCED POLYMER MEMBRANES FOR WASTEWATER TREATMENT, DRINKING WATER PURIFICATION AND BIOMEDICAL SEPARATION

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Conventional synthetic polymer membranes are often susceptible to membrane fouling due to their hydrophobic character and low surface energy. In order to develop antifouling and biocompatible polymer membranes with high permeability and good selectivity, a serial of amphiphilic copolymers composed of hydrophobic backbones and hydrophilic side/end chainswere designed as the blending additives of PVDF, PSF, PES ultra-/micro-filtration membranes prepared by traditional phase inversion process. The effects of amphiphilic macromolecules addition on membrane morphologies and properties were investigated in detail (Fig.1). The hydrophilic chains in amphiphilic macromolecules are often immiscible with host polymers and thus are segregatedonto membrane surface spontaneously during membrane preparation due to microphaseseparation. The hydrophobic part of amphiphilic additive is generally miscible with host polymer and able to anchor onto membrane surface. Based on the above work, a methodology “surface modification is achieved by simple blending” was established for the fabrication of high performance polymer membranes. The mechanisms of the surface segregation of amphiphilic macromolecules during membrane formation and application were revealed. Some novel membrane materials were developed and applied in many fields such as drinking water purification, wastewater treatment, biomedical separation etc[1-3].

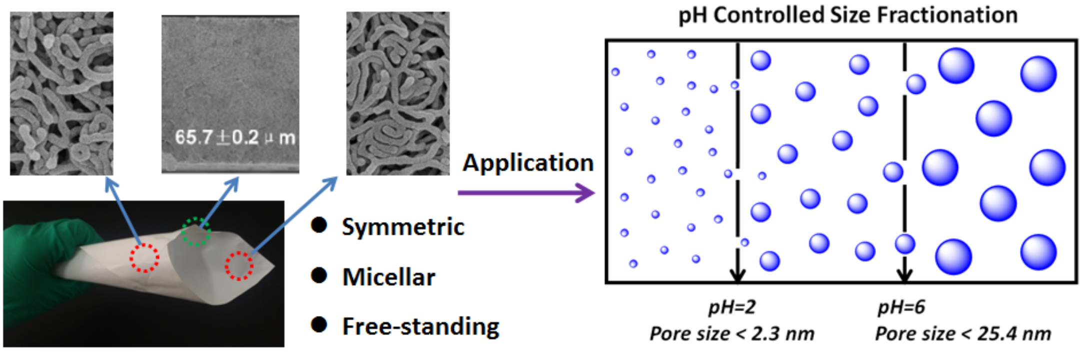

Fig.1 pH-responsive symmetrical membranes composed of block copolymer micelles used for nanoparticle size fractionation

STUDY OF THE POSSIBILITY OF USING MECHANICAL PROCESSING WASTE OF CARBON PLASTICS AS A FILLER OF POLYMER BASED COMPOSITE MATERIALS

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The mechanical method of recycling for polymer composite materials (PCM) is the most traditional method among physical ones. The main advantages of the mechanical method for processing of carbon fiber waste are the comparative simplicity of the technological process, the simultaneous processing of fibers with a polymer matrix without chemical and thermal processing, the absence of harmful emissions and fumes, the possibility of processing PCMs of various types (textolites, prepregs, dispersed composites). However, mechanical method for processing of carbon plastics can limit secondary use of recycled materials. This is due to the complexity of regulation of the fractional composition of shredded waste, the presence of a hardened polymer matrix on shredded carbon fibers,

The main aims of this work are investigation of the possibility of using of mechanical processing waste of polymer composite materials based on carbon fibers as a filler for "secondary" composites based on epoxy resins, and also testing of tribotechnical, mechanical and other properties of the composites produced.

The classification of mechanical waste particles for structural carbon plastics on the basis of carbon tape and epoxy resin has been made by size, composition and shape. With the help of Differential Thermal Analysis (DTA-analysis), possible processes of destruction of the filler from carbon fiber wastes during secondary processing have been investigated. It was shown that the features of the structure of dispersed waste particles influence upon tribotechnical properties: from the properties of solid lubricants to the predominant effect of solid crystallite particles.

The complex of the obtained characteristics will make it possible to formulate the recommendations concerning using of waste polymeric composites based on carbon fibers in engineering.

A NOVEL GRAPHENE-BASED ADDITIVE FOR MEMBRANE SURFACE MODIFICATION

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Graphene oxide was grafted with polyethylenimine (PEI) and subsequently blended with polyethersulfone (PES) to fabricate functional membranes with design surface properties. The synthesized GO-PEI additive was characterized with FTIR and XPS to confirm the successful grafting of PEI on GO. Zeta potential and size of GO-PEI were also analyzed. Subsequently, GO-PEI was mixed with PES in three different ratios to fabricate membrane through non-solvent phase inversion. Morphology of the prepared membranes was observed with both SEM and AFM. The chemical composition of the prepared membranes was characterized with XPS, indicating the presence of GO-PEI. More importantly, surface properties including hydrophilicity and surface charge of the prepared membranes were studied. The results indicated that with the increase of GO-PEI the membrane became more hydrophilic and more positively charged. Thus, we purposely prepared three membranes bearing negative, net zero and positive charges. The adhesion force between the prepared membranes and the negatively charged SiO2 AFM tip was studied through AFM force spectrometry. Four typical pollutants including phenanthrene, bovine serum albumin (BSA), Lysozyme and E.coli were used to evaluate the performance of the prepared membranes. In the static adsorption, surface charge more obviously affected the adsorption amount of pollutant than hydrophilicity. However, hydrophilicityindicated more obvious effect to prevent pollutant fouling in the dynamic filtration tests. In short, a novel graphene-based additive was synthesized to modify membrane surface property for different applications.

CARBONIZATION OF CARBON-CARBON COMPOSITES IMPREGNATED WITH A LIQUID PHASE UNDER HIGH PRESSURE

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Carbon-carbon composites are used to work in extreme environments because of their erosion resistance, ablative ability, and high mechanical characteristics at extremely high temperatures. The production of such materials includes several cycles of gas-phase or liquid-phase densification of initially porous carbon fibers reinforcement. High-temperature thermal stabilization (graphitization) is necessary to obtain a material with high, stable characteristics and can be carried out several times during the densification process. The main parameters of the processes occurring in the LP HPIC and graphitization of C/C composites are considered. A method for predicting the characteristics of C/C composites depending on the densification/graphitization routs and regimes is proposed.

FABRICATION AND OPTIMIZATION OF ZRC-BASED ULTRAHIGH TEMPERATURE CERAMIC COATINGS

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The development of hypersonic vehicles provokes outstanding structural materials for applications in extreme environments. Ultra-high temperatureceramics (UHTCs)have been paid attention to and developed due to their extremely high melting points above 3000^{o}C and acceptable mechanical properties. However, the shortcomings like poor toughness and thermal shock resistance limit the applications of bulk UHTCs. Carbon fiber reinforced composites (C/C, C/SiC) are usually considered as attractive engineering materials in the aerospace due to their excellent mechanical property and low density. However it is important to endow the composites with reliable anti-oxidation protection at high temperature environment containing oxygen. Therefore, the UHTCs coatings on C/C or C/SiC substrates have been extensively studied.In our laboratory, we have do some research work on the fabrication and high temperature properties characterization of UHTC coatings using vacuum plasma spray technique.

There are mainly three parts in this presentation:in the first part, the microstructure characters and some thermal and mechanical properties of air and vacuum plasma sprayed ZrC coatings were introduced. In the second part, the work relating to the interlayer coating between the top ZrC coating and C/C substrate were introduced. In the third part, the work relating to the function and influence of second phase (SiC, $MoSi_2$) on the oxidation/ablation behaviors of ZrC-based composite coatings were introduced.

INNOVATIVE PULSED DISCHARGE TECHNOLOGIES IN THE FIELD OF MATERIALS SCIENCE

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The analysis of pulsed discharge technologies (PDT), used in oil production, engineering, instrumentation, metallurgy, chemical industry, mining complexes, etc is performed in present review.

The use of high voltage electric discharge in different mediums allows impacting both the geometrical size and the structure of objects in order to give it certain mechanical and physical properties.

The Institute of Pulse Processes and Technologies of NAS of Ukraine designed and tested more than 40 different pulsed discharge technological processes for the industry: stimulation of oil wells; synthesis of hydrocarbon nanomaterials; removing rods from castings; crushing and grinding of materials; destruction of oversized and old foundations; regeneration of molding compounds; preparation of structured liquids; dispersion of mineral environments; activation of water and cement mortar; hardening of machine parts and stamping; fixing the pipe ends in the tube sheets of heat exchangers; calibration; compaction of the powder material; metal forming (rolling, drawing, extruding); processing of salt slag; intensification of the processes of casting and solidification of metals and alloys, etc.

Evolution of PDT and creation of new electric discharge devices is directed upon development of new pulsed technological processes for processing and obtainment of new materials.

MULTI-ACTION SELF-HEALING COATINGS FOR CORROSION PROTECTION

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Self-healing coatings inspired by biological systems possess the ability to repair physical damage or recover functional performance with minimal or no intervention. In protective coatings, the autonomous healing mechanisms are often enabled by embedding polymerizable healing agents or corrosion inhibitors in the coating matrices. For non-autonomous mechanisms, the healing effects are induced by external heat or light stimuli, which trigger the chemical reactions or physical transitions necessary for bond formation or molecular chain movement.

In this report, a new self-healing shape memory polymer (SMP) coating was introduced to protect the aluminum alloy 2024-T3 from corrosion by the incorporation of dual-function microspheres containing polycaprolactone and the corrosion inhibitor 8-hydroxyquinoline (8HQ). The self-healing properties of the coatings were investigated via scanning electron microscopy, electrochemical impedance spectroscopy, and scanning electrochemical microscopy following the application of different healing conditions. The results demonstrated that the coating possessed a triple-action self-healing ability enabled by the cooperation of the 8HQ inhibitor, the SMP coating matrix, and the melted microspheres. The coating released 8HQ in a pH-dependent fashion and immediately suppressed corrosion within the coating scratch. After heat treatment, the scratched coating exhibited excellent recovery of its anticorrosion performance, which was attributed to the simultaneous initiation of scratch closure by the shape memory effect of the coating matrix, sealing of the scratch by the melted microspheres, and the synergistic effect of corrosion inhibition by 8HQ.

INCREASE OF RELIABILITY OF ROLLERS OF ROLLING MILL AFTER RESTORATION OF THEIR COATINGS

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Rollers of the rolling mill are subjected to significant mechanical and thermal stresses during their operation and therefore have a limited service life. The extension of the resource of the rollers can be achieved by restoring them. The solution of this problem involves the use of cheap recovery technology while guaranteeing the quality of its results. Such a guarantee can be ensured by non-destructive detection of defects that are critical for reliable operation in the restored rollers. In mass production, the flaw detection method used must ensure high reliability of detection of defects with a short evaluation time of the product and minimum financial costs. Such problems can be solved with the help of ultrasonic flaw detection, however, each specific case requires individual methodological studies.

The paper presents the results of the development of a technique for ultrasonic diagnostics of the defect condition of a small batch of rolls that have been reconstructed after destruction of their surface during the exploitation. The rollers were cylinders of 40X steel with a height of 20...50 and a diameter of 50...60 mm with a cylindrical cavity 10...15 mm in diameter in the center. When restoring a roller on his side surface, a groove 6 mm deep, symmetrically disposed along the height of the cylinder, was cut out and the formed cavity was fused with liquid metal. As a result, pores could form in the welded part and cracks on its border with the base metal of the roller.

A measuring acoustic chamber has been developed in which the sensor is fixed coaxially with the roller on one of its flat surfaces for echo-sounding of its restored part. To sounding the entire near-surface area of the product with possible defects, a roller rotating device was used with respect to the sensor.

INVESTIGATION OF MODIFIED BASALT FIBERS

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Due to the unique multicomponent mineral and chemical composition of the raw material, the rock fibers are characterized by a successful combination of high performance properties such as temperature resistance and mechanical strength, low thermal conductivity, high vibration resistance and resistance to aggressive environments.

Of the developed basalt fibers, the most promising are continuous fibers that can be used as reinforcing elements of composite materials with the use of polymeric and inorganic binders, products made from multifunctional composites.

Previously conducted studies mainly determined the suitability of rocks for the production of fibers, which is represented by a complex of properties: homogeneity of the mineralogical composition, the absence of refractory minerals, the ability to form a homogeneous melt at a temperature (1400–1450) °C; the viscosity of the melt, the temperature of the upper limit of crystallization, the temperature interval of the production of fibers.

A special role is assigned to the chemical composition of the rock. The chemical composition of basalts of different deposits was studied by many researchers with the aim of revealing the possibility of their effective application in various branches of the economy.

For the production of fibers with certain characteristics (for example, more temperature, alkali or acid resistant), there is the possibility of artificial selection of raw materials or modification of natural rock.

Researches on receiving continuous basalt fibers from batch of rocks of the basic composition (basalts) and acid composition are done. Correction of the initial chemical composition of rocks (basalts) with a natural additive with a large viscosity modulus made it possible to obtain homogeneous melts with good forming properties and continuous fibers based on them. Correction of the composition of raw materials allows to receive fibers more chemically resistant in aggressive environments.

The conducted studies indicate the possibility to expand the base of raw materials for obtaining fibers with increased chemical resistance in corrosive media by adjusting the composition of basalt raw materials of the basic composition with a natural additive of acidic composition.

MATERIAL REMOVAL MECHANISM AND ORIGIN AND EVOLUTION OF DAMAGES AT NANOSCALE OF BRITTLE MATERIALS

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A novel approach of ultraprecision grinding is proposed by a single diamond grain at nanoscale depth of cut. A setup is developed on an ultraprecision grinder, which realizes relatively long scratches with continuous variable depth of cut at nanoscale with grinding speeds at m/s. This obtains the onset of chip formation and brittle-to-ductile transition point. A relationship is proposed among the force, depth of cut and grinding topography. A novel phenomenon is confirmed by high resolution transmission electron microscopy that a solely amorphous layer is obtained on Si wafers induced by a diamond wheel grinding. This is different from previous reports, in which there is an amorphous layer at the top, followed by a damaged crystalline layer beneath. To verify the grinding results by a single diamond grain, new diamond wheels are developed, obtaining a solely amorphous layer on Si wafers with thickness of 47 nm.

To overcome the disadvantages of traditional CMP slurries, fixed-abrasive lapping and environment-friendly CMP are developed. The novel CMP slurries consist of mainly hydrogen peroxide, silica, malic and citric acids.

INFLUENCE OF SURFACE SULPHIDES ON ELECTRODE PROCESSES AND HYDROGENATING OF STEELS IN CHLORIDE-ACETATE ENVIRONMENTS

Khoma M., Golovej S., Vasyliv Ch.

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Corrosion and hydrogenating of steels in hydrogen This suggests that sulfides of various compositions have different effects on the rate of partial hydrogen release reactions, in particular on the reaction of catalytic recombination of hydrogen atoms, which determines the surface concentration of adsorbed hydrogen atoms and is a prerequisite and driving force of their absorption. All investigated sulfides contribute to hydrogenating of Armco iron. Therefore it is possible to assume their slowing effect on this partial reaction.

Catalysts $[Fe\ (HS)]^{+}_{ads}$ are formed on the surface of steels in the *media containing* hydrogen sulfide. It promotes intensive hydrogenating and accelerated destruction of steels. At the same time, the oxidation-reduction reactions occur and various sulfide-containing corrosion products are formed, the composition of which depends on many factors. Initially unstable macinavit ($Fe_{x+1}S$) is formed on steels. Macinavit is subsequently converted into pyrite (FeS_2), troilite (FeS) or kanzite (Fe_9S_8), what is primarily determined by the concentration of hydrogen sulfide. Sulfides can affect the nature of corrosion damage, the allocation and absorption of hydrogen and the further development of corrosion-mechanical destruction.

Sulfide-containing environments depend on the nature of surface sulfide films. The influence of surface sulfides on electrode processes and hydrogenating of armco-iron in the chloride-acetate solution 5% NaCl + 0.5% CH_3COOH has been studied.

No direct relationship between the values of the cathode reactions overvoltage and the volume of the released and absorbed hydrogen was found. The Fe-FeS_2 electrode with the highest cathode overvoltage produces about 5.5 times more hydrogen than Armco iron, and hydrogenating increases by only ~ 30%. Reduction of hydrogen at Fe-Fe_9S_8 electrode with the lowest overvoltage is about ~7.1 times more, but hydrogenating increases only ~ 2.1 times.

MACROSCALE SUPERLUBRICITY ENABLED BY HYDRATED IONS

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Lubrication by hydration shells that surround and are firmly attached to charges in water provide a new mode for the extreme reduction of friction in aqueous media, which can be called hydration superlubricity. Several different microscale systems which exhibit hydration lubrication have been reported using a mica surface force balance. Nevertheless, how to obtain the hydration superlubricity under macroscale conditions with higher load-carrying capacity still remains a challenge and the mechanisms governing macroscale superlubricity with hydrated ions are still not well comprehended. Here we demonstrate that macroscale superlubricity based on hydrated alkali metal ions (Li+, Na+, K+) can be realized under high contact pressure between the Si3N4 ball and sapphire disc, extending earlier studies significantly to shed new light on the nature of this mechanism. The ultralow friction coefficients of 0.005 are obtained under average contact pressure up to 0.25 GPa by a universal micro tribometer (UMT-5) after a running-in period with acid solutions. Different conditions including concentration, load, pH values and velocity are studied in order to explore the nature and limits of the macroscale superlubricity of hydrated ions. The results reveal that running-in stage with acid solutions can not only make the worn region smoother, but can generate a silica layer easy to shear which provides excellent boundary lubrication. The hydration superlubricity originates because hydration shells surrounding the alkali metal ions could generate the hydration repulsive force to sustain a large normal load and have a fluid response to shear simultaneously. These findings pave the way to the scale-up of hydration superlubricity and thus to the wide application of new water-based lubricants.

A GRAPHICAL-ANALYTICAL METHOD HAS BEEN DEVELOPED FOR THE DAMAGES CRITICAL SIZE ESTIMATION IN ANODE COATING ON STEEL IN HYDROGEN SULFIDE ENVIRONMENT

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The corrosion potentials of coatings with the different damages area were determined. The values of cathode current of steel and anode current of coating were determined on the basis of the Volt-Amper dependencies for the corrosion potentials. The dependence of the ratio of these currents as a function of the ratio of the coating area to the defect area was constructed:

$I_{k\ (steel)}/I_{a\ coating)} = f\ (S_{steel}/S_{\ coating})$,

where: $I_{k\ (steel)}$ - cathode current (steel 20); $I_{a\ (coating)}$ - anode current (coating); S_{steel} - defect area (steel 20); $S_{\ coating}$ - coating area.

The ratio S_{steel} / $S_{coating}$ is considered critical, for which $I_{k\ (steel)} = I_{a\ (coating)}$. If the cathodic current of the steel does not compensate the anode dissolution of the coating, the steel begins to dissolve and the coating does not protect the steel. The critical size of corrosion damages in aluminum coating on steel 20 has been evaluated in the free aerated see water, and in the sulfur hydrogen saturated see water and in the solution of NACE. They are 0,061, 0.052, 0.043 respectively.

The theoretical calculations are completely corresponded to the experimental ones for the free aerated see water, for the sulfur hydrogen saturated see water the error is ~ 18%, for the NACE solution ~ 23%.

CAVITATION WEAR OF THE MAX-PHASE Ti_2AlC AND VACUUM-ARC COATINGS ON ITS BASIS

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Due to the development of new energy and transport systems, it became necessary to obtain quantitative data on the resistance of materials under the conditions of micro-impact, which are created by cavitation in different environments. One of the advanced materials may be the MAX phase of Ti_2AlC, which belongs to the class of nanolayered materials, where M is the transition metal, A is the element III-A or IV-A group of the periodic table, and X is the C or N. The MAX phase engaged by unique properties combination of metals and ceramics, which allows them to be used in extreme conditions. It is also interest to obtain protective coatings based on MAX phases. However, data about resistance of these materials and coatings in conditions of cavitation impact is absent.

The aim of this work is the study of cavitation wear of bulk MAX-phase Ti_2AlC and coatings, obtained by the vacuum-arc evaporation method from cathode with the same composition.

Samples and cathode for vacuum-arc deposition of coatings from the MAX phase Ti_2AlC were prepared by hotpressing. Coatings, 15-20 μm thickness were deposited on polished stainless steel 410 samples on a “Bulat-6” system. Investigation of the structure of bulk material and coatings was carried out using SEM and X-ray diffraction analysis. The sustainability of materials was investigated at the apparatus developed at the NSC KIPT under the conditions of micro-impact. In this apparatus, the cavitation zone was created in water by an ultrasonic radiator (frequency 21 ± 1 kHz, wave amplitude 30 ± 1 μm).

It is shown that cavitation wear of the MAX phase of Ti_2AlC in the massive state is 4 times higher than for Ti6Al4V alloy samples. At the same time, the resistance of $Ti_{65}Al_7C_{28}$ coatings to cavitation is 3 times higher than for Ti6Al4V alloy and 1.5 times than for TiN coating. The obtained data shows a further prospect for studying the processes of protective coatings synthesis using cathodes based on MAX phases.

SUPERLUBRICITY OF CARBON FILMS AND THE APPLICATION UNDER HIGH PRESSURE AND HIGH SPEED

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Friction and wear are still the primary means of triggering energy dissipation and component failure in the mechanical systems. Achieving superlubricity between two sliding surfaces (the friction force and wear are close to zero) is a significant mean to essentially deal with the problems mentioned above. Carbon film is one of the most promising solid lubricant coating in various tribological applications, for it can remarkably reduce friction and even achieve superlubricity under certain conditions and environments. Common view holds that superlubricity of carbon films is attributed to shear-induced graphitic tribofilm formation at rubbing interfaces. However, since the graphitic carbon has many allotropes with diverse structures and friction properties, it hints that the superlubricity of carbon films is related to graphitic transformation but not limited to this. In this report, a reasonable mechanism of superlubricity of carbon films will be introduced through analyzing the friction-induced phase transformation and interfacial structural evolution, and the potential application of carbon films with superlubricity under special working conditions like high pressure and high speed will be discussed.

DECORATED GRAPHENE AS EMERGING 2D MATERIAL FOR CORROSION PROTECTION AND WEAR REDUCTION

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Graphene is a typical two-dimensional layered material (2DLM) processing excellent mechanical, thermal, electric and superior barrier properties and showing many potential applications. In this talk, we will present some of our recent research on preparation of organo- or water-dispersible graphene nanosheets via noncovalent and chemical modification approach, and the integration of graphene sheets to polymer matrix for enhancing the corrosion protection, friction reduction and wear resistance performance. The utilization of graphene as additive to enhance the lubricating and wear resistance performance of PAO and water-based fluids will also be discussed.

ZINC OXIDE FILMS AS A MULTIFUNCTIONAL MATERIAL FOR ELECTRONIC APPLICATIONS

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Zinc oxide (ZnO) as a wide-bandgap semiconductor is a promisingmaterial for the design of optical devices such as transparent electroconductive films, electrochromic devices, light-emitting diodes,laser diodes and ultraviolet detectors, owing to the unique opticalproperties as well as a relatively low cost, non-toxicity, technologicaladvantages and resistance to radiation damage. In our work we use the reactive magnetron sputtering method for the deposition of textured nitrogen doped ZnO films on p-silicon substrates. We obtain the high quality of crystalline ZnO structure that gives intensive monochromatic UV photo and cathodoluminescence.It was developed the detectors of the UV radiation based on the high quality phototransistor structure Ni/ZnO:N/p-Si/Al. Those phototransistors provide a significant bending of the zones on the Ni/n-ZnO:N contact, which leads to an effective injection of carriers in n-ZnO:N. In the created phototransistors, the mechanism of internal amplification of current was realized and a significant photo sensitivity was reached at the level of 210 A/W at $\lambda = 390$ nm and high speed with a time constant of 100 ns. The main application areas are health care, biotechology, ecology and space applications.

ESR POSSIBILITIES FOR MANUFACTURING OF MODERN RAILS FOR HIGH-SPEED AND HEAVY HAUL RAILWAYS

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The high performance rails usage is one of the main preconditions to provide both the efficiency and safety of the modern railroads, playing main role in the transportation of various cargo and passengers. Today's requirements of railroad operators to the rails mechanical properties and service life become tougher because the speed of transportation and loads are growing. For durable exploitation in severe service conditions, the rail steels have to have high wear-resistance, strength and plasticity simultaneously that is quite challenging task for material scientists and metallurgical companies.

There are three main causes are recognized reducing the performances and service life of the modern premium rails. There are nonmetal inclusions of big size and unfavorable morphology, vast interlamelar spacing of the pearlite, the presence of proeutectoid cementite on the grain boundaries and austenite grain size.

The previous experience of electroslag remelting (ESR) usage for high quality steel production was analyzed and taken as the base of the two improved technological process: low speed continuous casting (CC) with the ESR heating of the meniscus and a high melting rate ESR.

Taking into consideration the known advantages of the ESR for high quality steels manufacturing the experimental melts with standard and two times increased melting rate (to increase ESR process productivity) were performed. Thesufficiently higher level of the rail steel quality (full absence of segregation, shrinkage and any other critical defects) after ESR in compare with theinitial rail was proven. The rail steel ingots made by ESR in all cases had fine dendrite macrostructure and very low sulfur content distributed evenly.

The speed of withdrawing increasing in compare with typical for ESR more than twice does not reduce metallurgical quality of the ESR ingot (no any indications of segregation were revealed) and dispersion and cleanness of microstructure. On the base of made experiments and previous experience the hybrid process CC+ESR was also proposed and preliminary tested. The base approaches to the pilot scale realization of the steel continuous casting in combination with the Electroslag heating are formulated and proposed.

HOW TO PREDICT THE CYCLIC LIFE OF MATERIALS SUBJECTED TO HIGH TEMPERATURE CREEP

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The world is now facing more than ever the energy and environmental challenges. The working conditions of the chemical and energy equipment are going much extreme in order to increase the efficiency and better utilize the natural resources. The failure of materials under cyclic loading and high temperature prior to the design life has been a fatal occurrence in many energy and chemical conversion processes, which may include aero engine, ultra-supercritical power generation, ethylene cracking, fuel cell system, power transmission devices and so on. The cyclic life prediction is fundamental to avoid the catastrophic failure. However, the creep and oxidation at high temperature reduces greatly the cyclic life which represents a significant challenge in the design and operation of the plants. The lecture summarized recent progress on the understanding of the failure mechanisms of a Nickel-based alloy due to creep-fatigue interaction. More than 160 specimens were used in the creep-fatigue tests with strain-controlled triangular and trapezoidalloading waveforms. Then, a modified strain energy density exhaustion (SEDE) model on the basis of linear damage summation (LDS) rule was proposed to predict the creep-fatigue lives. The effects ofmean stress and stress relaxation were considered in this model. Results showed that most of the predicted and experimental livesfell into a scatter band of ± 2. Furthermore, the cycle-by-cycle changes in material response.

PHASE COMPOSITION OF Ti-Cr-Al-Si-O COATINGS PREPARED BY DIFFERENT METHODS

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Quasicrystalline phases and their approximants are perspective materials for use as coatings because they have a high hardness and low friction coefficient. An attempt to obtain a coatings with a quasicrystal icosahedral structure from a three-component $Ti_{60}Cr_{32}Si_8$ alloy by flame and plasma spraying has been reported by another authors. First coating has the metallic phases based on β-Ti and the Laves $TiCr_2$ (type C14) and the other coating contains a large number of oxide.

In the present work we investigated the phase composition of $Ti_{60}Cr_{30}Al_3Si_2(SiO_2)_5$ coatings prepared by different methods: detonation, plasma spraying and magnetron sputtering.

The $Ti_{60}Cr_{30}Al_3Si_2(SiO_2)_5$ alloy was obtained by arc melting from high purity elements in a high purity argon atmosphere. Then it was made a powder and target for further spraying. The phase composition of coatings have been investigated by X-ray analyses in monochromatic Cuk_α-radiation.

In the initial state the $Ti_{60}Cr_{30}Al_3Si_2(SiO_2)_5$ alloy has two phase -the1/1 approximant α-TiCrSi and $TiCr_2$ Laves (C14). The coating obtained by the detonation spraying has many phase and contains $TiCr_2$(C14), Ti_3Al, TiN and oxide Me_2O_3 type. The diffraction pattern of coating obtained by plasma spraying shows two phase - 1/1 approximant α-TiCrSi and TiN. Since this coating is thin, the reflexes from stainless steel substrates was fixed also. Formation of an amorphous single phase was observed in a coating obtained by magnetron sputtering. The annealing at 750 °C leads to formation of 100% quasicrystal phase.

The method of automatic indentation was used to determine of the mechanical properties of the coating. The coating in an amorphous state has unusually high mechanical characteristics - in particular, the hardness reaches 23 GPa. After annealing its value decreases to 19 GPa.

DESIGN AND APPLICATION OF FRICTION PAIR SURFACE MODIFICATION COATING FOR REMANUFACTURING

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Friction, wear and contact fatigue are the main reasons for energy consumption, material wastage and equipment damage. So how to reduce wear, alleviate fatigue, extend service life and improve operational reliability is the major technical problem to guarantee the long-term security service of friction moving components. Based on the surface science theory and the design idea of structure-function integration, we comprehensively apply the latest achievement of surface engineering technology to design the surface modification coatings which can endow the function of solid lubricating, anti-fatigue, wear resistance and automatic sense to the surface of key friction pair. Relevant basic-research findings are the complement and deepening of the tribology basic theory. And the design, deposition and evaluation technology of the friction pair surface modification coatings achieves a great improvement in working performance, service life and real-time monitoring of service condition of the equipment key moving components. Besides, our studies have been successfully applied to the manufacturing, strengthening and repair of the key moving components of heavy equipment engine, machining and forming tools, oil and gas drilling equipments and etc. In general, our work can provide theoretical and technical supports for modification, strengthening, and remanufacturing of key friction pairs.

INVESTIGATION OF ALUMINOTHERMY USING FORGE-PRESS PRODUCTION WASTES

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Aluminothermy as a reduction of iron oxides by aluminum, one of the varieties of metallothermy, has found the greatest application in the industry. Exothermic mixtures are widely used for the melting of refractory additives, getting of cast iron and cast parts, welding and reduction of metals, and so on. As a main component of the exothermic charge, various wastes containing a large number of oxides are often used. To study the parameters of the combustion process of exothermic mixtures, 18Kh2H4MA steel scales were used as the main component of the charge. This scale is a waste of forging and stamping production of PJSC "Kovelsilmash". The chemical composition of steel scales 18Kh2H4MA: 41-33% FeO, 36-27% Fe_2O_3 and 23-40% Fe_3O_4 and 1.5-2.0% of oxides of alloying elements. As a reducing agent, a powder of aluminum PA is taken due to GOST 6058-73. Since the waste has a variety of oxides, the use of aluminothermy processes in the industry leads to a detailed study of their essence, patterns of reaction and comprehensive study of properties of the material obtained as a result of the reaction. Due to the content in the scale of three types of iron oxides, the theoretical calculation of the composition of the charge is complicated, so it was determined experimentally based on the optimum combustion temperature and the yield of a decent metal.

In experiments, the oxides were not separated by chemical composition and the composition of the charge varied according to two main components: scale plus aluminum powder. The component variation in percentage ratio of the charge varied for ten parties of samples as follows: scale/aluminum from 81%/19% to 72%/28%. It is established that from percentage ratio of components of the charge depend such parameters as, the combustion temperature, the reaction time and the output of the metal. The highest combustion temperature is typical of the ratios of scale/Al - 81%/19% - 79%/21% and was 3000-2900 °C. At the same time, the burning time fluctuated within 3.5-2.8 seconds, the output of metal about 44%. The lowest burning temperature was recorded for the percentage ratio of 74%/26% to 72%/28%, namely 2500–2400 °C, the output of the metal is about 50%. The optimal combustion temperature and metal outlet is a mixture with a proportion of scale/A%, 77/23 and 76/24%. With an increase in the content of scale, it is likely that due to increased caloric content of termite and the occurrence of excessive heat, the evaporation of iron occurs. With an increase in aluminum, there is not enough oxygen to pass the reaction, which leads to an uneven spread of the reaction and incomplete combustion of the components of the charge.

To determine the effect of compacting on the combustion process of termite, a combustion rate study was conducted on the density of the mixture and the dispersion of particles. The density varied from 0.47 to 8 g/cm^3. The density of 0.47 g/cm^3 is the density of the non-pressurized mixture. It was established that during compaction of samples, the combustion rate decreases. This is explained by the fact that the reaction of iron recovery with aluminum is slowed down due to the weakened oxygen supply to the combustion zone. The dispersion of the charge has minor effect on the change in the combustion rate, but the most stable passage of the reaction occurs when the powder size is 400-500 microns.

Metallographic studies were performed according to the standard method, ESEM Philips XL30-FEG was used for raster electron microscopy. In order to obtain a clear image of the grain boundaries, the grafts were etched with 4% H_2SO_4. The analysis of microstructure showed that this metal is more subjected to eutectic structure. This is due to the fact that the reaction temperature exceeds the temperature of the eutectic transformation ($\text{Р}_\text{C} \rightarrow \text{Л}(\text{А}_\text{Е}+\text{Ц})$. According to the phase rules, C = 2-3 + 1 = 0, this transformation occurs at constant temperature. The average chemical composition of the material obtained during combustion mixtures in the proportion of scale/Al,%: C-0.43, Si-0.21, Cr-0.22, Mo-0.19: Fe-98.94%.

Conclusions. The composition of the exothermic mixture with the most optimal combustion parameters has been experimentally determined. It has been determined that the dispersion of the powder of the charge does not have a significant effect on the combustion rate of the mixture, and when combustion of the compressed mixture with a density greater than the density of the filling a decrease in the combustion rate occurs. It is proved that the composition of the charge is significantly influenced by the yield of a worthy metal, as with increasing the content of scale, and, accordingly, Fe_2O_3, the caloric content of termite increases, which leads to the formation of excess temperatures.

TRIBOLOGY OF SURFACE OF THERMAL STEEL AFTER FRICTION

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Parts working in reverse friction are subjected to high dynamic, shock and temperature loads. Knowledge of rheological properties is necessary for estimating the stability of the material under the influence of high temperatures, dynamic and static loads, and also allows predicting the possibility of adhesion of contacting bodies.

Tribological researches were carried out on termite material obtained from scale of steel, aluminum powder and additives: copper powder, potassium nitrate, ferromanganese and ferrosilicion.

Chemical composition of scale: 58-59% of iron oxide Fe_3O_4, 40-48% of iron-ferrite Fe_2O_3 and 1.5–2.0% of alloying elements oxides.

As a result of the combustion of the proposed charge, ingots were obtained, a mass fraction of iron in which 56–58%.

The strength of the material, which was determined by the dynamic hardness meter TD-42M, is 870–920 MPa. An important characteristic of structural strength of materials is the impact strength. It depends both on the strength and on the plasticity of the material. Impact viscosity was investigated on a pendulum koper MK-30. According to the results of tests of U-like samples with a similar cutting zone on impact viscosity, the lowest impact strength of the material was observed at –20 °C, which is 150 J/cm^2, which is sufficient for materials working in reverse friction and temperatures of 90–120 °C.

As a counter body, a material with the same properties and the same initial roughness was used. In order to obtain more accurate results, the surface of the samples was mechanically treated to increase the contact area. The friction route was 5 kilometers, the sliding speed was 1.2 m/s, the specific load was 1.2 MPa.

According to the results of the analysis of microstructures, it was found that friction occurs the plastic fracture of the material with the formation of scratches, and in certain places crumbles that have a rounded shape and are unevenly distributed throughout the surface of the sample. The appearance of such types of wear-off indicates the implementation of the mechanism of abrasive wear. Studies have shown that the intensity of wear increases with increasing load and decreases with increasing slip speed.

The temperature in the contact zone at a slip speed of 1.2 m/s and a load of 1.2 MPa reached 90–120 °C, which ensures the course of physical and chemical transformations during the formation of a stable transfer film and does not cause degradation of the matrix. This film provides the stability of the friction process due to the self-organization of the structure of the surface layers of the friction pair.

Conclusion. It is established that the proposed thermite material is suitable for the manufacture of parts that operate under reverse friction, which provides the basis for a detailed study of its tribological characteristics.

DIMENSIONAL DESIGN OF MULTI-SCALE COATINGS

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Multi-scale coatings are widely used for various parts to functionalize the material surface or significantly improve the surface properties/performance of materials. However, coating design often suffers from great contradictions resulting from multiple requirements of coatings, for example, simultaneous high hardness and high toughness for wear resistance, simultaneous high thermal barrier effect and long lifetime for thermal barrier coatings in air engines and turbines, simultaneous ultrathin film thickness and huge in-plane size for thin films in solar cells.

In this talk, we will introduce dimensional design strategy of multi-scale coating interface/boundary towards simultaneously achieving a balance of those contradictory problems. First, grain boundary design strategy enables us to produce high quality large area but ultrathin films achieving highly efficient and stable perovskite solar cells with the world largest area of >0.4×0.6m. Second, phase boundary design strategy in cermet coatings help us to develop a superior wear resistance WC-Co coating with simultaneous high stiffness, high toughness and high bonding strength. These coatings have been successfully applied in turbine blades prolonging lifetime of hydroelectric power stations by several times. Third, layer boundary design strategy in thermal barrier coatings promote the simultaneous improvement of thermal barrier performance and thermal cyclic lifetime. In brief, dimensional design strategy of multi-scale coating based on interface/boundary engineering provides new insights and opportunities for the development of high performance coatings for various industry fields.

ADVANCED MATERIALS FOR GETTING HEAT-RESISTANT PROTECTIVE COATING UNDER SHS CONDITIONS

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Practical use of carbon-carbon composite materials (CCCM) in high-temperature processes is very limited due to strong oxidation, as well as erosion and burn-up in gas streams. In this regard, protecting the CCCM from oxidation and burn up is an important scientific and technical task.

The aim of the work is to search for optimal powder SHS-charges, which allow forming doped chromium-plated protective coatings on CCCM under self-propagating high-temperature synthesis.

Known methods for obtaining coatings have a number of disadvantages and advantages. Implementation of the application of protective coatings on high-carbon materials is difficult for a number of reasons. This concerns not high wettability of the surface of carbon by refractory metals, low adhesion of the coating to the substrate, which depends to a large extent on the thermal properties of the coating, and also the choice of coating components depending on the operating conditions of the finished product. However, to date, many technologies have been developed for applying protective coatings to carbon materials using chemical-thermal treatment methods (CTM), as well as impregnation from the liquid phase.

One of the most promising methods of CTM today is self-propagating high-temperature synthesis (SHS). From the analysis of the requirements for coatings on the CCCM, a diffusion method of surface saturation from the solid phase in the active gas medium in the SHS mode was chosen. Under the conditions of SHS, it is possible to obtain coatings of different chemical composition, varying the amount and content of alloying additives.

Analysis of the reactions taking place in the SHS process, as well as the results of experiments and metallographic studies, allowed to obtain a scheme for the formation of protective coatings. The process of formation of protective coatings in the regime of thermal autoignition can be conditionally divided into five stages-inert heating of the SHS mixture to the autoignition temperature, thermal autoignition, heating of the parts, isothermal aging and cooling.

For tests on the heat resistance of protective coatings, flat samples (thickness = 3 mm, length = 30 mm, width = 20 mm) made of CCCM were used. The test temperature was: 900–1100 ºC. The tests were carried out in an electric muffle furnace.

The best heat resistance among the coatings under consideration are chromoaluminosilicate coatings. Their heat resistance is 1.5–1.7 times higher than in uncoated samples.

REGULARITIES OF SOLID SOLUTION HARDENING OF SURFACE LAYERS OF TITANIUM ALLOYS (A, PSEUDO-A AND A+B) DEPENDING ON CONDITIONS OF THERMO-DIFFUSION SATURATION IN RAREFIED GASEOUS MEDIUM CONTAINED OXYGEN

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The aim of work was to determine regularities of solid-solution hardening of surface layers of titanium alloys (α, pseudo-α, α+β) depending on the conditions of thermodiffusion saturation in rarified gas medium containing oxygen. Object of investigation was system “titanium alloys - rarified gas medium containing oxygen”. To achieve the formulated aim the following methods were used: thermodiffusion saturation of titanium alloys in rarified gas medium containing oxygen in the wide range of temperature-time ($\boldsymbol{T}$ = 650, 700, 750ºC, τ = 1, 3, 5 h) and gas-dynamical ($\boldsymbol{P} = 6.6\times10^{-2}$, 1.33×10^{-2}, 6.6×10^{-3} Pa, $\boldsymbol{I}_H \approx 5\times10^{-5}\cdot\text{Pa}\cdot\text{s}^{-1}$) parameters. Kinetics of saturation was determined by methods of discrete thermogravimetry. Optical metallography, durometry, X-ray diffraction and electron probe micro analyses were also used.

It is determined that under the same conditions of saturation ($\boldsymbol{T}$, τ, $\boldsymbol{P}$) the hardened layers with various parameters ($\boldsymbol{H}$, $\boldsymbol{l}$) are formed on the titanium alloys. The monophase α-titanium alloys VT1-0, VT5 and pseudo-α-alloy OT4-1 are the most sensitive to the conditions of gas-saturation: surface hardness and its gradient in the hardened layer increases substantially. Hardness of near-surface layer is less sensitive to the changing of the parameters of chemico-thermal treatment with increasing of β-phase (VT16, VT22), but the thickness of the hardened zone increases with increasing of the temperature and exposure time. Obtained results allow to calculate the profiles of solid-solution hardening of metal using the parameters of thermo-diffusion saturation and determine the parameters of thermal treatment to achieve the regulated level of hardening.

RELIABLE ELECTROCHEMICAL PHASE DIAGRAMS OF NICKEL COMPOUNDS FROM FIRST-PRINCIPLES CALCULATIONS

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Ni oxides and hydroxides have very wide applications in many important fields, e.g., corrosion resistance, catalysis, and energy. The performance and lifetime of these materials are largely determined by their stabilities in various electrochemical environments, which can be effectively understood/predicted by using the Ni electrochemical phase diagram in terms of solution pH and electrode potential (called *Ni Pourbaix diagram*). We develop a theoretical approach based on density-functional theory (DFT) to calculate accurate thermodynamic energies and Pourbaix diagrams of materials, and obtain reliable Ni Pourbaix diagrams lacking for over 50 years. Furthermore, Ni (hydr)oxides grown/used in electrochemical conditions may have different spatial dimensions (e.g., from bulk to nanoscale). Thus, we comprehensively simulate the thickness-dependent Pourbaix diagrams of Ni-compound nanofilms, as well as reveal the roles of water adsorbates and metal substrate. Our theoretical results are systematically consistent with many electrochemical observations reported in recent decades, and also closely validated by further experimental measurements using electrochemical impedance spectroscopy (EIS), surface-enhanced Raman spectroscopy (SERS), and polarized neutron reflectometry (PNR). Our new Ni Pourbaix diagrams will be highly useful for the design, synthesis, and application of related materials in the future.

BIOACTIVE CERAMICS AND NEW TECHNOLOGIES FOR ITS APPLICATION

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Technologies have been developed for the production of powders, granules and wares from bioactive ceramics based on calcium phosphate with different physicochemical and biological properties and different functional effects (antibacterial, antitumor, osteoinductive).

The powders are used for the manufacture of products according to the shape of the defect and for coating titanium implants. Granules are used to restore bone tissue in various clinical cases.

Given the active development of theregenerative medicine and new medical technologies for the restoration of large fragments of the affected bone, a need has emerged for new biomaterials with specific requirements for interaction with the cells of the body.

For the restoration of bone tissue in regenerative medicine, donor bone or animal bone is mainly used. Such operations are very expensive and a number of complications are possible, both with moral and legal support, and with overcoming tissue incompatibility, which could be completely eliminated when using bioactive ceramics, which is a synthetic analogue of the mineral component of bone tissue.

Calcium phosphate biomaterials have a high potential for use in bone tissue engineering due to their high biocompatibility and ability to be replaced in a defect with full-fledged bone, but they are subject to very high demands on bioactivity, resorption, strength, pore architecture, and three-dimensional form.

New approaches to tissue engineering using bioactive ceramics for the treatment of post-traumatic bone defects of critical size will successfully restore the integrity of bone tissue, increase the effectiveness of treatment, significantly reduce treatment time and cost of the technique.

STIMULI-RESPONSIVE BIOMEDICAL HYDROGELS

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Stimuli-responsive hydrogels have been widely developed due to their handily and readily tailored properties under various external stimuli, such as pH, temperature, electricity, redox, and light. However, preparation of the customized high-performance biocompatible hydrogels is still a challenge. Herein, we present a disulfide-exchange-based controlled cross-linking strategy to dynamically tune crosslinking process and properties of hydrogels, and realize controlled formation of hydrogels, microgels and nanogels for construction of customized biomedical hydrogels. Further, we disclose a novel formation mechanism of reversible chitosan physical networks, and construct physical-chemical hybrid double network hydrogels with high tensile strength, ultrahigh toughness, excellent load-bearing capacity and remarkable anti-crash capacity. Finally, we develop an *in situ* forming method to produce high-mechanical poly(ethylene glycol) hydrogels, and explore their biomedical applications in wound-sealing, hemostatic and antibacterial materials. Overall, the controlled cross-linking strategy provides a facile approach to producing hydrogels with adjustable structures and properties, opening up design possibility, flexibility and complexity of hydrogels with customized properties and applications.

NON-COVALENT INTERACTIONS-STRENGTHENEDHYDROGELS FOR BIOMEDICAL APPLICATIONS

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Hydrogels resemble human's soft tissues in many physical ways; however, the weak mechanical strength intrinsic to conventional hydrogels has severely hindered their practical applications. Over the past decade, encouraging progress has been made in fabricating high strength hydrogels. However, they are still far from real biomedical applications due to lack of careful design functions catering to tissue integration. Recently, our team developed a series of high strength hydrogel by introducing non-covalent interactions in the network. These dynamic non-covalent interactions reinforced hydrogels exhibited a myriad of intriguing properties, such as ultrastiffness, toughness, fatigue resistance, self-healing, thermoresponsiveness and/or pH responsiveness, self-recovery, shape memory, and remoldability/recyclability/reusability. We made an effort to explore their versatile applications in biomedical fields including artery embolization, cartilage/bone scaffold, mammoplastic filler, and so on [1, 2].

TRADITIONAL AND STATE-OF-THE-ART TECHNOLOGIES OF POWDER METALLURGY IN THE PRODUCTION OF DENTAL AND ORTHOPEDIC IMPLANTS

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Traditional technologies, i.e. pressing and sintering of powders made it possible to produce new titanium alloys with a lowered Young's modulus which is close to bone tissues, as well as to produce porous one-piece implants and porous coatings. Their pore sizes are optimized for ingrowth and full functioning of newly formed bone tissues, as well as reliable and hard fixation of implants. MIM technology (Metal Powder Injection Molding) has made it possible to master the mass production of inexpensive parts of implants of a new generation: the body of artificial heart valves, the parts of the bracket correction system, dental implants, cutting elements and endoscope captures, etc., which have a complex shape and precise dimensions. New MIM technologies allow producing loaded structures of orthopedic implants: hip stems, cannulated (hollow) screws for fastening the fractures and others. HIP technology (Hot Isostatic Pressing) is used for postcompaction of implant blanks produced by traditional casting, MIM technology, AM, as well as to produce high-density and strong blanks of ceramic heads for hip stems, blanks of metal parts for orthopedic and dental implants from alloys of new generations: nickel-free austenitic steels with an increased content of nitrogen, titanium alloys which do not contain vanadium, etc. Additive Manufacturing (AM) is applied more and more nowadays to produce individual implants which have sufficient mechanical strength and biocompatibility and which replace significant fragments of the bones of the skull, jaw, pelvis, and so on. AM technologies are more widely used for the production of porous implants, new designs for dental implants, and even the first designs of hip stems have already appeared. Post HIPing of blanks produced by AM technology provides a level of properties that exceeds the requirements of ASTM or ISO standards.

CREATING SOY AND VEGETABLE COMPOSITIONS AND THE RECEIPT OF THEM FOOD POWDER

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A promising branch of food is the production of so-called functional foods that contain in their composition substances with a given physiological effect, as well as micronutrients including vitamins, antioxidants, phytoestrogens.

Vegetable products based on bean components make up more than 60% in the diet. The main protein-containing product is soy.

The high content of fat in legumes shortens the shelf life of crushed raw materials due to the oxidation of fats, increasing the acid number, which leads to the destruction of other biologically active substances.Therefore, to avoid increasing the acid number of fat, soya was combined in certain compositions with carotene-containing raw materials (carrots and spinach).

Carotenoids, in the process of preserving soya-vegetable compositions, help stabilize soybean fats and prevent their oxidation.

The preparation of phytoestrogenic raw materials for drying provides for such processes: soaking in soybean water under certain regimes with subsequent cooking to inactivate the anti-nutrient components of the raw material. Preparation of carrots and spinach, mixing of components, crushing and drying.

Experimental studies were conducted to dry the soybean-carrot mixture with heat-coolant temperatures of 70 and 100 ºC, soya-spinach, treated hygrothermically, at heat-coolant temperatures of 60 °C, 100 °C and 100/60 °C.

The process of drying the mixture takes place in the second period. With the deepening of the evaporation zone in the middle of the material, the temperature of its surface increases, and the rate of moisture yield decreases.The use of a high-temperature drying regime at 100 ºC results in an undesirable melaine reaction, which results in the burning out of biologically active substances, the qualitative characteristics of the raw materials change, with a characteristic substantial color clarification of the material.

The optimal mode of drying should be the regime behind which the temperature of the material for the soy-carrot mixture does not exceed 70–80 ºC, for soybean-spinach 60 ºC.

ANTIFOULING COATING WITH CONTROLLABLE AND SUSTAINED SILVER RELEASE FOR URINARY CATHETER APPLICATIONS

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Singapore, Kent Ridge, Singapore Catheter-associated urinary tract infections (CAUTIs) account for a large proportion of hospital-acquired infections. Bacterial colonization of the urinary catheter is a prime factor. Encrustation induced by urease-producing uropathogens like *Proteus mirabilis* causes further complications, including catheter blockage and increased risks of ascending infection and even death. In our presentation, we will describe a strategy for modifying the surfaces with antifouling coating with controllable and sustained release of silver over several weeks to combat bacterial infection and encrustation in urinary catheters. Silver nanoparticles (AgNPs) were deposited on polydopamine (PDA) pre-treated silicone catheter surface, and this was followed by another PDA coating. The number of AgNP-PDA bilayers could be manipulated to control the amount of silver loaded and its subsequent release. Poly(sulfobetaine methacrylate-*co*-acrylamide) was then grafted to provide an antifouling outer layer, and to ensure free diffusion of Ag from the surface. The micron-scale combination of an antifouling coating with two AgNP-PDA bilayers reduced *in vitro* colonization by uropathogens by ≥98%. The coated catheter was also able to resisted encrustation induced by *P. mirabilis* for up to 45 days, much longer than that of ~6 days with the commercial Dover™ silver-coated catheter. *In vitro* assay showed that the coated catheter has minimal or lower cytotoxic effects compared to the commercial Dover™ catheter. The antibacterial and anti-encrustation properties as well as the safety of the coating were further confirmed in mouse study and porcine study. The coating process was scaled-up for coating on full-length Foley catheters. Such anti-infective and anti-encrustation catheters can potentially have a large impact on reducing patient morbidity and health-care expenditure.

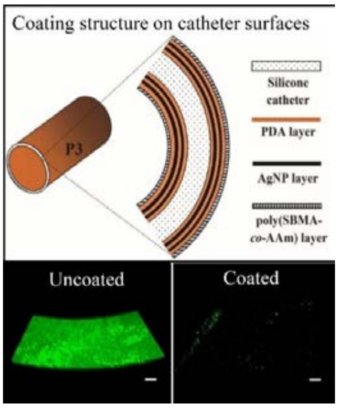

Fig. 1 Anti-infective and anti-encrustation coating on urinary catheter

COMPARATIVE PHYSICOCHEMICAL STABILITY OF COMPOSITION SYSTEMS OF HYDROXYAPATITE/POLYETHYLEN GLYCOL 400 AND 6000 IN BIOLOGICAL MEDIA

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The polyethylene glycol has a high using in medicine for treatment of infected wounds especially under wound of spinal cord which is a member of serious diseases of nervous system and surgical treatment very bad. The scientists from Purdue University (USA) showed that covering by polyethylene glycol of colloid solution of silicon oxide reducing the neurospasm through 15-20 minutes already injection shot of rats.

Interaction of composite systems on the bases of hydroxyapatite and polyethylene glycol (HAP + PEG) with molecular weights of HAP + PEG 400 10%, HAP + PEG 4000 10%, and HAP + PEG 8000 10% with physiological Ringer and Ringer-Locke solutions and NaCl has been investigated for following using of them in biological media of living organism. The study showed that PEG 4000 and PEG 8000 were covering the powders of HAP very densely and prevented liberation of calcium that is not good for our work.

By the methods of chemical analysis, it was established that the HAP + PEG 400 composite system interacts with biological media liberating calcium from a material step-by-step. The powder HAP + PEG 6000 system remained chemically stable during 100 h. By IR-spectroscopy, it was demonstrated that the spectrogram of surfaces of HAP + PEG 400 and HAP + PEG 6000 samples after the interaction with physiological solutions during 100 h contains valence vibrations in a range corresponding to the PEG presence. It can be supposed that the chemical activity of HAP + PEG 400 material relative to calcium and the prolonged presence of polyethylene glycol in the biological media help a reduction in both mineral metabolism and nervous impulses at bone defects. It is shown that the composite HAP + PEG 400 system is promising for the future development of materials for orthopedic applications.

NANODISPERSE SYSTEMS ON THE BASIS OF IRON IN THE COLLOID STATE FOR FODDER ADDITIVES

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Iron is an important element necessary for the development of the human and animal body. Deficiency of iron causes weight loss, growth and development of mental activity in children and inhibits the work of adults. Today, one third of the world's population suffers from a different type of anemia. One way to solve this problem is to introduce iron-based preparations as a fine powder in food products of daily use. In the world practice, food additives are carbonyl, electrolytic and reduced iron.

The authors developed nanopowders based on iron by the modified technology of decomposition / reduction of iron salts under special technological conditions of synthesis, which makes it possible to obtain nanodispersed iron systems in a colloidal state, which will allow them to be used as feed additives that will be easily assimilated by the organism of domestic animals.

The preliminary practical results of using experimental batches of the nanopowder of a ferromagnet, not in a colloidal state, obtained by the technology developed by the authors, in experiments in vivo on chickens of boilers by adding it to bird feed at certain concentrations, showed that it exhibits properties of a biologically active drug that affects hematological and biochemical indicators of meat and the increase in the body weight of the poultry (about 10 -15 mass%), normalizes metabolic processes of mineral substances and organoleptic and physiological ico - chemical characteristics of white and red meat of broiler chickens.

In parallel, in vitro studies on the stability of the obtained iron nanopowders in human gastric juice were carried out. It has been experimentally established that the synthesized nanopowder was dissolved in human gastric juice 3 times more intensively than in the case of Hoganäs powder (Sweden), without forming products that could have a side effect on the human body.

The iron nanopowder nanopowders obtained in the colloidal state suggested by the authors will make it possible to use it as a drink for the bird, which will make it possible to more accurately calculate experimentally the dose and time index for the drinking additive and obtain the meat enriched with iron, which will allow the prevention of iron deficiency in humans, its consuming.

POLY(LACTIC ACID) BASED BIOMATERIALS AND THEIR APPLICATIONS

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Poly(lactic acid) (PLA) is an aliphatic polyester derived from naturally-sourced lactic acid. Owing to the favorable biodegradability and excellent biocompatibility, PLA has become one of the most investigated biodegradable materials for a broad range of biomedical applications. In recent years, our research interests focus on the industrial production of PLA for use as green plastics and the development of PLA-based materials for use in bone fixation device, tissue-engineering scaffolds and drug delivery vehicles. In 2015, we have built a PLA plant with 15,000 ton/year capacity in Zhejiang Province, China. With a self-developed catalyst system, PLA is produced with high optical purity and high crystallinity, which can be readily processed into plastic sheets, films and foams for a variety of applications in green plastics. Besides, a GMP plant was also built in Jilin Province to produce “medical grade” PLA for various medical uses. A bioabsorbable bone fixation screw made from PLA-hydroxyapatite (HA) composite has been developed and approved by China Food and Drug Administration (CFDA). Other PLA-based medical devices, such as membrane for preventing postsurgical adhesions, porous scaffold for bone regeneration and microspheres for cosmetic use, are now under pre-clinical or clinical investigations. In laboratory, PLA is chemical coupled with other functionalized polymers for multifarious biomedical applications. For example, electroactiveoligoanilines have been incorporated into PLA to produce electroactive biomaterials for nerve or bone tissue engineering. Several amino acid-based monomers are designed and copolymerized with LA monomer to produce side-chain functionalized PLA materials, which can be further used for incorporation of bioactive molecules. Additionally, PLA-based injectable hydrogels and nanoparticles are also investigated for local and systemic anticancer drug delivery.

A NOVEL TITANIUM-BASED ALLOY FOR STOMATOLOGY AND IMPLANT SURGERY

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Recently the works on research, testing and application of special titanium alloys in medicine are intensified. The major aim of this work is the development of alloys without aluminum, vanadium and some other elements that are currently considered as toxic in human body. Another task for the elaborated alloys is the convergence of modulus of implant material and the elastic modulus of human bone.

As seen from the above information, the world is in searching for new alloys that would meet the requirements applying to biomedical materials. First of all, these materials should be non-toxic in the human body. Evidently, this requirement make effects on the works carried out in this direction, because the amount of alloying considered as bioinert to the human body is limited. The main of these are Zr, Ta, Nb, Pt та Si.

By using of a specific thermomechanical treatment and alloying the elastic modulus of the developed Ti-Si-X alloys can be decreased down to 60–75 GPa.

Unlike commonly used in the current practice Ti6Al4V alloy, containing undesirable elements V and Al, the new alloys use alloying elements which are completely biologically inert to the human body. Additionally, the corrosion resistance of the developed alloys are much higher compared to that of Ti6Al4V alloy.

The developed alloys have high mechanical properties: the ultimate strength - up to 1200 MPa, the yield stress – up to 1050 MPa, the ductility (elongation) 6-15% and elastic modulus 60-100 GPa (depending on the thermomechanical processing regime).

The new alloy can be used in stomatology, orthopedics and traumatology, oncology, maxillo-facial surgery and vertebrology, to produce hip joints and femoral stems (for implantation in the bone tissue), to manufacture arthroplasty items with a ratio of cross-section area to length of 1:100, in wide range of medical devices for orthopedics, plates, screws, pins, staples, needles.

TRANSLATIONAL RESEARCH OF OCULAR BIOMATERIALS

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The eye is an important organ of the human body. Cataract, keratopathy and uveitisare major or difficult ophthalmic diseases affecting the clinical treatment. The clinically therapeutic effect is greatly improved with the development of the ocular biomedical materials. For example, the clinical application of intraocular lens, artificial cornea or tissue engineered cornea brings brightness to more cataract and corneal blindness patients. However, there are still some problems to be solved urgently in the clinical application of exogenous ocular biomaterials, such as the secondary cataract after intraocular lens implantation, the scaffold in corneal tissue engineering, and long-term drug delivery in posterior segment diseases treatment, and so on. Arming to conquer these shortages of these ocular biomaterials, we have tried to improve the biocompatibility of the ocular implantable biomaterials and investigated new ocular biomaterials for translational applications. For example, surface biocompatibility modification of intraocular lenses via layer-by-layer assembly and surface-initiated free radical polymerization were carried out to inhibit the adhesion and proliferation of lens epithelial cells or bacteria after surgery, which effectively decreases the incidence of posterior capsular opacificaitonafter intraocular lens implantation [1]. Biocompatible tissue engineering hydrogel scaffolds were developed for corneal repair [2].Novel drug delivery systems were designed for posterior ocular diseases treatment, which reduces the risks of repeated intravitreal injections during conventional administration [3].

MEDIATING CELL MIGRATION BY GRADIENT CUES IN BIOMATERIALS

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The processes of tissue regeneration and remodeling depend strongly on the cell migration and differentiation. The cell migration is a very significant process in many physiological and pathological events such as embryonic development, morphogenesis, angiogenesis, wound healing, immune response, and tumor metastasis. Therefore, it would be very meaningful to study the cell migration behaviors in vitro by designing specific materials, especially the materials with gradient chemical, physical and/or biological cues, to understand the factors influencing cell mobility and further develop new strategy for designing regenerative materials. We have been focusing on the following topics in terms of gradient biomaterials and cell migration: (1) preparation and characterization of several types of gradient biomaterials with continuous changes in grafting density, chain length and swelling properties; (2) Influence of physicochemical properties of gradient biomaterials on cell migration in terms of rate and direction; (3) directional migration of cells under the guidance of gradient cues; (4) selective adhesion of targeted cells and directed migration; and (5) enhanced regeneration of endothelium of blood vessel and cartilage/subchondral bone by scaffolds that promote cell migration or infiltration. More recently, the in situ secreted chemokines by immune cells are integrated into the materials system for guided migration of tissue repair cells, enabling more adaptive systems that better mimic the microenvironments of host tissues.

INFLUENCE OF SEVERE PLASTIC DEFORMATION AND Ag DOPING ON STRUCTURE AND PROPERTIES OF MAGNESIUM ALLOY FOR BIODEGRADABLE IMPLANTS

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Magnesium-based implants a promising direction in cardiological surgery, orthopedics and traumatology due to their high solubility in biological tissues. Magnesium alloys have a great potential because they are completely biocompatible, have mechanical properties similar to the mechanical properties of natural bone, do not cause an inflammatory reaction, have the ability to osteointegration and stimulate the growth of new bone tissue. Moreover, due to their ability to dissolve, there is no need for repeated surgery to remove the implant.

The studies were conducted on the magnesium alloy WE43, which is one of the best industrial magnesium alloys strengthened by rare earth elements (Y, Nd, La). In addition to improve the corrosion properties and to increase the stability of the implant initial alloy was doped with silver (WE43+Ag).

Using methods of severe plastic deformation (ECAP, drawing and forging) samples of high purity WE43 alloy were obtained. These samples have fine-grained structure (3 μm) and a combination of high strength (σ_y = 295 MPa, σ_u = 353 MPa) and plasticity (δ = 22.5%).

SPD processing of WE43 alloy leads to the formation of the axial texture [10.0] in the samples with a predominant grain orientation by the crystallographic direction [10.0] along the axis of the samples. Texture is not uniform along the length of the samples - weakening of the texture from the upper part to the lower part is observed.

It is established that further deformation of such material can be accompanied by the increasing of the average grain size and a certain decreasing of mechanical properties. The purer the initial material, used to produce ingots of WE43 alloy, the more difficult the process of grains grinding by facilitating the relaxation processes in the stress field.

XRD studies have established that the value of crystallite domain size CDS is reduced to 150 nm in deformed alloys, but during the aging process at room temperature it increases by 1.5–3 times due to relaxation processes occurring under these conditions. At the same time the microstrain level decreases, but the texture remains practically unchanged.

Also, in vivo experiments were performed, where the samples of WE43 and WE43+Ag alloy were implanted to rats in the interdisk space at the base of the tail and subcutaneously. The animals were removed from the experiment after 15 days, 1, 2, 3, 4 and 5 months after implantation. The surface of the extracted samples is examined, the corrosion products and biological tissues are removed from the surface of the samples, the behavior and the rate of corrosion in vivo is assessed. It was found that the dissolution rate of the modified biodegradable magnesium alloy WE43+Ag in the body (in vivo) is about 2 times lower than the dissolution rate of the industrial alloy WE43.

FEATURES OF HYDRATION OF THE COMPOSITE SYSTEM SILICA-AMBER

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Amber is a natural organic mineral formed from a pine resin that has been petrified for several million years, the composition of which is a very complex mixture of supramolecular structures consisting of macromolecular and low molecular weight components. Amber is mainly used for jewelry and decorative art. A large amount of waste left after the manufacture of jewelry can be a valuable, natural, inexpensive, potentially bioactive raw material for veterinary, medicine and cosmetology. It has long been widely used in non-traditional medicine as a medicine for increasing immunity, treating inflammatory processes, and eliminating rheumatic pain. The main substances that can provide a therapeutic effect are succinic acid and some types of terpenes. However, the transition of biologically active substances from natural amber to biological fluids is limited by slow diffusion processes and poor solubility of its components in most biological fluids and organic solvents. A promising type of bioactive additives based on natural amber can be its composite systems with amorphous highly disperse silica. As a result, a composite material is formed in which the amber is evenly distributed over the surface of the silica particles. When creating such composites, a significant part of amber passes into a submicron state, which provides a significant increase in the contact surface with the environment. As an active biological additive, amber and composite systems based on it can be used either orally, or in transdermal therapeutic or cosmetic preparations. We have shown that for the amber/SiO_2 composite system there is no directly proportional relationship between the values of the water concentration and the interfacial energy, which is due to a change in the structure of the water clusters in the interparticle gaps of the composite with a change in its hydration. It is also shown that in the presence of strong acids on the boundary with a hydrophobic medium, some of the water bound to the surface of the amber/SiO_2 composite passes into a weakly associated state, which may serve as one of the signs of increasing bioavailability of succinates desorbed from the composite.

INJECTABLE HYDROGELS FOR SKIN WOUND REPAIR

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This talk presents the preparation of injectable polymer hydrogels based on dynamic bonds and applications for skin wound repair. Polysaccharides modified with functional groups form multiple dynamic bonds to create hydrogels. Rheological studies demonstrate the shear thinning and rapid self-healing. This feature enables injection and rapid re-gelation in vivo. In vivo studies show excellent biocompatibility and minimal inflammation. The gels degraded and were adsorbed in vivo in ten weeks. Meanwhile, the full skin wound model in the rats was excellently repaired with the presence of hydrogels, in comparison to the control.

HIGHLY-POROUS CERAMICS BASED ON BIOGENIC HYDROXYAPATITE FOR RECONSTRUCTIVE SURGERY

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Ceramics based on hydroxyapatite is most widely used for treatment of bone tissue defects in orthopedics, traumatology and dentistry thanks to its excellent biocompatibility and osteoconductive properties and similarity in chemical composition to the mineral component of natural bone.

In the present highly-porous ceramics based on biogenic hydroxyapatite with addition of 10, 25 and 40 wt. % of sodiumborosilicate glass (wt.%: 45.7 SiO_2, 28.2 B_2O_3, 26.1 Na_2O) have been prepared by foam replication method at 700-1000 °C.

The composition of prepared samples was controlled by XRD analysis (X’Pert PRO (PANalytical)), IR spectroscopy (FCM 1202 (Infraspectr)) and energy-dispersive X-ray fluorescent element analysis (Expert 3L (INAM)). The structure was examined by SEM using Zeiss Ultra Plus (Carl Zeiss Meditec AG) microscope. The total porosity of the samples was calculated using the skeleton density values measured by helium pycnometer AccuPyc II 1340 (Micromeritics). Open porosity measurement of the samples was performed in ethanol using the Archimedes principle. The dissolution rate of the samples was evaluated by means of weight loss measurements in saline at 36–37°C for 2 days.

According to the XRD results it was established that amount of glass did not influence on the phase composition of highly-porous glass ceramics. Using of sodiumborosilicate glass keeps the phase of hydroxyapatite during the sintering that was confirmed by IR spectroscopy. All prepared samples are characterized by a permeable structure with porosity of 93-97 %. The dissolution rate of ceramics is equal to 0.002-0.025 wt.%/day and increases with increasing of amount of glass in ceramics composition.

The publication contains the results of studies conducted by Grant for monthly visits of Ukrainian scientists to Poland according to the Protocol to the Agreement on Scientific Cooperation between the National Academy of Sciences of Ukraine and Polish Academy of Sciences.

DETERMINATION OF INFLUENCE BY FERROMAGNETIC ADDITIVES ON PHYSICAL AND MECHANICAL PROPERTIES OF BIOGENIC HYDROXYAPATITE MATERIALS

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The effect of ferromagnetic additives in the form of 1% magnetite into biogenic hydroxyapatite have been studied asacontrasting images in MRI, diagnosis of various diseases on the early stages, in purification and separation of various biological substances, as well asin treatment of malignant tumors and targeted drug delivery. Determination of the influence of ferromagnetic additives on the physical and mechanical properties of such materials has been investigated.Determination of dynamic characteristics of elasticity for the materials were carried out based on the results of measuring the elastic wavevelocity, which excitation parameters were chosen taking into account the structural characteristics of compact samples. The velocity was determined according to the time of the passage of the elastic momentum through the sample that was studied. Measurement of the passage time was carried out at a frequency of 0.6 MHz by the method of the radio pulse with a discrete delay in the shock excitation of the transducer and the through sound of the samples. For this purpose a hardware complex for precision acoustic measurements, developed in the Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine was used.The characteristics of elasticity of BHA, BHA / Fe_3O_4, obtained by physico-mechanical and chemical methods make up 15 GPa, 7.8 GPa and 4.3 GPa accordingly. These values are close to the dynamic characteristics of cortical bone tissue. Their elasticity characteristics differ almost twice: 15 GPa in the case of BHA and 7.8 GPa in the case of BHA/Fe_3O_4.Taking into account the above mentioned data BHA/Fe_3O_4 composite systems have different characteristics, and therefore it is possible to pick up the material and its shape according to the needs for implantation in different parts of the musculoskeletal system.

BIOMEDICAL POLYMER MATERIALS AND THEIR INFUSION AND INTERVENTIONAL MEDICAL DEVICES: FROM SCIENCE TO INDUSTRIALIZATION

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Aiming at the common problems of infusion and interventional medical devices including plasticizer precipitation ofpolyvinyl chloride, ethylene oxideresidue of ethylene oxide sterilization, bacterial infection and blood coagulation. Our group have conducted full chain research ranging from science, technology, to industrialization. Systematic work has been carried out on materials such as biomedical thermoplastic elastomers, radiation-resistant medical polymers,anti-bacterial and anticoagulantbiomedicalpolymers. The above materials have been used in some kinds of infusion and interventional medical devices, and put into industrialization in WEGO Group Co., Ltd.

COMPUTER IDENTIFICATION OF BIOCOMPATIBLE TI-BASED POWDER ALLOYS

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Currently, a large number of dental implants and medical devices are being developed and produced. The most promising areas in the development of biocompatible materials with a porous structure are the combination of fast prototyping with powders casting or sintering.

Materials, intended for the implants production must have a high biocompatibility and specific strength. According to numerous fundamental and applied research, the best material for the production of such products is titanium and its alloys.

The investigating, associated with the processes of the biocompatible material development and the manufacture of medical products from it, and the ability to manage them, contributes to the obtaining of material with specified properties. Currently, there is a large database of materials for medical products. On the one hand, this allows as to correctly selecting the implant material individually for each patient, and, on the other hand, it increases the time and financial resources. Therefore, to create new materials and coatings with specified properties and to improve the reliability of servicing of known materials, it is necessary to combine experimental diagnostic methods and methods of computer modeling.

The use of supervised learning, in this case, allows us to reduce the task of titanium alloys selection to the classification problem. An important result of the solution of this problem is the possibility of constructing a material from a powder titanium alloy with predefined properties (microstructure parameters, elemental and fractional composition).

It should be noted that simulation based on existing classification methods (Logistic regression, Support Vector Machine) shows poor accuracy (63.54 and 62.5% respectively). The same applies to a PNN-based classifier (80% accuracy). That is why increasing the accuracy of these methods remains an important task. This will enable to reduce financial losses in case of incorrect identification of biocompatible material and possible consequences of harm to health.

One of the variants for improving the accuracy of the identifying the biocompatible material's conformity tasks is the use of the Ito decomposition (Wiener polynomial). Based on this, the new approach to solving such problems is proposed. The idea of the method is to use the Ito decomposition to increase the number of input parameters. Classification occurs by searching for members of this polynomial. Different algorithms of machine learning are used for this purpose.

NANOSIZE EFFECTS AND ITS APPLICATION AT COMPOSITES CONSTRUCTION FOR MEDICINE AND BIOTECHNOLOGY

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By using the unique physical-chemical properties of substances in a clustered condition, wascreateed nanocomposite and bionanocomposite systems, as adaptogenic, immunomodulatory and medical nanocomposites for prevention and treatment of many diseases, which allow stimulating the development of crop seeds and activating cell metabolism; methods of remediation of contaminated with hydrocarbons water and soil; enterosorbents and dietary supplements for treatment of diseases in farm animals and birds; caused by violation of ecological systems under the influence of anthropogenic and natural factors

The innovative idea which was used is the application of activated composites with nanosilica instead of individual substrates such as drugs, mineral fertilizers, microbiological cultures, or biologically active compounds. The activation occurs by development a close contact between silica nanoparticles and their substrates, and depending on the type of substrate it takes place by mechanical-chemical activation, impregnation, or joint dispersion. Due to influence of the surface forces of the nanoparticles which affect the distance between 1-20 nm, the properties of the substrate change significantly due to transition to nanostate. The effectiveness of the influence of the substrate on drugs, bacterial cultures, seeds in the sprouting stage increases significantly.

The basis may be the hydrophilic or mixture of hydrophilic and hydrophobic nanosilicas (SiO_2 and $MeSiO_2$) which with a certain ratio act as carriers ofmedicinal or biologically active substances, natural or mineral fertilizers, nanofungicides, microbial preparations, natural growth stimulators for plants and related substances. The multidirectional nanocomposite materials can be produced within close technological cycles.

CATALYTIC EFFECT OF TRANSITION METALS TI, FE AND SI ON THERMAL STABILITY AND KINETICS OF DECOMPOSITION OF MGH$_2$ SYNTHESIZED BY REACTIVE MECHANICAL ALLOYING

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With the aim of lowering the temperature, improvement the kinetics of the decomposition of stoichiometric MgH_2 hydride the possibility of its complex doping by Si, Ti, Fe using the method of reactive mechanochemical alloying (RMA) has been investigated. Mg+5%wt.Si+5%wt.Ti+2%wt.Fe(MA1), Mg+5%wt.Si+5%wt.Fe+2%wt.Ti(MA2), Mg+10%wt. Si+2%wt.Ti+2%wt.Fe(MA3) mechanical alloys have been synthesized and their phase composition, structure, hydrogen-sorption properties, thermal stability and desorption kinetics of hydrogen from them have been investigated employing the X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermodesorption spectroscopy (TDS) mmethods. For comparison, we synthesized an additional composite alloy in the same ball mill and at the same condition that were used for obtaining the MA1, MA2, MA3 samples, however, without any Si, Ti, Fe additives. We shall refer this sample to MA4.

To evaluate the influence of complex alloying by Ti, Fe transition metals and by Si on decomposition temperature and thermal stability of MgH_2 phase hydrogen desorption isobars have been obtained at the first heating after RMA synthesis of MA1-MA4 samples and after the next cyclic hydrogenation from gas phase. All isobars were obtained at hydrogen pressure in the reactor 0.1 MPa and sample heating rate of 3 ^{o}/min. and were used to determine both the hydrogen desorption beginning temperature ($T_{beg.}$) from hydride phase MgH_2 of MA1-MA4 and temperature T_{max}, that corresponds to the maximum speed of hydrogen release. The kinetic curves of hydrogen desorption from MA1, MA2, MA3 mechanical alloys-composites has been obtained at the constant hydrogen pressure of 0,1 MPa in the reactor and temperature 310 and 330 °C and were used to determine both the hydrogen time release of half of hydrogen quantity ($\tau_{1/2}$) and total hydrogen quantity release (τ_t) for all MAs. This date of hydrogen time release for MA1-MA3 and for MA4 to be compared. It was established that:

- By reactive grinding during 20 h of magnesium with the additives of Si, Ti, Fe the hydrogen capacity of 5,7 wt.%; 5,6 wt. % and 5,4 wt. % can be achieved for MA1, MA2, MA3 samples respectively; and after the first hydrogenation from the gas phase - of 5,3 wt.%; 5,1 wt. % and 4,1 wt. % respectively.

- The temperature (^{0}C) of hydrogen desorption beginning (T_{beg}) from MA1-MA4 mechanical alloys after their RMA synthesis is 288, 290, 290, 288 and after the first hydrogenation from the gas phase – 288, 313, 310, 320 respectively.
- The best kinetics of hydrogen desorption at pressure of 0,1MPa in the reactor and a temperature of 330 °C had MA2 and MA3 alloys- composites, for which $\tau_{1/2}$ is 12 and 6,3 min and τ_t - 28 and 10 min respectively. For MA4 (MgH_2 without Si, Ti, Fe) $\tau_{1/2}$ and τ_t equal 31 and 75 min respectively.

It is found that Si, Ti, Fe additives to magnesium significantly improve hydrogen desorption kinetics process of MgH_2 hydride phase of obtained MAs. However, the effect of thermodynamic stability reducing of MgH_2 hydride phase as a result of its complex doping with silicon, titanium, and iron was not observed. The developed materials allow their use at stationary application conditions.

ADVANCEMENT IN NON-PRECIOUS METAL CATALYSTS FOR FUEL CELLS

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The development of high-performance and low-cost catalytic materials for the oxygen reduction reaction (ORR) has been a major challenge for the large-scale application of fuel cells. Currently, platinum and platinum-based alloys are the most efficient ORR catalysts in fuel-cell cathodes; however, they cannot meet the demand for the widespread commercialization of fuel cells because of the scarcity of platinum. Thus, the ongoing search for platinum-free catalysts for the ORR has attracted much attention. Graphene, single-layer sheets of sp2-hybridized carbon atoms, has attracted tremendous attention and research interest. The abundance of free-flowing p electrons in carbon materials composed of sp2-hybridized carbon atoms makes these materials potential catalysts for reactions that require electrons, such as the ORR. However, these p electrons are too inert to be used directly in the ORR. In N-doped electron-rich carbon nanostructures, carbon p electrons have been shown to be activated through conjugation with lone-pair electrons from N dopants; thus, O2 molecules are reduced on the positively charged C atoms that neighbor N atoms. Recently, we reported a novel strategy for the selective synthesis of pyridinic- and pyrrolic-nitrogen-doped graphene (NG) by the use of layered montmorillonite (MMT) as a quasi-closed flat nanoreactor, which is open only along the perimeter to enable the entrance of aniline (AN) monomer molecules. The flat MMT nanoreactor, which is less than 1 nm thick, extensively constrains the formation of quaternary N because of its 3D structure but facilitates the formation of pyridinic and pyrrolic N. Nitrogen is well-known to be incorporated into quaternary N in tetrahedral sp3 hybridization but incorporated into pyridinic and pyrrolic N in planar sp2 hybridization. The confinement effect of MMT ensures that N is doped in planar pyridinic and pyrrolic N. The results indicate that the content of the planar pyridinic and pyrrolic N is inversely proportional to the interspace width (d) of MMT. Electrochemical evaluations showed that planar pyridinic and pyrrolic N are much active for catalysis of the ORR than 3D quandary N doped NG. We improve the earlier method by “shape fixing via salt recrystallization” method to efficiently synthesize nitrogendoped carbon material with a large number of active sites exposed to the three-phase zones, for use as an ORR catalyst. Self-assembled polyaniline with a 3D network structure was fixed and fully sealed inside NaCl via recrystallization of NaCl solution. During pyrolysis, the NaCl crystal functions as a fully sealed nanoreactor, which facilitates nitrogen incorporation and graphitization. The gasification in such a closed nanoreactor creates a large number of pores in the resultant samples. The 3D network structure, which is conducive to mass transport and high utilization of active sites, was found to have been accurately transferred to the final N-doped carbon materials, after dissolution of the NaCl. Use of the invented cathode catalyst in a proton exchange membrane fuel cell produces a peak power of 600 mW cm^{-2}, making this among the best nonprecious metal catalysts for the ORR reported so far.

ELECTRON CONCEPT OF HYDROGEN-ENHANCED LOCALIZED PLASTICITY AS A TOOL FOR DESIGN OF NEW HYDROGEN-RESISTANT STRUCTURAL ALLOYS

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The hydrogen embrittlement (HE) phenomena in 3d transition metals-based structural materials are considered. Peculiarities of hydrogen effect on the electron structure, phase transformations and dislocation properties in Fe-, Ti- and Ni- based alloys were studied and the consequences for macroscopic mechanical properties of corresponding materials were derived.

Using nitrogen and carbon as indicators of correlations between electronic structure and mechanical properties, the verification of electron concept of hydrogen enhanced localized plasticity (HELP)has been performed. The proposed concept allows taking into account the chemical nature of interstitial elements and correctly predicting their influence on dislocation properties that is the main point of hydrogen-caused brittleness model. An additional advantage of the proposed concept, in comparison with the classical HELP model, developed within the framework of continuum mechanics, is the possibility to propose practical recommendations for the increase in materials resistance to hydrogen brittleness.

Using mechanical spectroscopy, the Snoek-Koester relaxation was studied and it was shown that nitrogen atmospheres assist dislocations mobility, whereas, in contrast, carbon atoms retard dislocations slip. Using first principle calculations, a correlation between the carbon and nitrogen effects on the Fe electronic structure and dislocation properties is established. Correspondingly, similarly to hydrogen, the nitrogen-caused increase in the concentration of free electrons should assist mobility of dislocations, which is in a perfect consistency with experimental data.

By means of theoretical and experimental studies, it was shown that there is similar effect of hydrogen on the electron structure and dislocation properties in Ti- and Ni-based alloys, which is an additional confirmation of correctness of the electron approach to hydrogen-enhanced localized plasticity and shows a general character of this approach for HE. Particularly, on this basis, the explanation is given for different appearance of HE in Ti alloys and austenitic steels, which allows using hydrogen as a temporary alloying element during technological treatment of Ti alloys in single-phase state, to provide their better deformational characteristics.

R&D OF ELEVATED TEMPERATURE METHANOL FUEL CELLS

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Among the advanced sustainable power source technologies, hydrogen based energy is widely considered as the most promising substitute technology for transportation, residential, and industrial applications with zero emissions. However, we still face barriers of the generation, storage, and transport of hydrogen. The related infrastructures are also far from commercialization. So, to find an interim solution is of great importance.

The energy circulation of methanol is thought to be a good substitution of hydrogen.Firstly, the massive production of methanol is easy tobe realized from fossil fuels, biomass, and even the conversion of carbon dioxide. The transportation and distribution of the liquid methanol is similar as that ofthe fossil fuels. So, how to use methanol to generate electricity with fuel cell technology is the key point. Direct methanol fuel cell (DMFC) is of remarkable energy density, but the power density is still lower than other power sources, such as lithium ion batteries. The methanol fuel cells at operation temperature of 150 to 200 could be a promising solution to improve the specific power of DMFCs. Our group have focused on the research of elevated temperature methanol fuel cells for a few years.Based on the critical issues of fuel cells, performance, durability, safety, and costs, we carried out different levels of researches, from materials, components, to system integration, and process controls. What's more, the reliability and security of fuel cell demonstrations is also studied.

CATALYTIC APPROACH FOR IMPROVING THE SOLID FUELS GASIFICATION AND HYDROGEN OR HYDROCARBONS PRODUCTION FROM BIO RESOURCES OR THE ORGANIC WASTES

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Application of the catalytic technologies is a key for the majority of the chemical processes, deep oil refining, production of cleaner motor fuels, petrochemicals and chemicals, engineering plastics, fertilizers, plant protection products, producing a new generation of high-quality medical products, environmentally friendly food production, other types of high value-added products, and all levels of redistribution. Here we report on the catalytic approaches that has been developed in the L.V.Pisarzhevky Institute of Physical Chemistry of NAN Ukraine. The approaches are directed towards development of the heterogeneously catalytic process for the hydrogen production from solid or liquid bio resources as well as for the hydrocarbons production from syngas.

The ethanol steam reforming (ESR) gives a promising way for hydrogen production from renewable feedstock.Our results show that spinel-type ferrites exhibit an appreciable performance in the ethanol steam reforming. The ESR reaction over ferrites allows to produce CO-free hydrogen that is of importance for hydrogen application in fuel cells.

For the hydrocarbons production from syngas, we show that carbon number distribution of C_{4+}products, resulting on $Co/SiO_2{\cdot}Zr(IV)$ catalyst at evaluated pressures is a superposition of two different distributions. Analysis of products show that olefin content in C_3–C_6 products decreases with increasing the carbon number, whereas the productivity is very high.

The third approach is based on a development of catalysts to improve the process of the wastes gasification. Using metal ions oxides, we have developed the catalyst that allows obtaining pure hydrogen and char coal from the organic and polymeric wastes.

Our approach to the development of the catalysts for the hydrogen production as well as for the hydrocarbons production gives a promising way for the development of new technologies for the fuel production from renewable sources of the 1-st and 2-nd generation.

FROM POWDER TO POWER: UKRAINIAN WAY

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A short surwey of the R&D activity of Laboratory for Ceramic Fuel Cells at Frantcevych Institute for Problems of Materials Science on their way from zirconia powders to Ceramic Fuel Cells is presented. The research topics, which are important for enhancing CFC, like 1Ce10ScSZ zirconia powders, formation of structure and strength of zirconia electrolytes, structure and properties of EB-PVD films, conductivity of bulk and film zirconia electrolyte, catalitic activity of zirconia powders, reduction of nickel, redox of Ni–ZrO_2 composites, and structural optimization of CFC, are discussed. Comparative test of developed CFC and commercial one as well as the investment proposal to establish pilot productions of zirconia powders, fuel cells and energy systems are completing the review.

Zirconia doped with 10-mol. % Sc_2O_3 and 1-mol. % CeO_2 (1Ce10ScSZ) is considered now as a promising alternative to yttria stabilized zirconia (8YSZ) ceramic electrolyte usedwidely. Different types of zirconia powder, newly developed and available on the World market, were studied extensively.

It was found, that at short-term testing, our 1Ce10ScSZ powder consisting of nanosized, 9-13 nm, particles and doped with aluminum and silicon may provide almost one order of magnitude higher conductivity than its the purest industrial counterpart. At long-term testing, ~1500 hours, the electrolytes, made of newly developed and industrial powders, purity of which differs for more than one order of magnitude, have the same conductivity.

The NiO-ZrO_2 anode based on our 1Ce10ScSZ powder ensures above 100 MPa mechanical strength and near zero electrical resistance at >30 % porosity in reduced state.

As to the 8YSZ composition, it ensures also higher properties realized in CFC made with tape-casting technique. It was found that our 8YSZ CFC tested with the model fuel gas, 5-

vol. % H_2 in Ar, at 800 ^oC ensures better (~50 %) result than analogous CFC available on the World market.

For the investment, an organization of pilot production of three products is proposed as follows: scandia and yttria stabilized zirconia powders specified for electrolyte and electrodes; 600 °C fuel cells; portable and stationary 5-kW SOFC-CHP systems to utilize hydrogen or natural gas.

AN ANODE-SUPPORTED SOLID OXIDE FUEL CELL BASED ON DOUBLE-SIDED CATHODES

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Anode supported planar solid oxide fuel cells (SOFCs) have been extensively studied during the past few decades for high efficiency and zero pollution. However, the commercial application of anodesupported planar SOFCs has been plagued by sealing and cell structural stability. Therefore, many methods, such as substituting the tubular structure for planar structure, updating the anode materials, and adjusting the thickness of each layer of SOFCs, are used to overcome the two weaknesses. Combining the advantages of tubular SOFCs and planar SOFCs, an anode-supported SOFC based on double-sided cathodes was developed by NIMTE.

The anti-fracture load of new structural SOFCs is 20 times stronger than that of traditional cells. Meanwhile, the electrochemical performance of new structural SOFCs is close to that of traditional large-scale, ultra-thin cells.In addition to high strength in structure, anode-supported flat-tube SOFC also has strong stability in redox. Under 2 redox cycles, the anode-supported flat-tube half cells were compared with traditional ultra-thin reference half cells in both reduction and oxidation states.After the first redox cycle, the reference half cells bended towards the electrolyte, displaying evident warping and deformation. After the second redox cycle,the cell with the electrolyte side facing the setter broke, whereas the other cell with the electrolyte on top seriously deformed.The DSC-SOFC maintained consistent completeness and flatness through the 2 redox cycles. The DSC-SOFC demonstrated excellent redox stability and uniformity in comparison with traditional ultra-thin, dissymmetric, anode-supported cells.The structure and preparation technology of DSC-SOFC cells were optimized, based on the testing results, with an output power density improvement up to 0.33 W cm^{-2} at 0.7 V under 750 °C.After 6 thermal cycles, the electrochemical performance slightly decreased. The testing results showed the satisfactory redox stability of anode-supported flat tube SOFCs, which withstood thermal cycles during operation without sudden failure.

The results of imitations are the same as those of the experiment, which show that in redox, the displacement of DSC-SOFCs is nearly 0, whereas that of T-SOFCs is significantly larger.

NOVEL MG-BASED COMPOUNDS, ALLOYS AND COMPOSITES AS EFFECTIVE HYDROGEN STORAGE MATERIALS

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Practical use of magnesium and its alloys in hydrogen storage systems is limited by slow kinetics and elevated temperatures of hydrogen absorption-desorption (>300 °C). Many recent studies were focused on the improvement of these parameters, including preparation of MgH_2 by reactive ball milling or other methods and synthesis of novel Mg-based alloys or composites. New Mg-Ti, Mg-TiO_2 and Mg-Ti/Zr suboxide composite materials have been synthesized in our recent studies. They demonstrated 6…6.5 wt.% hydrogen storage capacity and the substantial decrease of absorption-desorption temperature. The ternary Mg-IMC-C composites have shown higher cyclic stability than Mg-IMC materials.

The phase equilibria in the Mg-M-Ni (M = Ti,Mn) systems and hydrogenation properties of the selected alloys have been studied. The hydrogenation behavior of new Mg_3MNi_2 (M = Ti,Mn,Al) ternary compounds will be discussed in the report. The enhancement of hydrogen absorption-desorption properties will be demonstrated for the $Mg_{88}M_4Ni_8$ alloys.

The review on the R–Mg–(Ni,Co) systems and the hydrogenation properties of the selected intermetallic compounds will be presented. The crystal structures of new $RMgCo_4$, $RMgNi_2Co_2$, $R_2Mg(Ni,Co)_9$ (R = Y,La,Nd,Tb), $NdMg_2Co_9$ and other compounds have been studied. Hydrides of the selected compounds have been synthesized and their crystal structures were determined for the first time. Hydrogen sorption-desorption properties, which were studied from the gas phase and electrochemically, will be analyzed.

ATOMIC SCALE STRUCTURE CONTROL OF ENERGY CONVERSION CATALYSTS AND THE SITE STRUCTURE EVOLUTION INVESTIGATION

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The sluggish nature of oxygen reduction reaction and cost associated with Platinum based catalysts have long been regarded as the major impediment to the commercialization of polymer exchange membrane fuel cells (PEMFCs). Therefore, enormous research efforts have been devoted to search for non-noble metal catalysts with comparable electrocatalytic performance of Pt, including carbon-supported transition metal/nitrogen compounds, heteroatom-doped carbon materials and nitrogen-doped carbon with transition metal/metal carbide encapsulated in graphitic layer structure. Among the vast non-precious metal catalysts, our research group is particularly interested in the M/N/C catalysts due to its respectable activity.

Herein, we present a microporous metal-organic-framework-confined strategy to precisely control the material's structure at atomic level, preferentially forming single-atom dispersed Fe-N-C structure. As shown in Figure 1, the catalyst shows excellent ORR performance with an onset potential of 0.92 V in acidic electrolyte, which outperformed most non-precious-metal catalysts reported to date. The 57Fe Mössbauer spectrum and X-ray absorption spectroscopy for Fe L-edge revealed the high-spin Fe^{3+}-N_4 configuration in the pyrolyzed Fe-N-C catalyst. In-situ X-ray absorption spectroscopy showed a Fe^{3+}/Fe^{2+} redox transition at a low potential, demonstrating that the active site structure was the in-situ reduced non-planar Fe^{2+}-N_4 moiety embedded in distorted carbon matrix. The five coordinated OH-Fe^{2+}-N_4, which resembles the D3 structure, owns ultra-high turn-over frequency (TOF) of 3.98 e s^{-1} $sites^{-1}$. The ultra-high TOF of our catalyst can be ascribed to its optimized Fe^{2+}/Fe^{3+} redox potential that balanced the site-blocking effect and O_2 dissociation.

Meanwhile, for the first time, we designed and successfully fabricated a novel binuclear active site structure, $Co_2N_xC_y$, as ORR catalyst site, which was achieved by precisely controlling precursor's structure at atomic level. Two-atom sites with Co-Co distance at 2.1-2.2 Å were directly observed in the catalyst from aberration-corrected scanning transmission electron microscopy (STEM). Additionally, a novel shortened Co-Co path (2.12 Å) was found in X-ray absorption spectroscopy, attributable to the binuclear Co_2N_X site. Its configuration was further confirmed as Co_2N_5 combined with density functional theory (DFT) calculation. Excitingly, dramatic enhancement on the ORR activity was obtained on the Co_2N_5 site, which exhibits approximately 12 times higher activity than the conventional single CoN_4 site. Theoretical density functional theory calculations were applied to reveal the mechanism of ORR on the novel binuclear site, on which thermodynamic barrier towards ORR was considerably reduced, thus contributing to the much higher intrinsic activity of the dual atom center site. Our finding is of significance for rational designing non-noble metal catalysts to completely replace Pt for ORR in the future.

RECENT DEVELOPMENT OF SCALABLE HYDROGEN STORAGE TECHNOLOGY BASED ON THE CONCEPT OF LIQUID ORGANIC HYDROGEN CARRIER

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The rapid depletion of fossil fuels and the sharp rise of carbon emission have raised increasing energy and environmental concerns worldwide on energy sustainability, global warming and climate change. Low carbon manufacturing is playing an increasingly important role in sustainable development of future energy economy. To promote more extensive utilization of renewable energy sources, greener production processes and less green house gas emission, innovative energy technologies are imperative.

In the present lecture, we will outline our recent efforts to develop efficient hydrogen technologies for scalable energy storage, especially for automotive applications. As the lightest atom in the periodic table, hydrogen possesses the highest energy density and can serve as one of the most efficient energy carriers. Hydrogen can be produced via a wide variety of sources. It has been widely used in petrochemical, pharmaceutical and agrichemical processes. Most recently, hydrogen has been broadly recognized as one of the most efficient energy storage media to regulate smart grids and renewable energies and to power portable and mobile electric devices. It enables combustion of hydrocarbon materials, such as fossil fuels, municipal wastes and biomass, to undergo more complete oxidation and thus facilitates drastic improvement of air quality. Unfortunately, the major obstacle preventing hydrogen technologies from being broadly applicable to industrial applications has been a lack of high capacity, reversible and commercially viable hydrogen storage materials at neat ambient conditions. We have developed a highly scalable hydrogen storage technology based on the concept of liquid organic hydrogen carrier. High capacity, room temperature hydrogen storage can be realized through catalytic hydrogenation of selected polycyclic aromatic compounds; hydrogen release can be carried out catalytically at a temperature moderately higher than the waste heat temperature of proton exchange fuel cell devices. The storage media and their hydrogenated forms remain in a liquid state at room temperature and ambient pressure with high flash points and thus facilitate both safe storage and transport, similar to or better than the existing petroleum-based technologies. More importantly, the hydrogen storage technology requires a minimum energy infrastructural change and enables a long driving range if it is utilized to power electric vehicles. Implications of the technology deployment in the market place to future energy economy and environmental impact will be discussed.

IMPROVEMENT OF SILICON CARBIDE CERAMICS MECHANICAL PROPERTIES BY DIFFERENT ADDITIVES

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Dense silicon carbide (SiC) ceramics and composites are very attractive engineering ceramics at the extreme operating parameters, in particular for high temperature and nuclear applications, such as advanced nuclear fuel forms, structural components for fission reactor systems, blankets for fusion energy systems, and matrices for nuclear waste immobilization. As alternative of the mechanical properties improvement by SiC fibers reinforcing, the different additives to the SiC matrice were investigated at present paper. The SiC matrices reinforced by additives of amorphous B, Cr, Si were fabricated using High-Speed Hot Pressing Method (HSHP). Additives content was in the range from 0,5 to 3 wt %. Microstructural characteristics of silicon carbide ceramics were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM) and elemental distribution analyses (EDX). Results demonstrate the influence of different additions on the SiC ceramic sintering process. A fine-grained and dense ceramics with advanced mechanical properties were produced at optimal processing conditions. SiC ceramics with Cr and Si additives possess the best structural and mechanical characteristics: micro hardness 28.0 – 30 GPa and fracture toughness K_{1C} = 6.2 – 4.7 MPa·$m^{1/2}$, respectively. The sintering process by HSHP method leads to increase of the fracture toughness of ceramics. It is mean that structural and mechanical properties of SiC ceramics can be improved by effective additives content controlling.

ADVANCED TECHNOLOGY FOR FABRICATION OF NICKEL-PLATED HEXAGONAL BORON NITRIDE POWDER

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The powder of hexagonal boron nitride coated with layer of nickel is widely used as a component of the powder mixtures used for applying for tightening coatings to the parts of gas turbine plants (turbine blades and the flow of the engine diaphragm). Its use in the coating makes it possible to increase the heat resistance and surface finishability and to increase the life of the engine parts up to 2 times.

When using nickel-plated boron nitride for gas-plasma spraying, it is important to observe a number of physical and technological characteristics of the material. The grain size should correspond to a fraction of + 20–160 μm. In this case, the integrity of the grains is important, since when passing through the plasmatron the grains that are glued together during granulation are scattered into the original smaller ones and do not reach the target. This leads to significant losses of expensive powder during production.

The technology of 20 % BN – 80 % Ni composite material fabrication is developed which consists of the next operations: granulation of the initial boron nitride powder; classification of boron nitride granules; activation of the granules surface of by depositing a thin nickel sublayer on the boron nitride granules, which allows preserving the integrity of granular grains in subsequent operations chemical nickel plating of the granules.

Application of the developed technology allows to obtain grains of nickel-plated boron nitride powder with a dispersion of +40-160 μm (about 90%) oval-like shape, which ensures good powder flowability during spraying. The stable bulk density of the resulting powder is 1.4÷1.65 g /cm^3 (when required of 1÷2 g/cm^3). The known analogues of this material differ markedly less in the bulk density – up to 1.1 g/cm^3, which causes considerable loss of material during spraying. The grains of nickel-plated boron nitride powder fabricated by the developed technology, are unbroken, do not disintegrate under plasma spraying. The sprayed layer is dance and uniform. It correspond to all requirements of hardness, lack of cracks and flaking.

For manufacturing of the BN-Ni powder the raw materials and materials produced in China can be used. For each stage of the technological process, a technology has been developed for recycling or returning material to the production cycle.

Spray coatings obtained using this powder can be operated at temperatures up to 1150 °C.

ENHANCING PERFORMANCE OF Li-S BATTERIES WITH SOLID ELECTROLYTES

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Li-S batteries have been regarded as one of the most promising candidates for the next generation energy storage devices due to their high theoretical energy density, however, conventional Li-S batteries with liquid electrolyte suffer from the serious shuttle problem caused by the dissolved discharge products of sulfur, or lithium polysulfides which can migrate to the anode side and react with Li metal anode, resulting in severe capacity loss and low Coulombic efficiency. In this report, various strategies based on solid state lithium ion conductors and hybrid electrode designs have been applied to solve the shuttle problem of the polysulfide, which have been proved effective in suppressing dendrite growth to a large extent and improve the cycling stability of the batteries effectively.

AUSTENITIC ODS STEEL AND ODS HIGH ENTROPY ALLOY FOR ENERGY APPLICATONS

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Austenitic steels are widely used in nuclear power and in other technical fields. In comparison with ferritic-martensitic steels they are characterized by higher high-temperature strength but have lower radiation resistance. The problem solution of austenitic steels radiation resistance improvement with simultaneous increasing of high-temperature resistance is possible by producing the nanostructured state in these alloys. This state characterized by the presence of nanosized particles (~2–10 nm) with high density ($\sim 10^{15}$–10^{16} cm^{-3}) and uniform distribution into the matrix. Thermodynamically stable oxides may serve as such nanoparticles, and steels, strengthened by such particles, are named oxide dispersion-strengthened steels (ODS steels).

Other class of promising radiation-resistant materials for new generation nuclear reactors and future fusion reactors is so-called high entropy alloys (HEA’s) or concentrated multicomponent alloys that have simple BCC or FCC lattices. Single-phase HEAs with FCC lattice in recrystallized state have usually very high plasticity with relatively low strength characteristics, particularly yield strength. This fully applies to the "classical" equiatomic five-component FCC alloy CoCrFeNiMn (Cantor’ alloy). In this work we proposed to improve the strength characteristics of HEAs by using oxide dispersion-strengthening technique, i.e. creation of ODS HEA’s. The realization of this idea is demonstrated on Cantor’s alloy.

Commercial austenitic steel 08Cr18Ni10Ti and experimental equiatomic CoCrFeNiMn alloy were used as initial materials. Powders of steel or HEA were mixed with 0.5%wt of oxide nanopowder and mechanically alloyed in argon in high-energy ball mill. The oxide nanopowder composition was 80%mol Y_2O_3–20%mol ZrO_2; particle size was 16 nm and lattice parameter was $a = 10.528 \pm 8 \cdot 10^{-3}$ Å. All kinds of mechanical treatment from powder compacting to rolling of compacted blank were carried out at room temperature. In addition, mechanical treatments were alternated with short-time high temperature annealing. As the result, the bars of 08Cr18Ni10Ti ODS steel and CoCrFeNiMn ODS HEA 200 μm thickness were obtained. The specimens’ structure analysis was conducted by electron microscopy using JEM-100CX and JEM-2100 microscopes. X-ray diffraction studies were performed by DRON-2 diffractometer using Fe-Kα radiation. Mechanical tension tests were conducted at temperature range of 77 – 1000 K.

It was established that the ODS steel after the final thermal treatment had austenitic matrix in which complex oxide precipitates were uniformly distributed. The precipitate’s density was $7–8\cdot10^{15}$ cm^{-3} and their average size was near 10 nm. Strength characteristics of ODS steel were significantly higher than the initial steel ones. Especially substantial gain was observed at high temperatures (1000 K), where the yield strength of ODS steel was 2.3 times higher than for initial 08Cr18Ni10Ti steel.

Also, yield strength of the CoCrFeNiMn ODS HEA at temperature range of 77–800 K was 2.5÷3 times higher than for initial alloys, though average oxide precipitates was bigger and their distribution uniformity was poorer than in ODS steel. Thereby, oxide dispersion strengthening is effective not only for steels but also for high entropy alloys.

HIGH-ENERGY MATERIALS WITH CERAMIC NANOSCALE COATING FOR ELECTRODES OF NEW GENERATION LITHIUM-ION BATTERIES

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In severe conditions (temperature rise and increase of charge voltage) active electrode materials of state-of-the-art lithium-ion batteries (LIBs) quickly deteriorate, and their interfaces with the electrolyte lose stability. The first is mainly due to phase transformation of cathode material sand transition-metal dissolution. The second is connected with the problem of the passivating layer on the surface of the electrodes, which creates kinetic barriers for the insertion–extraction of lithium ions. Both problems arise due to the direct contact of electrode materials with electrolyte and modifying the surface of active electrode materials is effective strategy to solve them.

As inorganic coatings for electrodes LIBs use carbon, Al_2O_3, SiO_2, TiO_2, ZnO, MgO, ZrO_2, Li_2CO_3, LiF, AlF_3, LaF_3, Li_3PO_4, $AlPO_4$, $Li_4Ti_5O_{12}$. Although they inhibit side reactions between the electrode and the electrolyte the electrochemical parameters of the modified electrodes are not always sufficient for practical application especially at elevated temperatures and high charging potentials. One of the reasons for this is the unevenness and inhomogeneity of the coverage of individual particles of active materials. In the case where the coating is uniform blocking the electron transport pathways leads to an increase in impedance.

In order to overcome these short comings we have developed a method for joining nanoparticles of the active material with an electro- and ion-conducting heteronanostructured ceramic matrix/coating composition SiOC&C that is chemically inert and mechanically strong. This coating guarantees the protection of electrode materials from the powerful action of HF (which is always present in traditional organic electrolytes in a small amount and also generated on the surface of electrodes at high potentials, resulting in the ions of transition metal positive electrode dissolved in the electrolyte and then sedimented on surface of negative electrode LIBs).In addition the chemical inertness of the ceramic coating allows suppressing the side reactions of the electrodes with the electrolyte preventing the formation of a thick passivating layer on their surface and increasing the impedance.The ionic conductivity SiOC&C provides an efficient transfer of lithium ions between the electrolyte and the active particles of the electrodes.

SUSTAINABLE NUCLEAR ENERGY – RESEARCH AND DEVELOPMENT OF COATINGS IN ATFC CONCEPT

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Zirconium alloys are used as a base material of fuel claddings in the LWR-type thermal neutron reactors. The Zr-based alloys, possessing a high chemical stability provided by the zirconium oxide film, are widely applied due to their low thermal-neutron capture cross-section, good mechanical properties and high waterside corrosion resistance at normal operating temperature up to 350 °C. However, in the case of accidents with increasing temperature, the zirconium cladding can no longer operate as a reliable barrier preventing fuel release into the coolant and the environment. The use of zirconium alloys in the GenIV reactors is also limited due to their low corrosion resistance in supercritical water. To prevent fuel cladding damage, it is necessary to protect the zirconium alloy from the high-temperature corrosion in steam as well in air. For protection of the zirconium cladding in case of an accident scenario like loss of coolant accident (LOCA) it is proposed to utilize corrosion resistant coatings.

The report presents the results on the development of coatings for the protection of zirconium claddings of the fuel rods in the case of LOCA, and under normal operating conditions. Results of own research into the effect of ion-plasma treatment on mechanical properties, corrosion resistance of zirconium alloy tubes, saturation of the hydrogen from gas phase, as well as resistance to high temperature oxidation in air and steam flow of the layouts of gas-filled fuel rods are presented. Information review on the international experience of development of such coatings is also given.

EXPLORATIVE INVESTIGATION OF HIGH-ENERGY BATTERIES

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Recently, high-energy batteries draw the tremendous attractions in order to prolong the one-drive distance of electric vehicles. Among the known chemistries, the batteries with Ni-rich cathodes and lithium metal is one of the most proming high-energy systems. In this presentation, I shall introduce the progresses on $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ and lithium protection in our group. In cathode part, we have proved the improtatnce of the oxygen defects and also developed the novel structure to address its challenges. In anode part, we have developed the concept and structure of Li^+-ion filtration membrance, which should be a novel direction to improve the stability between electrolyte and Li metal. Our approaches should be helpflu to develop the protatype cells of lithium metal batteries.

ADVANCE ELECTROSLAG TECHNOLOGIES FORCOMPOSITE ROTOR MANUFACTURING

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The results of the development of a novel ESR based process for composite ingot with a shallow transition zone between layers for heavy-weight rotors for steam turbines are presented. The nowadays efficient rotors for steam turbines for power plants are monoblock or two or more layer in length composite part facilitating operation in different zones withstanding various loads and working medium. However, the joining of various steel in composite rotors by welding has low productivity. The ESR now is recognized as the best available technology for the big-diameter and mass forgings for power generating machines, including rotor ones. The ESR affords the most favourable conditions of solidification resulting in homogenous low-segregation ingot with a smooth surface and high-quality structure. The step ahead is the ESR for composite. The two-layer model ingot had produced from steel grades 12Cr13 and 35NiCrMoV12-5 were manufactured using the electroslag process with the liquid metal (ESR LM) in the CSM of 180 mm in diameter with ingot withdrawing. The transition zone in two-layer ingot had had the shallow shape and low depth with the even macrostructure without defects of the same type as both joined steels. The metal of the transition zone fully satisfies standard requirements for properties of both steel grades in the boththe heat-treated and as-cast conditions. The ESR LM can provide both the monobloc heavy ingots with uniform structure and composites with the low-stress connection between metal layers for heavyweight rotors and other critical products manufacturing.

ADVANCED SODIUM-ION BATTERIES BASED ON NASICON-TYPE MATERIALS

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Na-ion batteries (NIBs) have attracted rapidly increasing attention because sodium is abundant resources, low cost and their better safety. However, the development of NIBs is greatly hampered due to the lack of appropriate active materials for both cathodes and anodes, because of the large radius of Na+. NASICON-type Na3V2(PO4)3 (denoted as NVP) has recently been investigated as a promising cathode material for NIBs. While it is difficult to reach high rate performance of Na3V2(PO4)3 cathode due to the poor electronic conductivity of phosphates. For anode materials, NaTi2(PO4)3 has shown promising electrochemical performance.

Here, we reported electrode materials for NIBs based on porous carbon with excellent rate performance: Carbon-coated nanosizedNa3V2(PO4)3 embedded in the porous carbon matrix. The double carbon coating NVP could deliver high rate performance (44 mAhg-1 at 200C). This ultrahigh rate performance is comparable to that of supercapacitor, but with much higher energy density. We also designed NaTi2(PO4)3 particles embedded in micro-sized 3D graphene network to improve its electrochemical performance.

The outstanding electrochemical performance of electrode materials with porous carbon network for NIBs is attributed to the special structure design, which confined a variety of advantages: hierarchical porous channels facilitating fast ions and electrons transport, carbon coated structure resulting in low resistances, good mechanical properties leading to the excellent morphology stability.

INVESTIGATION OF MULTICOMPONENT HEAT-RESISTANT PROTECTIVE COATINGS FOR GAS TURBINE ENGINE BLADES

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Heat-resistant protective coating on the surface of turbine blades must be created because of the increased requirements for the operation of engine parts. Increase in operating temperatures, as well as long-term and reliable operation under conditions of exposure to corrosive media are some of the main requirements when choosing blade materials. Now, an effective solution to this problem is the use of high-temperature nickel alloys, and materials based on Si–Nb.

High-temperature oxidation of high-temperature nickel alloys in combination with sulphide and vanadium corrosion, as well as erosion, substantially limit the life of the blades. In this regard, it becomes necessary to create a heat-resistant coating on the entire outer surface of the blade, including the interior cavity and the perforations.

The method of vacuum activated diffusion saturation for the protection of heat-resistant nickel alloys is simpler and cheaper than other methods. Diffusion saturation was activated in gas and liquid media under the influence of self-propagating high-temperature synthesis (SHS).

Multiphase coating was obtained to protect the heat-resistant nickel alloy ZhS26 from oxidation at 1250 °C using this method. The effect of the composition and the conditions for the formation of protective coatings on their heat resistance was studied. This method allowed coating on a gas turbine engine blade including internal cavities with a diameter of less than 1 mm. The coatings can protect the ZhS26 alloy from high-temperature corrosion for a long time.

To further increase the operating temperatures of the blades, the use of Si–Nb-based materials is effective. Such materials can operate at temperatures of 1350 °C, provided there are protective coatings that will protect against high-temperature corrosion. Currently, our laboratory is developing and researching such coatings.

THE MOST PROBABLE MECHANISMS OF MATERIAL CHARACTERISTICS DEGRADATION DUE TO ACCUMULATION OF HYDROGEN AND PREDICTING THE POSSIBLE SCENARIOS OF MAINTAIN ITS RESOURCE

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Prediction of material properties under conditions of interaction with hydrogen is an important direction of modern physics and mechanics of deformed solids. Of greatest interest is the study of the features of hydrogen interaction with metals and its effect on the mechanical characteristics of the material, since hydrogen accumulating in the metallic parts of the construction encourage the development of defects, and as a consequence promotes the destruction - the manifestation of hydrogen embrittlement phenomenon.

The review considers the results of theoretical and experimental studies of hydrogen solubility, diffusion and penetration; the nature of hydrogen bonding with defects; critical levels of hydrogen accumulation, its distribution in the volume and mechanisms of interaction with the material. Changes of material structure in the presence of hydrogen are discussed, as well as the influence of external thermo-irradiation fields and the duration of annealing on these processes.

Hydrogen localization in the material bulk and possible mechanisms of hydrogen-induced material destruction are analyzed. Recommendations for minimizing the negative effect of hydrogen and for preventing the reduction of operating characteristics of structural materials are considered.

MODERN PROBLEMS OF RADIATION MATERIALS SCIENCE

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According to data of IAEA nuclear power makes now 20% of world production of electric power and guarantees the decrease of the level of CO_2.

In spite of accidents in Chernobyl and Fukusima realities of economy and ecology force to return to priority development of nuclear power because now doesn't exist another source of production of cheaper and ecologically pure electric power.

Realization of the programs of development and construction of nuclear plants of new generation (INPRO, Gen IV, fast reactors BN-800 and BN-1200, Terra Power, traveling wave reactors and so on) and also the improvement of operational characteristics of nuclear reactors under operation is possible only on the condition that problems of nuclear material science will be solved. Materials in nuclear power play extremely important role. The more important is the fact that fuel and structural materials of nuclear power plants in comparison with materials used in traditional power plants operate in specific and more severe conditions. Just the behavior of structural materials of nuclear reactor cores limits the achievement of commercially necessary rate doses (150–200 dpa), operational temperatures (500–600 ^{o}C) and make difficult the achievement of higher burn-up of the fuel.

In the proposed report the modern problems of radiation resistance of materials in operating reactors and in reactors of next generation will be considered.

On the base of analysis of the problems of radiation material science, study of microstructure evolution and its effect on degradation of initial physical-mechanical characteristics of materials the following new methodologies will be considered:

- Production of new generation of radiation-tolerant materials with increased radiation and corrosion stability (reactor steels and functional nano-structurized ceramics) hardened by nano-sized oxides of Y and Zr.
- Increase of corrosion stability and decrease of hydrogen saturation of zirconium alloys by modification of surface at the expense of ion-plasma treatment.
- Overhaul-period renewal of pipe-lines and other welded elements of equipment of NPS by development of complex of welding technology with controlled formation of welded joints.
- Development of transient processes in prospective fast reactor with traveling wave of nuclear burning and in materials of the core of reactor of IV generation.

Increase of the temperature of operation and life extension of fuel elements at the expense of modifying of the surface of structural materials by ion-plasma methods, synthesis of coatings, plasma-chemical and diffusion activated deposition.

TECHNOLOGY OF PURIFICATION OF RAW MATERIAL FOR PRODUCTION OF MICROPOWDER POLYCRYSTALLINE NANODIAMOND

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The main area of its use is the polishing of:

- LED substrate
- sapphires and leucosapphires
- glass of mobile phones and other gadgets
- fingerprint buttons
- glass of scanners
- lasers
- watch glass (swiss watches)

Also polycrystalline nanodiamond is used for production of complicated diamond tools, composite material with special properties and other application.

Features of existing technologies:

- formation of a low liquid and highly liquid fraction of product of synthesis.
- increase of the part of the low liquid fraction in the process of removal of non-diamond carbon.
- high content of inorganic impurities in the final product (up to 2%).
- difficulties of removing the intermediate product of conversion graphite into diamond – lonsdaleite.

The proposed technology allows to eliminate this shortcomings:

- Special processing of materials of explosive charge and the addition of special additives to the explosive at the stage of charge formation for detonation synthesis increases the percentage of yield of the highly liquid fraction to 20%.
- Separate processing of low liquid and highly liquid fraction allows to reduce the consumption of reagents and shorten the time of their cleaning.
- The stage of cleaning the diamond-graphite – provides a high degree of purification of final product from graphite and other impurities. The technology provides – 0.2–0.6% of inorganic impurities (according to technology – 2%) and not more than 0.1% graphite.
- Cleaning is carried out by patented technology with oxidizing reagents that do not require high pressures, under temperatures not exceeding 350 °C and with using of equipment from inexpensive materials.

- Technological conditions do not lead to the destruction of polycrystals, and as a result, the properties of diamond of detonation synthesis become comparable to the diamond of static synthesis by its heat resistance, which expands the scope of its use.
- Key feature of the technology is the possibility of removal of lonsdeylite from polycrystals, which reduces the need for additional crushing of raw materials and increases the abrasiveness of diamond detonation synthesis up to 2 times
- The technology does not require toxic, expensive reagents of high purity, does not form waste with special methods of utilization or processing. Wastes from the production process can be processed into liquid products, which significantly reduces the cost of the final product.

The technology has passed industrial tests, the key solutions have patent protection.

SULFIDE ELECTROLYTES FOR ALL-SOLID-STATE RECHARGEABLE BATTERIES

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Increasing concerns on the safety issues of commercial lithium ion batteries as the power sources for portable electronics and electric vehicles impel the exploration of the new battery systems with high reliability and safety. All-solid-state rechargeable batteries employingnonflammable inorganic solid electrolytes have been considered as the ultimate solution to combustion and leakage safety issues. Compared with oxide electrolytes, sulfide electrolytes are considered to be promising ion conductors due to their high ioinc conductivities and favorable interface compatibility with sulfide or sufur-based electrodes.

A series of sulfide solid electrolytes with room temperature ionic conductivity of 10^{-3} ~ 10^{-2} S/cm are successfully synthesized. The electrochemical stability and compatibility with lithium can be improved with oxide or halogen doping. The effect of ionic conductivity as well as particle size of sulfide electrolytes on the electrochemical performances will be discussed. Meanwhile, a battery construction containning a solid electrolyte bilayer, *i.e.* $Li_{10}GeP_2S_{12}$ and $70\%Li_2S-29\%P_2S_5-1\%P_2O_5$, have been designed, well addressing the compatibility between electrolyte and metallic lithium.

Furthermore, different type transition metal sulfides or sulfur-based materials are employing as electrodes for all-solid-state rechargeable batteries. The intimate contact interface can be realized by coating sulfide electrolytes evenly on the surface of active materials, which enables the battery to withstand the large stresses/strains during repeated charging/discharging, leading to significant improvements in energy density and cycle life.

COMPUTER SIMULATION OF THE EVOLUTION OF DISLOCATIONS AND THE MECHANICAL PROPERTIES OF METALS

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Computer modeling is an important part of theoretical materials science, since the behavior of a large number of particles or defects is unsolvable problem within the framework of the classical mechanic. Therefore, without computer modeling it is impossible to understand exactly how dislocations influence on the behavior of a material and how formed such characteristics as fracture toughness, strength, yield strength and how they depend on temperature, loading rate and material parameters.

In this work, the process of evolution of dislocations ensemble under the action of applied stress is considered. The process of multiplication of dislocations from several sources is taken into account. Variants of both cause the load constancy of time (creep) and the growth of the applied stress versus time are considered. In the letter case, the total movement of the dislocations is analyzed and the stress versus deformation is obtained (the loading curve).

The interaction of the ensemble of dislocations with the grain boundary for a smooth sample and a sample with a crack is considered. In the latter case, the formation of a plastic zone and its effect on fracture toughness in quasi-brittle materials are considered. The influence of a dislocation wall (disclination) on the evolution of a dislocation ensemble in a neighboring grain is studied. The reliability of the results obtained is tested by comparison with experiment.

MAGNETOCALORIC EFFECT OF HIGH-NUCLEARITY 4*f* AND 3*d*-4*f* METAL CLUSTERS

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Magnetocaloric effect (MCE) is a magneto-thermodynamic phenomenon in which a change in temperature of a suitable material is caused by exposing the material to a changing magnetic field. Since first observed by a German physicist Warburg in 1881,[1] the MCE of magnetic materials has attracted much interest in the field of cooling technology. High-nuclearity4*f* and3*d*-4*f*metal clusters, a unique class ofcompounds, are regarded as a promising candidate to replace the expensive andincreasingly rare helium-3 in ultralow-temperature (<<1 K).2In this work, we introduce our recent research progress in the magnetocaloric effect of high-nuclearity 4*f* and 3*d*-4*f* metal clusters, including in, 1) How to efficiently construct high-nuclearity 4*f* and 3*d*-4*f* metal clusters;[2-7] 2) How to reveal the magnetic interaction in the system of high-nuclearity 4*f* and 3*d*-4*f* metal clusters;[8,9] and 3) how to improve the magnetocaloric effect of the high-nuclearity 4*f* and 3*d*-4*f* metal clusters.[10]

COORDINATION SPACE WITH DYNAMIC BEHAVIORS

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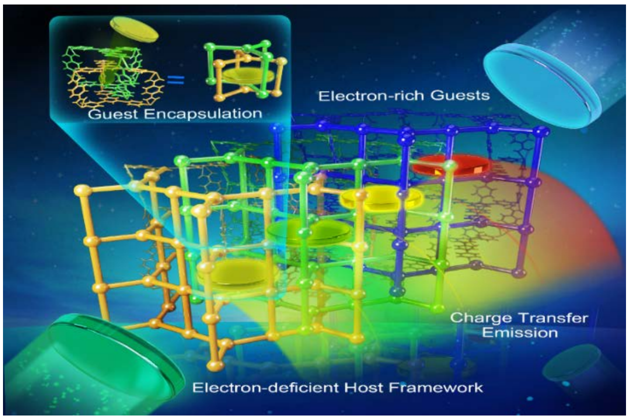
Coordination space could be considered as the structural and functional basic of coordination bonding based materials, such as porous coordination polymers (PCP), metal-organic frameworks (MOFs), and metal-organic polyhedral (MOP). One of the most attractive characters of coordination space is its dynamic transformation between multistable states with distinct properties. This behavior has great potential applications in many fields. However, compared with the well-developed strategies and methods for the structure oriented construction of coordination space, the rational achievement of dynamic behavior is still a great challenge. This should be due to the fact that the successful introduction of dynamic factors into a coordination space and the realization of the anticipated dynamic properties are somewhat random.

We herein report some of our new results in the construction and properties investigations of dynamic coordination space. Some other related results in our group will also be reported. [1-10]



ABSORPTION OF WATER VAPORS BY SINGLE LAYERS OF DICHALKOGENITES OF TRANSITION METALS – THE FIRST PRINCIPLES CALCULATIONS

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In the field of investigation of nanomaterials after an active development of graphene topic the prime accents of researchers worldwide are mainly being shifted to single layers of graphene-like compounds. Thus, the applications of materials enclosed with elements of these structural units, typically are similar to those traditional ones of basic materials.

Therefore, this effort using the first principle pseudo potential calculations, studies an adsorption of water molecules with the single layers of $MoSe_2$, and WSe_2. The calculations have been done for two types of exchange-correlation potential: a local density approximation (LDA) and a generalized gradient approximation (PBE).

Four potential centers of adsorption -T_H – hexagon center, T_M – Me atom, T_{Se} – Se atom and T_B – mid of the bond Me-Se were considered. It was established that adsorption centers are only T_H and T_M. The obtained results enable to turn to more effective targeted choice of 2D, 2D/2D, 2D/3D nanocomposites based on dichalkogenites of transition metal for experimental solution of specific physical problems with water vapors, such as gas nano-sensors of water vapors and nano-photo-catalysators for water purification.

CREATION OF A HETEROGENEOUS STRUCTURE BY PLASTIC DEFORMATION

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1. Analytical transmission electron microscopy studying of nanolayers in contact zone of bimetal after hot rolling in vacuum. Studying of “cross-section” samples of interface copper-niobium after hot rolling in vacuum was carried out by analytical transmission electron microscopy. Formation of the transition zone with width of some interatomic distance in process of plastic deformation was shown.

2. The results of precision chemical analysis of near boundary areas of the two-component powder composites 70Ni–30Mo and 50Fe – 50Cr, which demonstrate high tendency to alloy formation under high temperature severe deformation have been studied. It is established, that a sharp change in concentration occurs in a very narrow (about 20 nm) near boundary area. There are almost unalloyed particles refractory elements (concentration of about 90%) in the solid solution, which corresponds to a given composition of the composite

3. The effect of plastic deformation on the structure and mechanical properties in the temperature interval 77 ... 1123 K of high-enthalpy alloys (HEA) will be presented. Despite of the high strength characteristics after casting, HEAs are deformed by rolling at room temperature. Nanostructure of deformed HEAs significantly increases the strength characteristics of the material.

4. Severe plastic deformation methods: equal channel angular pressures (ECAP), twist extrusion (or their combination), high pressure torsion (HPT), accumulative roll-bonding (ARB) were developed for producing of nanostructures in “soft” one-component materials (unalloyed Cu, Al, Ti, Fe). Application of the mentioned methods for the ultimate strengthening states production in multicomponent materials and high-strength materials processing practically impossible. It requires high-power and sophisticated equipment of the large dimensions. Producing of gradient structure in near-surface layers of metals discovers an opportunity of nanostructural state formation, and accordingly functional characteristics unattainable for materials with conventional deformation structure. Methods of nanostructure formation in near-surface layers for gradient strengthening will be presented. These methods allow to receive hardness up to 11–13 GPa for carbon steel.

EMERGING MATERIALS FOR ELECTROCATALYSIS IN ENERGY CONVERSION

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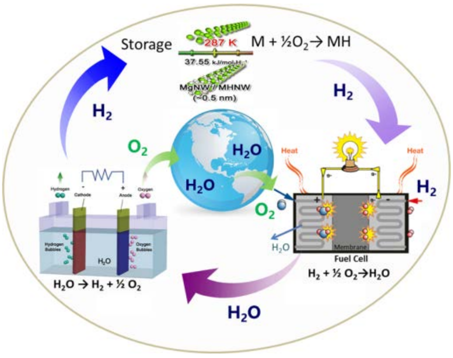
Platinum-based materials are highly active as the electrocatalysts for both hydrogen evolution reaction (HER) in water splitting and oxygen reduction reaction (ORR) in fuel cells, but high cost limits their wide applications. Thus, the exploration and design for high-activity non-precious metal ORR catalysts are urgent. Also some key models should be set to study the HER mechanism in detail.

In this talk, the reporter summarized the recent research progress of designing and preparing novel nanostructured electrocatalysts toward the HER and ORR in his group. Some key reaction mechanisms and relationships of structures, compositions and properties are also proposed and concluded. [1-6]



COMPOSITES CONSISTING OF NANOCARBON AND METAL NANOOXIDES; UNIQUE MATRICES FOR DEVELOPMENT OF EFFECTIVE CATALYRIC SYSTEMS FOR THIN ORGANIC SYNTHESIS

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Some ideas and collaborative researches, which were performed by the IGIC and Moscow State University (prof. M.A. Bumagin group), are considered. The investigations were stimulated by the Nobel Prize (2010) in the field of physics on the development of a two-dimensional graphene material (A. Geim, K. Novoselov). Other source of our stimulus is the Nobel Prize in the field of chemistry (R.F. Heck, E. *Negishi*, A. Suzuki, 2010), which has been awarded for fundamental researches directed to homogeneous catalysis of the reactions of cross-coupling of carbon atoms and the "construction" of larger molecules from individual parts, At last, our investigations were induced by increasing demands of "Green Chemistry", which provide rejection of toxic and harmful substances in industry.

The problems of Heck-*Negishi*-Suzuki reactions are discussed. For instance, the difficulties are stabilization of dimensional properties of catalyst through the use of new carbon nanostructures, providing selectivity of reactions, problems with separation and recycling of catalyst, toxicity of reagents.

The scheme of synthesis of new hybrid catalysts, which involves inorganic hydrophilic-hydrophobic nanomatrices based on nanocarbon and metal nanooxides. is proposed.

Nanosized heterogeneous catalytic nanosystems have been developed. The nanosystems are based on pyrogenic aluminum oxide, titanium dioxide or silica with carbon coating. Further the nanoparticles of zero-valence palladium are formed on this coating. Thus, the structure of the nanosystems is "core-carbon shell-palladium". Modern physical methods for investigation of these nanosystems, which allows us to control synthesis on the level of molecular design, are considered.

Main advantages of heterogeneous palladium catalysts have been established: their catalytic activity reaches 90–99 %. Moreover, it is possible to use water (or its mixture with lower alcohols) as a reaction medium instead of toxic, expensive, fire and explosive organic solvents. Lower alcohols can be recycled repeatedly and easily separated from reaction products.

COPPER-CNTs COMPOSITE MATERIAL FOR RELIABLE HIGH-CURRENT CONTACT

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Development of new composite materials and improvement of existing ones are the prospective issue of modern science and technology. Recently, the carbon nanotubes (CNTs) evoke big interest because of a unique combination of their properties. It is known, that CNTs have close or even bigger electrical conductivity than copper, and their thermal conductivity is almost 5 times more. It is evident that such characteristics are of interest for the development of materials for high-current (interrupting and sliding) electrical contacts. These materials have to demonstrate very incompatible properties and the use of CNTs can contribute positively.

The experimental program on the manufacturing of the copper-CNT (0.5; 1.0; 1.5 wt%) composite material was performed. Composites were produced by standard methods of powder metallurgy (mixing, pressing, sintering in the inert (argon) and reducing (hydrogen) atmosphere. It was shown, that the sintering under hydrogen leads to weight reduction of the samples, indicating the reduction of oxide films from the surface of the copper powder particles.

The CNTs were found in the matrix material on the grain boundaries of the powder (in the form of clusters as well). All composites with CNTs had the electrical conductivity of almost two times bigger in compare with samples of pure copper produced by the same technology. The effect of increasing the electrical conductivity was the most stable for the composite with 1.5 wt % CNTs. It was also revealed, that the microhardness (measured by Vickersand Berkovichnano-indenting) of copper-CNT composites is higher than pure copper that in view of the absence of the precipitating phases formation is a prerequisite for improving the wear resistance of the eventual electrical contacts.

MULTIFUNCTIONAL LUMINESCENT MATERIALS: STRUCTURAL DESIGN AND PERFORMANCE TUNING

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Rare-earth luminescence materials have important applications in display, lighting, marking and other fields. This project chooses inorganic luminescence materials as the research subject, aiming at the key problems existing in white LED phosphors and long-afterglow luminescence materials. (2) The monochrome color of long afterglow phosphor and the mechanism of afterglow have not been settled. On the one hand, a large number of experimental examples are used to preliminarily reveal the key factors affecting the performance of luminescence materials and the inner mechanism. On the other hand, based on these mechanisms and practical experience, a series of excellent LED phosphors and long-afterglow luminescence materials were developed. The details are as follows:

1. Luminescence materials for white light LED: a series of multi-color luminescence materials with excellent performance were designed and developed and spectral color tuning was realized through energy transfer and ion replacement, which further revealed its inner luminescence mechanism, providing reference for the design and development of LED luminescent materials;
2. Long-afterglow luminescence materials: a series of multi-color long-afterglow luminescence materials were developed and the effect of the inherent ‘defects’ of matrix such as oxygen vacancy on the material's afterglow performance was studied through reasonable experimental design, which provided direct and strong experimental evidence for the mechanism of long-afterglow.

Acknowledgements:

This work is supported by the Fundamental Research Funds for the Central Universities (lzujbky-2018-34), the National Natural Science Funds of China (No. 51672115 and No. 51502122) and Gansu Province Development and Reform Commission (NDRC, No. 2013, 1336.)

IMPROVING ELECTROCHEMICAL PERFORMANCE FOR RECHARGEABLE BATTERIES BY NANOTECHNOLOGY

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Electrochemical rechargeable batteries have been extensively used in portable electronic devices due to acceptable energy density and cycle life. In recent years, the fast development of electric and hybrid electric vehicles has largely promoted the global research interest to pursue for the batteries with high energy density, excellent rate capability and stable cycle performance.

Electrode materials are crucial for the high-performancerechargeable batteries. Searching for novel electrode materials or optimizing the current materials requires fundamental understanding or effective preparation methods. Nanotechnology is a very helpful strategy to improve the electrochemical performance for Li-ion/Na-ion batteries, Li-S batteries, supercapacitors.

Here, we introduce some strategies of nanotechnologies to design nano-based electrode materials to enhance specific capacity, rate capability, cycle life, etc. for rechargeable batteries.

Microstructure, surface and boundary can create additional active access to energy storage. Traditional Li insertion in graphite demonstrates that 6 carbon atoms storage 1 Li ion. In order to enhance the capacity, new energy storage mechanism should be discovered. By combining the effects of heteroatom doping and porous microstructure, the N-doped hierarchicalcarbon exhibitssuperhigh capacity and excellent rate capability, delivering a reversible capacity as high as 943 mAh g^{-1} at a current density of 2 A g^{-1} even after 600 cycles. Such high capacity cannot be controlled by chemical stoichiometric ratio. Similar strategy is also applicable for Na-ion batteries, Li-S batteries and supercapacitors. In addition, fabrication of nanoscaled electrode materials or nanocomposites with desired microstructure can greatly improve cyclabilityby alleviating the volume change during charge/discharge, and achieve excellent rate capability.By employing nanotechnology, diffusion- and capacitive-controlled storage mechanismswork synergistically for Li/Na and Li-S batteries and supercapacitors.

EFFECT OF CONCENTRATED LIGHT ON BORON AND BORON–METAL POWDERED MIXTURES TRANSFORMATION

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Concentrated light of a high-flux optical furnace is one of cleanest energy sources available for the nanotechnology. Optical furnace presents a number advantage such as high heating and cooling rates, versatility and ability to adjust temperature profile along each axis, maximum operating temperatures and environmental adaptability. Moreover, this technique is appropriate for both conducting and non-conducting materials.

Transformation of boron nitride and boron powders and boron-metal powdered mixture (25 wt. % In, Al, Cu, Fe, Ni, Si) in flow of nitrogen was considered. It was demonstrated an effect of melting, boiling and evaporation/sublimation processes on architecture formation of new nanostructures and proposed “gaseous model” for explanation based on evolution of a bubble. Burst of the bubble results in graphene-like structures formation. The stepwise transformation of bubbles of proper composition leads to threads formation because of their growth upwards by the heated gases. The distribution of temperature across an experimental camera and temperature gradients effect on different bubbles formation and in the result on change of the architecture and properties produced powdered materials.

Presence of metals (Al, Fe, Ni, Si) and formation of boron-rich borides simultaneously with amorphized boron nitride contribute to the formation of nanostructured powder of BN. Fullerene-like and core-shell structures were produced in consequence of In and Cu presence, which do not form borides. Encapsulation by h-BN of In and Cu promotes stability InN and high anti-oxidation properties of Cu nanoparticles that can be useful for maintains their high catalytic activity.

NANOSIZED MATERIALS FOR HIGH-RATE LITHIUM-ION BATTERIES

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Lithium-ion batteries (LIBs) are widely used in smart grids, energy storage supplies, electric vehicles, etc. The latter application requires high specific power (great charge/discharge rates), so as to ensure the starting acceleration of a vehicle. Practice of electromotive industry and environmental concerns have lead to the quite harsh selection of electrode materials employed in electric and hybrid cars. Toxic $LiCoO_2$ widely used in first commercial LIBs is now shifted by more environmentally benign $Li(Ni_xCo_{1-x})O_2$, $Li(Ni_xCo_yAl_{1-x-y})O_2$, $Li(Ni_xMn_yCo_{1-x-y})O_2$, and $LiMn_2O_4$. All these materials are synthesized commercially by means of by means of traditional technologies (sintering and precipitation).

On the other hand, much attention is paid to obtaining electrode materials in a nanosized form. The power density of any battery is significantly governed by the diffusion of lithium ions into/from (and within) the grains of electrode material [1]. Subdivision leads to great increasing in the area of contact between electrode and electrolyte and to decreasing of distances passed by electrons and lithium ions upon diffusion in the electrode material. This means that obtaining electrode materials in a nanosized form may allow for attaining greater charge/discharge rates than in the case of the electrode materials of a large particle size.

In our previous works [2-6] partly reviewed in Ref. [7], a modified citric acid aided route has been employed, and nanosized spinel-type materials including $LiMn_2O_4$, $LiNi_{0.5}Mn_{1.5}O_4$, a gradient material containing a $LiMn_2O_4$ core and $LiNi_{0.5}Mn_{1.5}O_4$ shell, and $Li_4Ti_5O_{12}$ have been synthesized. Analysis presented in Refs [2-7] demonstrates that all these materials overwhelm existing commercial samples being able to sustain much greater current loads (up to 65C) without losing their electrochemical activity.

In this presentation, our efforts directed towards citric acid aided synthesis of materials of $Li(Ni_xMn_yCo_{1-x-y})O_2$ type are described. In particular, for $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$, DTA, surface area and porosity, XRD, SEM/TEM and EXAFS data are obtained, and impedance, galvanostatic and CVA studies are performed. High-rate electrochemical tests are compared with existing data, and some disadvantages of nanosized materials are put forward. It is stressed that a key role in attaining high-rate properties plays the perfectness of materials obtained. Further, nanosized samples have high reaction ability and, unlike their bulk counterparts, do not tolerate even small overdischarges possibly occurring in cases if a failure happens in a battery equalizing control scheme.

OBTAINING OF TUNGSTEN CARBIDE NANOPARTICLES BY PLASMA DISCHARGE IN ULTRASONIC CAVITATION FIELD

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Carbides, particularly those of the transition metals, have a number of valuable properties that make them promising materials for use in various new technology fields. The principal application for carbides is as the major constituent in the so-called cemented carbide. The cemented carbides are combinations of carbides such as WC, TiC, and TaC with binder metals such as cobalt and nickel. These are mass produced as materials for cutting tools and wear-resistant parts. The tungsten carbide–cobalt (WC–Co) composite is the most important for these applications. The increase in the dispersion of the structural components of the composites facilitates the creation of new types of materials which combine high strength and ductility. Recent experiments [Fang, Z. Z., Wang, X., Ryu, T. et al. *Int. J. Refract. Met. Hard Mater.* 27 (2009): pp. 288–299; Dvornik, M. I., *Int. J. Refract. Met. Hard Mater.* 28 (2010): pp. 523–528] have demonstrated that nanostructured WC–Co composites have superior mechanical properties because of their improved hardness and increased ductility and plasticity.

In this study the tungsten carbide nanoparticles were obtained using plasma discharge in organic liquids (ethanol and benzene). Generation of plasma discharge began with an ultrasonic cavitation. The effervescent ultrasonic cavitation field may enhance the electrical conductivity of organic liquids due to high energy species (such as radicals, atoms, ions and free electrons) that form within the cavitation bubbles. The voltage between tungsten anode and iron-titanium cathode was held at 55 V and the upper current limit of DC power supply was set at 3.0 A throughout the experiment. The side products in the synthesized carbon powder sample consisting of iron particles from ultrasonic iron tip and amorphous carbon were removed by treatment of concentrated hydrochloric acid and 10 % hydrogen peroxide solution, respectively. Hot alkali (8M KOH) was used to remove the tungsten oxide particles. The yield of purified carbide powder was no more than 5 wt. % with respect to the weight of as-synthesized powder before purification treatment.

The electron microscopy and X-ray diffraction observations allowed recognizing spherical tungsten carbide (WC_{1-x} W_2C, WC) nanoparticles ranged from 5 nm to 1000 nm. The HRTEM images revealed that many tungsten carbide nanoparticles were separated from each other by graphite layers or were covered by graphite shells. The number of covering graphene layers is dependent on the particle size.

Electrochemical properties were determined by cyclic voltammetry and galvanostatic charge-discharge tests. Electrochemical measurements of the obtained powder showed a rectangular shape of cyclic voltammograms with specific capacitance of 92.5 F/g. Hence the prepared material has potential application as an electrode material for electrochemical supercapacitors [Liu, W., et al. *Carbon* 45 (2007): pp. 2759–2767].

SYNTHESIS OF REFRACTORY SIC NANOFIBERS ON HIGH-POROUS 3-D SUBSTRATES

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The first attempts to create high-performance filters using one-dimensional nanostructures show the promise of such products. Thus, in (A.Srivastava et al. Carbon nanotube filters, Nature Materials-2004, Vol. 3, P. 610-614), the creation and testing of a fine-purification filter using carbon nanotubes synthesized by CVD has been studied. Such filters were used both for cleaning gasoline from heavy hydrocarbons, and for purifying drinking water from bacteria Tscherichsa coli or polyvisirs (the size of the latter is about 25 nanometers). In both cases, good results were achieved.

In another work (D. Jayaseelan et al., In Situ Formation of Silicon Carbide Nanofibers on Cordierite Substrates, the Journal of the American Ceramic Society - 2007. - Vol. 90 Issue 5. - P. 1603-1606) British and Japanese scholars significantly increased the specific surface of cordierite by carbothermal reducing.

In recent years, a few papers on the synthesis of SiC nanofibers on carbon fiber substrates have been published. Such voluminous structures can be used in the development of new composites, filters and others. Thus, in [Wu R. et al. Growth of Tapered SiC Nanowires on Flexible Carbon Fabric: Toward Field Emission Applications // *J. Phys. Chem. C*, 2012, 116 (23), pp 12940–12945.], the growth of SiC nanowires on the surface of flexible carbon tissue by CVD is investigated. The results of the study have shown that SiC nanofibers grown on carbon fabric are potentially used in electronic devices and flat displays.

In recent years, the IPMS of the National Academy of Sciences of Ukraine also carried out works on the synthesis of SiC fibers by the CVD method on high-porous substrates (cordierite, the nickel foam, carbon fabric). The obtained results show that high-porous substrates filled with silicon carbide nanofibres can be successfully used both for the use of filters for fine purification of liquid and gaseous substances, as well as for reinforcement of new composite materials.

SUB-1NM ULTRATHIN NANOCRYSTALS

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When their sizes approach near 1nm, the surface atoms in ultrathin nanostructures will become dominant as compared with those in bulk or traditional nanocrystals with bigger sizes. As a result, the influence of surface effects on the inherent properties of the whole structure will become more remarkable. In this talk, we demonstrate the synthesis of ultrathin nanowires and nanoribbons with diameter/thickness less than 1 nm, a size comparable to that of a polymer chain. We found that the size reduction of the inorganic nanostructures brought them great similarity to macromolecules: the ultrathin nanowires mimicked the polymeric molecules in chain entanglement, non-Newton rheologicalbehavior, gelation phenomenon and electrospinning viability; the ultrathin nanoribbons demonstrated interesting conformational diversity through energy balance among organic ligand, inorganic structure and solvent which can be compared to the conformational variety in biomacromolecules. We have also tried to bring two different compounds together at sub-1 nm scale, based on which different heteronanostructures have been designed, including Ni-Co complex/1T MoS_2 and Au-Ni nanocrystals, which have shown multifunctional catalytic properties for full water splitting.

NANOSCALE METAL-ORGANIC FRAMEWORKS: EMERGING MATERIALS FOR CATALYSIS

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Distinct from classic inorganic nanoparticles of solid cores, nanoscale metal-organic frameworks (NMOFs) are of ordered crystalline pores with tunable composite, size and volume, which provide an ideal platform not only to manipulate the reaction active sites but also to understand the structure-functionality relationship.

In this presentation, we will introduce two recent works involving catalytic application of NMOFS.

ADVANCED TECHNOLOGIES FOR PRODUCTION OF BULK CERAMIC NANOCOMPOSITES

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Spark plasma sintering (SPS) and microwave sintering (MWS) are most applicable technologies to produce nanocomposites faster and cheaper. The microwave sintering is a rapid rate sintering technique suitable for various classes of materials including nanomaterials. MWS utilizes an ability of materials directly absorb microwave energy resulting in rapid volumetric selfheating. Spark plasma sintering (SPS) is a widely recognized field assisted sintering technique, enabling quite rapid consolidation of desired materials under pressure. High rate of consolidation for various ceramics during the SPS and MWS processes makes this methods attractive for the production of nanostructured materials based on high melting point compounds. The effect of technological parameters (heating rate and pressure) for SPS, together with structural design of composites for MWS, on the consolidation of various high melting point compositions (TiN, TiCN, TiB_2, Si_3N_4 etc.) were under our investigation.

It was discovered that non-linear regimes for SPS process and special preparation of nanocompositions for MWS are capable to suppress the grain growth to higher temperatures making possible to obtain near fully dense nanocrystalline ceramic with average grain size below 100 nm. In addition, the relationship coupling microstructural characteristics (grains size, grains boundary) with mechanical properties of nanostructural ceramics obtained via both sintering techniques is under discussion.

DESIGN OF ELECTRONIC NANODEVICES WITH NOVEL LAYERED NANOSTRUCTURES

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Due to the prospect of the 2D materials to be applied in electronic nanodevices, the discovery of a desirable 2D material with a moderate band gap, satisfactory intrinsic thermal conductivity and high carrier mobility is a primary goal of research in materials science. Recently, the 2D transition metal carbides/carbonnitrides (MXenes) have attract significant interest of research. By our first-principles calculations, the semiconducting MXene members with high thermal conductivities and high carrier mobilities have been determined. From our works, the electronic band structures of the M_2CT_2 MXenes (T=O, OH, F) are calculated. According to our data, the scandium MXenes with all termination groups and the M_2CO_2 type MXenes with M=(Ti, Zr, Hf) are determined to be semiconducting. Employing theoretical investigations, the Sc_2CF_2 and $Sc_2C(OH)_2$ MXenes both show excellent electron mobilities and thermal conductivities. The thermal conductivity along the armchair direction of the Sc_2CF_2 MXene is higher than that of the best conductor silver. In regard to the M_2CO_2 (M=Ti, Zr, Hf) MXenes, we find all of the three members present high hole mobilities, which is consistent with the previous reports. Therefore, it is demonstrated from our works that some members of MXene do possess the promising properties that merits their potential application in next generation electronic devices. With the properties of MXene well established, the calculation on the electron transport of the semiconducting Ti_2CO_2 MXene nanoribbons is carried out and their I-V characteristics are evaluated. We demonstrate that the energy gaps in patterned Ti_2CO_2 nanoribbons can be tuned by appropriate designs of crystallographic orientation and widths.

MULTIFUNCTIONALTWO-DIMENSIONAL TRANSITION METAL DICHALCOGENIDESNANOSHEETS AND THEIR NANOHETEROSTRUCTURES:NANOSTRUCTURE, SURFACE AND INTERFACE ENGINEERING

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This review provides a summary of recent progress of oursystematic interdisciplinary studies onfew-layer 2D Transitional Metals Dichalcogenides (TMDs) nanosheets and their nanoheterostructures as graphene inorganic analogues.

It was developed competitive, scalable laboratory 2D nanotechnologies of few-layer TMDs (2H-$MeCh_2$: Me=Mo, W, Re; Ch=S, Se) nanosheets and some van-der-Waals nanostructures (2D/2D (3D) with controlled properties. These 2D nanotechnologies were elaborated on the basis of own (IPMS) industrial technology of some TMDs micron powders which haven't word analogies.

Our approaches to 2D TMDs nanotechnologies parameters and 2D surface-, nanostructure-controlled properties are basis on engineering of real nanostructures, surfaces and interfaces (for example, interdisciplinary studies of surface- and structure-controlled (semiconducting) properties, functionalization of active surface, edge states (environment influences), application of active interface states in TMDs heterostructures synthesis.

It was shown that few-layer TMDs nanosheets with active surface states are solid 2D nanolubricants withexcellent lubricating properties. These 2D TMDs nanolubricants are perspective functional additives to industrial greases (benthonitic) and oils (industrials, aircrafts) for tribological properties enhancementsat extreme temperatures and pressures in comparison with natural micron 2H-MoS_2 powders present-day using (engineering, transport, aerospace, so an).

It was established that few-layer TMDs nanosheets with active surface states are perspective for important water-related environmental applications such as contaminant ultrafast 2D nanosorbents, 2D nanophotocatalysis in visible light for waste water treatment (organic pollutants) and gas sensing (humidity).

Finally, we suggest possible solutions to challenges concerning future developments of 2D TMDs nanosheets and nanomaterials emerging applications.

METAL (OXY)NITRIDE FUNCTIONAL MATERIALS

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Metal oxynitrides have shown prodigious potential in many fields including photocatalytic water splitting, optical detection and electrochemical applications. This is due to the physical and chemical properties of oxynitrides that can be easily tuned by varying their nitrogen and oxygen contents. Here we present series of our investigations on metal oxynitrides, from crystal structure studies to their applications. The works shown here include the crystal structure and anion ordering studies of metal oxynitrides as well as a simple process for preparing mesoporous transition metal nitrides without the use of nano-patterning or other template. Furthermore, these materials show remarkable properties for the fields of clean energy and sensing applications.

TITLE: MULTIFUNCTIONAL INORGANIC NANOPARTICLES FOR CANCER THERANOSTIC APPLICATIONS

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Cancer, uncontrolledgrowth of abnormal cells in the body, is a serious threatening disease which has been defeating many important lives every year. The tumor, mass of tissue, clotting of abnormal cells, is started when old cells do not die and grow in uncontrollable behavior. Proper diagnosis at early stage can increase the survival rate. Therefore, scientists and medical experts are putting their efforts for early detection for premature tumor and proper treatment to improve the life of cancer patients. Nanotechnology has been applying extensively in the field of cancer research, particularly nanotheranostics for the advancement of effective approaches for diagnosis and treatment. Multifunctional inorganicnanoparticles, combining noninvasively molecular imaging probe with therapeutic particles, have been contributing significantly towards magnetic resonance imaging and phototherapy for cancers. Magnetic inorganic nanoparticles are successfully applied as MRI contrast agents and excited photosynthesizers are able to produce cytotoxic reactive oxygen species (ROS), such as singlet oxygen ($^1O_2$) which can oxidize cellular macromolecules leading to tumor cell ablation. In this talk, I will presentsome magnetic and titanium based multifunctional inorganic nanoparticles for positive contrast agent in magnetic resonance imaging MRI and phototherapy applications of cancers.

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