



## *ЦІЛЬОВА КОМПЛЕКСНА ПРОГРАМА НАУКОВИХ ДОСЛІДЖЕНЬ НАН УКРАЇНИ*

*Розвиток наукових засад отримання,  
зберігання та використання водню в системах  
автономного енергозабезпечення*

## *USE OF HYDROGEN ACCUMULATORS IN MOTOR TRANSPORT*

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Грудень 2020

# National Academy of Sciences of Ukraine Institute of Problems of Materials Science



**Hydrogen materials science and  
chemistry of carbon nanostructures**

Щур Дмитрий Викторович

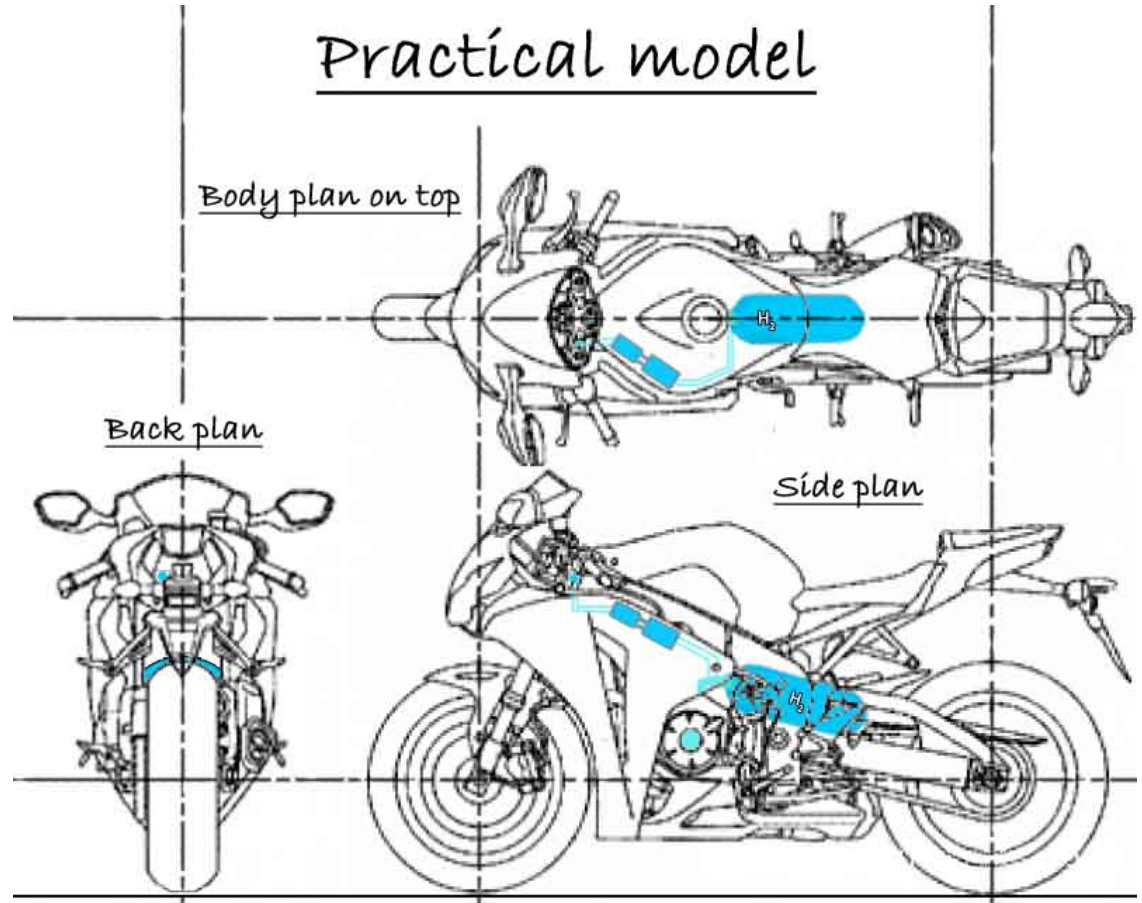
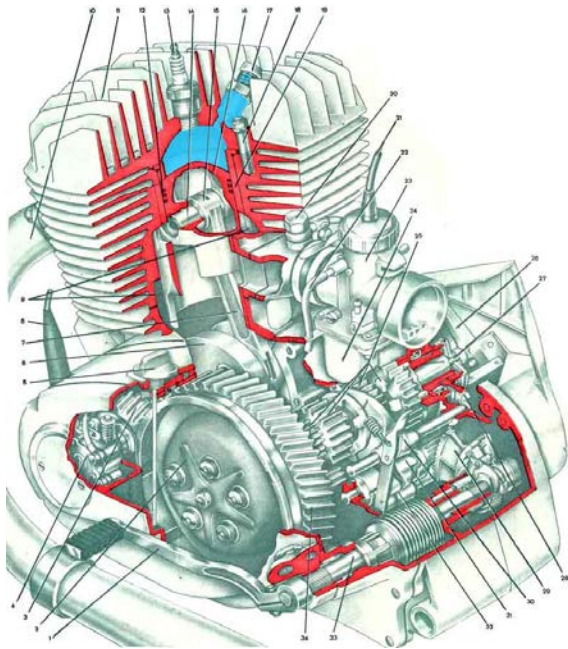
ООО "АРГУС СЕРВИС",



### **Speed Lake: Bonneville Salt Lake**

Speed records are registered for 33 body types, 13 engine classes and 12 engine types.

Modeling and design of the hydrogen supply system to the engine was carried out.

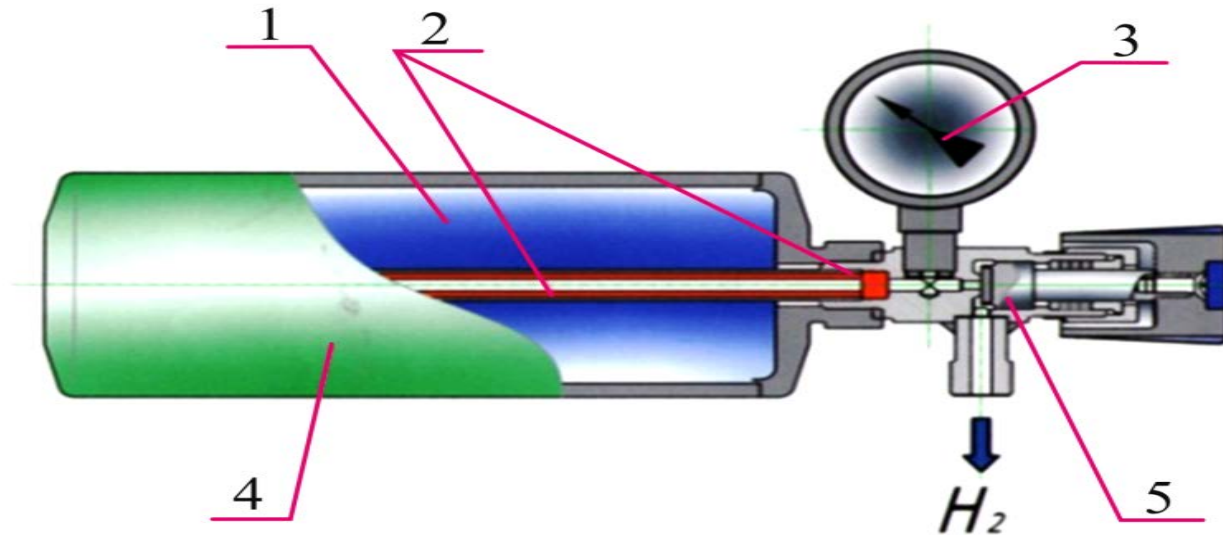


Modeling and design of the hydrogen supply system to the engine was carried out.



Motorcycle IZH-49, with a two-stroke engine 350 cm<sup>3</sup>

# Scheme of a metal hydride source of particularly pure hydrogen



1 - metal hydride; 2 - ceramic filter; 3 - manometer with a safety membrane; 4- stainless steel cylinder; 5- shut-off valve.

The passive protection system is equipped with a safety membrane designed for a pressure of 18.5 MPa.

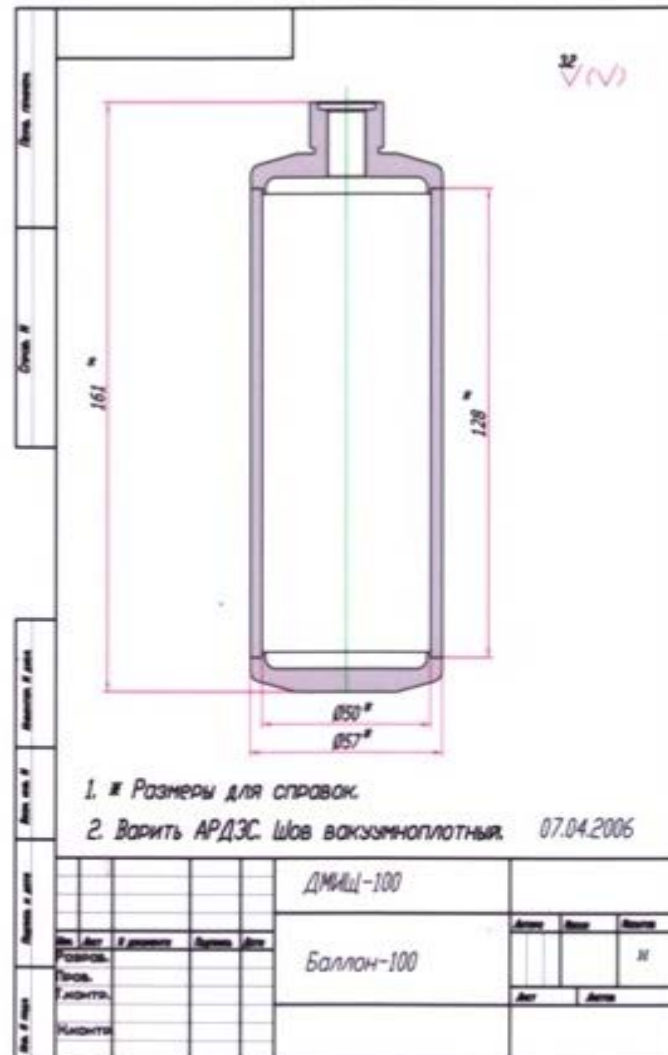
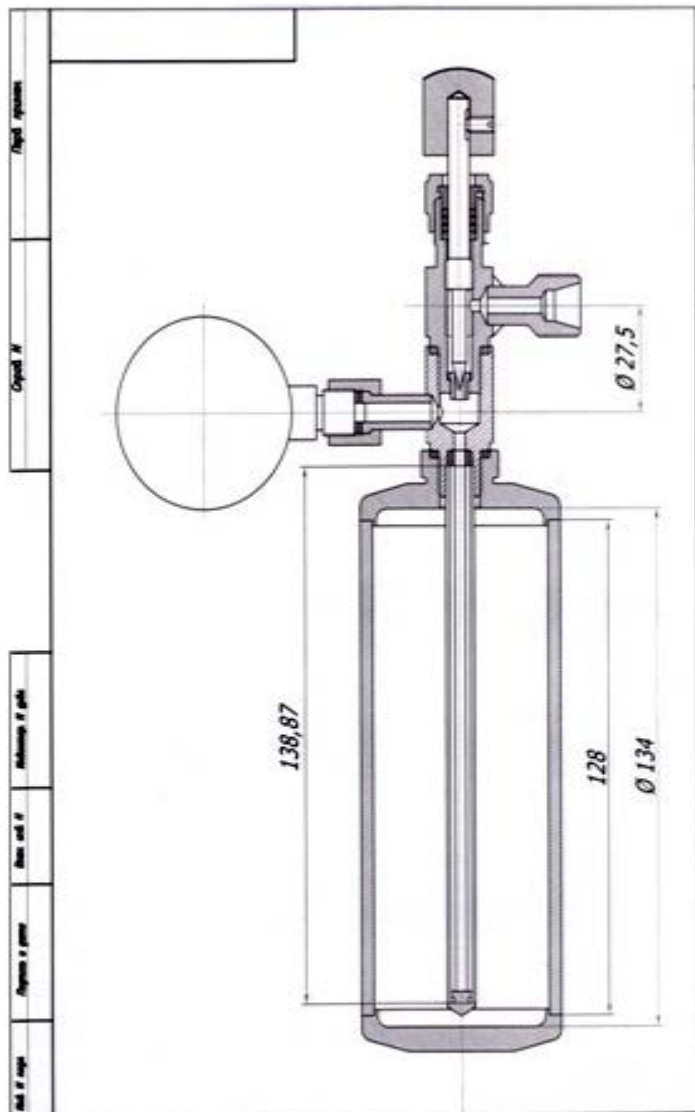


Рис. 13 – Креслення загального вигляду накопичувача водню



**Рис. 16 – Сосуд високого тиску накопичувача водню**



# Drawings are created and the test bench for certification of vessels of a high pressure is constructed

## 1. Destination

The desk is designed to conduct strength and leakage tests of the high-pressure vessels used in manufacture of hydride storage units.

## 2. Performance attributes

### 1. Overall dimensions:

Height ... 1350 mm

Dimension in the lay-out... 490mm x 500 mm

2. Maximum working pressure 55 MPa (force/cm<sup>2</sup>)

3. Mass ... 32 kg.

4. Force on the lever of a hand-power press force

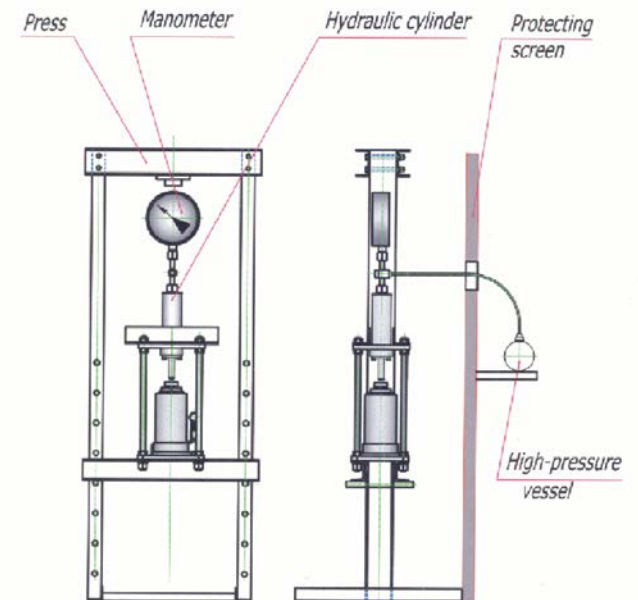
### 3. Configuration of the article

1. Hand-power press for 12 ton

2. Hydraulic cylinder

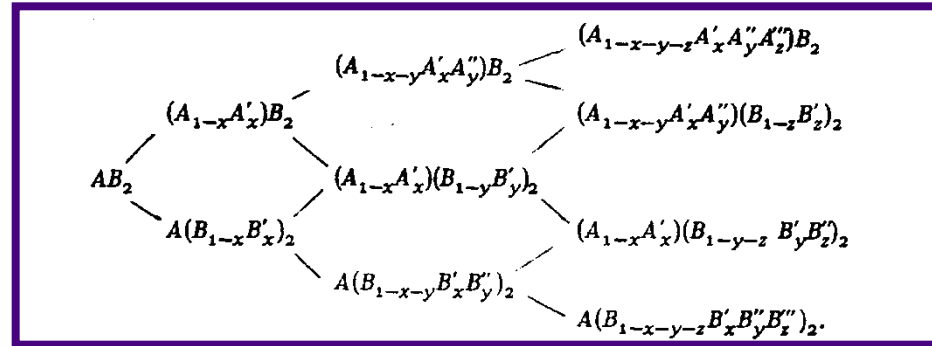
3. Manometer

4. Shield

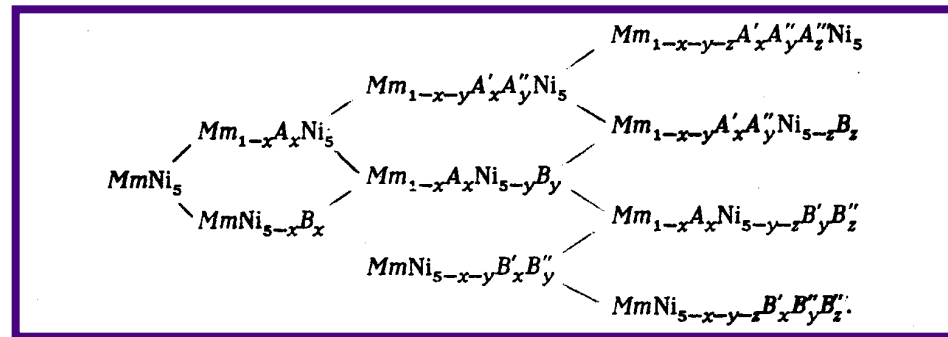


# Schemes of synthesis of new alloys of type AB<sub>2</sub> and AB<sub>5</sub>

I



II



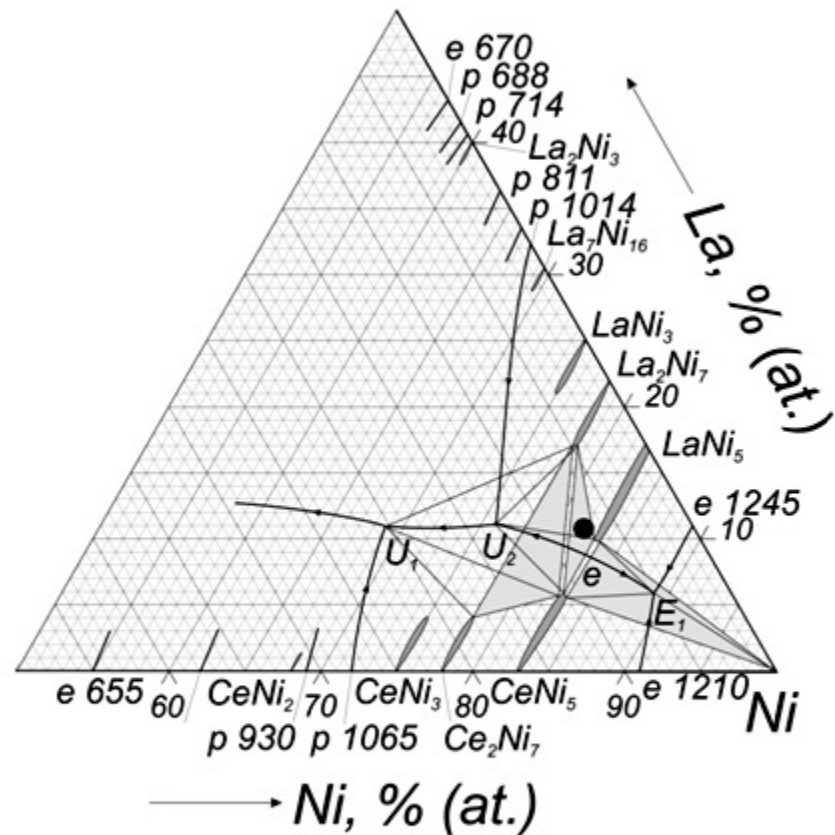
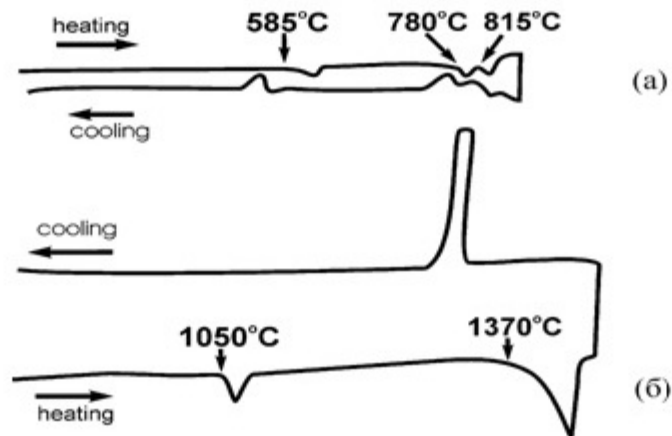


Рис. 10 – Фрагмент діаграми фазових рівноваг у нікелевому куті системи Ce-La-Ni при температурах плавлення (кристалізації сплавів) ● Сплав  $\text{Ce}_{7,5}\text{La}_{9,3}\text{Ni}_{83}$  % (ат.).



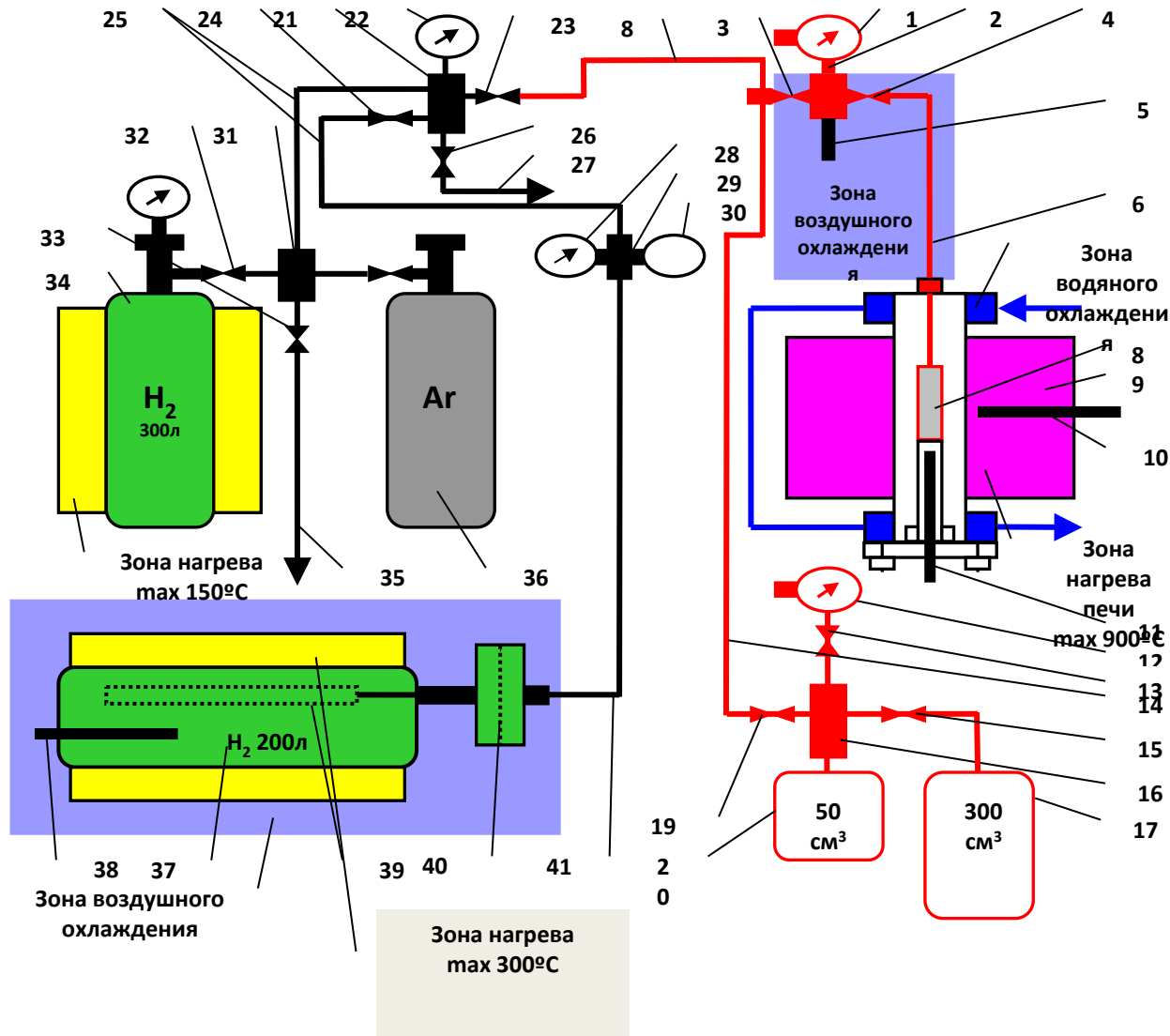
(а) – вихідний мішметалл; (б) – сплав складу  $Mn_{0.2}Ce_{7.5}La_{9.3}Ni_{83}$ , вибраний для використання у накопичувачі.

**Рис. 11 – Термічні криві**

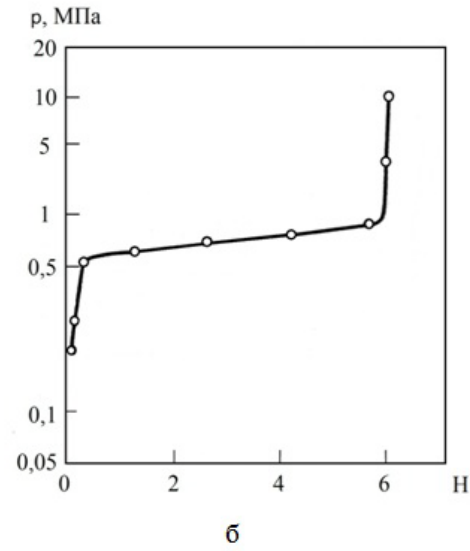
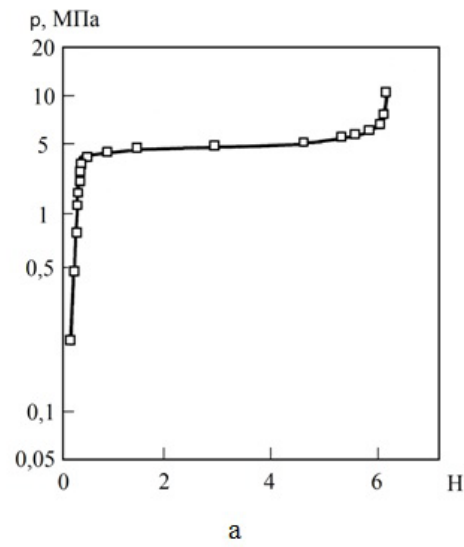
***The synthesized materials are investigated for water capacity.  
Their working characteristics are investigated***



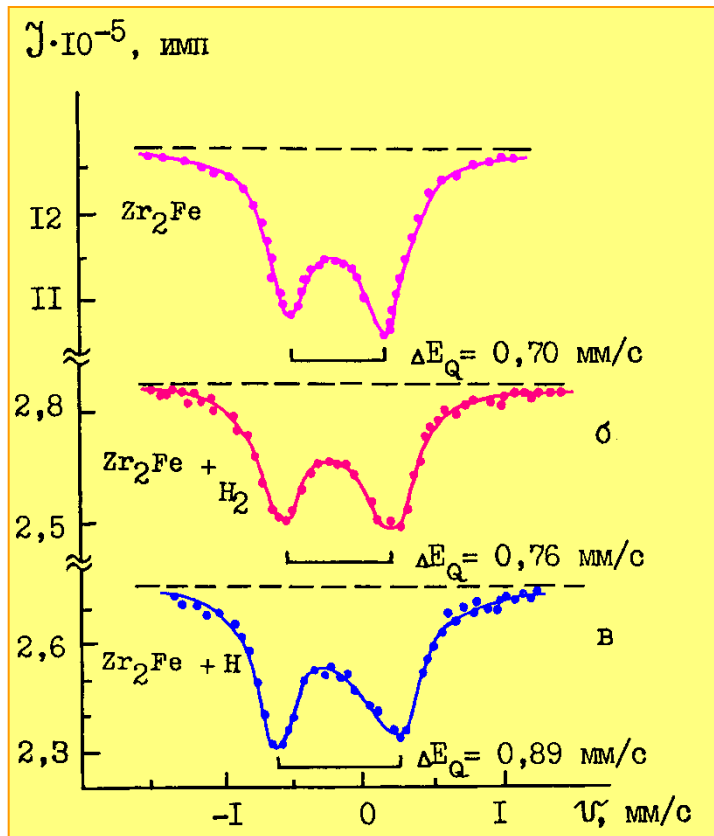
# General scheme of the installation for the study of hydrogen-sorption characteristics



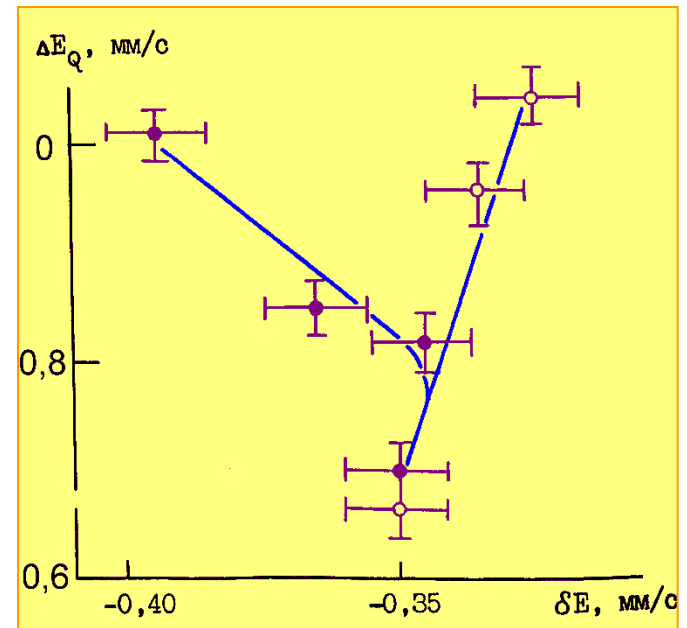
# Isotherms of sorption (a) and desorption (b) of hydrogen for intermetallic $Mm_{0,2}Ce_{7,5}La_{9,3}Ni_{83}$ ( $T = 393K$ )



**Destruction of metal gratings during hydrogenation takes place at internal stresses exceeding 109 Pa ..**



**Mössbauer absorption spectra  $\text{Zr}_2\text{Fe}$  compounds. Change the value quadrupole splitting from the content of H.**



**Dependence of the change in the isomeric shift on the hydrogen concentration for the compound  $\text{Zr}_2\text{Fe}$  (tetr.), Located on the surface of the Zr substrate (o) and in the volume Zr matrices (●)**













MPS-PF	Tim Cyrus & Family	H/D	8 /06	121.267
MPS-PG	Jenkins-Shogun	BSA	8 /04	108.213
MPS-VF	Chkalov Team	Izh-49	8 /18	92.023
MPS-VG	Kenneally	Yamaha	8 /95	128.537
P-P	Shogun - Jenkins	Moto Morini	8 /00	90.746



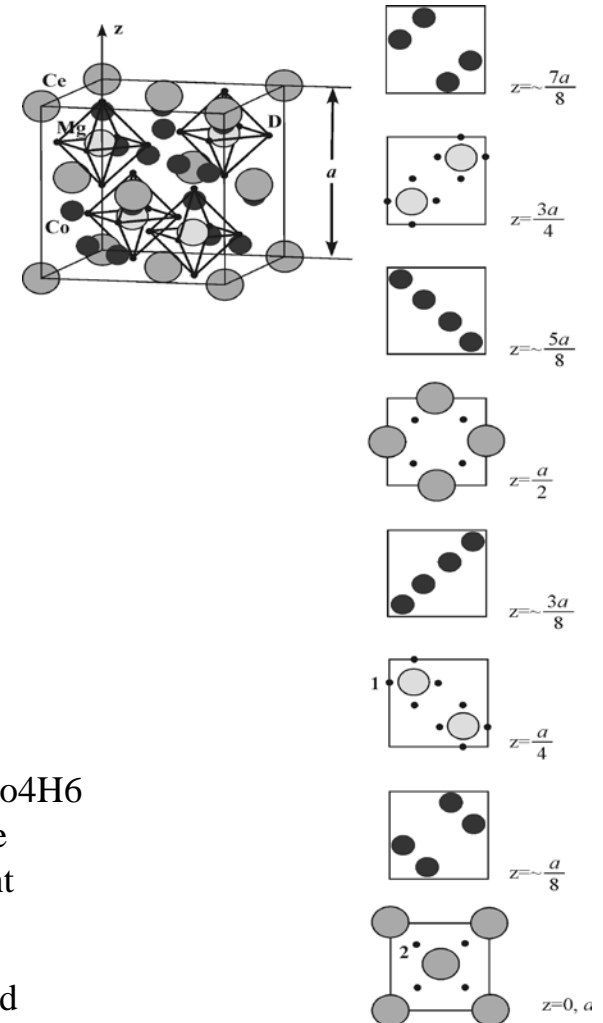
# Magnesium hydride MgH<sub>2</sub>

- Magnesium hydride MgH<sub>2</sub> due to its high hydrogen content (more than 7.5 wt.%) is considered one of the most promising materials for hydrogen storage. However, unsatisfactory kinetics of hydrogen absorption and desorption and excessive thermal stability create obstacles to its practical use. Magnesium intermetallic compounds, primarily with nickel and rare earth metals, obtained by traditional metallurgical methods, are characterized by improved interaction kinetics with hydrogen, but reduced sorption capacity due to the high concentration of heavy elements. Thus, the problem is to select such components and such a preparation procedure that can provide a qualitative modification of the kinetic and thermodynamic parameters of the reactions of formation and decomposition of hydrides in the presence of a small amount of alloying impurities.



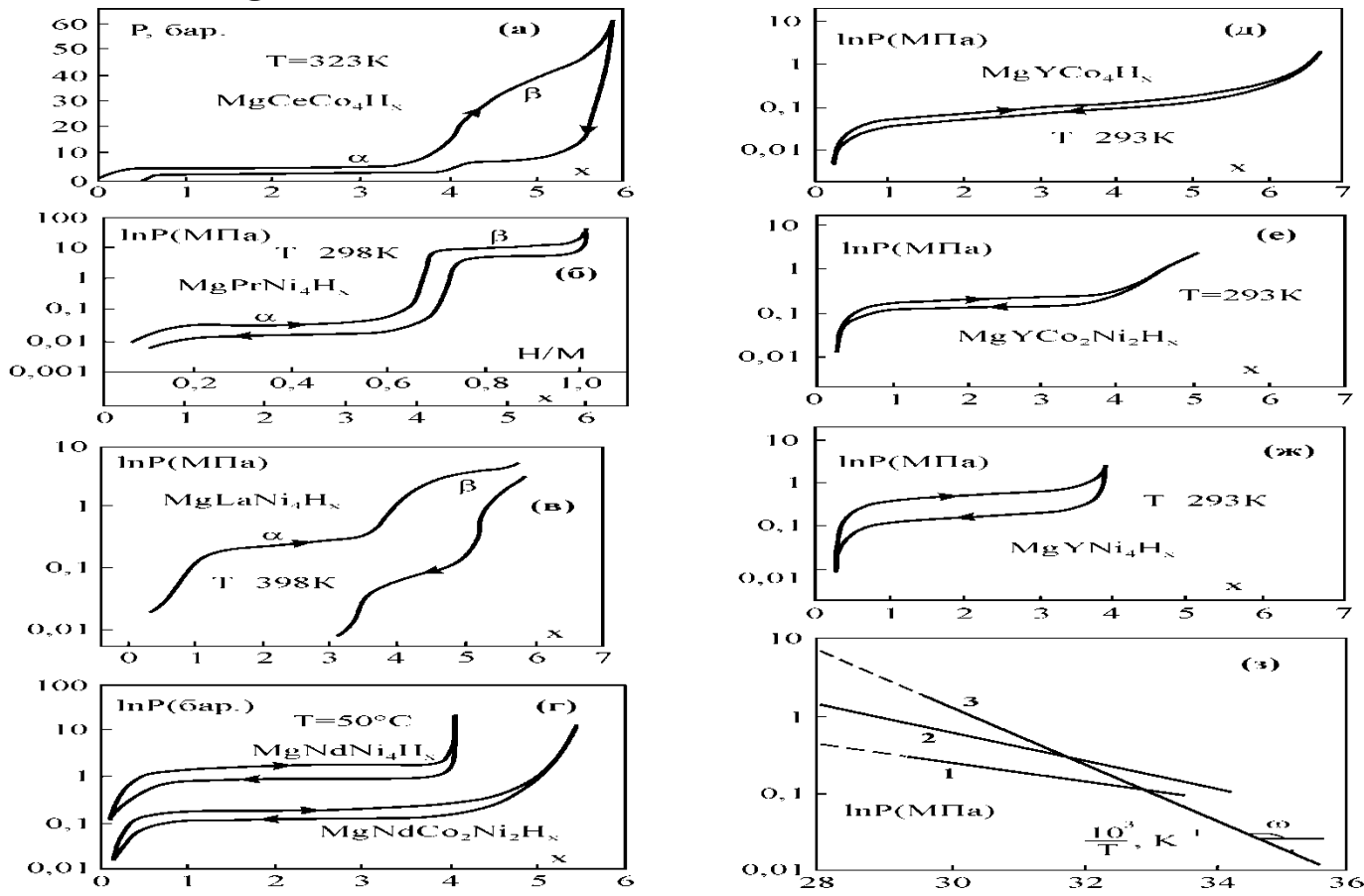
## The calculations were performed in accordance with the structure in the figure

As can be seen from the figure, the unit cell of the alloy contains 4 magnesium atoms, 4 cerium atoms, 16 cobalt atoms (24 metal atoms) and 24 positions of hydrogen atoms, some of which are vacant. The locations of hydrogen atoms form octahedra around magnesium atoms. The positions of hydrogen atoms in the vertices of octahedra are not equivalent, because they differ in the configuration of metal atoms around them, although the number of metal atoms, their grade and interatomic distances, they are the same. Each hydrogen atom is surrounded by five metal atoms: one Mg atom, two Ce atoms and two Co atoms. The positions of the hydrogen atoms in the vertices of the octahedra, which are in the planes with coordinates  $z = a/4$  and  $3a/4$  (there are four such positions for each octahedron), are surrounded by cerium and cobalt atoms, one above and one below these planes. The positions in the vertices of the octahedron, which are in the planes with coordinates  $z = 0$ ,  $a/2$  and  $a$  (such positions are one in these planes for each octahedron), are surrounded by cerium and cobalt atoms differently. Both cerium atoms fall in the same planes, and both cobalt atoms are above or below these planes



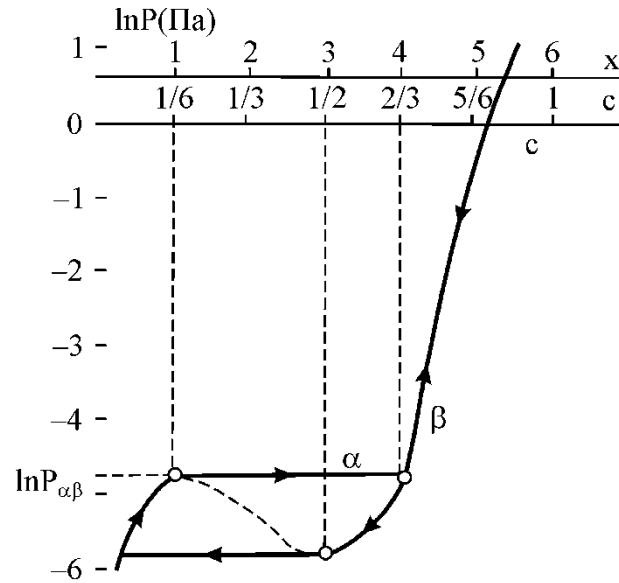
Cubic lattice C15b type  $\text{MgSnCu}_4$  crystal  $\text{MgCeCo}_4\text{H}_6$  in the spatial image (a) and in the projection on the planar area perpendicular to the  $z$  axis, for different values of the  $z$  coordinate.

# The experimental isotherms (a, b, c, d, e, f), isopleths (c) of hydrides of magnesium intermetallics are studied:



It is interesting to develop a statistical theory of the considered alloys in order to substantiate and explain the experimentally observed patterns in the RT diagram of these systems.

Graph of hydrogen absorption-desorption isotherm in  $\text{MgCeCo}_4\text{H}_x$  crystal taking into account the  $\alpha \rightarrow \beta$  phase transition

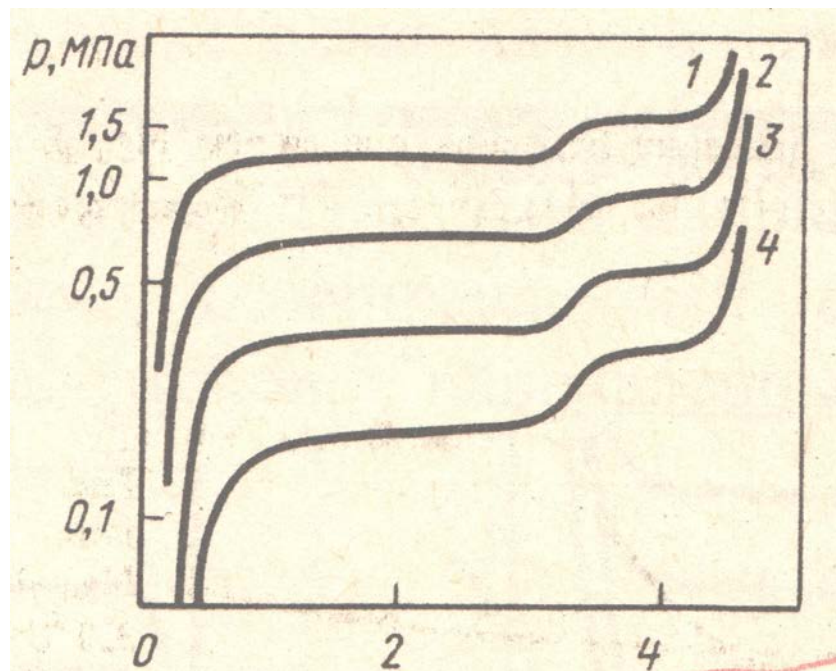


The calculated graph of the isotherm of hydrogen absorption-desorption of the  $\text{MgCeCo}_4\text{H}_x$  crystal during the implementation of the  $\alpha \rightarrow \beta$  phase transition, constructed without taking into account the constant term according to the formulas for energies  $U_{HH} / kT = 2.6$ ;  $U' / kT = -7$ ;  $U'' / kT = -2$ . The dotted part of the curve corresponds to the nonequilibrium state. The circles indicate the extreme points of the curve and the point of the phase transition  $\alpha \rightarrow \beta$ .

# **MgCeCo4Hx hydride desorption isotherms**

**1,5 масс.%**

**Desorption isotherms of MmLaMg16Ni hydride at  
temperature: 1-340; 2 - 310; 3 - 290; 4 - 280 0C**



При  $T=285^{\circ}\text{C}$  и  $P= 3 \text{ МПа}$  поглощает 5 масс.% Н

При  $T=285^{\circ}\text{C}$  и  $P= 0,2 \text{ МПа}$  десорбирует 2,5 масс.% Н





ООО "АРГУС СЕРВИС",



**Speed Lake: Bonneville Salt Lake**



## ***PUBLICATIONS ON THE PROJECT***

- .A. Matysina, N.A. Gavrylyuk, A. Veziroglu, T.N. Veziroglu, A.P.Pomytkin, D.V. Schur, T.S. Ramazanov, M.T. Gabdullin, An.D. Zolonarenko, Al.D. Zolonarenko «HYDROGEN SORPTION PROPERTIES OF NEW MAGNESIUM INTERMETALLIC COMPOUNDS WITH MgSnCu<sub>4</sub> TYPE STRUCTURE», **International Journal of Hydrogen Energy**, 2021, 46, 25520-25532
- An.D. Zolonarenko <sup>а\*</sup>, Al.D. Zolonarenko, A. Veziroglu, T.N. Veziroglu, A.P.Pomytkin, N.A. Gavrylyuk, D.V. Schur, T.S. Ramazanov, M.T. Gabdullin « USE OF ATOMIC HYDROGEN IN APPARATUSES OF ARTIFICIAL LUNG VENTILATION IN THE FIGHT AGAINST VIRUS COVID-19», **International Journal of Hydrogen Energy**, 2021, HE-S-20-07038
- Al.D. Zolotareno<sup>к\*</sup>, An.D. Zolotareno, A. Veziroglu, T.N. Veziroglu, A.P.Pomytkin, N.A. Gavrylyuk, D.V. Schur, T.S. Ramazanov, M.T. Gabdullin, «METHODS OF THEORETICAL CALCULATIONS AND OF EXPERIMENTAL RESEARCHES OF THE SYSTEM ATOMIC HYDROGEN – METAL» **International Journal of Hydrogen Energy**, 2021, HE-D-20-05424
- Nazym Akhanova a,b, Yerassyl Yerlanuly a,c, Didar Batryshev a,d, Timur Kulsartov a, Yevgeniy Chikhray a, Tlekkabul Ramazanov b, Ayfer Veziroglu e, Dmitry Schur b,f, Wanli Kang g, Maratbek Gabdullin a,b The study of deuterium permeability of filmforming inhibitors with the addition of fullerenes **International Journal of Hydrogen Energy**, 2021, 46, 25520-25532
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- 2. Д.В Щур, СЮ Загинайченко, А Везироглу, ТН Везироглу, АД Золотаренко, МТ Габдуллин, ТС Рамазанов, Ал Д Золотаренко, Ан Д Золотаренко [Особенности изучения систем атомарный водород–металл](#), **Альтернативная энергетика и экология (ISJAEE)**, 2019, 13-15, 62-87.
- СЮ Загинайченко, ДА Зарицкий, ДВ Щур, ЗА Матысина, ТН Везироглу, МВ Чимбай, Л.И. Копылова [Теоретическое исследование водородно-сорбционных свойств борокарбидов лития и магния](#) **Альтернативная энергетика и экология (ISJAEE)**, 2019, Issue13-15 Pages 52-61.
- ZA Matysina, S Yu Zaginaichenko, DV Schur, Al D Zolotareno, An D Zolotareno, MT Gabdulin, LI Kopylova, TI Shaposhnikova, [Phase Transformations in the Mixed Lithiummagnesium Imide Li<sub>2</sub>Mg \(NH\)<sub>2</sub>](#), 2019/4, **Russian Physics Journal**.

**THANK YOU ALL !!!**



**Thank you all for attention and interest in our research. We hope for cooperation.**