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NUMERICAL SIMULATION OF METAL HYDRIDE BATTERY HEAT CONDUCTING MATRIX HEAT-STRESSED AND DEFORMED STATE

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The problem of safe and effective storage of hydrogen is dealt with by many researchers in different countries. The method of storing hydrogen in a chemically bound state in metal hydride accumulators has a number of advantages in comparison with the storage methods in compressed or liquefied form. The use of metal hydrides makes it possible to achieve high packing density of hydrogen, which today reaches from 0.09 to 0.19 g/cm³, and for intermetallic hydrides – up to 0.56 g/cm³. The high safety of hydrogen storage in metal-hydride batteries should also be noted, which is especially important when using hydrogen in transport. When using numerical methods, the heat-stressed state of the heat-conducting matrix of a cylindrical metal hydride battery is considered. The matrix is made of an aluminum alloy and has rectangular cells filled with metal hydride in the form of a fine powder. The matrix is heated by two electric heating elements: a rod-type central element and a cylindrical peripheral one. The radial and axial expansions of the matrix in a body are limited by elastic elements made of heat-resistant steel. The simulation of the heat-conducting matrix heat-stressed and deformed states is performed for a hydrogen desorption regime for 900s at a temperature of 350 °C. As a metal hydride, magnesium hydride (MgH2) is chosen. The packing density of hydrogen in a metal hydride is assumed to be 0.11 g/cm³. The problem can be solved in Cartesian coordinates in a three-dimensional stationary setting. Calculation results show that during the hydrogen desorption process, the maximum temperature difference in the radial direction of the heat-conducting matrix is about 40 °C. The maximum radial expansion of the heat-conducting matrix reaches 0.56 mm, which is not critical for the reliable operation of a metal-hydride battery. The level of equivalent von Mises stresses varies within 10-60 MPa on the sections of the heat-conducting matrix cell-based structure, which does not exceed the level of the stress boundary values for the aluminum alloy, i.e. for these matrix design parameters there is a reserve for increasing heat exchange intensity.

Keywords: metal hydride, hydrogen, heat-conducting matrix, heat-stressed state, temperature level.

Introduction

The problem of safe and effective storage of hydrogen is dealt with by many researchers in different countries [1–11]. The method of storing hydrogen in a chemically bound state in metal hydride accumulators has a number of advantages in comparison with the storage methods in compressed or liquefied form [1, 3–5]. The use of metal hydrides makes it possible to achieve high packing density of hydrogen, which today reaches from 0.09 to 0.19 g/cm³, and for intermetallic hydrides – up to 0.56 g/cm³. The high safety of hydrogen storage in metal-hydride batteries should also be noted, which is especially important when using hydrogen in transport.

Magnesium hydride (MgH2) is one of the most promising chemical compounds for creating hydrogen batteries. As is known, MgH2 is a high-temperature metal hydride (hydrogen absorption and desorption can only occur at elevated temperatures of 250–350 °C), which requires high energy costs for implementing the hydrogen desorption process.

Analysis of publications

A metal hydride battery is a tubular body with a heat exchanger inside [1, 6, 7]. The metal hydride powder is placed in the annular gap between the body walls and the heating element [1]. The use of heaters / heat exchangers is both due to the need to supply heat to the metal hydride during hydrogen desorption and the low thermal conductivity of a metalloid powder, on average up to 2 W·m/K [1].

The recommended thickness of the metal hydride layer is limited to 5−6 mm, and the amount of its filling in the battery body should not exceed 40–50 % [1, 7]. If metal-hydride batteries are large, then heat-conducting matrices of different configurations are used [1, 7].

Taking into account the large coefficient of the metal hydride volumetric expansion (from 20 to 30 %) during the absorption and desorption of hydrogen, such heat-conducting matrices should have sufficient mechanical strength and compensate for the expansion of the metal hydride during the operation [1, 10].

From the above review, it can be concluded that studying heat and mass exchange processes in metal hydride accumulators, increasing the hydrogen packing density, improving the design and thermo-physical properties of heat-conducting matrices are important and promising directions in the development of hydrogen energy.
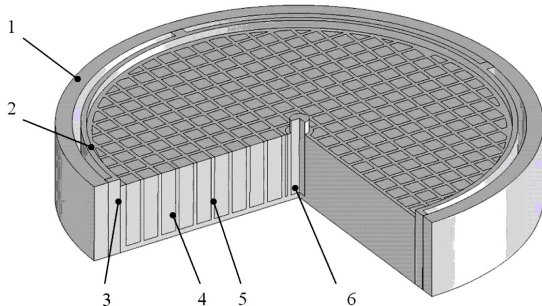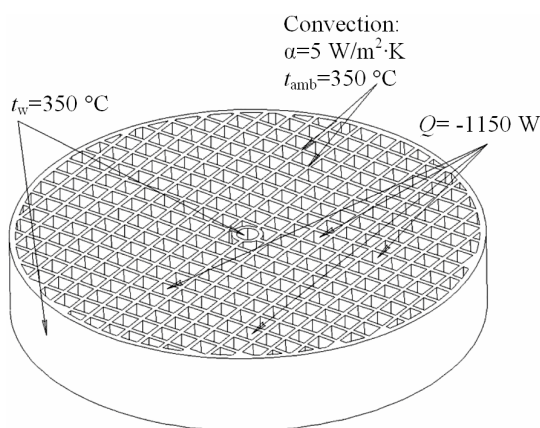

Fig. 1. Metal‑hydride battery design features:
1 − body; 2 and 6 − heating elements; 3 − elastic element; 4 − metal hydride (MgH2); 5 – heat-conducting matrix
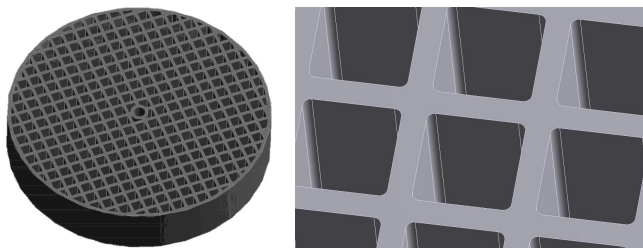
Fig. 2. Metal hydride battery heat-conducting matrix computational domain

t_w is wall temperature; Q is heat flux; convection: t_{amb} is ambient temperature; α is heat exchange coefficient

Fig. 3. Diagram of setting the heat-exchange BCs on heat-conducting matrix sections

Purpose and objectives of the study

The aim of this paper is to estimate the heat-stressed and deformed state of a metal-hydride accumulator heat-conducting matrix during the desorption of hydrogen.

The work had the following tasks:

− to conduct a literature review on modern technologies of hydrogen storage in metal hydrides;

− to develop a design of a metal-hydride battery heat-conducting matrix;

− to synthesize the computational domain and mesh describing the heat-conducting matrix configuration;

− to calculate the heat-conducting matrix heat-stressed and deformed state for the hydrogen desorption regime;

− to draw conclusions and recommendations on the use of a heat-conducting matrix to intensify the heat and mass exchange processes in a metal-hydride battery.

Figure 1 shows the construction of a metal hydride battery fragment. Heat rejection during hydrogen absorption can be realized by blowing on the battery body outer surface. The heat-conducting matrix is made of the AL25 aluminum alloy. The matrix is a cylindrical cellular structure with a diameter of 150 mm and height of 28 mm. The cells are 6 by 6 mm in size and 25 mm in height.

The computational domain describing the configuration of a heat-conducting matrix is shown in figure 2. In the computational domain, fillet radii are taken into account.

The calculations of the heat-conducting matrix heat-stressed and deformed state were performed using the finite element method implemented in open source software − the Caelinux Salome Meca complex [12].

The scheme for specifying the boundary conditions of heat exchange and the values of the specified boundary conditions (BC) are shown in figure 3. Both on the lateral surface of the heat-conducting matrix and on the surface of the hole under the heating element (at the place

of installation of the heating elements 2 and 6), the first-order BCs were set – their temperature. On the sections of the heat-conducting matrix cellular structure, the BGs were set in the form of a heat flux (equivalent to heat rejection during hydrogen desorption [1] – the software package capabilities make it possible to specify the heat flux or specific heat flux). On the heat-conducting matrix outer surface, the third-order BCs were set, taking into account the recommendations in [1].

The heat-conducting matrix heat-stressed and deformed state is considered in a stationary three-dimensional setting. The density of metal hydride saturation with hydrogen is taken equal to 0.11 g/cm^3. The hydrogen desorption process lasts for 900 s.

To calculate the heat-conducting matrix temperature field, the equations of stationary thermal conductivity are used in the form

$$\frac{\partial}{\partial x}\left(\lambda_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda_z \frac{\partial T}{\partial z}\right) + R \cdot T + Q = 0 ; \tag{1}$$

$$T\big|s_T = T_0 ; \tag{2}$$

$$q\big|s_q = -\left(\lambda_x \frac{\partial T}{\partial x} n_x + \lambda_y \frac{\partial T}{\partial y} n_y + \lambda_z \frac{\partial T}{\partial z} n_z\right); \tag{3}$$

$$\alpha_{cp}(T - T_{amb})\big|s_\alpha = -\left(\lambda_x \frac{\partial T}{\partial x} n_x + \lambda_y \frac{\partial T}{\partial y} n_y + \lambda_z \frac{\partial T}{\partial z} n_z\right), \tag{4}$$

where T is the temperature; Q is the heat source density; $R \cdot T$ is the source component, proportional to the temperature; t_{amb} is the ambient temperature; $\lambda_x, \lambda_y, \lambda_z$ are the coefficients of thermal conductivity in the direction of the anisotropy axes, (in the case of isotropy $\lambda_x = \lambda_y = \lambda_z$); n_x, n_y, n_z are the direction cosines of the outer normal; q is the heat flux at the outer boundary of S_q.

The boundary conditions (4) correspond to the heat exchange with the external environment according to the Newton-Richmann law. For the case of the third-order BCs, we find the solution by minimizing the corresponding functional for the temperature field $T(x_1, x_2, x_3)$:

$$\Phi(T) = \frac{1}{2}\iiint\limits_V \left(\lambda_x \left(\frac{\partial T}{\partial x}\right)^2 + \lambda_y \left(\frac{\partial T}{\partial y}\right)^2 + \lambda_z \left(\frac{\partial T}{\partial z}\right)^2\right) dv + \frac{1}{2}\iint\limits_S \alpha_{cp}(T - T_{cp})T dS \to \min. \tag{5}$$

The results of the numerical study of the field and specific heat flux in a metal hydride battery heat-conducting matrix during hydrogen desorption are shown in figure 4. As can be seen from the results shown in figure 4, a the temperature difference along the radius of the heat-conducting matrix between the heat supply and rejection zones is of the order of 40 °C, and the specific heat flux density distribution is of the order of 1.1–1.82 W/mm^2 (Figure 4, b).

When describing the scheme of fixing a heat-conducting matrix in the areas of its contact with an external heating element (Fig. 1, item 2) and the matrix fasteners in a metal hydride battery body (not shown in figure 1), efforts were made from the action of the elastic elements (figure 1, point 3).

The results of calculating the stress-strain state of a heat-conducting matrix, taking into account the thermal load effect, are shown in figure 5. The radial thermal expansion of the heat-conducting matrix along its outer surface reaches 0.56 mm (Fig. 5, a). The level of equivalent von Mises stresses varies from 10 to 60 MPa on the matrix cellular structure sections (Fig. 5, b).

The resulting values of stresses and deformations in a heat-conducting matrix that arise during the desorption of hydrogen are consistent with the results obtained by other authors [13, 14].
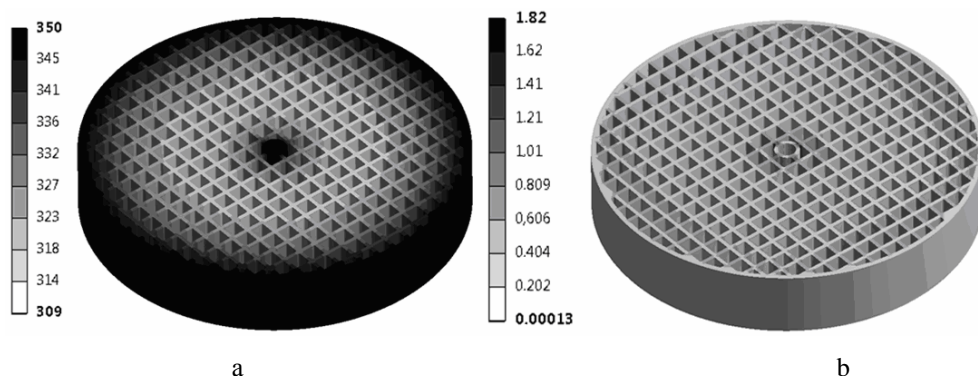
Fig. 4. Numerical simulation results:
a – is temperature distribution, °C; b – is specific heat flux distribution W/mm² in a metal-hydride accumulator heat-conducting matrix during hydrogen desorption
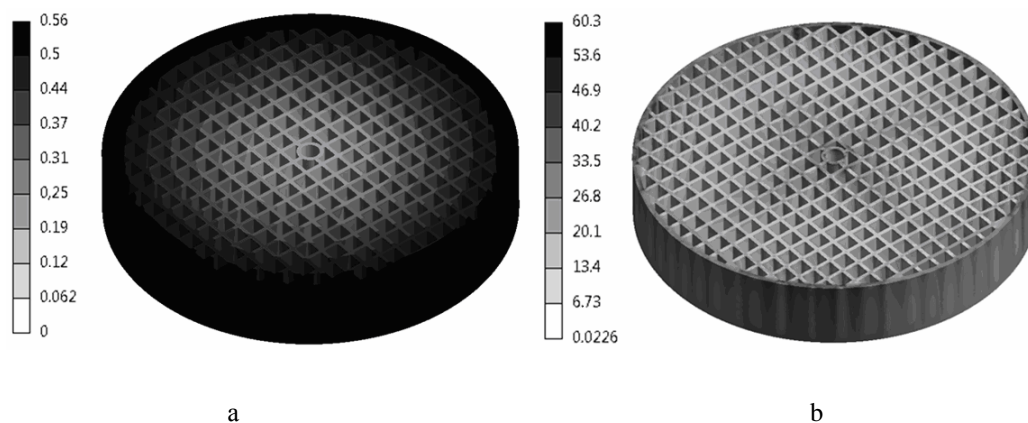
Fig. 5. Stress-strain state numerical simulation results:
a – heat-conducting matrix radial expansion, mm; b – level of equivalent von Mises stresses, MPa in a metal-hydride accumulator heat-conducting matrix during hydrogen desorption

Conclusions

Based on the results of a literature review and a computational study, it has been established that:

– studying the intensification of heat and mass exchange processes and ways to improve the heat-conducting matrices of high-temperature metal hydride accumulators is a promising direction in the development of hydrogen energy;

– for a heat-conducting matrix with selected geometric and thermo-physical parameters, the maximum temperature difference in the radial direction during hydrogen desorption is about 40 °C;

– the maximum increase in the heat-conducting matrix outer diameter reaches 0.56 mm, which is not critical for the reliable operation of a metal-hydride battery;

– the level of equivalent von Mises stresses varies within 10–60 MPa on the heat-conducting matrix cellular structure sections, which does not exceed the level of the stress boundary values for the aluminum alloy, i.e. for these matrix design parameters there is a reserve for increasing heat exchange intensity.

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Чисельне моделювання теплонапруженого й деформованого стану теплопровідної матриці металогідридного акумулятора

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Проблемою безпечного і ефективного зберігання водню займаються багато дослідників в різних країнах. Спосіб зберігання водню в хімічно зв'язаному стані в металогідридних акумуляторах має низку переваг порівняно зі способами зберігання в стиснутому і зрідженому вигляді. Використання гідридів металів дозволяє домогтися високої щільності упаковки водню, яка на сьогодні сягає від 0,09 до 0,19 г/см³, а для інтерметалевих гідридів – до 0,56 г/см³. Також слід зазначити високу безпеку зберігання водню в металогідридних акумуляторах, що особливо важливо під час використання водню на транспорті. З використанням чисельних методів розглядається теплонапружений стан теплопровідної матриці металогідридного акумулятора циліндричної форми. Матриця виконана з алюмінієвого сплаву і має комірки прямокутного перерізу, які заповнюються металогідридом у вигляді дрібнодисперсного порошку. Нагрівання матриці здійснюється двома електронагрівальними елементами: центральним стрижневого типу і периферійним у вигляді циліндра. Радіальне і осьове розширення матриці в корпусі обмежені пружними елементами, виконаними з жаростійкої сталі. Моделювання теплонапруженого та деформованого стану теплопровідної матриці виконується для режиму десорбції водню протягом 900 с за температури 350 °C. Як металогідрид обрано гідрид магнію (MgH2). Щільність упаковки водню в металогідриді дорівнює 0,11 г/см³. Задача розв'язується в декартових координатах у

тривимірній стаціонарній постановці. В результаті розрахунку встановлено, що в процесі десорбції водню максималь-ний перепад температури в радіальному напрямку теплопровідної матриці становить близько 40 °C. Максимальне радіальне розширення теплопровідної матриці досягає 0,56 мм, що не є критичним для надійної роботи металогідрид-ного акумулятора. Рівень еквівалентних напружень за Мізесом змінюється в межах 10 – 60 МПа ділянками комірчас-тої структури теплопровідної матриці, що не перевищує рівня граничних значень напружень для алюмінієвого сплаву, тобто для даних конструктивних параметрів матриці є резерв підвищення інтенсивності теплообміну.

Ключові слова: *металогідрид, водень, теплопровідна матриця, теплонапружений стан, рівень температур.*

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