DEFINITION OF FIRE AND EXPLOSION HAZARD OF TECHNOLOGICAL PARAMETERS OF STORAGE SYSTEMS AND SUBMISSION OF HYDROGEN ON THE BASIS OF CONVERTIBLE HYDRIDES OF INTERMETALLIDE

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Statement of a problem. One of ways of storage of hydrogen is its storage in the form of hydrides of metals and intermetallides which use is characterized by change of temperature and pressure. So it is necessary to determine interrelation and allowable limits for parameters of technological processes of hydrogen storage and hydrogen generation.

These limits influence on Fire and Explosion Hazard (FEH) of System Of Hydrogen Storage and Submission (SOHSS).

The analysis of last achievements and publications. The analysis of results of many researches testifies perspectives of use of intermetallide $LaNi_5$ for storage of hydrogen [1,2].

Processes sorption and desorption of hydrogen are accompanied by thermal effects ((25-50) κJ/moll), this fact causes necessity of definition of parameters of technological process of hydrogen storage and hydrogen generation [2,3].

All existing models of phase equilibrium do not reproduce observable peculiarities of phase diagrams (shift and asymmetry PCT - curves). One of last works in the field of definition of the processes occurring in metalhydrides is work [4]. It takes into consideration the above-mentioned disadvantages. In this work on the basis of the modified theory of indignation it is offered the method of definition of thermodynamic properties of a non-ideal hydrogen subsystem of intermetallides.

Statement of a task and its decision. In the given work on the basis of offered in [4] models PCT - diagrams for $LaNi_5H_x$ are received.

According to [4], PCT - diagrams for LaNi5Hx can be described the following equation:

$$\ln P_{H_2}(\theta,T) = \ln P_{H_2}^{(PL)}(T) + 2\left[\beta\mu_H^+(\theta,T) - \beta\mu_H^{+(PL)}(T)\right], \quad (1)$$

where $\ln P_{H_2}^{(PL)}(T)$ is pressure of decomposition β - phases; $\mu_н^+(\theta,T)$ is chemical potential; $\mu_H^{+(PL)}(T)$ is height of a plateau on concentration dependences of isotherms $\mu_H^+(\theta)$.

Fig. 1 presents the PCT-diagram of dependence of pressure from temperature and concentration of hydrogen in LaNi5Hx, received according to expression equation (1).

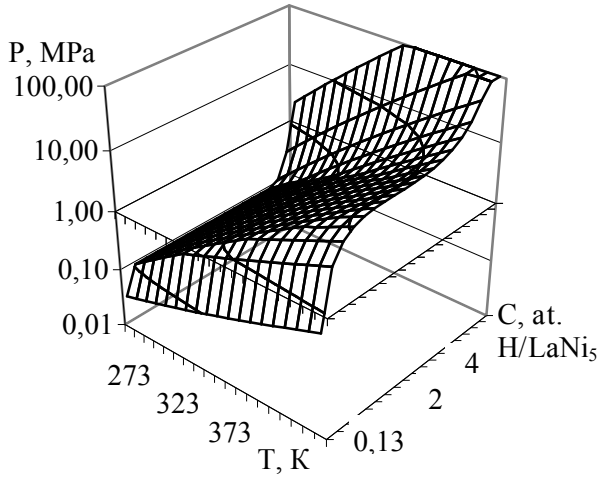

Figure 1 - Isotherms of balance of hydrogen in $LaNi_5$ received according to (1)

According to fig. 1, the pressure in system rises when temperature and concentration grows. The analysis shows, that taking into consideration FEH, temperature rise is more dangerous at approached to a maximum concentration of hydrogen in hydride.

Pressure of decomposition of β - phases $\ln P_{H_2}^{(PL)}(T)$ is determined according to equation:

$$\ln P_{H_2}^{(PL)}(T) = -\frac{\Delta H_{\beta\to\alpha}}{RT} + \frac{\Delta S_{\beta\to\alpha}}{R}, \quad (2)$$

where $\Delta H_{\beta\to\alpha}$ is enthalpy of β→α-transition; $\Delta S_{\beta\to\alpha}$ - entropy of β→α-transition; R - a universal gas constant; T is temperature in system.

The chemical potential $\mu_н^+(\theta,T)$ was determined according to equation:

$$\beta\mu_н^+(\theta,T)=\ln\frac{\theta}{1-\theta}+\frac{W_1\theta}{T(1+\alpha c_s\theta)}+\frac{W_2\theta^2}{T^2(1+\alpha c_s\theta)^2} \quad (3)$$

The value $\mu_H^{+(PL)}(T)$ corresponding to height of a plateau on concentration dependences of isotherms $\mu_H^+(\theta)$, is determined according to equation:

$$0=P_H^{(\beta)}-P_H^{(\alpha)}=\frac{c_s}{\Omega}\int_{\theta_\alpha}^{\theta_\beta}\left[\mu_н^{+(PL)}-\mu_н^+(\theta)\right]d\theta \quad (4)$$

On fig. 2 the schedule of definition of pressure is constructed depending on concentration of hydrogen in intermetallide and temperature. Besides this figure presents curves of changes of concentration θ_α, θ_β depending on temperature, where pressure does not depend on change of concentration of hydrogen in hydride.

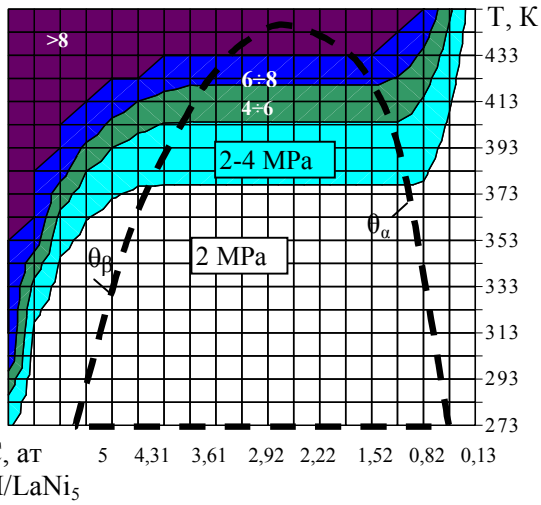

Figure 2 - Allowable areas of temperatures depending on pressure and concentration of hydrogen in intermetallide

Conclusions: In work with use of the modified thermodynamic theory of indignation it is determined:

- Concentration limits of β→α - transition for which it is observed, the field of plateau depending on pressure and also graphic dependence θ_α and θ_β from temperature is constructed;
- Dependence of pressure increase from temperature in the field of a plateau;
- The schedule of pressure (fig. 2) depending on concentration of hydrogen in intermetallide and temperature.

On the basis of received PCT - diagrams of interaction of hydrogen with LaNi5Hx it is possible to define the most dangerous modes of technological processes sorption and desorption of hydrogen and to develop the preventive measures.

The safest modes are mates which technological parameters are characterized by field of constant pressure are optimum. This field on fig. 2 is specified by a dashed line.

Thus, on the basis of the thermodynamic theory of indignation for FEH on basis $LaNi_5H_x$, it is received the PCT-diagram. The ranges of values for technological parameters of processes sorption and desorption the hydrogen, garanteering the safest level for systems of storage and submissions of hydrogen are determined on the basis of the given intermetallide combination.

Referernces

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