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ANALYSIS OF HEAT AND MASS TRANSFER PROCESSES IN A METAL HYDRIDE LAYER WITHOUT SIMPLIFICATION OF LOCAL THERMODYNAMIC EQUILIBRIUM

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A system of differential equations for thermophysical processes involving the interaction between a metal hydride layer and hydrogen is obtained by the averaging method. The system includes two energy equations, of energy namely, for solid and gas phases. The thickness of the transition layer beyond which local thermodynamic equilibrium is established is estimated.

Hydrides of intermetallic compounds (IMC) such as $LaNi_5H_x$, $FeTiH_x$, etc. are studied extensively nowadays owing to their promising use in creating safe hydrogen cells (an alternative to storage of liquid hydrogen) and highly efficient thermochemical compressors and ecologically pure hydride cooling systems (an alternative to Freons used) and in power machines with the purpose of converting low-potential thermal energy into the potential energy of hydrogen pressure. These compounds are characterized by a number of unique properties, first of all, by the capability of reversible sorption (only of hydrogen) under normal conditions (the ambient temperature and a pressure measured in atmospheric units) and an extremely high hydrogen capacitance [1].

In order to design efficient installations that use metal hydride elements, it is important to have a mathematical model that adequately describes the main physical-chemical processes in an element, namely, heat supply or removal from the hydrogenation zone, hydrogen filtration through a porous hydride matrix, and chemical processes involving hydrogen sorption-desorption by a hydride.

Many works are devoted to mathematical simulation of heat and mass transfer processes in IMC hydrides. In [2], the dynamics of operation of an $LaNi_5$-based metal hydride element is analyzed under the assumption that at each point of the IMC the equilibrium is established between the temperature, pressure, and mass content of the bound hydrogen. The presence of characteristic isobaric areas that comprise a major part of the sorption capacity in the region of moderate temperatures has allowed the authors of [2] to formulate a frontal model of heat and mass transfer in a metal hydride layer. According to this model, equilibrium isotherms are reduced to horizontal areas covering the entire IMC sorption capacity. Mathematically, the frontal model leads to a Stefan-type problem with a movable boundary.

In [3], a program is described for calculating the operational dynamics of metal hydride elements of different configurations based on an analysis of the thermal processes. The finite-difference method has been used for solving one-dimensional problems, the finite-element method for solving two-dimensional problems.

The effect of hydrogen filtration through a porous matrix of a metal hydride on the dynamics of processes in the metal hydride layer is discussed in [4-6]. The filtration exerts a substantial influence on these processes if the porosity of the hydride matrix is low. It should be noted that no unified opinion exists on whether the Darcy law holds exactly for hydrogen filtration (such an approach is adopted in [4, 6]) or its modifications must be used [5]. It is the opinion of the authors of [4] that the apparent departure from the Darcy law in hydrogen filtration is due to compaction of disperse material in the experimental setup. Based on experimental results the following equation for the mass flow rate of free hydrogen is proposed in [4, 6]:

$$G = -2.37\cdot 10^{-3}\left[\frac{\Pi^3}{\mu}\rho_\gamma\left(\frac{d}{1-\Pi}\right)^2 \operatorname{grad} P\right]. \tag{1}$$

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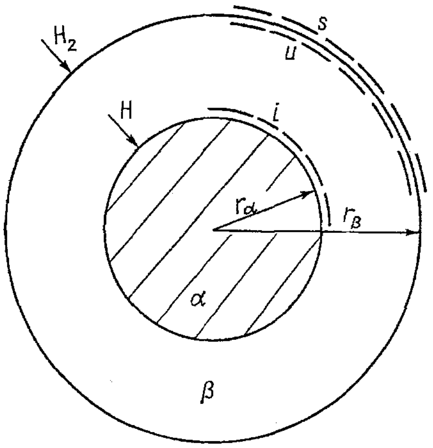

Fig. 1. Sheme for the hydrogenation rate calculation in a spherical IMC particle.

To describe the kinetics of the sorption-desorption reaction of hydrogen, different equations are suggested [5, 7]. The approach suggested in [5] seems to be most substantiated theoretically and experimentally. There, a spherical IMC particle (Fig. 1) whose core consists of an intermetallic compound (α-phase) and shell consists of a hydride (β-phase) is considered. It is assumed that the reaction of hydrogen sorption includes four stages:

1) sorption of H_2 molecules by the s-surface;
2) $H_2 \rightarrow 2H$ dissociation on the u-surface;
3) diffusion of H atoms through a hydride phase to the core surface;
4) the phase transition $\alpha + H \rightarrow \beta$ on the i-surface.

In [5], it is assumed that the third stage is the limiting one. An equation for the reaction kinetics is obtained from consideration of the diffusion of hydrogen atoms through a spherical hydride layer in a quasi-stationary approximation [8]:

$$\langle \dot{m} \rangle = K \exp\left(-\frac{E_a}{RT} \right) \frac{(P_u^{1/2} - P_i^{1/2})}{[(1-\omega)]^{-1/3} - 1}, \tag{2}$$

where P_u and P_i are the pressure on the u- and i-surface, respectively.

Thus, by now the literature on simulation of processes in metal hydrides is quite extensive. Nevertheless, none of the models considered allows a satisfactory account of heat transfer between hydrogen and a hydride in hydrogen filtration through a hydride matrix. In [6], an attempt is made to take into account this interaction (using a mathematical model with one energy equation); however, the authors report no experimental or theoretical estimates of the "coefficient accounting for the departure from thermal equilibrium in convective interaction between hydrogen and the hydride" introduced for this purpose. In essence, all the models discussed proceed from the hypothesis of local thermodynamic equilibrium between hydrogen and the intermetallic compound. We think that it is important to study how this equilibrium is attained since the hydrogen temperature at the inlet to a metal hydride layer (in a heat-sorption compressor or a metal hydride cooler) may differ substantially from the IMC temperature.

To investigate the physics of this process, it is necessary to develop a more complete mathematical model that includes two energy equations, namely, for gas and solid phases. Moreover, these equations must account for convective heat transfer between the filtered hydrogen and the intermetallic compound.

Mathematical Model. The equations of the mathematical model are constructed by performing local averaging of the equations of continuity, momentum, and energy [9-12]. In writing these equations, two different types of averaging of physical quantities are employed. The local volume average of a quantity Φ related to the phase Ψ is defined as

$$\langle \Phi \rangle = \frac{1}{V} \int_{V_\Psi} \Phi dV ,$$

where V_Ψ is the portion of the averaging volume V occupied by the phase Ψ.

The local phase average of a quantity of Φ related to the phase Ψ is defined as

$$\langle \Phi \rangle^{\Psi} = \frac{1}{V_\Psi} \int_{V_\Psi} \Phi dV .$$

To construct the mathematical model, we make the following assumptions:

1) gaseous hydrogen is in the superheated state and the equation of state of an ideal gas is valid for it;

2) the effect of natural convection is negligible compared to forced convection in the gas phase;

3) an IMC matrix does not change its shape or volume during interaction with hydrogen, and it is isotropic and has homogeneous porosity;

4) radiative heat transfer between hydride particles is negligible;

5) the Darcy law in the form of Eq. (1) may be used to describe hydrogen filtration;

6) the kinetics of the hydrogenation reaction is described by Eq. (2).

The mathematical model includes the following equations:

I. The continuity equation for hydrogen

$$\frac{\partial}{\partial t} (\Pi \langle \rho_\gamma \rangle^\gamma) + \nabla (\langle \rho_\gamma \rangle^\gamma \langle \mathrm{v}_\gamma \rangle) = - \langle \dot{m} \rangle . \tag{3}$$

II. The momentum equation for the gas phase (hydrogen) obtained from formula (1):

$$\nabla \langle P_\gamma \rangle^\gamma = - \frac{\mu_\gamma}{\Omega_\gamma} \langle \mathrm{v}_\gamma \rangle , \tag{4}$$

where

$$\Omega_\gamma = \frac{\Pi^3 d^2}{421.92 \, (1 - \Pi)^2} .$$

Substituting Eq. (4) into (3), we may combine Eqs. (3) and (4):

$$\frac{\partial}{\partial t} (\Pi \langle \rho_\gamma \rangle^\gamma) = \nabla \left(\frac{\Omega_\gamma}{\mu_\gamma} \langle \rho_\gamma \rangle^\gamma \nabla \langle P_\gamma \rangle^\gamma \right) - \langle \dot{m} \rangle . \tag{5}$$

III. The energy equation for the gas phase

$$\begin{aligned} \Pi \langle \rho_\gamma \rangle^\gamma (c_p)_\gamma \frac{\partial \langle T_\gamma \rangle^\gamma}{\partial t} + \langle \rho_\gamma \rangle^\gamma (c_p)_\gamma \langle \mathrm{v}_\gamma \rangle \nabla \langle T_\gamma \rangle^\gamma = \\ = \nabla \, [\lambda_{\gamma \, \mathrm{ef}} \nabla \langle T_\gamma \rangle^\gamma] + h_{\sigma\gamma} \, a_{\sigma\gamma} \, [\langle T_\sigma \rangle^\sigma - \langle T_\gamma \rangle^\gamma] - \\ - \langle \dot{m} \rangle (c_p)_\gamma \, [\langle T_\sigma \rangle^\sigma - \langle T_\gamma \rangle^\gamma] \, \theta \, (- \langle \dot{m} \rangle) , \end{aligned} \tag{6}$$

where $\theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x \le 0, \end{cases}$ is a function accounting for the sorption ($\langle \dot{m} \rangle > 0$) or desorption ($\langle \dot{m} \rangle < 0$) process.

The coefficient of convective heat transfer between the solid and gas phases $h_{\sigma\gamma}$ entering Eq. (6) may be calculated by relations given in [13]:

$$\frac{1}{h_{\sigma\gamma}} = \frac{d}{\mathrm{Nu}_{\sigma\gamma}\lambda_\gamma} + \frac{d/\beta}{\lambda_\sigma},$$

where, according to experimental data of [14], at small Re numbers (which usually corresponds to the regimes realized in hydrogen sorption-desorption by metal hydrides) $\mathrm{Nu}_{\sigma\gamma} \approx 0.1$, $\beta = 10$ for spherical IMC particles.

The specific surface $a_{\sigma\gamma}$, according to [11], is estimated as $a_{\sigma\gamma} = 6(1 - \Pi)/d$, and the effective thermal conductivity of the gas phase may be assumed equal to $\lambda_{\gamma\mathrm{ef}} = \Pi\lambda_\gamma$ [10-12].

IV. The energy equation for the solid phase (hydride)

$$(1 - \Pi)\langle\rho_\sigma\rangle^\sigma (c_p)_\sigma \frac{\partial\langle T_\sigma\rangle^\sigma}{\partial t} = \nabla\,[\lambda_{\sigma\,\mathrm{ef}}\nabla\langle T_\sigma\rangle^\sigma + Q^* D_{\mathrm{ef}}\nabla\langle\rho_{\mathrm{H}}\rangle^\sigma] -$$

$$- h_{\sigma\gamma}\,a_{\sigma\gamma}\,[\langle T_\sigma\rangle^\sigma - \langle T_\gamma\rangle^\gamma] + \langle\dot m\rangle\,\Delta H - \tag{7}$$

$$- \langle\dot m\rangle (c_p)_\gamma\,[\langle T_\sigma\rangle^\sigma - \langle T_\gamma\rangle^\gamma]\,\theta(\langle\dot m\rangle),$$

where $(c_p)_\sigma$ includes the heat capacity of the IMC and that of the bound hydrogen;

$$\lambda_{\sigma\,\mathrm{ef}} = (1 - \Pi)\,\lambda_\sigma + \frac{\lambda_\sigma}{|\nabla\langle T_\sigma\rangle^\sigma|}\,\frac{1}{V}\int_{A_{\sigma\gamma}} T_\sigma\,\mathrm{n}_{\sigma\gamma}\,d\,\mathrm{A};$$

where V is the averaging volume; $A_{\sigma\gamma}$ is the interface of the solid and gas phases; $n_{\sigma\gamma}$ is the unit normal. But calculation of $\lambda_{\sigma\mathrm{ef}}$ by this formula is extremely difficult. Therefore $\lambda_{\sigma\gamma}$ is usually determined experimentally. To calculate $\lambda_{\sigma\mathrm{ef}}$ theoretically, it is necessary to make some assumption on the structural regularity of a porous intermetallic compound. Such an approach is described in [15], where the effective coefficients for a specified regular model of a porous hydride are calculated by solving cellular problems of averaging theory. The term $\nabla\,[Q^* D_{\mathrm{ef}}\nabla <\rho_{\mathrm{H}}>^\sigma]$ in Eq. (7) ($<\rho_{\mathrm{H}}>^\sigma = (<\rho_\sigma>^\sigma M_\gamma/2M_\sigma)\,<\kappa>^\sigma$) takes into account the fact that a heat flux in a metal hydride matrix may be caused not only by a temperature gradient but also by a concentration gradient of hydrogen atoms (the Dufur effect [16]: in the case of a zero heat flux a concentration gradient causes the temperature gradient $\nabla<T_\sigma>^\sigma = -[Q^* D_{\mathrm{ef}}/\lambda_{\sigma\mathrm{ef}}]\nabla<\rho_{\mathrm{H}}>^\sigma$).

In [17], it is suggested that the hydrogen diffusion effect be taken into account by introducing a correction for the effective thermal conductivity of the hydride:

$$\lambda_\sigma' = \lambda_{\sigma\,\mathrm{ef}} + Q^* D_{\mathrm{ef}}\frac{d\rho_{\mathrm{H}}}{dT} = \lambda_{\sigma\,\mathrm{ef}} + Q^* D_{\mathrm{ef}}\frac{\rho_\sigma}{2M_\sigma}M_\gamma\frac{d\kappa}{dT}.$$

Estimation of $Q^* D_{\mathrm{ef}}\rho_{\mathrm{H}}$ from data of [16] yields 50 W/m. This means that the diffusion effect of the bound hydrogen on heat transfer may be substantial in the region where $d\kappa/dT$ is high, i.e., in the region of low saturation of the IMC with hydrogen, and in the region of saturation close to the limiting one.

V. The equation of state of free hydrogen

$$\langle P_\gamma\rangle^\gamma = \langle\rho_\gamma\rangle^\gamma R\,\langle T_\gamma\rangle^\gamma/M_\gamma. \tag{8}$$

VI. The continuity equation for bound hydrogen (in the hydride)

$$\frac{\partial}{\partial t}((1 - \Pi)\langle\rho_{\mathrm{H}}\rangle^\sigma) = \nabla\,(D_{\mathrm{ef}}\nabla\langle\rho_{\mathrm{H}}\rangle^\sigma) + \langle m\rangle. \tag{9}$$

VII. The rate equation of the hydrogenation reaction based on formula (2):

$$\langle \dot{m} \rangle = K \exp\left(- \frac{E_a}{R \langle T_\sigma \rangle^\sigma} \right) \frac{(\langle P_\gamma \rangle^\gamma)^{1/2} - P_{\text{eq}}^{1/2}}{[(1-\omega)]^{-1/3} - 1}, \tag{10}$$

where P_u in formula (2) is replaced by $\langle P_\gamma \rangle^\gamma$, and P_i by P_{eq}.

System of equations (5)-(10) is used to determine all the basic characteristics of interaction between hydrogen and the intermetallic compound – the dynamics of the fields $\langle T_\gamma \rangle^\gamma$, $\langle T_\sigma \rangle^\sigma$, $\langle P_\gamma \rangle^\gamma$, and $\langle \rho_H \rangle^\sigma$.

Estimation of the Thickness of the Transition Layer. To estimate the influence of the convective interaction between hydrogen and the metal hydride on the processes in the IMC layer, we consider the simplified problem (Fig. 2) where hydrogen (at the pressure P_0 and the temperature T_0) is supplied from the same side of a plane IMC layer from which heat is removed (hydrogen is supplied through a gap, reinforced with a heat-conducting material, between the IMC layer and the element casing). To solve this problem, we make the following additional assumptions:

7) $\lambda_\gamma = 0$: heat transfer in the gas phase is accomplished totally by the convective gas flow;

8) $h_{\sigma\gamma} = \text{const}$ (this is correct at small Re; generally speaking, $h_{\sigma\gamma}$ depends on the rate of hydrogen filtration);

9) the frontal model is valid;

10) the quasistationary approximation is applicable.

With these assumptions the mathematical formulation of the problem is reduced to the following system of equations (for simplicity the averaging operator will be omitted below):

$$\frac{d}{dx}\left(\frac{P_\gamma}{T_\gamma} \frac{dP_\gamma}{dx} \right) = 0, \tag{11}$$

$$\frac{P_\gamma}{T_\gamma} \frac{dT_\gamma}{dx} = \beta_1 [T_\sigma - T_\gamma], \tag{12}$$

$$\frac{d^2 T_\sigma}{dx^2} = \beta_2 [T_\sigma - T_\gamma], \tag{13}$$

where

$$\beta_1 = \frac{h_{\sigma\gamma} a_{\sigma\gamma}}{(c_p)_\gamma v_\gamma} \frac{R}{M_\gamma}; \quad \beta_2 = \frac{h_{\sigma\gamma} a_{\sigma\gamma}}{(1 - \Pi) \lambda_\sigma}.$$

If we now consider a regime where filtration is only slightly hindered: $P_\gamma \approx P_0 = \text{const}$ (this regime occurs when the pores are large and the IMC particles are coarse; concrete estimates are given in [18]), then after some transformations system of equations (11)-(13) is reduced to the system:

$$\frac{d^2 T_\sigma}{dx^2} = \beta_2 \left[T_\sigma - T_0 \exp\left(\frac{\beta_1}{P_0 \beta_2} \left(\frac{dT_\sigma}{dx} - \frac{dT_\sigma}{dx}\bigg|_{x=0} \right) \right) \right], \tag{14}$$

$$T_\gamma = T_0 \exp\left(\frac{\beta_1}{P_0 \beta_2} \left(\frac{dT_\sigma}{dx} - \frac{dT_\sigma}{dx}\bigg|_{x=0} \right) \right). \tag{15}$$

If we expand the exponent in Eq. (14) in a Taylor series and retain only the zeroth and first terms of the expansion (as is seen from formula (15), such an approximation is permissible if $T_\gamma / T_0 \approx 1$, i.e., the hydrogen temperature changes by no more than 20% as hydrogen filtration proceeds in the metal hydride matrix), then Eq. (14) becomes an ordinary second-order differential equation. With boundary conditions of the first kind at the

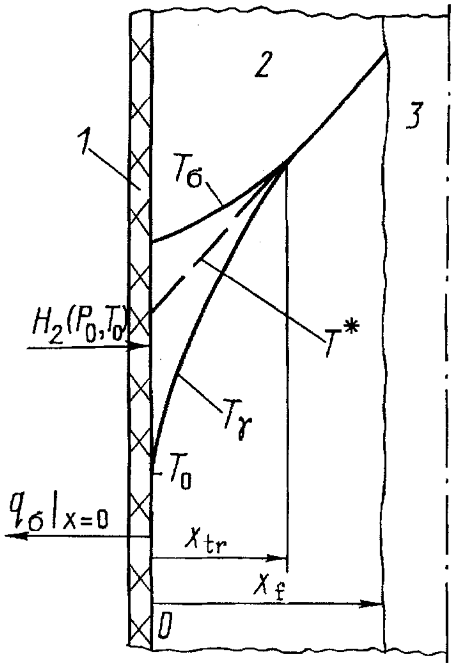

Fig. 2. Sheme for the temperature distribution calculation in a symmetric IMC plane layer: 1) gap, reinforced by a heat-conducting material, between the IMC layer and the element casing through which hydrogen is supplied and heat is removed; 2) hydrogen-saturated IMC; 3) IMC not saturated with hydrogen.

phase transition front (T_σ $(x = x_f) = T_f$) and of the second kind on the layer surface (the specified gradient $(dT_\sigma/dx)|_{x=0}$) its solution is

$$T_\sigma = -\left[\frac{T_\sigma\beta_1}{P_0\beta_2}\frac{dT_\sigma}{dx}\bigg|_{x=0} - T_0\right] + C_1\exp\left(-\frac{T_0\beta_1}{P_0}x\right) + C_2\exp\left(\frac{P_0\beta_2}{T_0\beta_1}x\right), \tag{16}$$

where

$$C_2 = \frac{T_f + \left[\dfrac{T_0\beta_1}{P_0\beta_2}\dfrac{dT_\sigma}{dx}\bigg|_{x=0} - T_0\right]}{\exp\left(\dfrac{P_0\beta_2}{T_0\beta_1}x_f\right)}, \quad C_1 = \frac{\dfrac{dT_\sigma}{dx}\bigg|_{x=0} - C_2\dfrac{P_0\beta_2}{T_0\beta_1}}{-\dfrac{T_0\beta_1}{P_0}}.$$

The term $C_1\exp(-T_0\beta_1 x/P_0)$ differs substantially from zero only in a small neighborhood of the layer boundary $x = 0$, i.e., in the region where the temperatures of the solid and gas phases differ substantially. As soon as local thermodynamic equilibrium is established, the behavior of the solution is determined by the summand $C_2\exp(P_0\beta_2 x/T_0\beta_1)$.

To clarify the physical meaning of Eq. (6), we consider its reduction to the solution obtained under the assumption of local thermodynamic equilibrium. Ignoring the summand with C_1 in (16), which is responsible for the behavior of the solution in a small neigborhood of the boundary, and expanding the exponent in the summand with C_2 in a Taylor series, with the zeroth and first terms of the expansion being retained (analogously to what was done in integrating Eq. (14)), we may write formula (16) as follows:

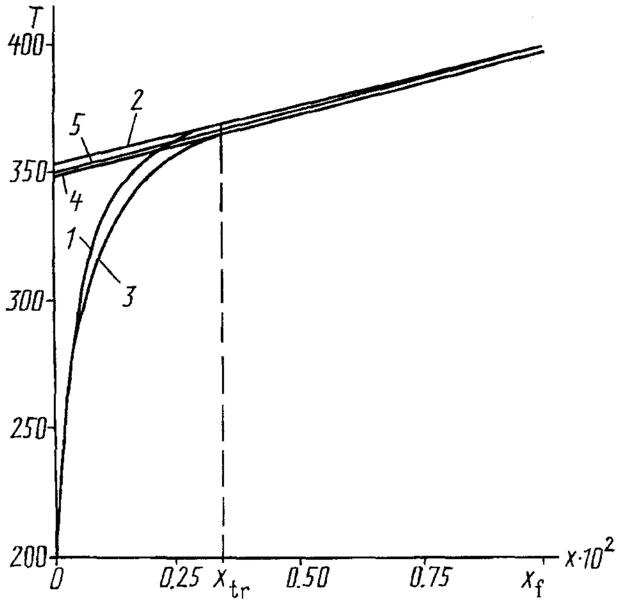

Fig. 3. Temperature distribution in the IMC layer: 1, 2, numerical calculation: 1) $T_\gamma(x)$; 2, $T_\sigma(x)$; 3, 4, approximate solution (16): 3) $T_\gamma(x)$; 4) $T_\sigma(x)$; 5) calculation in the approximation of local thermodynamic equilibrium (by formula (17)): $T^*(x) = T_\sigma(x) = T_\gamma(x)$. T, K; x, m.

$$T^* = -\left[\frac{T_0\beta_1}{P_0\beta_2}\left.\frac{dT_\sigma}{dx}\right|_{x=0} - T_0\right] + \frac{T_f + \left[\frac{T_0\beta_1}{P_0\beta_2}\left.\frac{dT_\sigma}{dx}\right|_{x=0} - T_0\right]}{\left(1 + \frac{P_0\beta_2}{T_0\beta_1}x_f\right)}\left(1 + \frac{P_0\beta_2}{T_0\beta_1}x\right). \qquad (17)$$

The function $T^*(x)$ describes the solution of the problem under consideration under the assumption of local thermodynamic equilibrium. Indeed, $T^*(x_f) = T_f$ and

$$\left.\frac{dT^*}{dx}\right|_{x=0} = \frac{\frac{P_0\beta_2}{T_0\beta_1}[T_f - T_0] + \left.\frac{dT_\sigma}{dx}\right|_{x=0}}{\left(1 + \frac{P_0\beta_2}{T_0\beta_1}x_f\right)} = \left.\frac{dT_\sigma}{dx}\right|_{x=0} +$$

$$+ \frac{(c_p)_\gamma\, v_\gamma \rho_\gamma}{(1-\Pi)\lambda_\sigma}\left[T_\sigma|_{x=0} - T_0\right] = \left.\frac{dT_\sigma}{dx}\right|_{x=0} + \frac{q'}{(1-\Pi)\lambda_\sigma},$$

where q' is the additional heat flux induced by the temperature difference between the IMC layer surface and the hydrogen supplied.

The solution of Eq. (14) differs from that of (15) by the presence of the term $C_1 \exp(-T_0\beta_1 x/P_0)$. An estimate of the depth at which local thermodynamic equilibrium may be expected, is the value x_{tr} at which the exponent in this summand differs only slightly from zero. As such an estimate, we may choose:

$$x_{tr} = 5\frac{P_0}{T_0\beta_1}. \qquad (18)$$

Figure 3 shows the temperature distribution in an $LaNi_{4.4}Al_{0.6}$ layer calculated with the aid of numerical and approximate analytical (formula (16) for T_σ and formula (15) with account for "linear" expansion of the exponent for T_γ) solutions of the problem (11)-(13) as well as the temperature distribution corresponding to the

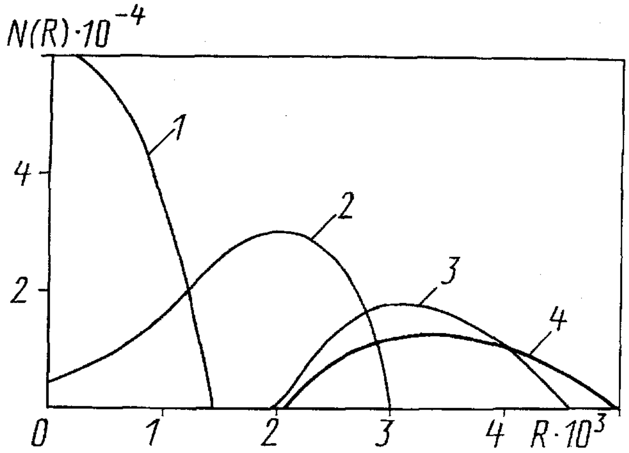

Fig. 4. Temperature distribution in the IMC layer versus T_0: 1, $T_\sigma(x)$; 2-5, $T_\gamma(x)$ for $T_0 = 330$ (2), 250 (3), 150 (4) and 50 K (5).

hypothesis of local thermodynamic equilibrium (formula (17)). As the initial data we have chosen: $d = 3\cdot 10^{-3}$ m (granules), $\Pi = 0.4$, $P_0 = 5\cdot 10^5$ Pa, $T_0 = 200$ K, $x_f = 0.01$ m, $\lambda({}_\sigma dT_\sigma/dx)|_{x=0} = 3.4\cdot 10^3$ W/m^2. Approximate solution (16) is seen to fit sufficiently well the temperature distribution in the layer, as follows from its closeness to results of the numerical solution, while formula (18) estimates the depth of the transition layer sufficiently accurately. From Fig. 3 it also follows that the local thermodynamic equilibrium approximation introduces an appreciable error only into the calculation of the temperature distribution in the gas phase T_γ. However, this approximation exerts an insignificant influence on the temperature calculation for the solid phase T_σ even within the transition layer. This is due to the fact that at the hydrogen flow rates realized in practice in metal hydride elements convective heat transfer is considerably lower than heat transfer by conduction in the solid phase.

It is also worth noting that approximate solution (16) describes quantitatively and qualitatively correctly the temperature distribution in the IMC layer only when the condition $T_\gamma/T_0 \approx 1$ is fulfilled. Figure 4 shows results of a numerical study of the thickness of the transition layer as a function of the gas temperature T_0 at the inlet to the metal hydride layer. The temperature distribution is calculated for the same conditions as for Fig. 3 but for different T_0 values. It is seen that at relatively small deviations of T_0 from $T_\sigma|_{x=0}$ (curves 2 and 3), the thickness of the transition layer increases with a decrease in T_0, as might be expected according to formula (18). However, with a further decrease in T_0 (curves 4 and 5) the situation is reversed – the dimensions of the transition layer begin to diminish with a decrease in T_0.

In conclusion, a mathematical model is developed for calculating the interaction between hydrogen and an intermetallic compound with account for the temperature difference between hydride and gas phases. The thickness of the transition layer is determined beyond which local thermodynamic equilibrium is established. It is found that the approximation of local thermodynamic equilibrium introduces a substantial error only into the temperature distribution calculation for the gas phase and exerts an insignificant influence on the temperature calculation for the solid phase.

NOTATION

P, pressure, Pa; T, temperature, K; t, time, sec; c_p, specific heat capacity at constant pressure, J/(kg·K); ΔH, heat of the hydrogenation reaction, J/kg; Q^*, heat of transfer (characterizes the heat flux accompaning the diffusional flow of the bound hydrogen), J/kg; D, diffusion coefficient of the bound hydrogen in the hydride, m^2/sec; M, molecular mass, kg/kmole; Π, porosity, vol. fractions; ρ, density, kg/m^3; μ, coefficient of dynamic viscosity of hydrogen, Pa·sec; λ, thermal conductivity, W/(m·K); d, mean diameter of hydride particles, m; κ, content of bound hydrogen in the hydride, katom H/kmole IMC; $\omega = \kappa/\kappa_{\max}$, relative concentration of the bound hydrogen; $\dot{m}$, sorption rate, kg/(m^{3}sec); $R = 8314$ J/(kmole·K), universal gas constant; $a_{\sigma\gamma}$, specific surface area of the pores, m^2/m^3; $h_{\sigma\gamma}$, heat transfer coefficient for an IMC particle in the hydrogen flow, W/(m^2·K); **G**, mass flow rate of hydrogen, kg/(m^2·sec); v, velocity of the hydrogen flow, m/sec; q, heat flux density, W/m^2; E_a, activation energy for hydrogen diffusion through the hydride phase, J/kmole; K, constant characterizing the hydrogenation rate, (kg/m^5)$^{1/2}$; x, current linear coordinate, m; x_{tr}, thickness of the transition layer beyond which local thermodynamic equilibrium is established, m; T^*, temperature calculated in the approximation of the local thermodynamic equilibrium, K; Re, Reynolds number; Nu, Nusselt number; < >, averaging operator. Subscripts and superscripts: γ, gaseous hydrogen in the hydride pores; σ, hydride; H, chemically bound hydrogen; ef, effective value corresponding to a thermophysical coefficient in the averaged equation; eq, equilibrium value; f, hydrogenation front; 0, the state of hydrogen in the metal hydride layer.

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