INFLUENCE OF THERMAL STRESSES ON THERMAL DIFFUSION OF HYDROGEN

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Introduction

Internal stresses of the various physical nature have an essential effect on the diffusion processes in materials. The main types of the internal stresses are thermal [1], residual and those to structural defects [2]. The diffusion kinetics is described by a parabolic equation under corresponding initial and boundary conditions. The thermal stress field is caused by non-uniform distribution of temperature. In the general case, thermal stresses have a complex dependence on coordinates. Therefore, taking into account their effect on the diffusion processes kinetics generally introduces significant mathematical difficulty. However, in some cases thermal stresses have a logarithmic spatial variation. Thermal stresses in a hollow cylinder are an example of such dependence. Such dependence allows the exact solution of the diffusion kinetics problem to be obtained. The objective of this paper is simulating the thermal diffusion of atoms of hydrogen in zirconium taking into account thermal stresses.

Results and discussion

The elastic interaction of the impurity atoms with the thermal stresses is defined by known relation [2]

$$V = -\frac{\sigma_{ll}}{3}\delta\upsilon\,, \qquad (1)$$

where σ_{ll} is the first invariant of tensor stresses, $\delta\upsilon$ is the change of material volume at an impurity atom placement. For σ_{ll} >0 (tension stresses) and $\delta\upsilon$ >0 (an impurity atom increases a crystal lattice parameter) potential V takes a negative value. It corresponds to attraction of an impurity atom to the tension stresses area and its displacement from the compession stresses area. The relation (1) takes into account only dimensial effect in the energy of the impurity atom connection with the thermal stresses. The other types of interactions (module, electrostatic, chemical ones) can be easily estimated by renormalization of the constants in the relation (1).

The diffusion flow of hydrogen atoms in the hollow cylinder depends linearly on both the concentration and temperature gradients (thermal diffusion) [3]

$$\vec{j} = -D\left(\nabla C + \frac{C\nabla V}{kT} + \frac{QC\nabla T}{kT^2}\right), \qquad (2)$$

where D is the hydrogen atom diffusion coefficient, k is Boltzmann's constant, T is the absolute temperature, Q is the heat of transport of hydrogen in solid solution, V is the interaction potential of hydrogen atom with the thermal stresses. The hydrogen concentration is determined the solution of the equation of a parabolic type under the corresponding initial and boundary conditions

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\nabla(C\nabla V)}{kT} + \frac{Q\nabla(C\nabla T)}{kT^2}\,,$$

$r_0<r<R$, (3)

$C=C_0$ at t=0, $C=C_p^1$ at $r=r_0$, $C = C_p^2$ at r=R,

where C_0 is the initial concentration of hydrogen atoms, C_p^1 and C_p^2 are equilibrium concentrations of the hydrogen atoms on the boundaries of the hollow cylinder, r_0 and R are inner and outer radii of a hollow cylinder. Physical meaning of the initial and boundary conditions of problem (3) is quite evident. At start time the hydrogen atoms concentration is equal to an initial value. The equilibrium hydrogen concentration is quickly set on the area boundary and then kept in a accordance with potential V and temperature T. From the equation (3) one can see that segregation of the hydrogen atoms are proportional to the gradient of the potential V and the temperature T. Therefore, the constants in the relations for σ_{ll} and T disappear when differentiating. It simplifies the solution of the equation (3). We will assume also, that temperature difference (T_1-T_2) it is essential less than value of average temperature T_0 in the hollow cylinder, that is $\frac{T_1 - T_2}{T_0} << 1$, T_1 and T_2 are temperatures of inside and outside of a hollow cylinder correspondingly ($T_1>T_2$).

The potential V and the temperature T are a harmonic functions ($\Delta V=0$, $\Delta T=0$), and its gradient are inversely proportional to the radius in the polar coordinate system ($\nabla V \sim r^{-1}$ and $\nabla T \sim r^{-1}$). It leads to the following mathematical formulation of a problem (3)

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1-\beta_1-\beta_2}{r}\frac{\partial C}{\partial r}, \quad r_0<r<R, \tag{4}$$

$C=C_0$ at $t=0$, $C=C_p^1$ at $r=r_0$, $C=C_p^2$ at $r=R$,

where dimensionless parameters β_1 and β_2 look like

$$\beta_1 = \frac{4\alpha(T_1-T_2)\mu(1+\nu)\delta\upsilon}{3kT_0(1-\nu)\ln R/r_0},$$

$$\beta_2 = \frac{Q(T_1-T_2)}{kT_0^2 \ln R/r_0}, \tag{5}$$

where α is the coefficient of linear expansion, μ is the shear module, ν is the Poisson's ratio.

The first of them considers influence of the thermal stresses, and the second - the thermal diffusion. These relations defines the contribution of characteristics of a material in the diffusion kinetics taking into account the thermal stresses and the thermal diffusion

$$\frac{\beta_1}{\beta_2} = \frac{4\alpha T_0\mu(1+\nu)\delta\upsilon}{3(1-\nu)Q}. \tag{6}$$

Keeping a generality, we will accept following values of constants: $\alpha=10^{-5}K^{-1}$, $T_0=10^3K$, $\mu=4\cdot10^{10}$ Pa, $\nu = 0.3$, $\delta\upsilon = 3\cdot10^{-30}$ m^3, Q = 0.4 eV($0.64\cdot10^{-19}$ J). For these values we will receive β_1/β_2 =0.05. Physically it means, that for the accepted conditions the thermal diffusion in comparison with influence of the thermal stresses prevails.

Conclusions

Thermal diffusion of atoms of hydrogen in zirconium taking into account thermal stresses has been investigated. As a mathematical model the steady-state temperature in the hollow cylinder has been considered. The kinetics of the diffusion processes has been described by a parabolic equation under corresponding initial and boundary conditions. The first invariant of the tensor of thermal stresses and the temperature in the hollow cylinder has a logarithmic dependence on the radial coordinate. Such dependence permits to obtain an exact analytical relations for the hydrogen atoms concentration in the hollow cylinder. It has been shown that for the accepted conditions the thermal diffusion in comparison with influence the thermal stresses prevails.

References

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