HYDRIDES FORMATION IN HOLLOW CYLINDER

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Introduction

Hollow cylinders have a significant place among construction elements of atomic engineering. Fuel elements claddings of nuclear reactors can be considered as an example. The claddings material interacts with hydrogen. After dissociation hydrogen atoms penetrate into the material and cause degradation of mechanical properties. Physical mechanisms of the properties change are rather various: surface energy reducing, corrosion cracking, hydrogen embrittlement. If the hydrogen concentration exceeds a solubility limit at given temperature, hydrides are formed in some metals (for example, in zirconium). Volume changes of the latter ones lead to forming microcracks on interphase boundaries. The hydride formation process depends on the level and nature of stresses distribution. They occur in the places of the hollow cylinders bends and have an effect on kinetics of hydride phase growth. The objective of given paper is to analyze kinetics of zirconium hydride growth about the hollow cylinder bend.

Results and discussion

The stresses at the hollow cylinder bend have a logarithmic dependence on a radial coordinate [1]. Such dependence allows obtaining an exact analytical solution of a diffusion equation taking into account the stresses field. The hydride growth kinetics is described by an equation of a parabolic type under corresponding initial and boundary conditions. On the interphase boundary a mass balance condition is carry aut [2]

$$\frac{1}{D}\frac{\partial C}{\partial t} = \Delta C + \frac{\nabla(C\nabla V)}{kT},$$

$$C(R,t) = C_1,\ C(r,0) = C_o,\ C(\infty,t) = C_o \qquad (1)$$

$$\left(C_p - C_1\right)\frac{dR}{dt} = D\left(\frac{dC}{dr} + \frac{C}{kT}\frac{\partial V}{\partial r}\right)_{r=R},$$

where D – diffusion coefficient of hydrogen atoms, k- Boltzman constant, T- absolute temperature, C_0 - initial concentration of hydrogen atoms, C_p and C_1 - concentration of hydrogen atoms on the interphase boundary in a hydride and matrix ($C_p > C_0$, $C_1 < C_0$), V- energy of hydrogen atoms binding with the stresses field. Value of V can be found from the expression

$$V = -\frac{\sigma_{ll}}{3}\delta\upsilon,$$

where $\delta\upsilon$ - change of the material volume when placing a hydrogen atoms, σ_{ll} - first invariant of the stresses tensor when bending a hollow cylinder. Hydrogen atoms belong to interstitial impurities. They increase a parameter of a crystal lattice. For $\delta\upsilon>0$ and $\sigma_{ll}>0$ (positive dilatation) binding energy V takes a negative value. It corresponds to attraction of a hydrogen atom to the area of tensile stresses and its displacement from the compression stresses area. The interphase boundary catches the hydrogen atoms from the solution and supplies them into a new phase having a higher concentration. Binding energy V is a harmonic function, and its gradient is inversely to a radius in a polar coordinate system. These features of function V considerable simplify task (1)

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1+\alpha}{r}\frac{\partial C}{\partial r},$$

$$C(R,t) = C_1,\ C(r,0) = C_o,\ C(\infty,t) = C_o \qquad 2)$$

$$\left(C_p - C_1\right)\frac{dR}{dt} = D\left(\left|\frac{dC}{dr}\right| + \left|\frac{\alpha C}{r}\right|\right)_{r=R}.$$

A dimensionless parameter $|\alpha| \approx 1$ defines the relation of the binding energy of a hydrogen atom with the stresses field to the energy of heat motion. For $\alpha = -1$ the stresses field converts the coordinate dependence of the diffusion equation. Hydride of cylindrical shape grows according to the plane symmetry law. If change of the hydride size is defined by hydrogen atoms diffusion, its radius is changed according the law $R(t) = \beta\sqrt{Dt}$,

where β - dimensionless parameter. Its value is found from a mass balance equation on the interphase boundary. For $\alpha = -1$ we have a quadratic equation for definition β

$$\beta^2 - \frac{2\beta}{\sqrt{\pi}}\left|\frac{C_1 - C_0}{C_p - C_1}\right| - \left|\frac{2C_1}{C_p - C_1}\right| = 0. \qquad (3)$$

If in task (2) $\alpha=0$ is taken, we will obtain under other equal conditions the following

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r},$$

$$C(R,t) = C_1,\ C(r,0) = C_o,\quad C(\infty,t) = C_o \qquad (4)$$

$$\left(C_p - C_1\right)\frac{dR}{dt} = D\frac{\partial C}{\partial r}\Big|_{r=R}.$$

In this case, the stresses field under the hollow cylinder bending is not taken into account. Writing down kinetics of the hydride phase growth as $R = \beta_1 \sqrt{Dt}$, we obtain a transcendental equation for defining the dimensionless parameter β_1

$$\beta_1 = \frac{2}{\pi}\left|\frac{C_1 - C_0}{C_p - C_1}\right| \frac{K_1\left(\beta_1 \frac{\sqrt{\pi}}{2}\right)}{K_0\left(\beta_1 \frac{\sqrt{\pi}}{2}\right)}, \qquad (5)$$

where $K_0(x)$ and $K_1(x)$ -modified Bessel functions of the second kind of the zeroth and first orders correspondingly. Keeping generality, we take $C_0 = 2\cdot10^{-4}$ (atm), $C_1 = 10^{-4}$ (atm), $C_p = 3\cdot10^{-4}$ (atm). For these values of the hydrogen atoms concentration we will obtain

$$\beta^2 - \frac{\beta}{\sqrt{\pi} - 1} = 0, \; \beta_1 = \frac{1}{\sqrt{\pi}} \frac{K_1\left(\beta_1 \frac{\sqrt{\pi}}{2}\right)}{K_0\left(\beta_1 \frac{\sqrt{\pi}}{2}\right)}, \qquad (6)$$

The computational solution of equations (6) gives $\beta=1.3$; $\beta_1 =0.8$. It means that the stresses field under the hollow cylinder bending increases a growth rate of the hydride phase centre. As the typical size of a new phase increases, depletion of the solid solution takes place. The rate of hydride growth slows down. In addition, volume changes of the hydride phase are accompanied with occurrence of the stresses on the interphase boundary. The latter ones change kinetics of the diffusion process. However, it is possible not to take into account such influence under little volume changes and on the early stages of the process.

Conclusions

The stresses fields occur about the hollow cylinder bending. They have a logarithmic dependence on a radial coordinate. It allows obtaining an exact analytical solution of a diffusion kinetics equation taking into account the stresses field. The analytical dependences for changing a hydride radius are given taking into account the stresses field and without doing it. The rate of formation of the hydride phase considerably increases when the stresses field available about the hollow cylinder bending. The results of a theoretical analysis are attracted for explaining hydrogen embrittlement of the alloys on zirconium base.

References

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