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The Boundary Value Problem of Determining Hydrogen Concentration and the Stress State in a Titanium Shell

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Abstract. Decreasing physical and mechanical properties of materials in contact with an aggressive environment is one of the factors determining the strength and service life of various structures. In this paper, the effect of a hydrogen-containing medium on the mechanical properties and stress state of a titanium alloy shell is shown. For this purpose, the diffusion boundary-value problem is solved and the distribution of hydrogen concentration over the shell wall thickness is determined. Then the boundary-value problem of statics is solved, and the stress state of the shell structure is determined before and after hydrogenation. The object of study is presented in the form of a shell of revolution loaded with internal pressure and working in a hydrogen-containing medium.

INTRODUCTION

Structural elements made of titanium alloys are widely used as structural elements in various fields of technology. Such structural elements generally work under the action of external mechanical loads and thermal loads, and sometimes come in contact with aggressive environments. The negative influence of an aggressive environment on the mechanical properties of metals during the operation of structures is one of the important factors determining the design and residual life of many potentially dangerous objects.

The interaction of hydrogen with metals and alloys has been studied since early 1900s and, therefore, a vast theoretical and experimental experience has been accumulated. However, the interaction of titanium structural elements with hydrogen-containing media has its own specific features. It is known that hydrogen interacting with titanium alloys can change their mechanical properties both positively and negatively. The negative effect of hydrogen manifests itself in the form of hydrogen embrittlement characterized by the degradation of the mechanical properties of titanium alloys at a hydrogen concentration exceeding critical.

The effect of hydrogen on a titanium alloy was observed in numerous tensile experiments, which show a change in the shape of the strain diagram. Therefore, in loaded structural elements subjected to hydrogenation, it is necessary to take into account these phenomenological effects.

PROBLEM STATEMENT AND RESOLVING EQUATIONS

A numerical experimental method for determining the stress state of a thin-walled structure operating in an aggressive environment is proposed. It is assumed that the structure is a shell of revolution, with a thickness h, with variable geometric and mechanical parameters along the generatrix, on which a distributed mechanical load may act. We assign the shell to a continuous median surface with curvilinear orthogonal coordinates s, θ, γ , where s is the

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meridional coordinate and θ is the circumferential one, γ is the direction of the external normal to the shell surface ($-h/2 \le \gamma \le h/2$).

Suppose that one of the shell surfaces is in contact with a hydrogen-containing medium, from which hydrogen diffuses into the shell at an excess pressure *P*. It is necessary to evaluate the limiting state of the shell taking into account the mechanical properties of the material changing under the influence of hydrogen.)

The boundary-value problem of determining the stress state of a thin-walled structure is solved using a model of the classical theory of shells in a geometrically linear and physically nonlinear formulation. In general terms, the solution to this related non-stationary problem can be represented as the following sequence: 1) solving the boundary-value problem of hydrogen diffusion with defining the distribution of hydrogen concentration over time $c(t)$; 2) implementing an experiment and obtaining dependences relating stress, strain, and hydrogen concentration $\sigma=f(\varepsilon, c)$ for a uniaxial stress state of a sample; 3) solving the boundary value problem of defining the stress state of the shell, taking into account the physical and mechanical properties of the material, depending on the concentration of hydrogen $\sigma=f(c, P)$.

Since the shell is in contact with hydrogen, it begins to diffuse into the metal wall. The process of diffusion movement of matter is described by Fick's diffusion equations. The change in the concentration of the diffusing substance at each point in the medium is described by the equation [1, 2]

$$\frac{\partial c}{\partial t} = D\Delta(c)\ ; \tag{1}$$

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \text{ (the Laplace operator),}$$

where *D* is the diffusion coefficient, *c* is the concentration of hydrogen in the wall of the shell.

It is known that the diffusion equation is completely identical to the heat equation [1–3]. Therefore, the methods for solving diffusion and thermal conductivity problems are the same. The differential diffusion equation, by analogy with the differential heat equation for a thin shell, will have the form [4]

$$\frac{1}{H_1 H_2}\left[\frac{\partial}{\partial s}\left(\frac{H_2}{H_1}\frac{\partial c}{\partial s}\right) + \frac{\partial}{\partial \theta}\left(\frac{H_1}{H_2}\frac{\partial c}{\partial \theta}\right) + \frac{\partial}{\partial \gamma}\left(H_1 H_2 \frac{\partial -}{\partial \gamma}\right)\right] = \frac{1}{D}\frac{\partial c}{\partial t}\ , \tag{2}$$

Where H_1, H_2 are the Lame parameters.

To solve the boundary value problem (2) on the surface of the shell, it is necessary to set some physically justified boundary conditions through the values of hydrogen concentration *c*. The concentration of hydrogen in metals is measured by its content in ppm (1 cm^3/100 g). It is known that titanium alloys interact very actively with hydrogen and that the solubility of hydrogen can reach 40,000 ppm [5, 6]. The boundary can be set in several ways. We distinguish between boundary conditions of kinds I, II, III, and IV. In the boundary conditions of the first kind, it is required to find solutions of the equation in a certain region of space that takes specified values at the boundary of the region. Here, the distribution of the diffusant concentration over the body surface is specified. If we assume that the hydrogen-containing medium is rapidly mixed, then boundary conditions of the first kind can be set, for example, the conditions on

$$c\left(\gamma = -\frac{h}{2}, t\right) = c_H\ , \tag{3}$$

where c_H is the initial concentration of hydrogen near the surface of the shell.

In the boundary conditions of the second kind, the distribution of the diffusant flux density is set for each point on the surface as a function of coordinates and time.

The boundary conditions of the third kind can be linear, nonlinear, and unsteady. We restrict ourselves to linear boundary conditions that determine the law of convective mass transfer between the surface of the body and the environment in the form of a relationship between the desired function and its normal derivative at the boundary

$$\frac{\partial c}{\partial \gamma} = k_s(c_H - c), \quad (4)$$

where k_s is the proportionality coefficient characterizing the intensity of the concentration interaction of the medium with a given concentration of the diffusant with the surface of the body.

The boundary conditions of the fourth kind determine the conditions on the contact surface of two solids. They correspond to the mass transfer of the surface of the body with the environment of contacting solids. The boundary conditions of the fourth kind are used in solving diffusion problems in multilayer bodies with different diffusion and absorption properties in each layer.

The mathematical formalization of the diffusion problem and boundary conditions has been well studied; it describes various computational cases of boundary value problems. However, in solving real applied problems, various physical constants are required, which must be obtained by experimental methods, this being difficult in many cases. The main problem in solving diffusion problems is the mismatch of experimental data and calculation results when mathematical models are used. The correct formulation of the initial and boundary conditions and the diffusion coefficient used in the calculations largely determine the non-stationary field of the distribution of hydrogen concentration in the body under study.

To solve the stress state of the shell, experimental dependences relating stress, strain, and concentration are necessary. The effect of hydrogenation on the mechanical properties of a titanium alloy was experimentally studied in [7]. The paper presents conditional strain diagrams for samples of the VT20 alloy in the hydrogenated and non-hydrogenated state. The dependences obtained in solving problems of determining the stress state of the shell must be approximated by piecewise linear segments for a titanium alloy with and without hydrogen. This approximation was presented in [8].

The boundary-value problem of solving the stress state of shells using the Kirchhoff–Love hypotheses is described by a system of the sixth-order ordinary differential equations [4, 9]

$$\frac{d\overline{Y}}{ds} = P_{ij}\overline{Y} + \bar{f}, (i, j = 1,2,....6), \overline{Y} = \{N_r, N_z, M_s, u_r, u_z, \vartheta_s\}, \quad (5)$$

with the boundary conditions

$$B_1\overline{Y}(s_0) = \overline{b}_1, B_2\overline{Y}(s_L) = \overline{b}_2 .$$

Here, N_r, N_z are the radial and axial forces; u_r, u_z are similar movements; M_s is the meridional bending moment; ϑ_s is the angle of rotation of the normal. The elements of the matrix P_{ij} and the column vector of the free terms f are not given due to cumbersomeness. B_1 and B_2 are the given matrices; b_1 and b_2 are the given vectors. Different variants of the boundary conditions are formulated through a combination of resolving functions.

PROBLEM SOLUTION METHODS

When solving diffusion problems for an axisymmetrically loaded shell for equations (2), we have the condition

$$\frac{\partial c}{\partial \theta} = 0 \quad (6)$$

Then, the obtained two-dimensional diffusion equation is replaced by the equivalent variational equation [9]. When solving the diffusion problem, we will use the developed method for solving boundary-value heat conduction problems based on the finite element method. The solution method and the results of the numerical solution of the diffusion thermal conductivity problem for a steel shell construction are given in [10].

When solving the system of equations (5), the discrete orthogonalization method proposed by S. K. Godunov [11] is used.

When solving this problem, taking into account possible plastic deformation, the physically nonlinear problem will be described by a system of differential equations (5), and the relationship between stress and strain will be linearized by the method of additional deformations. This relationship appears in the form of Hooke's law, but with additional terms taking into account the strain and temperature dependences of the mechanical properties of the material [4]. For the problem being solved, this relation will also take into account the variation of the mechanical properties with hydrogen concentration.

SOLUTION EXAMPLE

As an example, the stress state of a thin-walled shell of revolution made of the VT20 titanium alloy was determined. During operation, the inner surface of the shell is in contact with a hydrogen-containing medium. As a result of the operation of the apparatus, hydrogen diffuses into the wall of the body structure, and this leads to a change in the mechanical characteristics of the material and decreases its strength.

When calculating the structure, the boundary conditions on the inner surface of the shell were taken in the form of boundary conditions of kinds I and III, since they are most physically justified and often used in such problems. According to conditions (3), an initial hydrogen concentration c_H near the shell surface is required. This concentration depends on many factors, including the type of material and the surface quality of the shell, and it can only be determined experimentally. For the analysis of the studying shell, the surface concentration c_H = 100 ppm was assumed.

Figure 1 shows the distribution of hydrogen concentration over the wall thickness on the cylindrical part of the shell under boundary conditions of the first (a) and third kind (b) on the inner surface. Curves 1 to 5 (a) correspond to 33 min, 2.77 h, 5.55 h, 8.33 h, and 11.11 h of shell hydrogenation. Under the boundary conditions (4), the proportionality coefficient should be determined experimentally depending on the conditions of hydrogen contact with the shell surface (flow rate, temperature, and pressure). For the model representation of the influence of the boundary conditions in the calculation, it is assumed that k_s= 1. Curves 1 to 6 (b) correspond to 33 min, 2.77 h, 5.55 h, 11.11 h, 55 h, and 11 days of shell hydrogenation.

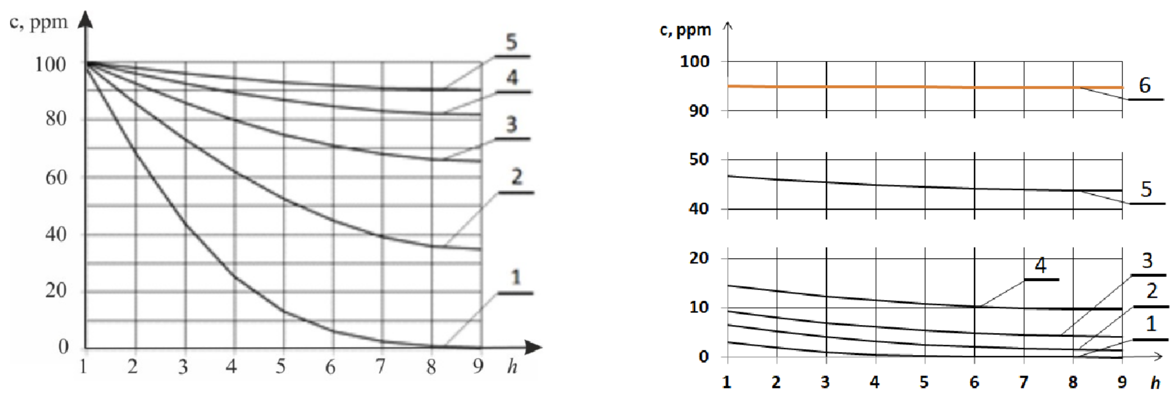

FIGURE 1. Distribution of hydrogen concentration over the wall thickness

It follows from Fig. 1a that, when the boundary conditions of the first kind are used, the shell is saturated with hydrogen within 11 hours. It follows from Fig. 1b that, when using the boundary conditions of the third kind, the shell is saturated with hydrogen within 11 days. Thus, during the long-term operation of the studied structure, it is necessary to use conditional diagrams of deformation of titanium alloy samples in a fully hydrogenated state to calculate the stress state.

For the structure under study, the boundary problem represented by the system of ordinary differential equations (5) for determining the stress-strain state of the shell is solved. The mechanical properties of the titanium alloy were assumed without hydrogen and after complete saturation with hydrogen. It follows from the calculation that, for the assumed mechanical properties at a pressure of P = 10 MPa, the shell material works in the elastic region of the diagram.

With increasing pressure, the problem becomes physically nonlinear. For example, at a pressure of P = 30 MPa, 5 approximations are required to solve a nonlinear problem in order to achieve the necessary solution accuracy of 1%.

Such integral energy characteristics as shear stress intensity and shear strain intensity are often used to evaluate the strength of a shell structure. It was shown in [8] that the danger point is on the outer surface of the shell.

CONCLUSION

The use of numerical methods and experimental results for samples has allowed us to determine the stress state of a titanium alloy shell affected by hydrogen. The influence of the boundary conditions of the diffusion problem on the hydrogenation time and the manifestation of the known effect of titanium alloy embrittlement in a shell structure have been demonstrated.

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