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ФОРМУВАННЯ МОДЕЛІ ВИЗНАЧЕННЯ НАПРУЖЕНЬ В МЕТАЛЕВИХ КОНСТРУКЦІЯХ ПІД ВПЛИВОМ КОНЦЕНТРАЦІЇ ВОДНЮ

У сучасних умовах промислової діяльності особливої гостроти набуває питання точного прогнозування експлуатаційних ресурсів металевих систем, зокрема їхньої витривалості та безвідмовності. Це зумовлено складним поєднанням корозійної деградації матеріалу та постійного механічного навантаження. На сьогодні механізми взаємозв'язку між водневим насиченням і перерозподілом напружень у металах досліджено фрагментарно. Процес абсорбції водню спричиняє деформацію структури тіла, що проявляється у зміні його лінійних параметрів та загального об'єму. Такі об'ємні трансформації за відповідних умов стають джерелом виникнення внутрішніх зусиль. У цій роботі розглядається модель, де взаємний вплив атомів водню вважається нехтовно малим. Ключовим завданням дослідження є визначення параметрів напружено-деформованого стану об'єкта, що виникає внаслідок дифузії та накопичення водню в його структур

Ключові слова: *конструкції, деформації, напруження, концентрація водню, метод скінченних елементів, суцільний циліндр.*

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FORMATION OF A MODEL FOR DETERMINING STRESSES IN METAL STRUCTURES UNDER THE INFLUENCE OF HYDROGEN CONCENTRATION

In modern industrial conditions, the issue of accurately predicting the operational resources of metal systems, in particular their durability and reliability, is becoming particularly acute. This is due to the complex combination of material corrosion degradation and constant mechanical stress. To date, the mechanisms of the relationship between hydrogen saturation and stress redistribution in metals have been studied fragmentarily. The process of hydrogen absorption causes deformation of the body structure, which manifests itself in a change in its linear parameters and total volume. Under appropriate conditions, such volumetric transformations become a source of internal forces. This paper considers a model in which the mutual influence of hydrogen atoms is considered negligible. The key objective of the study is to determine the parameters of the stress-strain state of an object resulting from the diffusion and accumulation of hydrogen in its structure.

Keywords: *structures, deformations, stress, hydrogen concentration, finite element method, solid cylinder, cylindrical.*

Introduction. When using materials, residual stresses play a significant role, which is associated with a significant temperature gradient in the creation of the alloy, high cooling rates, etc. This, in turn, can cause residual stresses, which have not yet been sufficiently studied in materials.

Among the existing experimental methods for determining residual stresses, the most widely used are the method of N.V. Kalakutsky for disc-type parts, the method of N.N. Davidenkov's method for ring-type parts and prismatic bars, L.A. Glikman and D.I. Gregon's method for I-beam bars, D.M. Shur's method, i.e., the force method for determining residual stresses, which does not require measurements of part deformation based on approximate relationships between stresses and deformations, but it can only be applied to parts with a regular geometric shape, the Gunnert method, which requires drilling conical holes, milling ring grooves, and high-precision deformation measurements, which greatly complicates the measurement process, and the Zaks method for solid and hollow cylinder-type parts [1-3].

The authors set themselves the task of simulating the stress state of a cylindrical sample and studying the effect of hydrogen on the stress characteristics of the material using this model.

The presence of hydrogen in the structure of metallic materials significantly affects their mechanical properties, in particular, their resistance to destruction and service life. The key factor here is the ability of hydrogen atoms to freely migrate through the crystal lattice, causing its deformation expansion [4]. The results of the analysis of sorption and desorption processes confirm the formation of local inhomogeneities in hydrogen content [5]. These areas of uneven concentration become sources of internal forces known as concentration stresses. That is why the identification and calculation of such factors are critically important for modern engineering design of objects that come into contact with aggressive hydrogen-saturated parts.

It should be emphasized that previous scientific studies have mainly focused on how external mechanical stress affects hydrogen diffusion processes [6-10]. However, for the qualitative development of the theoretical basis, it is necessary to study in more detail the reverse feedback – the formation of a stress-strain state under the direct influence of a change in gas concentration. For example, study [11] analyses the stresses in a solid cylinder caused by hydrogen diffusion, but the algorithm proposed there is only effective for bodies of infinite size. This article presents the author's methodology, which allows for the proper assessment of stress indicators in bodies of finite geometric configuration.

Theoretical position and solution algorithm. The process of hydrogen saturation of metal is accompanied by a transformation of its geometric characteristics – both the linear parameters of individual elements and the overall volume of the structure. When free deformation is restricted, such volumetric changes become the root cause of internal stresses. Within the proposed approach, we base ourselves on the hypothesis of a negligible energy connection between individual hydrogen atoms. The key task is to calculate the parameters of the stress-strain state of a metal object formed under the direct influence of variations in hydrogen concentration.

The total deformation of the material resulting from a variation in hydrogen content by a value of C_H. Macroscopic deformation of the material resulting from a variation in hydrogen content by a value is accompanied by a change in the linear parameters of its structure. Thus, the edge of an elementary parallelepiped ds after transformation takes the form $\left(1+\alpha_{C_H}C_H\right)ds$, where α_{C_H} is the concentration expansion index [2]. In the case of an isotropic and homogeneous medium, this coefficient does not depend on the spatial orientation of the segment ds. If we assume that α_{C_H} is invariant with respect to the saturation level, this parameter can be considered a constant. Under these circumstances, the differential rectangular element retains its initial orthogonal configuration, since the elongation indices are identical in all directions. Thus, a change in hydrogen concentration C_H over a time interval Δt initiates the following increase in deformation components of a hydrogen nature:

$$\Delta\varepsilon_{ij}^{H}=\alpha_{C_H}C_H=\alpha_{C_H}[C(t+\Delta t)-C(t)], i,j=1{,}2{,}3; \varepsilon_{ij}^{H}=0 \text{ при } i\neq j. \tag{1}$$

According to the principle of superposition, the total increase in material deformation is determined as the additive sum of two components: the increase resulting from fluctuations in hydrogen concentration and the deformation changes caused by external force factors.

$$\Delta\varepsilon_{ij}=\Delta\varepsilon_{ij}^{P}+\Delta\varepsilon_{ij}^{H}. \tag{2}$$

To determine the hydrogen distribution profile in the material structure, the solution of Fick's diffusion equation will be used. This model takes into account an additional factor – the influence of the mechanical stress gradient on the migration processes of hydrogen atoms [11-13].

$$\frac{\partial C}{\partial t}=\nabla(D\nabla C)+\nabla\left(\frac{DV_H}{RT}\nabla\sigma_h\right), \tag{3}$$

The following symbols are used in the expression above: $\nabla=(\partial/\partial x,\partial/\partial y,\partial/\partial z)$ – Hamilton operator, represented by components $(\partial/\partial x,\partial/\partial y,\partial/\partial z)$; D is responsible for the intensity of diffusion processes (diffusion coefficient); R and T denote the universal gas constant and the absolute temperature, respectively. The parameter V_H reflects the partial molar volume occupied by hydrogen in the metal matrix, while σ_h characterizes the hydrostatic component of the internal stress tensor; the time coordinate is defined by the variable t.

The solution to mathematical model (3) is sought taking into account the following initial parameters:

$$\mathrm{C}(x,y,z,t)|_{t=0}=C_0, \tag{4}$$

The boundary state of the system is described as follows: for the outer boundary section S_c, a fixed hydrogen content C_0 is regulated, while on the segment S_N, the hydrogen flow intensity φ is determined. In this case, the total surface area of the object is the result of combining both of the specified zones $S_c\cup S_N=S$.

For one surface area, boundary conditions of the first kind (hydrogen content) are set, while for the other, the intensity of the hydrogen flow is determined.

Cylindrical samples were selected as objects of study for testing the developed algorithm for calculating the stress state caused by fluctuations in hydrogen concentration. The first model is represented by a solid body with a radius $r_1=b$ and a length of $2h$.

The analysis is performed for two types of mechanical fastening: in the absence of external constraints (free bodies) and in the case of rigid fixation of one end. For free samples, given their symmetry, the calculation scheme is limited to half of them. When modelling, the assumption of zero hydrogen flow intensity is made. The formulation of boundary and initial conditions for each scenario is given below:

$$\begin{gathered}C(r,z,0)=C_0, \text{при} r,z\in S_1,\\ C(r,z,t)=C_\text{c}, \text{при} r,z\in L_1\end{gathered} \tag{20}$$

In the above expressions, S_1 denotes the area of the meridian cross-section of the corresponding cylindrical bodies, and S_2 denotes the contours formed by the intersection of the plane of symmetry with the free lateral surface and the unfixed end face.

The calculations were performed for two boundary conditions: hydrogen saturation ($C_0 = 0, C_c = 5\,mol/m^3$) and dehydration ($C_0 = 5\,mol/m^3\,, C_c = 0$) of the samples. All calculations were performed using the following parameters: Young's modulus $E = 2.1 \cdot 10^5$MPa, Poisson's ratio ν=0.3, $D = 10^{-10}\,m^2/s$,, R=8.31 J/(*mol*·*K*), V_H=1,96 · 10^{-6} *m*^{3}/*mol*, *T*=295 *K*, *a*=5 *mm*, *b*=10 *mm*, R_1=2.5 mm, *h*=40 *mm*, h_1=9 *mm*.

The analysed areas were discretized using linear four-node finite elements. For the numerical implementation of mathematical models (14) and (17) in FORTRAN, software was developed that allows tracking the dynamics of hydrogen content and the corresponding increase in stresses at any time interval. The accuracy of the computational algorithm was verified by comparing the obtained data with the analytical solution [7] for hydrogen absorption and desorption processes in an infinite cylinder. The graphical analysis presented in Figs. 1 and 2 demonstrates a high degree of correlation between the results of the author's program and the theoretical data [7] with acceptable errors.

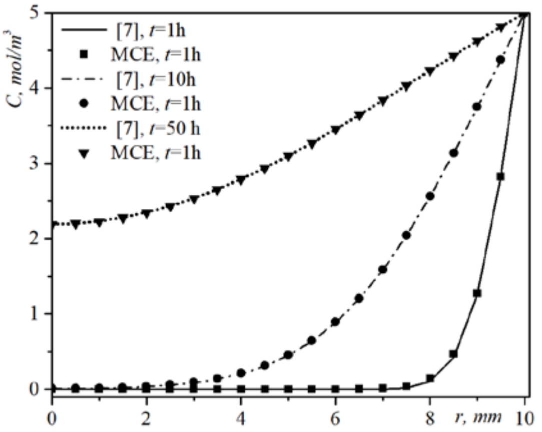

Fig. 1. **Comparison of data obtained by numerical method and by analytical solution of equation (14) for the case of hydrogen absorption by a long cylindrical body**

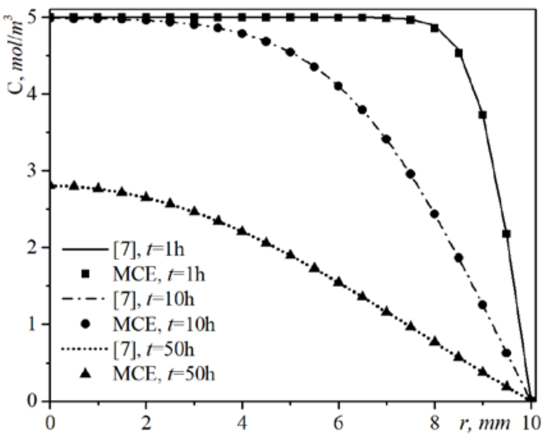

Fig. 2. **Assessment of the convergence of numerical results with the exact solution of equation (14) for modelling the process of hydrogen desorption from an elongated cylinder**

Modelling of the stress-strain state of a monolithic cylinder was performed using two calculation schemes. In the first approach, the boundary *L*₁ is identified with the contour that arises at the intersection of the end and side surfaces; at the same time, a restriction on axial displacements in the form of $u_z(r, 0, t) = 0$ is assumed. The second scheme is based on the assumption of rigid fixation of the object from the end face *z*=$-h$. This same section is considered isolated from diffusion exchange, which makes it impossible for hydrogen sorption or desorption processes to occur through it. For this case, the boundary conditions are formulated as $u_r(r, 0, t) = u_z(r, 0, t) = 0$.

Experimental results. Mathematical implementation of dependencies (14) and (17) was performed using an iterative step in time Δt=1 minutes. The finite element approximation of the unclamped cylinder model was based on the use of 900 four-node fragments (corresponding to 966 nodal points), while for the clamped configuration, the mesh density was increased to 1800 elements (1911 nodes). The calculation period for hydrogen saturation and desorption processes was 100 hours. Fig. 3 and 4 shows the spatial profiles of radial stresses σ_{rr} in the cross section *z*=0 for a free object at times *t*=10 and *t*=100 hours. The data obtained indicate that the amplitude values σ_{rr} during sorption and dehydration are mirror images: they coincide in absolute value but have opposite directions (different signs). Since a similar symmetry is inherent in all other components of the stress-strain state throughout the cycle, further interpretation of the results in the work is given only for the gas desorption scenario.

The graphical interpretation in Fig. 4 illustrates the distribution of radial stresses σ_{rr} for different cutting planes of clamped and free cylindrical objects. Evaluation of the obtained data confirms that the amplitude and nature of these forces demonstrate invariance with respect to the spatial coordinate of the cross section, remaining identical for both rigidly fixed and unfastened models.

Similar patterns have been established for the tangential components $\sigma_{\varphi\varphi}$.. However, it should be noted that such a correlation is not typical for axial stresses σ_{zz}: in this case, there are significant differences in distribution caused by the influence of boundary conditions and cross-section localization.

The construction of graphical dependencies and the execution of computational procedures are implemented using the author's software complex [14]. The development is based on the adaptation of classical theoretical models for an infinite solid cylinder [3, 7, 8, 11-13] to the specifics of analysing real experimental objects of cylindrical configuration.

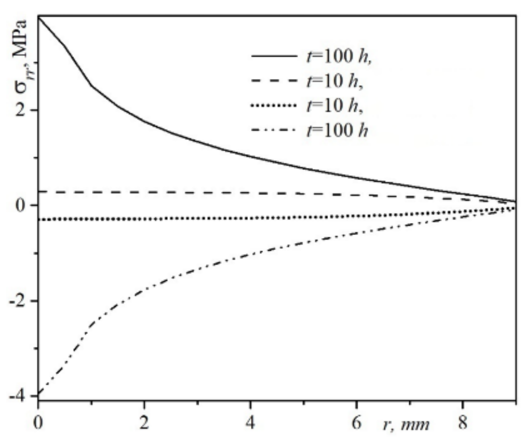

Fig. 3. **Nature of stress state change σ_{rr} in the plane z=0 of a monolithic cylinder during its hydrogen saturation and dehydration, recorded 10 and 100 hours after the start of diffusion**

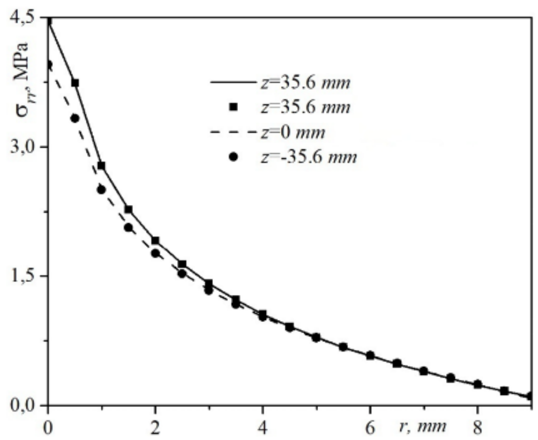

Fig. 4. **Comparative characteristics of stress fields σ_{rr} in different planes of clamped and unclamped cylindrical specimens after t=100 hours of exposure**

Conclusions. During the study, analytical patterns were derived and systematized, allowing the deformation components and stress vectors in metal media to be determined depending on the level of hydrogen saturation. This made it possible to conduct a series of numerical experiments to study the spatial distribution of hydrogen concentration and the corresponding force factors inside a cylinder of finite dimensions, taking into account the temporal dynamics of sorption and desorption processes. It was found that during hydrogen removal (dehydration), a compression zone forms in the central part of the sample, while the peripheral layers are subjected to tensile forces. During saturation (flooding), the opposite effect is observed: the inner zones are characterized by uniform stretching, while an increase in the intensity of compressive stresses is recorded near the outer surface.

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