THE INFLUENCE OF THE TRAPPING MODEL CHOICE ON THE ADEQUATE DESCRIPTION OF HYDROGEN DIFFUSION INTO METALS FROM EXTERNAL ENVIRONMENT

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Abstract: The paper considers the hydrogen diffusion into metals from their external environment. In order to properly describe a time-stable boundary layer (experimentally observed) with a hydrogen concentration being tens of times higher than that inside the body, the previously obtained hydrogen diffusion equation has been modified. This equation obtained from the first principles and taking into account the influence of the stress-strain state of solid on the transport process of the gas component, was supplemented with a stock term describing the diffusion with trapping modes. This modification was carried out in two ways: using the classical McNabb model and using the tensor of damageability. The boundary-value problem was solved for both approaches. The solution results were compared with published experimental data.

Keywords: hydrogen diffusion, trap model, solid, boundary layer, stress-strain state

ВЛИЯНИЕ ВЫБОРА ЛОВУШЕЧНОЙ МОДЕЛИ НА АДЕКВАТНОСТЬ ОПИСАНИЯ ДИФФУЗИИ ВОДОРОДА В МЕТАЛЛЫ ИЗ ВНЕШНЕЙ СРЕДЫ

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Аннотация. В работе рассматривается явление диффузии водорода в металлы из внешней среды. Для того чтобы наиболее корректно описать возникновение стабильного во времени пограничного слоя (наблюдается экспериментально), обладающего концентрацией водорода, в десятки раз превышающей его концентрацию внутри тела, модифицируется ранее полученное уравнение диффузии водорода. В это уравнение, учитывающее из первых принципов взаимовлияние между напряженно-деформированным состоянием твердого тела и процессом транспорта газового компонента, вводится стоковый член, который описывает диффузию по ловушечным модам. Указанная модификация выполняется двумя способами: с помощью классической модели МакНабба и с использованием тензора поврежденности. Для обоих подходов решается краевая задача, результаты решения сравниваются с опубликованными экспериментальными данными.

Ключевые слова: диффузия водорода, ловушечная модель, твердое тело, пограничный слой, напряженно-деформированное состояние

Introduction

The effect of hydrogen degradation on the strength properties of metals has remained one of the most pressing problems in mechanics for over a century [1]. It is known that metals can absorb hydrogen from the external environment, consequently losing strength and fracture toughness [2], which is especially critical for industrial applications, where increasingly stringent requirements are imposed on the strength characteristics of steels. Experimental estimates and measurements of hydrogen concentration profiles in metals [3−6] suggest that hydrogen concentration in the boundary layer is dozens or even hundreds of times higher than in the entire volume of the metal. Recent experimental studies [7−9] suggest that this thin layer (its thickness is about one micrometer) has the strongest influence on the elastic properties, brittleness and viscosity of the metal. Thus, there is much theoretical and practical interest in simulation of a thin boundary layer produced by hydrogen diffusion from the environment into the metal, providing descriptions for the mutual influence between the diffusion process and the mechanical properties of the metal.

No consensus has been reached in the literature as to how to take into account the influence of mechanical stresses on diffusion. One of the first models still widely used is based on empirical

evaluation of experimental data [10]. The next generations of widespread models are based on the thermodynamics of irreversible processes, representing a generalization of Fourier-type equations that describe irreversible processes by linear differential equations with constant coefficients. This approach assumes that the diffusion rate is proportional to thermodynamic forces, which can be expressed in terms of gradients of the corresponding potentials, depending, in particular, on the stress-strain state (see, for example, [11− 13]). These additional thermodynamic forces are generally associated with a change in the volume or stiffness of the solid material or a change in gas concentration. Some studies formulate the thermodynamic force accounting for the influence of stresses in terms of the chemical potentials of materials, using Eshelby's tensor as the chemical potential of the deformable solid [14−17]. However, such models are rarely used, due to some difficulties in determining model constants. Moreover, experiments indicate that hydrogen not only diffuses through the crystalline substance of the metal, but also redistributes in trap sites [4, 18−20].

Therefore, hydrogen diffusion in metals cannot be characterized as conventional grain-boundary diffusion. Many papers on hydrogen diffusion in metals consider the trapping mechanism for this diffusion (see the fundamental studies [21, 22] and many others, e.g., [17, 23−26]). Such models are very peculiar, failing to adequately describe the entire range of diverse experimental data. Consequently, hydrogen diffusion coefficients are given in handbooks with an accuracy up to the order of magnitude (see, for example, [27]). Notably, most models for trapping and bulk diffusion have been verified for small gradients of hydrogen concentration in the material. This does not allow to account for the observed boundary layer and requires significant modification of these models.

The experimentally observed near-surface layer contains a high concentration of hydrogen, is relatively time-stable and does not expand into the bulk of the metal due to diffusion. To describe this layer more accurately, we introduced the sink term into the equation of hydrogen transport inside the metal in a stress-strain state (the equation was obtained earlier in several studies, see, for example, book [28] and references therein).

Two models introducing the sink term are considered in the study. The first is the classical McNabb model [21]. The second is an alternative model of two-channel diffusion, separately accounting for the flow through inhomogeneities inside the metal.

Hydrogen diffusion by the trapping mechanism accounting for the influence of the stress-strain state in metal

Our previous studies (see, for example, [28] and references therein) explored the approach of linear non-equilibrium thermodynamics. Assuming that the chemical potential of diffusing gas depends on Eshelby's energy-momentum tensor, a modified diffusion equation was obtained, accounting for the dependence of gas transport process inside the solid on its stress-strain state. This equation was written as follows for the case of ideal gas and linear elastic body:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(D_{eff} \nabla c + \mathbf{V} c \right). \tag{1}$$

The effective diffusion coefficient D_{eff} was defined as

$$D_{eff} = D_0 \left(1 + \frac{cM}{RT\rho} \frac{E}{1-2\nu} \left[-\alpha \mathrm{tr}\boldsymbol{\varepsilon} + 3\alpha^2 c \right] \right). \tag{2}$$

The proposed additional term taking the form $\mathbf{V}c$ expresses a drag force proportional to the concentration, where the proportionality factor follows the expression

$$\mathbf{V} = \frac{D_0 ME}{RT\rho} \left(\frac{\nu}{(1+\nu)(1-2\nu)} \mathrm{tr}\boldsymbol{\varepsilon} \nabla(\mathrm{tr}\boldsymbol{\varepsilon}) - \frac{1}{1-2\nu} \alpha c \nabla(\mathrm{tr}\boldsymbol{\varepsilon}) + \frac{1}{2(1+\nu)} \nabla(\boldsymbol{\varepsilon} \cdot\cdot \boldsymbol{\varepsilon}) \right). \tag{3}$$

The following notations are used in Eqs. (2) and (3): c is the concentration of hydrogen in diffusive motion; T is the temperature; R is the universal gas constant; M, ρ are the molar mass and density of the solid; D_0 is temperature-dependent principal values.

Additionally, this notation of the diffusion equation takes into account that the diffusing gas induces internal strains ε_{diff}, proportional to the concentration and exhibiting isotropic behavior: $\varepsilon_{diff} = \alpha c \mathbf{E}$ ($\mathbf{E}$ is the unit tensor).

Evidently, the last term of expressions (2) and (3) can be discarded due to smallness in the case of linear theory, since the linear strain tensor is included. However, the diffusion equation also takes a non-classical form in this case; moreover, it contains additional terms aside from the widely used diffusion models, accounting for the stress-strain state by means of a pressure gradient (this is the factor $\nabla(\mathrm{tr}\varepsilon)$ for the proposed model).

The obtained diffusion equation does indeed yield high gradients of gas concentration inside the solid for solutions of specific boundary-value problems, while its concentration profile is equalized more slowly as the sample under consideration is saturated with the gas component. These results suggest that the proposed diffusion equation can be used to describe the transport of hydrogen into the metal from the external environment. However, no internal stresses can cause almost a hundred-fold difference in gas concentrations at the interface and in the bulk of the solid within this approach, which means that an additional diffusion channel needs to be taken into account.

As mentioned above, many studies into the processes associated with hydrogen degradation of metals assume that diffusion of hydrogen in the metal is governed by the trapping mechanism. The trapping mechanisms can differ in nature and depend on both the mechanical and thermodynamic characteristics of the metal-hydrogen system. Classical models accounting for trapping diffusion are the McNabb model of hydrogen interchange [21] or its simplified version, excluding the dependence of the interchange rate on time, proposed by Oriani [22].

We intend to use the McNabb model along with the modified diffusion equation (1) to more accurately describe the experimentally observed near-surface layer with a high concentration of hydrogen, which is relatively stable over time and is not diffused into the bulk of the metal over time. Although this trapping model is most commonly used to solve problems related to hydrogen diffusion, it has never been used this far to solve boundary-value problems accounting for the influence of the stress-strain state of the metal on the diffusion process from first principles.

The processes of bulk diffusion and trapping diffusion are believed to proceed independently from each other. Therefore, we can decompose the total hydrogen concentration into a sum of two concentrations:

$$c = c_{vd} + c_{trap}, \tag{4}$$

where c_{vd} is the concentration of hydrogen diffused by the bulk mechanism; c_{trap} is the concentration of hydrogen diffused by the trapping sites.

Hydrogen concentration in the traps is calculated by introducing two additional quantities: θ_{trap} is the degree of trap occupancy and N_{trap} is the density of trap distribution.

Accordingly, the hydrogen concentration in the traps is then expressed as

$$c_{trap} = \theta_{trap} N_{trap}. \tag{5}$$

The trap density N_{trap} is assumed to be known (from the experiment or additional constitutive equations). For consistency with the data published in the literature, we assume that the N_{trap} is a time-independent quantity.

To find the trap occupancy, we introduce an additional constitutive equation incorporating two more quantities, similarly to the approach for c_{trap} in Eq. (5): θ_{vd} is the occupancy of grain boundaries; N_{vd} is the density of grain boundaries into which mobile hydrogen can diffuse.

According to the data given in [21], the constitutive equation for θ_{trap} is as follows:

$$\frac{\partial \theta_{trap}}{\partial t} = p\theta_{vd}\left(1 - \theta_{trap}\right) - k\theta_{trap}, \tag{6}$$

where p, k are the parameters of the material (metal) determined experimentally.

To account for the dependences of the diffusion process and the concentration c_{vd} on the stress-strain state of the solid, we use Eq. (1). Only terms of first-order smallness are taken in expressions (2) and (3) The system of equations for finding the concentration profile of the gas component in the solid, taking into account diffusion by the trapping mechanism, is then written as follows:

$$\begin{cases} \dfrac{\partial c_{vd}}{\partial t} + N_{trap} \dfrac{\partial \theta_{trap}}{\partial t} = \nabla \cdot \left(D_{eff} \nabla c_{vd} + \mathbf{V} c_{vd} \right) \\[4mm] \dfrac{\partial \theta_{vd}}{\partial t} = p \theta_{vd} \left(1 - \theta_{trap} \right) - k \theta_{trap} \\[4mm] D_{eff} = D_0 \left(1 - \dfrac{cM}{RT\rho} \dfrac{E}{1-2\nu} \alpha \mathrm{tr}\varepsilon \right) \\[4mm] \mathbf{V} = \dfrac{D_0 M E}{RT\rho} \left(\dfrac{\nu}{(1+\nu)(1-2\nu)} \mathrm{tr}\varepsilon - \dfrac{1}{1-2\nu} \alpha c \right) \nabla(\mathrm{tr}\varepsilon) \\[4mm] c = c_{vd} + N_{trap} \theta_{trap} \\[4mm] \nabla \cdot \left[\dfrac{\nu}{1-2\nu} \left(\mathrm{tr}\varepsilon - 3\alpha c \right) \mathbf{E} + \left(\varepsilon - \alpha c \mathbf{E} \right) \right] = 0. \end{cases} \qquad (7)$$

The last equation in system (7) is the elasticity equation, accounting for the deformations induced by diffused hydrogen.

It is assumed in the available literature (see, for example, [29−31]) that trapping sites are associated with inhomogeneities within the metal (nanopores, dislocations, microcracks, etc.) where diffusing hydrogen accumulates. Recent experimental studies [32, 33] considering damage in metals provide data for distribution of damage over the bulk of metals. In particular, the concept of scalar damage is extended in [33] to proposes a damage tensor $\mathbf{D}$, defined as

$$\left(\mathbf{E} - \mathbf{D} \right) \cdot \mathbf{n} \delta S = \overline{\mathbf{n}} \left(\delta S - \delta S_T \right), \qquad (8)$$

where δS is the area of some site; δS_T is the area of damage in this site; $\overline{\mathbf{n}}$ is the normal defining the given flow; $\underline{\mathbf{n}}$ is the normal to the site.

Since trapping diffusion is in fact an additional flow through the defects in the solid (microcracks, pores, dislocations, etc.), multichannel diffusion can be suggested as an alternative to the McNabb approach, assuming flow of hydrogen through the metal defects in addition to the standard diffusion flow in the system; the gas component is deposited on these defects. Since the diffusive flow of gas $\mathbf{j}$ is expressed as

$$\mathbf{j} = \rho \mathbf{V} S,$$

where $\mathbf{V}$ is the flow velocity vector of the diffusing gas; ρ is the gas density; S is the area of the site through which this gas flows, we obtain that the additional flow through trapping sites $\mathbf{j}_{trap}$ is

$$\mathbf{j}_{trap} = \mathbf{D} \cdot \mathbf{j}, \qquad (9)$$

and thus the diffusion equation in this case takes the form

$$\frac{\partial c}{\partial t} = \nabla \cdot \left[\left(\mathbf{E} - \mathbf{D} \right) \cdot \left(D_{eff} \nabla c + \mathbf{V} c \right) \right]. \qquad (10)$$

The equivalent of the sink term here is

$$-\nabla \cdot \left[\mathbf{D} \cdot \left(D_{eff} \nabla c + \mathbf{V} c \right) \right]. \tag{11}$$

The system of equations for finding the concentration profile of the gas component in the solid, taking into account diffusion by the trapping mechanism, is then written as follows:

$$
\begin{cases}
\dfrac{\partial c}{\partial t} = \nabla \cdot \left[\left(\mathbf{E} - \mathbf{D} \right) \cdot \left(D_{eff} \nabla c + \mathbf{V} c \right) \right] \\[2mm]
D_{eff} = D_0 \left(1 - \dfrac{cM}{RT\rho} \dfrac{E}{1-2\nu} \alpha \operatorname{tr}\varepsilon \right) \\[2mm]
\mathbf{V} = \dfrac{D_0 ME}{RT\rho} \left(\dfrac{\nu}{(1+\nu)(1-2\nu)} \operatorname{tr}\varepsilon - \dfrac{1}{1-2\nu} \alpha c \right) \nabla(\operatorname{tr}\varepsilon) \\[2mm]
\nabla \cdot \left[\dfrac{\nu}{1-2\nu} \left(\operatorname{tr}\varepsilon - 3\alpha c \right) \mathbf{E} + \left(\varepsilon - \alpha c \mathbf{E} \right) \right] = 0.
\end{cases} \tag{12}
$$

Since most experiments are carried out with cylindrical specimens, where the tensile stresses are applied along their symmetry axes, we verify the model by considering a cylinder under uniaxial tension as a boundary-value problem (Fig. 1). It is assumed that the length of the cylinder along the z axis significantly exceeds its radius r_{out}, and hydrogen penetrates only from the lateral surface. Therefore, the deformations that occur in the cylinder and the concentration of hydrogen inside it depend only on the coordinate r, by virtue of symmetry.
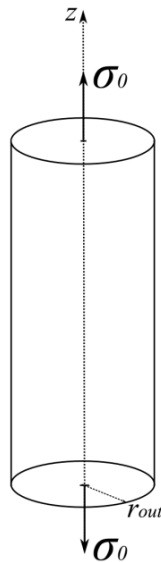

Fig. 1. Scheme for the formulation of the boundary-value problem: a cylindrical specimen with the radius r_{out} is exposed to axial tensile stresses σ_0 and gas flow from the lateral surface

The boundary conditions for finding the stress-strain state are given by the uniaxial tensile stress σ_0 and the stress-free lateral surface, and by the concentration of the gas component given on the lateral surface for the diffusion problem.

Notably, the elasticity equation contains components that depend on the concentration, and the diffusion equation contains coefficients that depend on deformations (both in r and in z directions). Thus, we obtain a conjugate problem, and these two equations cannot be solved separately. The boundary-value problem (both the elasticity problem and the diffusion equation) is solved numerically using an explicit finite difference scheme that corresponds to the finite volume method. To examine the surface effects in more detail, we constructed a mesh clustered to the surface of the specimen (i.e., with the coordinate r close to r_{out}). Discrete formulations of the corresponding integral balance equations were considered in the scheme instead of the differential equations for local balances. Displacements and concentration were given in the nodes of the mesh, and strains, stresses and diffusivities were given in the cells. The scheme itself is verified and analyzed for convergence for a particular case of a one-dimensional diffusion problem in a cylindrical coordinate system with a constant diffusivity in the absence of a stress-strain state.

Experimental data for the calculations are taken from [34] for T24 steel. The parameter α, corresponding to expansion due to hydrogen diffusion, is tailored so that all deformations of the solid remain within the linear-elastic range. The selected parameters are given in the table. The distribution of traps and vacancies for diffusively mobile hydrogen and the parameters p and k for the McNabb model are taken from [35, 36]; the values of damage depending on the coordinate and necessary for calculating the radial component of the tensor are taken from [32].

Table

Parameters of the simulated solid and gas component

Parameter	Notation	Unit	Value
Diffusion coefficient	D_0	mm/s²	3.5·10⁻⁹
Temperature	T	K	293
Young's modulus	E	GPa	182
Poisson's ratio	ν	–	0.295
Steel density ratio to molar mass	ρ/M	mol/m³	1.45·10⁴
External radius of cylinder	r_{out}	mm	1.1
Coefficient of thermal expansion	α	–	0.03

Fig. 2 shows the solutions to the diffusion problem accounting for the diffusion of hydrogen by the trapping mechanism. The concentration profile obtained by the McNabb model (Fig. 2,a) practically does not penetrate into the bulk of the metal over time, exhibiting the same locking effect and near-surface layer formation that was observed experimentally. Notably, however, this result was obtained using the phenomenological dependence N_{trap} on the coordinate [35], constructed assuming a highly uneven distribution of hydrogen throughout the sample as a result of its transport from the external environment. Varying the parameter N_{vd} does not produce a significant change in the concentration profiles and redistribution of hydrogen during diffusion.
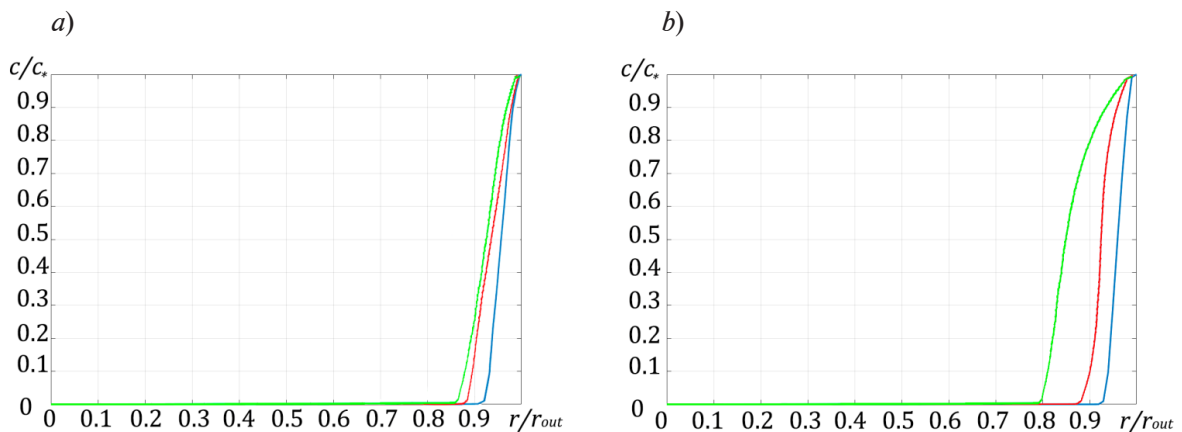

Fig. 2. Dependences of normalized hydrogen concentration in the solid on normalized radius at different times with a step of 600 minutes); the computational data are obtained using the McNabb trap model, provided that the distribution of N_{trap} is non-uniform (a), and a modified model accounting for flow through trapping sites by a damage tensor (b)

Accounting for hydrogen diffusion through traps based on the damage tensor (Fig. 2, *b*) eliminates a pronounced locking effect, while the concentration gradient tends to smooth out, and the hydrogen itself moves deep into the metal specimen. Apparently, the result obtained suggests that the components of the damage tensor are time-independent, so it is impossible to take into account the degree of occupancy of these traps, as well as the redistribution of hydrogen from the traps to the grain boundaries (and vice versa). However, this approach also remains attractive for further research, since the values of damage tensor components and their dependence on the coordinate can be calculated independently.

Conclusion

The paper theoretically investigates the diffusion of hydrogen into a solid in a stress-strain state, considering the mutual influence between the deformations inside the body and hydrogen transport from the external environment surrounding the solid. A modification of an earlier model is proposed to more accurately describe the experimentally observed near-surface layer with a high concentration of hydrogen, which is relatively time-stable and does not expand into the bulk of the metal due to diffusion. The diffusion equation obtained this way, taking into account the influence of the stress-strain state on the diffusion process, contains a sink term reflecting hydrogen flow by the trapping mechanism as the second diffusion channel. This modification was carried out in two ways: using the classical McNabb model and within the concept of damage.

A boundary-value problem was solved for the modified diffusion equation with the new sink term, the results were analyzed and compared. We have found that the results differ slightly, but movement of the diffusion front and 'smearing' of the near-surface hydrogen layer are slower for the McNabb model, which is more consistent with the experimental data.

Notably, the concept of damage allows to avoid some of the physical contradictions that inevitably arise within the McNabb model. These contradictions are removed if the flow of hydrogen is considered by the trapping mechanism within the concept of damage. However, because this model cannot account for the occupancy of traps and does not include a mechanism for redistribution of hydrogen within the solid (from trapping sites to grain boundaries and vice versa), the computational results are less consistent with the experimental data. We can thus conclude that the modification of the model is insufficient and requires further elaboration.

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