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ONE-DIMENSIONAL GOVERNING EQUATIONS FOR THE CREEP UNDER HYDROGEN DIFFUSION FLOW

Saturation with hydrogen of some metals, in particular α -iron, directly in the loading process can cause a great increase of their deformation response. The study is aimed at the macroscopic description of the phenomenon. The constructed governing equations are based on the concept of the equation of state with internal parameters. The modeled experiment lies in the saturation of a cylindrical specimen with hydrogen from the electrolyte, loaded torque. The analysis of both the literature and the experimental data justified the applicability of the linear boundary conditions of the first and third kinds. This made it possible to use the analytical solutions in the form of Fourier series of Bessel functions for the classical diffusion equation. It turned out that the scatter of the diffusivity, reported by different authors, can result in a significantly different interpretation of the experiments. For the most common value of D of the order $10^{-9} \text{ m}^2 \text{ s}^{-1}$, the calculated time for the complete saturation of the specimen was approximately a few minutes, which diverged from the characteristic times of the experiment. The explanation could have been either a lower value of the diffusivity, or the presence of the so-called "traps". Including into the model the limited capacity traps with the irreversible capture has also enabled us to explain the presence of a noticeable incubation period. From the time dependences of the concentration and its derivatives, the authors concluded that the hydrogen concentration should be the first to be considered as the parameter of the state. For this end, in the creep power law the stress exponent was kept constant but the creep coefficient was assumed to be dependent on the hydrogen concentration as well as on the accumulated plastic strain. The latter dependence was justified by the gradual strain rate deceleration for the loading below the macroscopic yield stress. The numerical results have demonstrated the principal possibility of the macroscopic modeling of the deformation synergistic effects under hydrogen absorption.

Key words: Creep, Diffusion of Hydrogen, Diffusivity, Governing Equations, Synergy Effects, α -Iron

INTRODUCTION

Simulation of the interaction of hydrogen with metals is an important issue in view of the prospects of hydrogen power engineering. There are many studies related to the consequences of undesirable but often unavoidable presence of hydrogen in metals. But it is also known that the high diffusivity of hydrogen atoms in certain transition metals can lead to devastating consequences directly in the process of the hydrogen saturation of loaded metal. Hence it is important to predict the mechanical behavior and assess a lifetime of the constructions under combined effect of stresses and hydrogen flux. For these calculations, the governing equations of the mechanics of solids are necessary to describe the stress-strain state of metal under this type of loading. The study is the first step towards a macroscopic modeling of loaded metals deformational behavior under the effect of hydrogen diffusion flux.

The experiments carried out since the 60-s of the last century have shown that the saturation of metals and alloys with hydrogen directly in the de-

formation process can cause some phenomena that did not exist during the deformation of metals, previously saturated with hydrogen. A comprehensive review of related publications is given in [13]. The basic feature of these effects is the synergistic nature of the phenomena: the deformations caused by the joint action of inhomogeneous stress field and hydrogen flux may be greater by orders of magnitude than those that occur under the influence of each of these factors separately. The physical nature of these phenomena is not the issue of our study. We only note that such effects are, by assumption, the result of a specific state of the material occurring under the super equilibrium concentration of hydrogen in microdomains of metal together with inhomogeneous stress field. The relevant discussion can be found in [13].

A triad of mechanical after-effects has been studied in the experiments: creep under a constant stress applied; relaxation of the stress and the reverse mechanical after-effect. To be specific, we focused on the first of these effects. Iron was selected for

investigation because the effect of pre-introduction of hydrogen on deformation properties of this material has been studied in detail.

The purposes of the modeling were to determine some calculable macroscopic parameters affecting the process and propose the equations usable to predict the appearance of synergistic deformation effect in the metal under the above loading. To this end, we, firstly, examined the experiments which were to be modeled. Being based on this analysis, the concentration of hydrogen and related quantities were calculated from the classical diffusion equation. After that, a more complicated diffusion equation together with a constitutive equation for creep was used for simulating the process.

EXPERIMENTAL BACKGROUND

Some details about the experiments which were modeled in this paper can be found in [7], [14] and the references cited therein. The specimens of Armco iron was annealed in vacuum at 600 °C for one hour. The form of the specimens was wire $8 \cdot 10^{-4}$ m in diameter and $8 \cdot 10^{-2}$ m in working length. Hydrogen was being introduced from the electrolyte into the specimen being under the torsional loading. The densities of the cathode current were varied within the range of 50–1000 A/m². The deformation was measured by an installation based on the principle of inverted torsional pendulum.

The creep of iron in torsion has been studied for the following loading modes: (a) loading below the macroscopic elastic limit, (b) the specimen unloaded after plastic deformation is subjected to repeated loading below the yield point of the underformed specimen, (c) on attainment of the prescribed level of plastic strains, the specimen is partially unloaded to stresses $\tau \approx 0,9 \tau_s$.

Since in actual structures the design stresses are usually well below the yield point, case (a) was chosen for simulating. The typical dependence corresponding to this loading model is as follows: the period of deformation acceleration is followed by the period with the strain rate gradually decreasing, and eventually the deformation stops rising. The following features in the behavior of the material which are important for our further modeling were identified [6], [7], [13], [14]:

- The deformation process is active only when hydrogen is fed and it stops immediately when the current is switched off.
- A necessary condition for plastic deformation development is the presence of tangential stresses. In this case the synergistic effect of plastic deformation is observed in loading both below and above the macroscopic yield point.
- The strain rate of the after-effect, all other things being equal, is determined by the rate of saturation. There is a critical value of the cathode current, below which the effects are not clearly visible. The composition of the electrolyte as well as the shape of the anode

affect the kinetics of the process, but there is a limiting deformation for the metal with a specified thermomechanical prehistory.

- The observed mechanical instability is not due to the discontinuity of the material upon saturation with hydrogen.
- The active process of creep deformation is preceded by some incubation period. This period decreases with applied load or with hydrogen introduction rate increase. For a sufficiently high intensity of the introduction the incubation period does not depend on the stresses.
- Synergistic effects are observed only in the metals with a sufficiently high (no less than $10^{-10} \text{ m}^2 \text{ s}^{-1}$) diffusivity (except for zirconium). Alloying iron with the elements which reduce the solubility and diffusivity of hydrogen leads to decreasing the deformational effects.

From these regularities, it follows that the parameters of state for pure torsion at a fixed temperature could be: the hydrogen concentration, the concentration gradient, the rate of the change in concentration and the amount of the accumulated plastic strain. It is to be investigated which of these variables have the greatest impact on the deformation behavior and should be included in the constitutive equation.

SIMULATION OF THE DIFFUSION PROCESS IN THE ELECTROLYTIC HYDROGEN ABSORPTION

The problem of the diffusion coefficient choice

The main parameter of the material which determines the hydrogen saturation rate is the diffusion coefficient, or diffusivity. There are many various values of a low temperature hydrogen diffusivity in α -iron reported by different research groups. The lack of agreement among them, even if the same electrochemical permeation technology was used, is very well known [10]. There are a few reasons for this disagreement. Firstly, the hydrogen permeability of a specimen which is saturated with hydrogen electrolytically is the characteristics which is difficult to reproduce. The kinetics of the process is influenced by the specificity of the electrolyte, the surface layer of the specimen and the cathode processes. Besides, some of these parameters are often difficult to control [2]. For example, it is shown in [11] that variations in the charging current density and the electrolyte can very well explain the variations in the reported values of diffusivity. Secondly, diffusivity is a function of trap density and the magnitude of the trap depth [12]. The third avowed reason is the surface problems [10]. In addition, the structure of the metal is changing under the process of saturation [2]. From the mathematical point of view, such a discrepancy in the diffusivity values indicates the ill-posedness of the inverse problem. It means that small deviations in the row data can lead to large variations in the solutions. The study [17] on this issue showed that estimation of hydrogen transfer pa-

rameters and identification of the type of boundary conditions should be performed simultaneously.

In the experiments under consideration the diffusivity of the material had not been determined previously as this is a problem which should be solved separately. That is why in the simulation the values of diffusivity which were determined by an electrochemical hydrogen permeation method under the same temperature ([8], [11]) were used. One can also find the values collected from different researchers in [10].

The Process with the Cathode Current Switched on

Taking into account the dimensions of the specimen given above we ignored the changes of any parameters along its length. In the polar coordinates with the independence of all the values on the angle the classical equation for Flick's diffusion is:

$$\frac{\partial c(t, r)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D(r) \frac{\partial c(t, r)}{\partial r} \right), \quad 0 \leq r < R, \quad t > 0. \quad (1)$$

Here $c(t, r)$ is concentration of hydrogen atoms at the points with radius r at time t , D – diffusivity, R – radius of the specimen. Generally the value of the D does not remain permanent during the process. For example, the results of [11] suggest a positive concentration dependence of hydrogen diffusivity in Armco iron. The research [16] indicates the dependence of diffusivity on the gradient of shear stress. But in this first study the value was assumed to be constant, so (1) is simplified:

$$\frac{\partial c(t, r)}{\partial t} = D \cdot \left(\frac{\partial^2 c(t, r)}{\partial r^2} + \frac{1}{r} \frac{\partial c(t, r)}{\partial r} \right). \quad (2)$$

Since before the experiment the specimen was dehydrogenated, the initial condition is

$$c(0, r) = 0, \quad 0 \leq r < R. \quad (3)$$

The important problem was to formulate the boundary condition properly. Hydrogen penetration in metals is the sequence of the successive processes occurring both on the surface of the metal and inside it. It includes adsorption, absorption, dissolution, desorption and diffusion. The most general form of the boundary conditions takes into account all these processes [9]. But adding any term describing the corresponding process into the equation requires the knowledge of the relevant constant (parameter). To get these parameters one needs to have data from some other experiments with the same material. On the other hand, not all of these processes can be equally important in each specific case. Since any direct measurements of the surface concentration or flux of hydrogen are impossible, it is only indirect information that enables us to draw conclusions about the influence of the surface processes on the diffusion. According to the results of the experiments [7], [13], [14] there exists some characteristic delay time t^* for the creep to start. For sufficiently high intensities of hydrogenation, in particular, for $i_c = 1000 \text{ A/m}^2$ this time does not depend on the stress level. According to [2], such intensity corre-

sponds to a pressure higher than 10 MPa. This suggests that at this level of the cathode current density, the high pressure suppresses desorption, and in the volume of the metal adjacent to the surface the maximum concentration of hydrogen atoms c_0 sets almost immediately. Therefore, in this case we can reasonably write the boundary condition as follows:

$$c(t, R) = c_0, \quad t > 0. \quad (4)$$

By using the technique of separation of variables [15] one obtains the solution of the problem (2)–(4) in the form of a Fourier series:

$$c(t, r) = c_0 \left[1 - 2 \sum_{n=1}^{\infty} \frac{1}{\mu_n^{(0)} J_1(\mu_n^{(0)})} \cdot J_0 \left(\frac{\mu_n^{(0)} r}{R} \right) \cdot \exp \left(-\frac{D \mu_n^{(0)2}}{R^2} t \right) \right]. \quad (5)$$

Here $J_0(x)$, $J_1(x)$ – Bessel function of the first kind of zero and first orders, and $\mu_n^{(0)}$ – the positive successive roots of $J_0(x)$.

Values of diffusivity at room temperature given in [9] vary from $5 \cdot 10^{-13} \text{ m}^2 \text{ s}^{-1}$ to $8 \cdot 10^{-9} \text{ m}^2 \text{ s}^{-1}$, and this is the most comprehensive range of the value we could find in the literature. (But the greater part of the experimental results is in the region $D \approx 10^{-9} \text{ m}^2 \text{ s}^{-1}$). One can verify numerically that for these orders of magnitude all the troubles connected with summation (5) lie in the region $t < 10 \text{ s}$. By “troubles” we mean a saw tooth curve for $c_r(t) \equiv c(t, r)$ for the values of r in the vicinity of R . Consequently, for the numerical values of the parameters we deal with, the use of analytical solutions for larger values of t is quite acceptable.

Fig. 1, reproduced from [13], presents the growth of creep shear deformations at $i_c = 1000 \text{ A/m}^2$ with the stress level $\tau = 180 \text{ MPa}$. (The author also reports that without hydrogenation at the given stress level the value of deformation, observed during 60 minutes, was invisible in the scale of the graph.) The curves substantiate that an active deformation process starts a few minutes after the beginning of saturation. So it was reasonable to follow the changing of the concentration during this time interval.

Fig. 2 demonstrates the distribution of a relative concentration $c(t, r)/c_0$ along the radius for different values of diffusivities after 60s of saturation, computed according (5). For $D = (1,8-7) \cdot 10^{-9} \text{ m}^2 \text{ s}^{-1}$

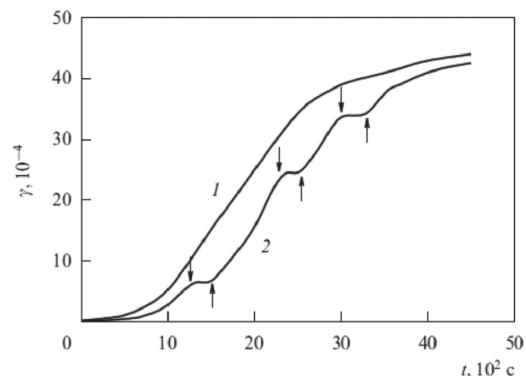


Fig. 1. Creep deformation (10^{-4}) in Armco iron: 1) continuous hydrogenation; 2) alternating switch on and switch off the cathode current. Reproduced from [13]

(the value was taken from [11] for Armco iron annealed in vacuum at 800 °C for 8 hours) hydrogen concentration in the cross section of the specimen reaches its limit values approximately in one minute. There are no gradients of concentration after this moment. It suggests that the actual value of diffusivity is less than this value. However, it is emphasized in [13] that the higher is the diffusivity, the more is the effect, and there is no effect for metals with low diffusivity. But in our opinion, it is unlikely that any processes take place in the material after saturation. Otherwise, we would have had the effect in the material, previously saturated with hydrogen. It is also unlikely that there exists some surface process the durability of which does not depend on the current density. So the logical conclusion is that if equation (2) is valid, the macroscopic diffusivity for this material is lower than the value mentioned above.

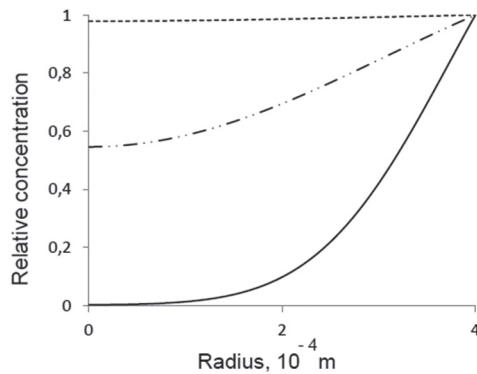


Fig. 2. Distribution of relative concentrations at $t = 60s$:
(---) $D = 2 \cdot 10^{-9} m^2 s^{-1}$, (- · - ·) $D = 5.8 \cdot 10^{-10} m^2 s^{-1}$,
(—) $D = 10^{-10} m^2 s^{-1}$

For $D = 5.8 \cdot 10^{-10} m^2 s^{-1}$ (the value is from [8] for pure iron, there is no information about heat treatment) the specimen is saturated in approximately five minutes. So we expect that this value of diffusivity is also too large for the investigated material. It is only the values near $D \approx 1 \cdot 10^{-10} m^2 s^{-1}$ that enable us to explain the curves in Fig. 1. In this case the $c(t, r)$ for the values of r in the vicinity of R reaches the saturation in a few minutes, and the whole specimen is saturated in nearly thirty minutes, when deformation no longer increases (Fig. 2). But as it was mentioned earlier, due to the surface processes the real values of concentrations are somewhat less, so the diffusivity from [8] could be true.

In [18], [19] a model for electrolytic permeability method, considering absorption and desorption processes, is proposed. Assuming the surface concentration to be constant, the authors have modified the general form of boundary condition to a linear one. The values of diffusivity, obtained from this model, are practically independent of sample thickness and surface treatment, confirming the correctness of the boundary conditions. The desorption rate constant and the absorption parameter have also been calculated there. Hence, for the smaller values of the current

density, the use of the boundary conditions, proposed in [19] instead of the condition (4), would be appropriate. Fig. 3a shows the changes in gradient at successive times. The values were obtained by differentiation of formula (5) with respect to r , constant factor was not taken into account. As expected, the major changes take place in the subsurface layer where the gradient decreases more than five times within the first five minutes. Such a drastic change in the gradient could, in principle, be the driving force of the process. Fig. 3b demonstrates the distribution of derivatives of (5) with respect to t , constant factor is also not taken into account. The hump of curve is characteristic of all similar processes ([17]) and can be derived from (5). The moving of this “hump” along the radius would also describe the phenomenon. The results, given above, lead to conclusion that the concentration of the hydrogen, as well as its derivatives in the subsurface layer, could be accepted as the parameters of the state in the governing equations. Finally, we note that the series (5) converges so fast that for $t > 100s$ it is sufficient to use only the first term of the series.

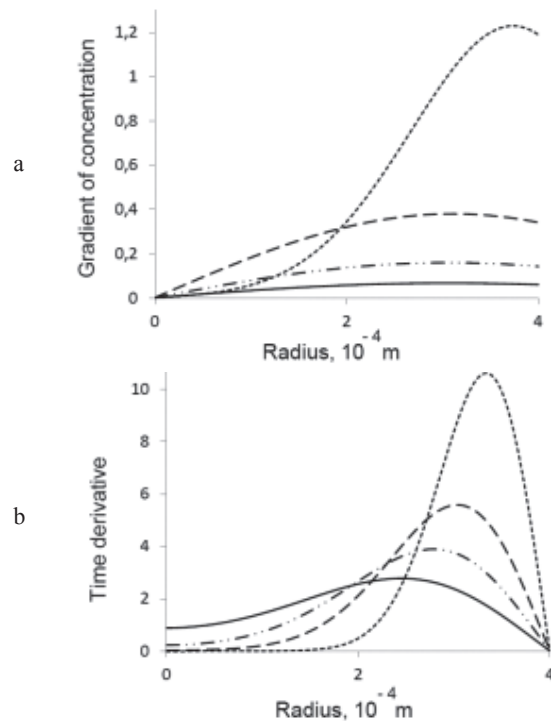


Fig. 3. Distribution of concentration gradients (a) and time derivatives of $c(t, x)$ (b) for $D = 1 \cdot 10^{-10} m^2 s^{-1}$:
(---) $t = 60s$, (- · - ·) $t = 300s$, (- · · - ·) $t = 540$, (—) $780s$

The Process with the Cathode Current Switched Off

The experiments show that after the cathode current is switched off, the creep deformation stops almost immediately. So we should follow the changes in the distribution of concentration along the radius of the specimen after this moment. Let t_1 be the time when the cathode current was switched off. To avoid confusion, we denote $f_1(r) = c(t_1, r)$ where $c(t_1, r)$ is calculated by (5) with $t = t_1$. So the initial condition for the diffusion equation in this case is

$$c(0, r) = f_1(r). \quad (6)$$

If desorption is neglected, no hydrogen leaves the specimen and the boundary condition for (2) is

$$\left. \frac{\partial c}{\partial r} \right|_{r=R} = 0. \quad (7)$$

The solution of the problem (2), (6), (7) obtained with the same separation of variables technique is:

$$c(t, r) = \phi_0 + \sum_{n=1}^{\infty} \phi_n \cdot J_0\left(\frac{\mu_n^{(1)} r}{R}\right) \cdot \exp\left(-\frac{D\mu_n^{(1)2}}{R^2} t\right), \quad (8)$$

where ϕ_0 and ϕ_n are given by the expressions:

$$\phi_0 = \frac{2}{R^2} \int_0^R r \cdot f_1(r) dr, \quad \phi_n = \frac{2}{R^2 J_0^2(\mu_n^{(1)})} \int_0^R r \cdot f_1(r) \cdot J_0\left(\frac{\mu_n^{(1)} r}{R}\right) dr$$

and $\mu_n^{(1)}$ are the positive successive roots of $J_1(x)$.

Fig. 4a demonstrates the changes in concentrations at successive times calculated from (8) for $t_1 = 780$ s. The presence of the intersection point follows from the properties of the series (8): in the points with the radius $r = R\mu_n^{(0)} / \mu_n^{(1)}$ the first term of the series vanishes, and $\mu_n^{(1)2}$ provides a rapid decrease of the exponent in the remaining terms of the series. Although the concentration in the near-boundary region decreases after the current is switched off, the small value of the change did not enable us to simulate further the effects when cathode current was alternatively switched on and off. That is why the linear boundary condition of the third kind, accordingly [19], was accepted in our study:

$$\left(D \frac{\partial c}{\partial r} + kc \right)_{r=R} = 0, \quad t > 0. \quad (9)$$

The solution of the problem (2), (6), (9) is:

$$c(t, r) = \sum_{n=1}^{\infty} \phi_n \cdot J_0\left(\frac{\mu_n^{(2)} r}{R}\right) \cdot \exp\left(-\frac{D\mu_n^{(2)2}}{R^2} t\right), \quad (10)$$

where ϕ_n are given by the expressions:

$$\phi_n = \frac{2\mu_n^{(2)2}}{R^2 [\mu_n^{(2)2} + k^2 R^2] \cdot J_0^2(\mu_n^{(2)})} \int_0^R r \cdot f_1(r) \cdot J_0\left(\frac{\mu_n^{(2)} r}{R}\right) dr$$

and $\mu_n^{(2)}$ are the successive positive roots of the equation $\mu \cdot J_0(\mu) + kRJ_0(\mu) = 0$.

Although the desorption rate constant k should depend on charging current density, as well as on electrolyte and material properties, it is unlikely equal to zero, even if the current is switched off, it is much more likely that for this case it is larger than when some current is applied. That is why the order of the value in (10) was taken from [19]. The results of these calculations have provided a more rapid decrease of the concentration (Fig. 4b), so they were used in simulating hereinafter.

The Process with the Cathode Current Switched On and Off Alternately

We also applied the formulas (5) and (10) one by one successively for successive times. The corre-

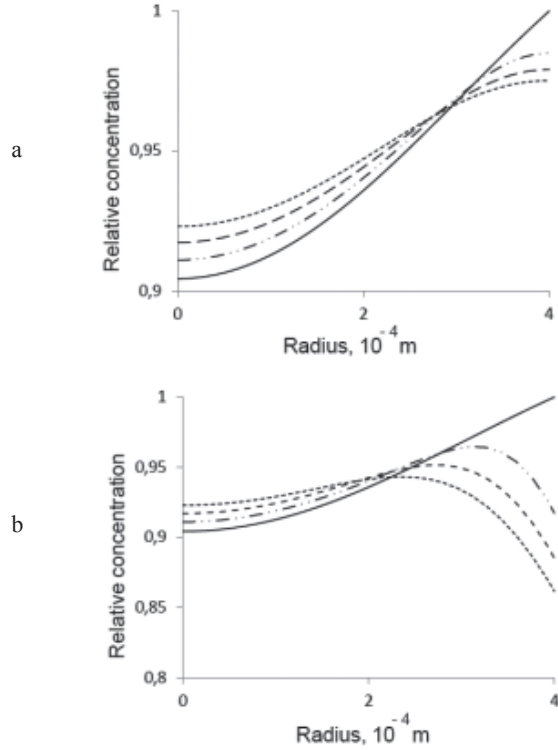


Fig. 4. Distribution of relative concentrations for $D = 1 \cdot 10^{-10} \text{ m}^2 \text{ s}^{-1}$ after current is switched off, for boundary condition of first (a) and third (b) kinds: (—) $t = 0$ s, (····) $t = 20$ s, (---) $t = 40$ s, (- - -) $t = 60$ s

sponding changes in the initial condition (3) are obvious. As a result, we got a picture of the changes in the concentrations in the near-boundary region (not presented). The concentration in the surface layer was changing in a stepwise manner; the step height was gradually reduced. In our opinion, it is the concentration in the near-boundary region that is likely to be the critical value for the process.

The Trapping Effect

Having supposed the validity of the diffusion model (2)–(4), we were unable to simulate clearly the existence of an incubation period. It is widely acknowledged that the trapping effect is one of the main causes for the delay of penetration, so the governing equation to describe the trapping should be added to Flick's second law. On the local equilibrium assumption the two equations are reduced to one with effective diffusivity [12]. But having no preliminary knowledge about the traps we suppose using this approach is incorrect. The different forms of the equations for various types of traps are presented in [1], [5]. Since the object of the paper was only the qualitative simulation, we tried to keep the number of the unknown parameters as small as possible. That is why we used the following diffusion model with irreversible capture and limited capacity of the traps:

$$\begin{cases} \frac{\partial c(t, r)}{\partial t} = D \cdot \left(\frac{\partial^2 c(t, r)}{\partial r^2} + \frac{1}{r} \frac{\partial c(t, r)}{\partial r} \right) - \beta \left(\frac{\bar{w} - w(t, r)}{\bar{w}} \right) \cdot c(t, r) \\ \frac{\partial w(t, r)}{\partial t} = \beta \left(\frac{\bar{w} - w(t, r)}{\bar{w}} \right) \cdot c(t, r) \end{cases}, \quad 0 \leq r < R, \quad t > 0. \quad (11)$$

where $w(t, r)$ is the concentration of hydrogen in the traps, \bar{w} – the capacity of the traps, β – the unknown coefficient. The initial condition

$$w(0, r) = 0 \quad (12)$$

is to be added to (3).

We supposed the linear dependence of traps capacity on the radius, because the number of the traps can depend on the plastic deformation which has the greatest value near the edge. Since the objective of the study was to obtain the governing equations of mechanics of solids, it is noteworthy that the concept of microstructure is alien in principle to the mechanics of the solids. Thus, by “traps” one can mean any internal state variable which is governed by the equations above.

THE COUPLED SYSTEM OF THE GOVERNING EQUATIONS

When a material is subjected to a stress that is below its yield stress, it deforms commonly only elastically. However, provided the temperature is relatively high, plastic deformation can occur even when the stress is lower than the yield stress. This deformation is time-dependent and known as creep. In our case, the similar phenomenon is observed having been caused not by temperature but by diffusion flux of hydrogen.

A creep elongation curve for the time dependence of the deformation has typically the three stages: 1) the stage of primary or reduced creep, 2) the stage of stationary creep, 3) the stage of accelerated creep. At the end of the third stage, creep rupture of the specimen occurs. In practice, steady-state creep often dominates in the creep behavior because the duration of this stage is usually much greater than of the first and third ones; therefore, most studies focus primarily on the second stage of the creep curve (although some unified nonlinear models for all stages of creep have also been suggested).

The applied stress provides a driving force for any creep mechanisms. When the stress is increased, the rate of deformation also increases. In the case of uni-axial stretching, the power creep law is often accepted:

$$\dot{\epsilon} = \alpha_1 \sigma^n, \quad (13)$$

([3], [4]) where $\dot{\epsilon}$ is the creep strain rate, σ – applied stress, α_1 and n are the constants. The stress exponent n depends on the creep mechanism, for dislocation creep it is usually in the range 3–8. The constant α_1 depends on the temperature, and it is determined from the experiments, too. Some other dependencies are also used instead of (13), but all of them have an empirical nature, the specific choice depends on the convenience of use.

Let us consider the steady-state creep of the cylinder of radius R under the torque with the magnitude M . Assume the cross sections remain plane, as in the case of elastic loading. In this case the angular

creep strain γ is connected with the relative angle of torsion $\theta = \theta(t)$ as follows [4]:

$$\gamma(r) = r \cdot \theta. \quad (14)$$

It is shown in [4] that for a steady torsion creep one can as well use the power law like (13):

$$\dot{\gamma} = \alpha \tau^n. \quad (15)$$

Here $\dot{\gamma}$ is the angular creep strain rate, τ – the resulting tangential stress, $\alpha = 3^{(n+1)/2} \alpha_1$. The tangential stresses are connected with the torque:

$$M = 2\pi \int_0^R \tau(r) \cdot r^2 dr. \quad (16)$$

From (14)–(16) one gets:

$$\tau(r) = M \cdot I \cdot r^{1/n}, \quad (17)$$

where $I = 2\pi n(3n-1)^{-1} R^{(3n+1)/n}$ is the resulted polar moment of inertia. But since the experiments show that in our case the dependence $\gamma(t)$ is far from a linear one (Fig. 1), we cannot use the steady-state law (15) directly.

Suppose, for simplicity that α is the only constant in (15) that is changeable under the diffusion and probably under the deformations, so the creep law is:

$$\dot{\gamma}(t, r) = \alpha(t, r) \cdot \tau^n(t, r) \quad (18)$$

(the dependence of $\alpha = \alpha(t, r)$ is not a direct one). Still assume the cross sections remain plane and θ does not depend on r , so (14) is valid for the total angle strain γ_{total} . The increment of this value $\Delta\gamma_{total}$ during the time interval $(t, t + \Delta t)$ is the sum of the increments of the creep and elastic strains:

$$\Delta\gamma_{total} = \Delta\gamma + G^{-1} \Delta\tau, \quad (19)$$

$\Delta\gamma_c$, $\Delta\tau$ – the increments of creep strain and tangential stress, respectively, G – shear modulus. Dividing by $\Delta\tau$ and letting Δt tend to zero, one gets the similar equation for the rates. Substituting the rates from (14) and (18), gives:

$$\frac{\partial \tau}{\partial t} = G(\dot{\theta} \cdot r - \alpha(t, r) \cdot \tau^n(r, t)), \quad 0 \leq r \leq R, \quad t > 0. \quad (20)$$

To close the equation we use the equilibrium condition (16). By differentiating (16), the torque is constant, and using the result together with (19), after transformations one obtains:

$$\frac{\partial \tau}{\partial t} = G \left[4R^{-4} \int_0^R \alpha(t, r) \tau^n(r, t) r^2 dr - \alpha(t, r) \tau^n(t, r) \right]. \quad (21)$$

The initial condition for (21) is the elastic stress distribution:

$$\tau(0, r) = G \theta_{el} r, \quad (22)$$

where θ_{el} is the initial elastic torsion angle.

As the creep strain grows considerably under the hydrogen flux, we choose the power dependence upon concentration for a creep coefficient. Since

there exists the maximum creep strain θ_{max} that can be attained for the specimen with a specified thermomechanical prehistory, the creep coefficient was taken in the form:

$$\alpha(t, r) = \alpha_0 \left(\frac{(c(t, r) - c_s)^+}{c_s} \right)^k \left(\frac{\theta_{max} - \theta(t)}{\theta_{max}} \right)^m \tau^n(t, r). \quad (23)$$

Here c_s is the critical concentration at which the effect starts, α_0 – the value for the metal without hydrogen saturation, the sign plus means that if the difference is less than zero, the value in brackets is taken for zero.

The model for the mechanics of the solids includes equilibrium equations, and equations of state. In our one-dimension case the two are combined in (21). The parameter in this equation depends on the concentration of hydrogen, hence diffusion equations (11) are to be included in the model. The initial and boundary conditions are (3), (12), (22) and (4) or (9).

The systems of coupled equations (2), (21) and (11), (21) were solved numerically by the explicit scheme. Although the diffusion equation has an analytical solution, it was also integrated numerically. After that, the values of the concentration were substituted into the equation (21). The derivatives were approximated with the second order of accuracy; the integral was calculated by a trapezoidal rule. The accuracy of the solution was controlled only by decreasing the time step. The parameter values are given in the Table. The results of the calculations, when the current was alternatively switched on and off, are presented in Fig. 5, where the dash line is for the model with trapping, the solid line is without trapping. The comparison of the Fig. 1 and Fig. 5 enables us to conclude that the proposed model provides a

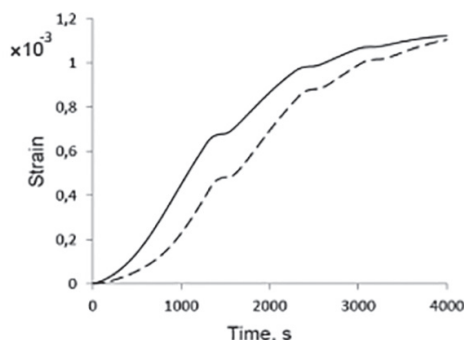


Fig. 5. Computed creep deformation at alternating switch on and switch off the cathode current: (—) without trapping, (---) with trapping

qualitative description of the synergistic effect of the creep under hydrogen absorption.

CONCLUSION

The macroscopic modeling of the interaction of hydrogen with metals requires a careful analysis of all the experimental conditions. The critical issue is the values of the penetration parameters, and especially, the value of diffusivity. A small discrepancy between the diffusivity used in calculations and the real one can result in qualitatively incorrect conclusions. The value of relative concentration of hydrogen in the near-boundary region is to be included, first of all, into the set of the state parameters. This conclusion is also consistent with the physical basis [13]. Some other related values can't not be excluded from consideration, either. The numerical results illustrate that the proposed equations can provide a qualitative description of the process.

The numerical data for simulating

Diffusion		Creep							
D	k/D	G	M	α_0	n	k	m	θ_{max}	c_s
$10^{-10} \text{ m}^2 \text{ s}^{-1}$	$2 \cdot 10^3 \text{ m}^{-1}$	$8 \cdot 10^{10} \text{ Pa}$	$1,8 \cdot 10^{-2} \text{ Nm}$	$4 \cdot 10^{-29}$	3	2/3	3	$1,5 \theta_0$	$0,8 c_0$

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ONE-DIMENSIONAL GOVERNING EQUATIONS FOR THE CREEP UNDER HYDROGEN DIFFUSION FLOW

Saturation of some metals with hydrogen, in particular α -iron, immediately in the process of loading can cause a great increase of their deformation response. The study is aimed at the macroscopic description of this phenomenon. The constructed governing equations are based on the concept of the equation of state with internal parameters. The modeled experiment involves saturation of a cylindrical specimen with hydrogen from the electrolyte, loaded torque. The analysis of both research literature and experimental data justified the applicability of the linear boundary conditions of the first and third kinds. This made it possible to use the analytical solutions in the form of Fourier series of Bessel functions for the classical diffusion equation. It turned out that the scatter of diffusivity, reported by different authors, can result in a significantly different interpretation of the experiments. For the most common value of D of the order $10^{-9} \text{ m}^2 \text{ s}^{-1}$, the calculated time for the complete saturation of the specimen was approximately a few minutes, which diverged from the characteristic times of the experiment. The explanation could have been either a lower value of diffusivity, or the presence of the so-called “traps”. Inclusion of the limited capacity traps with the irreversible capture into the model has also enabled us to explain the presence of a noticeable incubation period. The study did not take into account the dependencies of D on the accumulated plastic strain, the stress gradient, and concentration. From the time dependences of the concentration and its derivatives the authors concluded that the hydrogen concentration should be the first to be considered as a parameter of the state. Furthermore, the creep power index was kept constant but the creep coefficient was assumed to be dependent on hydrogen concentration as well as on the accumulated plastic strain. The latter dependence was justified by the gradual strain rate deceleration for the loading below the macroscopic yield stress. The numerical results have demonstrated the principal possibility of macroscopic modeling of deformation synergistic effects under hydrogen absorption.

Key words: creep, diffusion of hydrogen, diffusivity, governing equations, synergy effects, α -iron

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