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EFFECT OF ELECTRIC CURRENT ON MIGRATION OF POINT DEFECTS NEAR A CRACK TIP

D. N. Karpinskii and S. V. Sannikov

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The effect of direct current on migration of point defects dissolved in a crystal near the tip of a crack in tension is estimated. Calculations are carried out with allowance for the plastic strain near the crack tip of a loaded specimen, caused by the motion of dislocations in the active slip planes of the crystal, the Joule heat released, and the effect of gas exchange on the crack edges on the evolution of distribution of interstitial impurity atoms. A numerical analysis is performed for an α-Fe crystal.

Introduction. It is known that high-density current in a metal substantially decreases its deformation resistance and increases its plasticity [1, 2]. It is, therefore, of considerable interest to study the evolution of point defects near the crack tip under a combined action of mechanical and electrical forces. The authors [3] studied the distribution of point defects as a function of time in the absence of electric current. To develop methods of electrochemical filling by hydrogen [4] and to solve other applied problems, it is important to know the specific features of the effect of electric current on the strength of specimens, which strongly depends on migration of point defects. To the authors' knowledge, this topic was studied only in [5], where the evolution of the distribution of hydrogen atoms dissolved near a notch in a current-carrying rod was calculated. It was assumed, however, that the external load did not cause plastic strain and the gaseous impurity was not accumulated in the notch cavity.

The aim of the present paper is to calculate the evolution of the distribution of hydrogen atoms near the crack tip in a crystal under the action of direct electric current and mechanical load with allowance for gas exchange on the crack edges.

1. Formulation of the Problem and Method of the Solution. The problem of migration of point defects in a loaded specimen with cracks and pores has long been the subject of interest [6]. The authors [3] calculated the evolution of the concentration of interstitial impurity atoms $c(\boldsymbol{r}, t)$ and determined the contributions of dislocation mechanisms in the transfer of interstitial impurity atoms. A crack of length $2l$ located in the cleavage plane (010) (along the negative Ox half-axis) of an infinite crystal with a body-centered cubic (BCC) lattice was considered. The crystal planes $y \to \pm\infty$ are subjected to a uniform tensile stress $\sigma_{yy}(t) = \sigma'_a(t)$ (mode I) increasing monotonically to a certain value σ_a sufficient for plastic deformation of the crystal but insufficient for crack growth. Before loading, the interstitial hydrogen atoms are uniformly distributed in the crystal with a concentration c_0. In addition to [3], we assume that, far from the crack, direct electric current of density j_0 passes through the crystal in the normal direction to the crack plane [$j_x(\boldsymbol{r}) = 0$ and $j_y(\boldsymbol{r}) = j_0$ as $|\boldsymbol{r}| \to \infty$].

As in [7], we assume that the plastic strain of the BCC lattice of the crystal occurs due to displacement of the total dislocations with the Burgers vector $\boldsymbol{b} = (1/2)\langle 111\rangle$ over planes of easy slip $\{110\}$. Intersecting the Oxy plane, planes $\{110\}$ form two families of slip lines with uniformly distributed dislocation sources, which emanate rectilinear loops lying in the planes of easy slip. Using this model, the authors [7] calculated the evolution of plastic strain. In the calculations, only the sections of the loops normal to the Oxy plane were taken into account. In [8], the calculation of [7] was extended to the case of direct electric current passing through a loaded cracked crystal. The following three mechanisms by which the current affects the dislocations in the plastic zone near the crack were taken into account in [8]: the Joule heat, the Thomson effect, and the "electron wind." In [9], the following

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three mechanisms of transfer of interstitial hydrogen atoms near the crack tip were studied: the lattice diffusion, dislocation "sweeping-out" of point defects, and transfer of impurity atoms in the cores of dislocations that move in the plastic zone. The calculation results of [9] show that the first mechanism (lattice diffusion) makes the main contribution to the flow of impurity atoms.

It is of interest to refine the results of [3] by taking into account the action of direct electric current on hydrogen atoms dissolved in a crystal. The electric current acts on the atoms both directly and indirectly, through the change in the character of motion of dislocations. In accordance with [8, 9], we take into account the Joule heat released in a cracked crystal under the action of direct electric current passing there and the lattice diffusion of hydrogen atoms caused by the combined action of mechanical and electric fields.

We consider the equations governing electromechanical diffusion (see, e.g., [5])

$$\frac{\partial c}{\partial t} = -\nabla J, \qquad J = \frac{Dc}{k_{\mathrm{B}}T}\,\nabla\mu. \tag{1}$$

Here D is the diffusivity, k_{B} is the Boltzmann constant, T is the temperature, $\mu = k_{\mathrm{B}}T\ln(c/c_0) - V(\boldsymbol{r},t)$ is the chemical potential for a weak solution of impurities in the elastic-stress and electric fields, where $V(\boldsymbol{r},t) = \Delta v\sigma_{ii}(\boldsymbol{r},t) - eZ^*\varphi$ (Δv is the volume change of the crystal lattice cell that contains the interstitial atom, $\sigma_{ii}(\boldsymbol{r},t)$ is the spherical component of the effective-stress tensor [7], e is the elementary charge, Z^* is the effective charge number, and φ is the electric potential of the current in the crystal). It follows from [10] that $\varphi = -\rho j_0\sqrt{2lr}\sin(\theta/2)$ as $|\boldsymbol{r}|/l \to 0$. Here $\rho = \rho_0[1+\alpha(T-T_0)]$ is the specific electric resistance of the crystal (ρ_0 is the specific electric resistance of the crystal at room temperature T_0 and α is the temperature coefficient of resistance). As $|\boldsymbol{r}|/l \to 0$, the asymptotic values of the current density $j_x = j_0\sqrt{l/(2r)}\sin(\theta/2)$ and $j_y = j_0\sqrt{l/(2r)}\cos(\theta/2)$ [10] correspond to the electric potential φ. In this case, from Eqs. (1) with allowance for $\Delta V = 0$ we obtain

$$\frac{\partial c(\boldsymbol{r},t)}{\partial t} = D\nabla^2 c(\boldsymbol{r},t) + \frac{Dc(\boldsymbol{r},t)}{k_{\mathrm{B}}T}\,\nabla c(\boldsymbol{r},t)\nabla V(\boldsymbol{r},t). \tag{2}$$

The problem is solved under the initial condition $c(\boldsymbol{r},0) = c_0$ and the boundary conditions

$$\frac{\partial c(\boldsymbol{r},t)}{\partial y} = \frac{eZ^*c(\boldsymbol{r},t)j_0\rho}{k_{\mathrm{B}}T}\sqrt{\frac{l}{2r}} \qquad \text{for} \quad y=0,\ x>0; \tag{3}$$

$$D\,\frac{\partial c(\boldsymbol{r},t)}{\partial y} = k_m(c^2(\boldsymbol{r},t) - (\Gamma')^{-1}P(t)) \qquad \text{for} \quad y=0,\ x<0 \tag{4}$$

and $c(\boldsymbol{r},t) = c_0$ as $|\boldsymbol{r}| \to \infty$. Relation (4) expresses the Ziverts law [3]. In (4), k_m is the constant of mass exchange at the interface between gaseous and solid phases, $P(t)$ is the gas pressure in the crack cavity, and Γ' is the modified Henry constant [3]. It is assumed that the gas in the crack cavity is ideal and, therefore, its pressure inside the crack $P(t)$ is given by [3]

$$P(t) = \frac{1}{2}\,\sigma_a'(t)\Big[\Big(1 + \frac{4GTN(t)}{\pi(1-\nu)(2l)^2\sigma_a'^2(t)}\Big)^{1/2} - 1\Big]. \tag{5}$$

Following [11], we calculate the number of hydrogen molecules in the crack cavity $N(t)$ by summing the point-defect flow through the crack edges into the cavity $\boldsymbol{J} = k_m\displaystyle\int_{-\infty}^{0}\Big[c^2(x,0,t) - (\Gamma')^{-1}P(t)\Big]\,dx$ over time:

$$N(t) = \int_0^t J(t)\,dt. \tag{6}$$

We now consider the method of solving problem (2)–(6). Following [3], we change the variable $c(\boldsymbol{r},t)$: $F(\boldsymbol{r},t) = c(\boldsymbol{r},t)\exp(V(\boldsymbol{r},t)/(2k_{\mathrm{B}}T))$. Then, Eq. (2) yields

$$\frac{\partial F(\boldsymbol{r},t)}{\partial t} = D\nabla^2 F(\boldsymbol{r},t) - D\,\frac{\nabla V(\boldsymbol{r},t)}{2k_{\mathrm{B}}T}\,F(\boldsymbol{r},t). \tag{7}$$

This equation is supplemented by the initial condition $F(\boldsymbol{r},0) = c(\boldsymbol{r},0)\exp(V(\boldsymbol{r},0)/(2k_{\mathrm{B}}T))$ and the boundary conditions

$$\frac{\partial F(\boldsymbol{r},t)}{\partial y} = F(\boldsymbol{r},t)\,\frac{eZ^* j_0 \rho}{2k_{\mathrm{B}}T}\sqrt{\frac{l}{2r}} \qquad \text{for} \quad x>0,\ y=0,$$

$$\frac{\partial F(\boldsymbol{r},t)}{\partial y} = k_m\,\frac{F(\boldsymbol{r},t)^2 - (\Gamma')^{-1}P(t)}{D} \qquad \text{for} \quad x<0,\ y=0,$$

$$F(\boldsymbol{r},t) = F(\boldsymbol{r},0) \qquad \text{for} \quad |\boldsymbol{r}|\to\infty.$$

As in [3], to obtain an approximate solution of Eq. (7), we replace the time t in the function $F(\boldsymbol{r},t)$, which enters the second term on the right side, by $t-\Delta t$ and solve the equation in the intervals $[t_i, t_{i-1}]$ $(t_{i-1} = t_i - \Delta t_i)$:

$$\frac{\partial F(\boldsymbol{r},t)}{\partial t} = D\nabla^2 F(\boldsymbol{r},t) - D\,\frac{\nabla V(\boldsymbol{r},t)}{2k_{\mathrm{B}}T}\,F(\boldsymbol{r},t-\Delta t).$$

The initial condition becomes $F(\boldsymbol{r},0) = c_0 \exp\left(V(\boldsymbol{r},0)/(2k_{\mathrm{B}}T)\right)$. In a similar manner, we obtain the boundary condition

$$\frac{\partial F(x,0,t)}{\partial y} = k_m\,\frac{F^2(\boldsymbol{r},t-\Delta t) - (\Gamma')^{-1}P(t-\Delta t)}{D} \quad \text{for} \quad x<0,\ y=0.$$

The increment Δt_i was determined in [7] for different algorithms of calculating the evolution of plastic strain. Under these simplifying assumptions, the classical solution of problem (2)–(5) satisfying the initial and boundary conditions considered has the form [12]

$$F(x,y,t_i) = \int\limits_0^\infty \int\limits_{-\infty}^\infty F(x_1,y_1,t_{i-1}) G_2(x,y,x_1,y_1,t_i)\,dx_1\,dy_1$$

$$- k_m \int\limits_{-\infty}^0 \left[F^2(x_1,0,t_{i-1}) - (\Gamma')^{-1}P(t_{i-1})\right]\left[\int\limits_0^{\Delta t_i} G_2(x,0,x_1,0,\Delta t_i - \tau)\,d\tau\right] dx_1$$

$$- \frac{D}{(2k_{\mathrm{B}}T)^2}\int\limits_0^\infty \int\limits_{-\infty}^\infty (\nabla V(\boldsymbol{r},t_{i-1}))^2 F(x_1,y_1,t_{i-1})\left[\int\limits_0^{\Delta t_i} G_2(x,y,x_1,y_1,\Delta t_i - \tau)\,d\tau\right] dx_1\,dy_1. \tag{8}$$

The technique of calculating the quantity $F(\boldsymbol{r},t)$ in (8) is described in [3]. Using the inverse change of the variable in the function $F(\boldsymbol{r},t)$, we determine the evolution of the concentration of the interstitial impurity atoms near the crack tip $c(\boldsymbol{r},t)$.

Let us consider the evolution of the stress-intensity factor (SIF) in a loaded current-conducting crystal. We assume that the SIF of the crack can be written in the form [7]

$$K(t) = K^c(t) + K^p(t),$$

where $K^c(t) = (\sigma_a'(t) + P(t))\sqrt{\pi l}$ and $K^p(t)$ is the term that takes into account the effect of plastic strain [7].

2. Calculation Results and Discussion. The calculations were performed for an α-Fe crystal with the following constants: $2l = 10^{-3}$ m, $T_0 = 300$ K, $Z^* = 1$, $\rho_0 = 8.6\cdot 10^{-8}$ $\Omega\cdot$m, $\alpha = 3.3\cdot 10^{-3}$ K^{-1}, $D = 4.88\cdot 10^{-12}$ m^2/sec, $\Delta v = 2.06\cdot 10^{-30}$ m^3, $e = 1.6\cdot 10^{-19}$ C, and $k_m = 4.88\cdot 10^{-9}$ m/sec [3]. The remaining constants were the same as in [7, 8].

The loading rate of the crystal was chosen so that the maximum strain rate in the plastic zone was equal to 0.1 sec^{-1}. After the external load $\sigma_a'(t)$ reached the upper limit $\sigma_a = 5$ MPa, it remained constant, and stress relaxation near the crack tip was observed.

We analyze the effect of electric current on the evolution of the point-defect distribution near the crack tip. Figure 1 shows the time evolution of the SIF for brittle and plastic cracks in the crystal with and without current. One can see that electric current causes additional stress relaxation near the crack tip. The calculations show that electric current decreases the SIF by approximately 10% compared to stress relaxation due to plastic strain near the crack tip. It should be noted that the following two factors lead to the decrease in the SIF: 1) an increase in temperature due to the Joule heat released, which intensifies the development of the plastic strain and, hence, leads to additional stress relaxation near the crack tip; 2) an increase in the "disposal" of hydrogen into the crack cavity and its transfer to the tip by the dislocation mechanism (lattice diffusion). The latter factor may be the

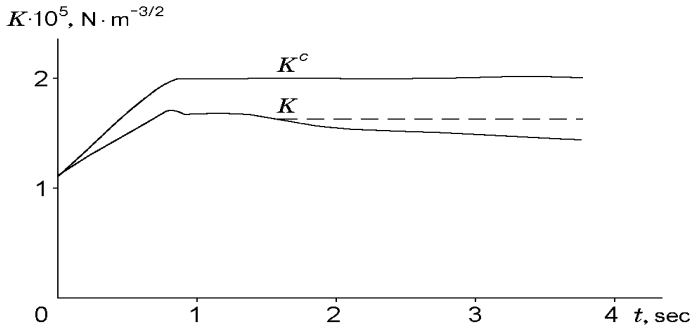

Fig. 1. SIF of the crack in the BCC lattice of the crystal in tension versus time: the curve K^c refers to the brittle crack, and the curves K refer to the crack with a plastic zone (the dashed curve corresponds to the case where electric current is absent, and the solid curve is obtained with allowance for direct electric current of density $j_0 = 5 \cdot 10^8$ A/m^2 at a large distance.)

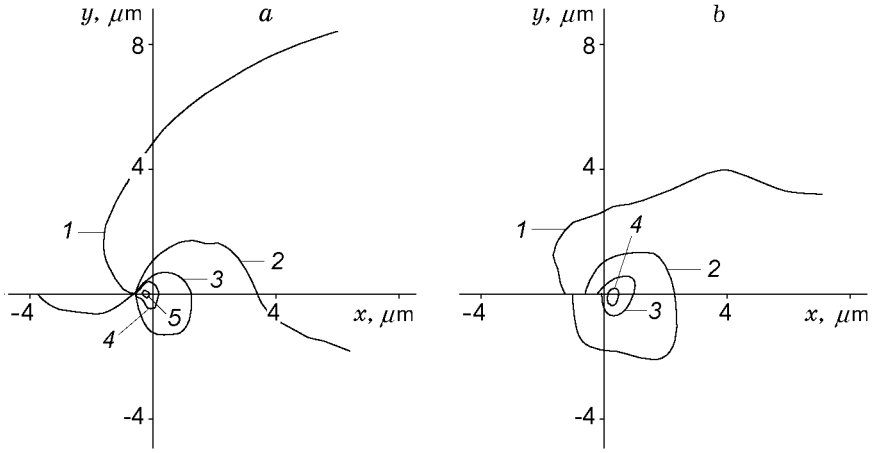

Fig. 2. Concentration of interstitial impurity hydrogen atoms near the crack tip for $j_0 = 10^8$ A/m^2 and $t = 0.268$ (a) and 5.715 sec (b): (a) $c(\boldsymbol{r}, t)/c_0 = 0.997$ (1), 1.01 (2), 1.03 (3), 1.04 (4), and 1.05 (5); (b) $c(\boldsymbol{r}, t)/c_0 = 1.02$ (1), 1.04 (2), 1.07 (3), and 1.10 (4).

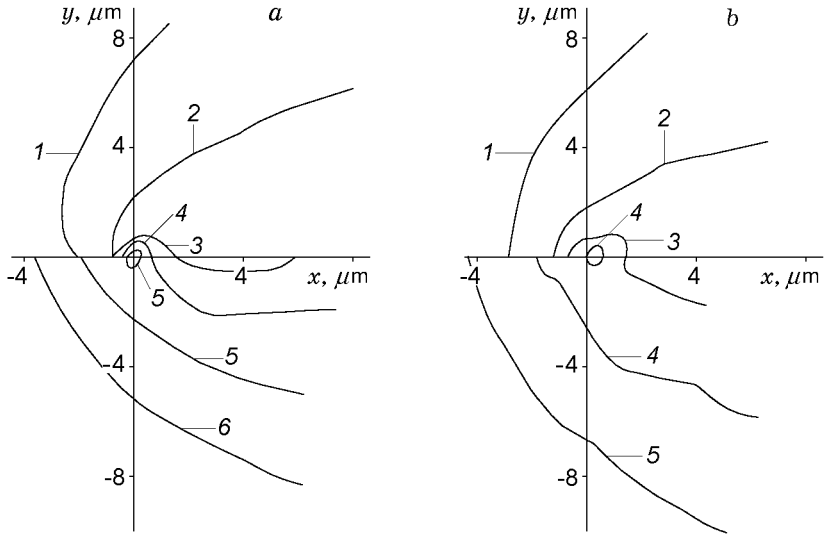

Fig. 3. Concentration of interstitial impurity atoms near the crack tip for $j_0 = 5 \cdot 10^8$ A/m^2 and $t = 0.143$ (a) and 4.1 sec (b): (a) $c(\boldsymbol{r}, t)/c_0 = 0.932$ (1), 0.957 (2), 0.983 (3), 1.01 (4), 1.03 (5), and 1.06 (6); (b) $c(\boldsymbol{r}, t)/c_0 = 0.936$ (1), 0.967 (2), 0.999 (3), 1.03 (4), and 1.06 (5).

reason for the increase in the SIF caused by "widening" of the crack. Figures 2 and 3 show the distribution of the concentration of interstitial hydrogen atoms near the crack tip for two values of electric-current density. One can see in Figs. 2 and 3 that the concentration of hydrogen is distributed asymmetrically about the line of crack. It is noteworthy that the sink of hydrogen atoms into the cavity of the crack through its contour containing the tip remains almost unchanged. In other words, the calculations show that, for reasonable current densities, it is experimentally impossible to reduce significantly the flow of hydrogen atoms filling the crack cavity.

REFERENCES

1. V. I. Spitsyn and O. A. Troitskii, *Electroplastic Deformation of Metals* [in Russian], Nauka, Moscow (1985).
2. V. E. Gromov, L. B. Zuev, and É. V. Kozlov, *Electrically Stimulated Plasticity of Metals and Alloys* [in Russian], Nedra, Moscow (1997).
3. D. N. Karpinskii and S. V. Sannikov, "Migration of point defects near a gas-filled crack," *Fiz. Metal. Metalloved.*, **85**, No. 2, 121–126 (1998).
4. S. M. Beloglazov, *Hydrogenization of Steel in Electrochemical Processes* [in Russian], Izd. Leningr. Univ., Leningrad (1975).
5. N. A. Ugodchikov and A. G. Berendeeva, "Numerical modeling of low-temperature nonstationary directed hydrogen diffusion," in: *Applied Problems of Strength and Plasticity: Methods of Solution* [in Russian], Izd. KMK, Moscow (1997), pp. 69–74.
6. S. D. Gertsriken and I. Ya. Dekhtyar, *Diffusion in Metals and Alloys in the Solid Phase* [in Russian], Fizmatgiz, Moscow (1960).
7. D. N. Karpinskii and S. V. Sannikov, "Calculation of the plastic-strain evolution near a crack tip and related phenomena," *Prikl. Mekh. Tekh. Fiz.*, **34**, No. 3, 154–160 (1993).
8. D. N. Karpinskii and S. V. Sannikov, "Effect of electric current on the evolution of plastic strain near a crack tip," *Prikl. Mekh. Tekh. Fiz.*, **42**, No. 5, 176–182 (2001).
9. D. N. Karpinskii and S. V. Sannikov, "Evolution of the point-defect concentration near a crack tip," *Fiz. Tverd. Tela*, **39**, No. 9, 1580–1585 (1997).
10. L. D. Landau and E. M. Lifshits, *Electrodynamics of Continuous Media* [in Russian], Nauka, Moscow (1995).
11. D. N. Karpinskii and S. V. Sannikov, "Plasticizing effect of hydrogen dissolved in a crystal on the evolution of plastic strain near a crack tip," *Fiz. Tverd. Tela*, **42**, No. 12, 2171–2174 (2000).
12. B. M. Budak, A. A. Samarskii, and A. N. Tikhonov, *Collected Problems of Mathematical Physics* [in Russian], Nauka, Moscow (1972).