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The effect of hydrogen on the mechanical properties of metals under conditions of high-speed deformation

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The movement of an ensemble of edge dislocations in metals with a high hydrogen content under conditions of high-speed deformation (high strain rate deformation) is theoretically analyzed. Within the framework of the theory of dynamic interaction of defects (DVD) (DID), an analytical expression is obtained for the dependence of the dynamic yield strength on the concentration of hydrogen atoms.

Keywords: dislocations, hydrogen, high-speed deformation, metals.

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Studying of hydrogen-charged metals and alloys is of great importance for both the development of fundamental science and for practical applications [1–11]. The interaction of hydrogen with metals is a very significant factors in nuclear power industry, steel-making, machine-building, oil-refining, and many other industries.

The presence of hydrogen in metals can result in negative (hydrogen embrittlement, hydrogen cracking, and hydrogen-induced destruction [3]), and positive consequences (plasticising of metals [11]). In addition, hydrogen is able to impact on metal properties with concentrations of about hundred thousandths of percent. There are tens of thousands of studies devoted to the impact of hydrogen on properties of metals and alloys.

However, there is a very interesting, yet insufficiently studied field of the interaction of hydrogen atoms with defects in the crystal, that is the field of high-speed deformation of hydrogen-charged metals where hydrogen concentration can be very high. This, first of all, is palladium, which is the most often used as a model metal when studying the interaction with hydrogen, as well as vanadium, niobium, tantalum and some other metals. High-speed deformation is implemented in both metal parts manufacture (forging, punching, cutting, dynamic channel-angular pressing) and operation in conditions of high-energy external impacts [12–17].

Hydrogen is the most frequently localized in interstices of the metal matrix, which results in the emergence of additional elastic stresses [2]. With high concentrations these stresses can be very strong. A hydrogen atom is a defect of dilatation center type. In case of high-speed deformation, mechanical properties of metals are strongly impacted by collective effects described in the theory of dynamic interaction of defects (DID) [18–23]. Due to high solubility in metals, hydrogen is able to impact significantly on the dynamics of dislocations, and, therefore, on the formation of mechanical properties of metals. At the same time an increase in the speed of plastic deformation leads to a higher impact of hydrogen atoms on mechanical properties of the metal, in particular, on the dynamic yield strength.

In this study an analytic expression for the contribution of hydrogen atoms to the dynamic yield stress of metals is derived and it is shown that this contribution can be quite considerable.

Let us assume that an ensemble of infinite edge dislocations under the action of a constant external stress σ_0 is uniformly moving in a metal that contains chaotically distributed hydrogen atoms. Dislocation lines are parallel to OZ axis, the Burgers vectors are parallel to OX axis, in the positive direction of which the dislocations slide with the constant velocity v. The sliding plane of the k-th dislocation coincides with XOZ plane, and its position is determined by the following function

$$W_k(y = 0, z, t) = vt + w_k(y = 0, z, t). \tag{1}$$

The vt term of the sum describes the motion of the dislocation center of mass at velocity v, and function $w(z, t)$ describes oscillations of the dislocation element arising from interaction with hydrogen atoms.

Equation of motion of the dislocation under study has the following form

$$m\left\{\frac{\partial^2 W_k}{\partial t^2} - c^2\frac{\partial^2 W_k}{\partial z^2}\right\} = b[\sigma_0 + \sigma_{xy}^{\mathrm{H}} + \sigma_{xy}^{dis}] - B\frac{\partial W_k}{\partial t}. \tag{2}$$

Here m — mass of dislocation unit length, b — modulus of the Burgers vector, B — damping constant due to phonon, magnon, electron or other dissipation mechanisms, characterized by the linear dependence of dislocation braking force on its sliding velocity, c — velocity of transverse sound waves in the crystal, $\sigma_{xy}^{p}, \sigma_{xy}^{dis}, \sigma_{xy}^{G}$ — components of the stress tensor created on the line of

κ-th dislocation by hydrogen atoms and dislocations of the ensemble, respectively.

The mechanism of dissipation in conditions of high-speed deformation consists in the irreversible transition of the external impact energy into the energy of lateral oscillations of dislocations in the plane of sliding. The efficiency of this mechanism depends on conditions of dislocation vibrations emergence. The higher is their amplitude, the higher is the loss of energy, the stronger is the force of dislocations braking and, respectively, the higher is the dynamic yield strength. The collective interaction of hydrogen atoms with a dislocation results in the formation of a potential well that moves over the crystal together with the dislocation. This well is the cause of a gap that appears in the dislocation oscillation spectrum, which is described by the following expression

$$\Delta = \Delta_{\mathrm{H}} = \frac{c}{b}\,(n_{\mathrm{H}}\chi^2)^{1/4}. \quad (3)$$

Here χ — parameter of hydrogen atom non-compliance, n_{H} — dimensionless concentration of these atoms.

Using the results of the DID theory, after necessary calculations we derive an expression for the contribution of collective interaction of hydrogen atoms with dislocations to the dynamic yield strength

$$\tau_{\mathrm{H}} = K\dot{\varepsilon}\sqrt{n_{\mathrm{H}}};\quad K = \frac{\mu\chi}{\rho bc}. \quad (4)$$

Here $\dot{\varepsilon}$ is the plastic deformation rate, ρ is the density of dislocations, μ is a shear modulus.

Let us make a numerical estimation. For $\mu = 5 \cdot 10^{10}$ Pa, $b = 4 \cdot 10^{-10}$ m, $n_{\mathrm{H}} = 10^{-2}$, $\chi = 10^{-1}$, $c = 3 \cdot 10^3$ m/s, $\dot{\varepsilon} = 10^6\,\mathrm{s}^{-1}$, $\rho = 10^{14}\,\mathrm{m}^{-2}$ we get $\tau_{\mathrm{H}} = 10^8$ Pa, i.e. the contribution of dynamic braking of dislocations by hydrogen atoms to the dynamic yield strength of hydrogen-charged metals in conditions of high-speed deformation can be tens of percents. Therefore, the dynamic braking of dislocations by hydrogen atoms impacts significantly on the mechanical properties of metals.

If, however, the density of dislocations achieves high values, then the main contribution to the formation of the gap is from their collective interaction. This takes place when the following inequality is satisfied

$$\rho > \frac{\chi\sqrt{n_{\mathrm{H}}}}{b^2}. \quad (5)$$

This case can be implemented with densities of dislocations $\rho = 10^{15}{-}10^{16}\,\mathrm{m}^{-2}$. Then the spectral gap can be described as follows

$$\Delta = \Delta_{dis} = \pi b\sqrt{\frac{\mu\rho}{6\pi m(1-\gamma)}} \approx c\sqrt{\rho}, \quad (6)$$

where υ is the Poisson ratio.

In this case the contribution of hydrogen atoms to the dynamic yield strength of metal depends linearly on the concentration of these atoms

$$\tau_{\mathrm{H}} = Dn_{\mathrm{H}}\dot{\varepsilon};\quad D = \frac{2(1-\gamma)\chi^2\mu}{\rho^2 b^3 c}. \quad (7)$$

Let us make a numerical estimation. For values of $\rho = 10^{15}\,\mathrm{m}^{-2}$, $\mu = 5 \cdot 10^{10}$ Pa, $b = 4 \cdot 10^{-10}$ m, $n_{\mathrm{H}} = 10^{-3}$, $\chi = 10^{-1}$, $c = 3 \cdot 10^3$ m/s, $\dot{\varepsilon} = 10^6\,\mathrm{s}^{-1}$ we get $\tau_{\mathrm{H}} = 10^8$ Pa.

Thus, the dynamic braking of dislocations by hydrogen atoms impacts significantly on the mechanical properties of metals under high-speed deformation.

Conflict of interest

The author declares that he has no conflict of interest.

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