HYDROGEN-DISLOCATION INTERACTIONS AND THEIR ROLE IN HELP MECHANISM OF HYDROGEN EMBRITTLEMENT

Y. Yagodzinskyy and H. Hänninen

Laboratory of Engineering Materials, Helsinki University of Technology,
FIN-02150 Espoo, Finland

ABSTRACT

Effects of hydrogen on elastic interactions in single dislocation dipole and dipole-like dislocation pile-up (DDP) were analysed. It was shown that there is no significant hydrogen shielding of elastic forces in the case of a single dislocation dipole, while hydrogen induces a notable effect on the elastic equilibrium of the DDP. Accumulation of hydrogen between adjacent dislocation pile-ups results in a reduction of external stresses which stabilises DDP. The tensile tests of hydrogen-charged austenitic stainless steel single crystals oriented for easy glide and observed hydrogen-induced strain localization are discussed in terms of such a dynamic softening. It is concluded that HELP takes place at the initial stages of plastic deformation.

1 INTRODUCTION

A significant progress in understanding of Hydrogen-Enhanced Localised Plasticity (HELP) mechanism has been recently achieved in studies based on the so-called hydrogen-induced localised softening effect [1,2]. Main idea of this approach takes into consideration material softening in micro-scale caused by enhanced dislocation mobility in the presence of hydrogen. This phenomenon has been evidenced in a variety of metals with different types of dislocations by using direct TEM observations with special environmental cells [1,3]. It has also been assumed that the dislocation mobility enhancement originates from hydrogen-induced elastic shielding of dislocation-dislocation(s) and dislocation-obstacles interactions.

Evaluations of the hydrogen elastic shielding effects for a single couple of edge dislocations evidence that its magnitude becomes substantial when the spacing between the dislocations is less than about ten lattice parameters [1]. Such a situation can be realised only in the case of severe plastic deformation, which results in an extremely high dislocation density. It has also been observed [4,5], that hydrogen affects the plastic flow of AISI 310 stainless steel and stable austenitic Cr-Ni-Mn steel single crystals at the initial stages, just after the yield point.

It seems that hydrogen has an effect on dislocation dynamics even at the stage of easy glide of dislocation. The purpose of the present study is to evaluate the hydrogen elastic shielding for typical cases of dislocation dipole configurations, which are characteristic at the initial stages of the plastic deformation.

2 HYDROGEN ELASTIC SHIELDING FORCES IN DISLOCATION DIPOLES AND DIPOLE-LIKE DISLOCATION PILE-UPS

Dislocation dipoles and dipole-like dislocation pile-ups are dominant elements of microstructures forming at the initial stages of plastic deformation of metals [6]. Dislocations emitted by a source stay on the same slip plane and interact elastically with dislocations produced by another source operating on an adjacent slip plane. Because of the attractive elastic forces, dislocations with opposite Burgers vectors, which are moving to opposite directions in the adjacent slip planes, can form dipole pairs or dipole-like dislocation pile-ups (DDP's). Both dislocation configurations are schematically shown in Fig. 1.

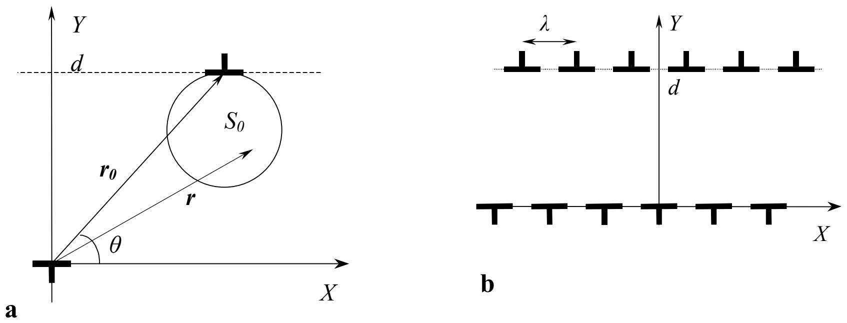

Figure 1. a) - Dislocation dipole with a dense hydrogen atmosphere in S_0, b) - Model of a DDP.

In the case of a dipole of edge dislocations with parallel Burgers vectors b_1 and b_2, the dislocation at the origin in Fig. 1a exerts on the dislocation on the adjacent slip plane a shear force [6]:

$$f_g = \frac{Gb_1 b_2}{2\pi(1-\nu)r_0}\cos\theta\cos 2\theta \ , \tag{1}$$

where G and ν are shear modulus and Poisson's ratio, respectively. One can see, that the dipole configuration of the opposite dislocations ($b_1 b_2 < 0$) has stable equilibrium position at $\theta = \pm\pi/4$ and an unstable equilibrium at $\theta = 0$. It is widely accepted that elastic shear forces (1) operating on the slip planes cause strain hardening at the initial stages of plastic deformation.

DDP (see Fig. 1b) has reduced elastic energy in comparison to the sum of the elastic energies of single dislocation pile-ups. The elastic stresses of DDP are mainly located between the opposite dislocation rows on the adjacent slip planes. When the distance between the slip planes $d >> \lambda$ (dislocation spacing, which is assumed equal within both rows), the elastic stresses σ between dislocation rows are approximated by [6]:

$$\sigma_i \approx \frac{2Gb}{\lambda(1-\nu)} \ , \tag{2}$$

where b is Burgers vector, which is the same for all of elemental dislocations in the rows.

Total energy accumulated per unit area of the DDP consists of a sum of the elastic deformation energy of the plane stresses (2) and the self-energy of the dislocation lines per unit area of both dislocation rows:

$$E_e + E_d \approx \frac{Gb^2}{(1+\nu)(1-\nu)^2}\frac{d}{\lambda^2} + \frac{Gb^2}{2\pi(1-\nu)}\frac{1}{\lambda}\ln\frac{d}{\rho_0}, \tag{3}$$

where $\rho_0 \approx b$ is the radius of the dislocation core.

The equilibrium hydrogen distribution in a non-uniform elastic stress field of a dislocation is described by an expression [6]:

$$c(\vec{r}) \approx \left(1 + \frac{1-c_0}{c_0}\exp\frac{w(\vec{r})}{k_B T}\right)^{-1}, \tag{4}$$

where k_B is the Boltzmann´s constant, T is temperature, c_0 is the average hydrogen content in metal expressed in H/Me units and

$$w(\vec{r}) = -\frac{1}{3\pi}\frac{1+\nu}{1-\nu}\frac{Gb\Delta V}{r}\sin\theta \tag{5}$$

is an energy of the elastic interaction of hydrogen (a dilatation centre inducing an extra volume ΔV) with a dislocation [6].

Edge dislocations of a dipole are subjected in the presence of hydrogen to an additional shear force per dislocation unit length:

$$f_H = a_0^{-3}\frac{\partial}{\partial x_0}\int_S d\vec{r}\cdot w(\vec{r})\cdot c(\vec{r},\vec{r}_0), \tag{6}$$

where a_0 is lattice constant. Taking into account only the contribution from S_0 one can obtain for the hydrogen shielding force (6) an approximation:

$$f_H(x_0) \approx -\frac{4}{9\pi}\frac{1+\nu}{1-\nu}\frac{Gb\Delta V}{a_0^3}\varsigma^2\frac{1-(\varsigma/2)}{(r_0^2-\varsigma d^2)^2}x_0 d^3, \tag{7}$$

where

$$\varsigma = \varsigma(c_0, T) = \frac{1}{3\pi}\frac{1+\nu}{1-\nu}\frac{G\Delta V}{k_B T\ln(1/c_0)}\frac{b}{d}.$$

It can be seen that the ratio f_H/f_g for typical parameter values of nickel, $\Delta V \approx 2$ cm^2/mol, G = 74 GPa, $a_0 = 3.54\times10^{-8}$ cm, $b = 2.5\times10^{-8}$ cm, and an average hydrogen concentration $c_0 = 10^{-3}$, is about $1.5\times10^{-2}\,b/d \ll 1$ at $T = 300K$ for any possible value of d. Conclusion is, thus, that hydrogen has no significant shielding effect on the elastic equilibrium dislocation dipole.

Using approximation (2) one can see, that the elastic energy change caused by a hydrogen atom association with a DDP:

$$w = \frac{1}{3}\sigma_i\cdot\Delta V \approx -\frac{2}{3}\frac{G\Delta V}{(1-\nu)}\frac{b}{\lambda} \tag{8}$$

depends strongly on the spacing λ between the dislocations in the pile-ups. It means that any variation of λ due to a variation of the external stresses stabilising the DDP will change the energy (8) and lead to hydrogen redistribution between the DDP (hydrogen trap) and solid solution by diffusion. In turn, if hydrogen starts to accumulate in a DDP, a reduction in dislocation spacing λ will occur, because the total elastic energy of the DDP starts to decrease. Finally, when λ is kept constant by an external stress and hydrogen concentration increases in the DDP, the magnitude of the external stabilising stress will decrease. The last effect may be interpreted as dynamic hydrogen-induced softening.

The total energy change per unit area of a DDP caused by accumulation of hydrogen in the case of its equilibrium distribution can be expressed as:

$$\Delta E_H = \frac{d}{a_0^3} w(\lambda) \cdot c(\lambda) , \tag{9}$$

where $c(\lambda) = c_0 \exp(w(\lambda)/k_B T)$ is the equilibrium concentration of hydrogen in the DDP. By using expression (9) together with (3) one can obtain for the elastic energy variation of a DDP in the presence of hydrogen:

$$\delta E \approx \frac{Gb^2}{(1-\nu)\lambda^2}\left[\frac{2d}{(1-\nu^2)\lambda} + \frac{1}{2\pi}\ln\frac{d}{r_0} - \frac{2}{3}\frac{\Delta V}{a_0^3}\frac{d}{b}\left(\frac{2}{3}\frac{G\Delta V}{(1-\nu)k_B T}\frac{b}{\lambda} + 1\right)c(\lambda)\right]\frac{\delta\lambda}{d} \ . \tag{10}$$

Since the elastic energy variation (10) is equal to the work $\delta R = \sigma_e \delta\varepsilon$ of plastic deformation done by the external stress σ_e, a softening effect $\Delta\sigma_e$ induced by hydrogen can be estimated as:

$$\Delta\sigma_e \approx \frac{2G}{3(1-\nu)}\frac{\Delta V}{a_0^3}\frac{d}{\lambda}\left(\frac{2}{3}\frac{G\Delta \nu}{(1-\nu)k_B T}\frac{b}{\lambda} + 1\right) \cdot \frac{c(\lambda)}{N} , \tag{11}$$

where N is the number of dislocations in the pile-up of a DDP. The expression (11) was obtained from (10) by assuming that plastic deformation $\delta\varepsilon$ corresponds to the variation in the dislocation spacing $\delta\lambda$ according to relationship $\delta\varepsilon \approx Nb\delta\lambda/\lambda d$. Comparison of the first and the third term in expression (10) using the above mentioned values of the parameters for nickel allows to conclude that hydrogen-induced softening can be up to 10 % of the magnitude of the external stress.

3 DISCUSSION

Plastic deformation of hydrogen-charged austenitic AISI 310 stainless steel [4] and Cr-Ni-Mn austenitic steel single crystals oriented for easy glide [5] demonstrates sharp yield point and increased flow stress (solid solution hardening) caused by hydrogen. The most important result obtained in [5] is the strain localization and reconstruction of the slip line heights caused by hydrogen already at the initial stages of deformation, when the planar slip of dislocations is predominant. Hydrogen induces more rough shear bands with a higher amount of slip, while between the shear bands plastic deformation is reduced.

Based on the above considerations, the softening effect described by expression (11) means that a higher amount of dislocations N can be involved in DDP´s and a higher local plastic deformation can be achieved within the shear bands in the presence of hydrogen. Actually, the hydrogen-induced enhancement of strain observed in the slip line relief [5] can reflect such a softening. The local enhancement of plastic deformation in glide the shear bands shifts the beginning of the macroscopic linear hardening, stage II, to higher strains as was also observed in [5].

The decrease of strain hardening coefficient in the stage II hardening of hydrogen-charged steel may originate from the fast climb reactions in the DDP's as proposed in [7]. In fact, the annihilation reactions caused by of opposite dislocations from adjacent pile-ups accompany generation of vacancies, which can, in turn, support many relaxation mechanisms leading to dynamic softening in the later stages of plastic deformation.

Due to trapping in DDP's, hydrogen will accumulate by diffusion redistribution in active shear bands and the areas adjacent to the shear bands become depleted of hydrogen. Such a redistribution of hydrogen may be a dominant process in the development of strain localization and various patterns of hydrogen effects on plastic flow, such as yield point, sharp Lüders bands and serrated flow. Any further progress in understanding these phenomena needs a more comprehensive and detailed study of hydrogen-DDP interactions.

4 CONCLUSIONS

Hydrogen does not provide any significant shielding effect on elastic interaction of edge dislocations in their dipole configuration while dipole-like dislocation pile-ups formed during planar slip can be effectively shielded by hydrogen. Hydrogen affects dynamic and elastic equilibrium of DDP's, that results in a notable softening effect under stabilising external stress and/or enhanced local plastic strain.

REFERENCES

1. Birnbaum H. K., Robertson I. M., Sofronis P., and Teter D., 'Mechanisms of hydrogen related fracture – A review', *Corrosion Deformation Interactions CDI'96*, *Nice, France, 1996,* The Institute of Materials, Great Britain, 172-195, 1996.
2. Sofronis P., Liang Y., and Aravas N., 'Hydrogen induced shear localization of plastic flow in metals and alloys', *Eur. J. Mech. A/Solids*, **20**, 857-872, 2001.
3. Robertson I. M., 'The effect of hydrogen on dislocation dynamics', *Engineering Fracture Mechanics*, **68**, 671-692, 2001.
4. Abraham D. P., and Altstetter C. J., 'The effect of hydrogen on the yield and flow stress of an austenitic stainless steel', *Met. Mater. Trans. A*, **26A**(11), 2849-2858, 1995.
5. Yagodzinskyy Y., Tarasenko O., and Hänninen H., 'Effect of hydrogen on plastic deformation of stable 18Cr-16Ni-10Mn austenitic stainless steel single crystal', *Hydrogen Effects in Materials and Corrosion Deformation Interaction*, A. W. Thompson and N. R. Moody eds., The Minerals, Metals & Materials Society, 201-210, 2003.
6. Hirth J. P., and Lothe J., *Theory of dislocations*, Malabar, Florida, 734 p., 1992.
7. Jagodzinskyy Yu. N., Larikov L. N., and Smouk A. Yu., 'Void formation in hydrogen charged metals induced by plastic deformation as the initial stage of embrittlement', *Hydrogen Effects in Materials*, A. W. Thompson and N. R. Moody eds., The Minerals, Metals & Materials Society, 375-384, 1996.