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C. R. Mecanique 337 (2009) 709–715

COMPTES RENDUS MECANIQUE

Plastic yielding and work hardening of single crystals in a soft device

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Received 17 June 2009; accepted 13 October 2009

Available online 22 October 2009

Abstract

An analytical solution to the problem of an anti-plane constrained shear of single crystals placed in a soft device within the continuum dislocation theory is found. The dependence of the nucleation stress on the grain size exhibits a modest deviation from the Hall–Petch relation. It is shown that, as soon as the dissipation is taken into account, the hardening behavior becomes nearly identical to that of single crystals in a hard device. ***To cite this article: K.C. Le, Q.S. Nguyen, C. R. Mecanique 337 (2009).***

Résumé

Déformation antiplane et écrouissage d'un monocristal lors d'un essai à bord libre. On propose une solution analytique du problème de déformation antiplane d'un monocristal lors d'un essai à bord libre dans le cadre de la théorie mathématique des dislocations. La dépendance de la contrainte limite en fonction de la taille du cristal dévie légèrement de la relation de Hall–Petch. On montre que le comportement d'écrouissage obtenu dans ce cas dissipatif est pratiquement identique au cas du monocristal sous déplacement controlé au bord. ***Pour citer cet article : K.C. Le, Q.S. Nguyen, C. R. Mecanique 337 (2009).***

Keywords: Continuum mechanics; Crystal; Twist boundary; Dislocation; Yielding; Hardening

Mots-clés : Milieux continus ; Cristal ; Joint de torsion ; Dislocation ; Déformation ; Écrouissage

1. Introduction

Plasticity in crystals and polycrystals is caused by nucleation, multiplication and motion of dislocations. Dislocations appear in the crystal lattice to reduce its energy. Motion of dislocations yields the dissipation of energy which, in turn, results in a resistance to their motion. The thermodynamics of gradient plasticity [1–3] must therefore reflect this physical reality: energy decrease by nucleation of dislocations and resistance to the dislocation motion due to dissipation. In recent years a number of problems have been solved within this continuum approach [4–8]. However,

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1631-0721/$ – see front matter
doi:10.1016/j.crme.2009.10.004

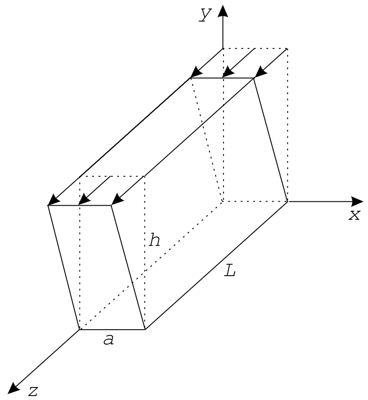

Fig. 1. Anti-plane constrained shear of single crystal in a soft device.

in all mentioned studies the crystals are always placed in a hard device which do not allow dislocations to reach the boundaries.

This paper aims at studying the plastic yielding and the work hardening of single crystals placed in a soft device representing the grain boundaries under an anti-plane constrained shear. Since screw dislocations may reach such boundaries, the energy of twist boundary must be taken into account in accordance with Read–Shockley formula [9]. This leads to the new type of the boundary conditions. We find the explicit solution to this problem which exhibits the energetic and dissipative thresholds for dislocation nucleation, the Bauschinger translational work hardening, and the size effect. The dependence of the nucleation stress on the grain size for crystals in a soft device turns out to be slightly different from that of Hall–Petch. Concerning the work hardening we show that, as soon as the dissipation is taken into account, the behavior of crystals is nearly identical to those in a hard device.

2. Anti-plane constrained shear

Consider a single crystal in form of a beam undergoing an anti-plane shear deformation. Let C be the cross section of the beam by planes $z = \text{const}$. For simplicity, we consider C to be a rectangle of the width a and height h, $0 < x \leqslant a$, $0 < y \leqslant h$. We place the crystal in a device with the prescribed displacement at the boundaries $y = 0$ and $y = h$ (see Fig. 1)

$$w = \gamma y \quad \text{at } y = 0 \text{ and } y = h$$

where $w(x, y, z)$ is the z-component of the displacement and γ corresponds to the overall shear strain. In contrary, the boundaries $x = 0$ and $x = a$ are "soft" in the sense that they may absorb dislocations, so, they model the true grain boundaries. The height of the cross section, h, and the length of the beam, L, are assumed to be much larger than the width a ($a \ll h$, $a \ll L$) to neglect the end effects and to have the stresses and strains depending only on one variable x in the central part of the beam. If the shear strain is sufficiently small, then the crystal deforms elastically and $w = \gamma y$ everywhere in the specimen. If γ exceeds some critical value, then the screw dislocations may appear. We allow only the slip planes parallel to the plane $y = 0$ and the dislocation lines parallel to the z-axis. For screw dislocations with the slip planes parallel to the plane $y = 0$, the tensor of plastic distortion, β_{ij}, has only one non-zero component $\beta_{zy} \equiv \beta$. We assume that β depends only on x-coordinate: $\beta = \beta(x)$. The plastic strains are given by

$$\varepsilon^{(p)}_{yz} = \varepsilon^{(p)}_{zy} = \frac{1}{2}\beta(x)$$

The only non-zero component of the tensor of dislocation density, $\alpha_{ij} = \varepsilon_{jkl}\beta_{il,k}$, is

$$\alpha_{zz} = \beta_{,x}$$

where the comma in indices denotes the spatial derivative with respect to the corresponding coordinate. Under the assumptions made the bulk energy density per unit volume of the crystal with dislocations takes a simple form

$$U = \frac{1}{2}\mu(\gamma - \beta)^2 + \mu k \ln \frac{1}{1 - \frac{|\beta_{,x}|}{b\rho_s}} \tag{1}$$

with μ the shear modulus, b the magnitude of Burgers' vector, ρ_s the saturated dislocation density, and k the material constant. The first term of (1) is the elastic energy, the second term the energy of the dislocation network [3]. The logarithmic energy term stems from two facts: (i) energy of the dislocation network for small dislocation densities is the sum of energy of non-interacting dislocations, and (ii) there exists a saturated dislocation density which characterizes the closest packing of dislocations admissible in the discrete crystal lattice. The logarithmic term [3] ensures a linear increase of the energy for small dislocation density ρ and tends to infinity as ρ approaches the saturated dislocation density ρ_s hence providing an energetic barrier against over-saturation. Since dislocations may reach $x = 0$ and $x = a$ forming there the twist boundaries, we ascribe to each of them the surface energy density [9]

$$\Gamma(\beta) = \Gamma_* \beta \ln \frac{e\beta_*}{\beta} \tag{2}$$

with $\Gamma_* = \frac{\mu b}{4\pi}$ and β_* the saturated misorientation angle. For $\beta > \beta_*$ we put $\Gamma = \infty$ which means that the grain boundary can no longer absorb dislocations.

If the resistance to the dislocation motion is negligible (and, hence, the dissipation is zero), the true plastic distortion minimizes the total energy, E, which is a functional of $\beta(x)$,

$$E\big[\beta(x)\big] = hL \int_0^a \left[\frac{1}{2}\mu(\gamma - \beta)^2 + \mu k \ln \frac{1}{1 - \frac{|\beta_{,x}|}{b\rho_s}}\right] \mathrm{d}x + hL\big[\Gamma\big(\beta(0)\big) + \Gamma\big(\beta(a)\big)\big] \tag{3}$$

among all admissible function $\beta(x)$. The integral in (3) is the bulk energy, while its last term corresponds to the energy of the free boundaries which may absorb dislocations. The total strain, γ, is regarded as a given function of time, so one can study the evolution of the dislocation network which accompanies the change of the total strain.

If the resistance to the dislocation motion cannot be neglected, then the energy minimization must be replaced by the variational equation

$$\delta E + hL \int_0^a \frac{\partial D}{\partial \dot\beta} \delta\beta \, \mathrm{d}x = 0 \tag{4}$$

For rate-independent plasticity we assume the dissipation potential in the form

$$D = K|\dot\beta| \tag{5}$$

From (4) and (5) one can obtain the evolution equation for β and the boundary conditions at $x = 0$ and $x = a$.

For small up to moderate dislocation densities the logarithmic term in (1) may be approximated by the formula

$$\ln \frac{1}{1 - \frac{|\beta_{,x}|}{b\rho_s}} \cong \frac{|\beta_{,x}|}{b\rho_s} + \frac{1}{2}\frac{\beta_{,x}^2}{(b\rho_s)^2}$$

We shall use further only this approximation.

3. Dislocation nucleation at zero resistance

We first analyze the situation when the resistance to the dislocation motion is negligible (and, hence, the dissipation is zero). In this case the determination of $\beta(x)$ reduces to the minimization problem (3). It is convenient to introduce the following dimensionless quantities

$$\bar x = xb\rho_s, \qquad \bar a = ab\rho_s, \qquad \bar\Gamma = \frac{b\rho_s \Gamma}{\mu}, \qquad \bar E = \frac{b\rho_s}{\mu hL} E \tag{6}$$

The functional (3) reduces to

$$E\big[\beta(x)\big]=\int_0^a\left[\frac{1}{2}(\gamma-\beta)^2+k\big|\beta'\big|+\frac{1}{2}k\beta'^2\right]\mathrm{d}x+\Gamma\big(\beta(0)\big)+\Gamma\big(\beta(a)\big) \tag{7}$$

where the prime denotes differentiation with respect to $\bar{x}$, and, for short, the bars over E, x, a and Γ are dropped.

Since β can be varied arbitrarily in the whole segment $[0,a]$, we first seek the minimizer in the form $\beta(x)=\beta_m$, where β_m is an unknown constant. Functional (7) becomes then a function of β_m

$$E(\beta_m)=\frac{1}{2}(\gamma-\beta_m)^2a+2\kappa\beta_m\ln\frac{e\beta_*}{\beta_m}$$

where $\kappa=\rho_s b^2/4\pi$. Its minimum is achieved when

$$\beta_m a+2\kappa\ln\frac{\beta_*}{\beta_m}=\gamma a \tag{8}$$

The function on the left hand side of (8) has a minimum equal to $2\kappa\ln\frac{e\beta_*a}{2\kappa}$ which is achieved at $\beta_m=2\kappa/a$. Thus, Eq. (8) has no positive root if $\gamma<\frac{2\kappa}{a}\ln\frac{e\beta_*a}{2\kappa}$. Returning to the original variables according to (6) we see that inequality $\gamma<\frac{2\kappa}{a}\ln\frac{e\beta_*a}{2\kappa}$ corresponds to the condition

$$\gamma<\gamma_{en}=\frac{b}{2\pi a}\ln\frac{e\beta_*2\pi a}{b} \tag{9}$$

Thus, for $\gamma<\gamma_{en}$ the minimizer β is zero and no dislocations are nucleated. Note that (9) is slightly different from that of Hall–Petch [10,11]. This can be explained by the fact that the Hall–Petch relation applies to polycrystals for which the grain boundary is not exactly the free boundary. The energy of the boundary between two adjacent grains will be the function of the jump in plastic distortion, so the Hall–Petch relation must be explained as a collective phenomenon of dislocation nucleation and pile-up. In our model the mechanism of dislocation nucleation is energy driven, and due to the specific expressions for the surface energy, it is preferable to have dislocations nucleated first at the grain boundaries, while no dislocations are formed inside the crystal. For $\gamma>\gamma_{en}$ Eq. (8) has two roots for $\beta_m>0$. By checking the second derivative of the energy, it can be shown that the only larger root minimizes the energy. So, as γ increases, $\beta=\beta_m$ increases up to the saturated value β_*, and dislocations are accumulated further at the grain boundaries.

After reaching the saturated value β_* (which corresponds to $\gamma=\beta_*$) the boundary conditions for β change to $\beta(0)=\beta(a)=\beta_*$. In this case we seek the minimizer in the form

$$\beta(x)=\begin{cases}\beta_1(x) & \text{for } x\in(0,l)\\ \beta_m & \text{for } x\in(l,a-l)\\ \beta_1(a-x) & \text{for } x\in(a-l,a)\end{cases} \tag{10}$$

where β_m is a constant, l an unknown parameter, $0\leqslant l\leqslant a/2$, and $\beta_1(l)=\beta_m$ at $x=l$. We have to find $\beta_1(x)$ and the constants, β_m and l. Since $\beta'>0$ for $x\in(0,l)$, the functional becomes

$$E=2\int_0^l\left[\frac{1}{2}(\gamma-\beta_1)^2+k\left(\beta_1'+\frac{1}{2}\beta_1'^2\right)\right]\mathrm{d}x+\frac{1}{2}(\gamma-\beta_m)^2(a-2l) \tag{11}$$

Function $\beta_1(x)$ is subject to the boundary conditions

$$\beta_1(0)=\beta_*,\qquad \beta_1(l)=\beta_m \tag{12}$$

The solution of (11) and (12) is quite similar to that found in [4]. In the interval $(0,l)$ we have

$$\beta_1(x)=\gamma+(\beta_*-\gamma)(\cosh\lambda x-\tanh\lambda l\sinh\lambda x) \tag{13}$$

where $\lambda=1/\sqrt{k}$. The length of the boundary layer l is the root of the following transcendental equation

$$2k=\frac{\gamma-\beta_*}{\cosh\lambda l}(a-2l) \tag{14}$$

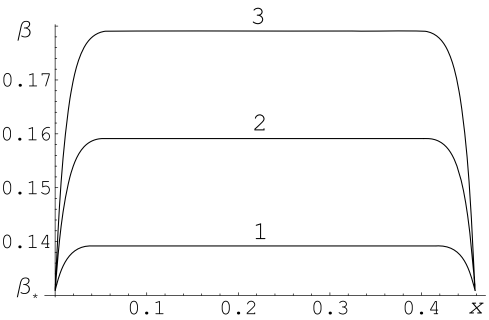

Fig. 2. Evolution of β: (1) $\gamma = 0.014$, (2) $\gamma = 0.016$, (3) $\gamma = 0.018$.

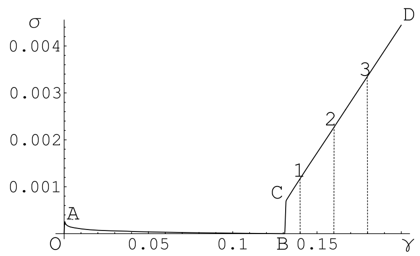

Fig. 3. Normalized average stress versus shear strain curve.

It turns out that Eq. (14) has no positive root if $\gamma \in (\beta_*, \beta_* + 2k/a)$, so $\beta(x) = \beta_*$ if γ lies in this interval. For $\gamma > \beta_* + 2k/a$ Eq. (14) has only one root in the interval $(0, a/2)$. Fig. 2 shows the evolution of $\beta(x)$ as γ increases ($\gamma > \beta_* + 2k/a$). For the numerical simulation we took $k = 1.56 \times 10^{-4}$, $\rho_s = 1.834 \times 10^{15}\ \mathrm{m}^{-2}$, $b = 2.5 \times 10^{-10}$ m, $a = 10^{-6}$ m, which are typical for aluminum, and $\beta_* = \pi/24$ so that $\bar{a} = ab\rho_s = 0.4585$.

Fig. 3 shows the normalized average shear stress

$$\bar{\sigma}/\mu = \frac{1}{a}\int_0^a \big(\gamma - \beta(x)\big)\,\mathrm{d}x$$

versus shear strain curve OABCD. There are a “softening” section AB for $\gamma \in (\gamma_{en}, \beta_*)$ according to the dislocation accumulation at the grain boundaries and a “work hardening” section CD for $\gamma > \beta_* + 2k/a$ due to the dislocation pile-up against the saturated twist boundaries, where points 1, 2, 3 correspond to the solutions shown in Fig. 2. Mention, however, that there is no residual strain as we unload the crystal by decreasing γ: the stress–strain curve follows the same path DCBAO, so the plastic deformation is completely reversible, and no energy dissipation occurs. In the course of unloading the dislocations nucleated annihilate, and as we approach the point A they all disappear.

4. Plastic distortion at non-zero resistance

If the resistance to the dislocation motion (and hence the dissipation) cannot be neglected, then the plastic distortion may evolve only in accordance with the variational Eq. (4), from which the following flow rule is implied

$$\left|\gamma - \beta + k\beta''\right| = \gamma_c \equiv K/\mu \tag{15}$$

Provided $\beta'(0) > 0$ and $\beta'(a) < 0$, this equation is subject to the boundary conditions

$$k + k\beta'(0) = \Gamma'\big(\beta(0)\big), \qquad k - k\beta'(a) = \Gamma'\big(\beta(a)\big) \tag{16}$$

which are also the consequences of the variational Eq. (4). Note that (15) and (16) are written in terms of the dimensionless variable $\bar{x} = xb\rho_s$, where the bar are dropped for short. We regard γ again as a given function of time (the “driving” variable) and try to determine $\beta(t, x)$. We consider the following close loading path: γ is first increased

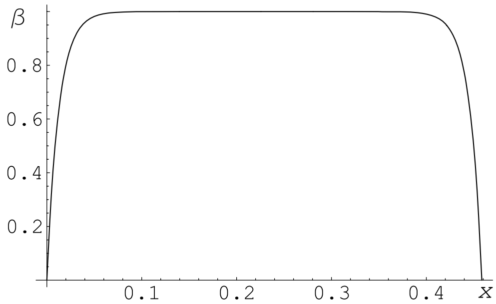

Fig. 4. The plot of $\beta(x)$ for $\gamma_r = 1$.

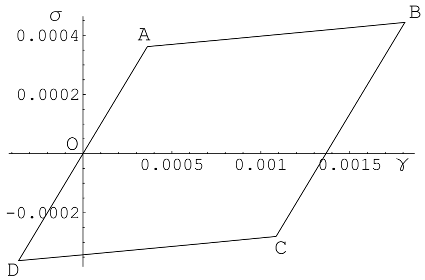

Fig. 5. Normalized average shear stress versus shear strain curve.

from zero to some value $\gamma^* > \gamma_c$, then decreased to $-\gamma_c$, and finally increased to zero. The rate of change of $\gamma(t)$ does not affect the results due to the rate independence of the dissipation. The problem is to determine the evolution of β as function of t and x, provided $\beta(0,x) = 0$. Since β is initially zero, we see from (15) that $\beta = 0$ as long as $\gamma < \gamma_c$. Thus, the dissipative threshold stress (the yield stress) $\sigma_y = K$ in this case.

For $\gamma > \gamma_c$ the yield condition

$$\gamma - \beta + k\beta'' = \gamma_c \tag{17}$$

takes place everywhere in $(0,a)$. It is convenient to introduce the deviation of $\gamma(t)$ from the critical shear, γ_c, $\gamma_r = \gamma - \gamma_c > 0$, and to seek the solution of (17) in the form

$$\beta(x) = \begin{cases} \beta_1(x) & \text{for } x \in (0, a/2) \\ \beta_1(a-x) & \text{for } x \in (a/2, a) \end{cases} \tag{18}$$

The boundary-value problem (17), (16) can be solved in exactly the same manner as in previous section. For $x \in (0, a/2)$ the solution reads

$$\beta_1(x) = \gamma_r + C\left(\cosh \lambda x - \tanh \frac{\lambda a}{2} \sinh \lambda x\right)$$

The constant C must be found from the boundary condition (16) yielding

$$k = kC\lambda \tanh \frac{\lambda a}{2} + \kappa \ln \frac{\beta_*}{\gamma_r + C}$$

Numerical calculations show that only the smaller root $C \approx -\gamma_r$ provides the assumed slops of $\beta(x)$ at the boundaries. Thus, $\beta(0) = \beta(a) \approx 0$, and the solution, which is proportional to γ_r, turns out to be quite close to that found for crystals in the hard device [4]. Fig. 4 shows the plot of $\beta(x)$ for $\gamma_r = 1$. The same can be said about the solution at the unloading. This property of the solution is due to the specific form of the Read–Shockley surface energy.

Fig. 5 shows the normalized average shear stress (or average elastic shear strain) versus shear strain curve for the above loading program. We took $\gamma_c = \gamma_{en}$, $\gamma^* = 5\gamma_c$, while all other parameters remain the same as in the previous section. The straight line OA corresponds to the purely elastic loading with γ increasing from zero to γ_c. The line AB corresponds to the plastic yielding. The yield begins at the point A with the yield stress $\sigma_y = K$. The work hardening due to the dislocation pile-up is observed. During the unloading as γ decreases from γ^* to $\gamma_* = \gamma^* - 2\gamma_c$ (the line BC) the plastic distortion $\beta = \beta^*$ is frozen. As γ decreases further from γ_* to $-\gamma_c$, the plastic yielding occurs (the line CD). The yield stress $\sigma_y = \mu\gamma^* - 2K$ at the point C, at which the inverse plastic flow sets on, is larger than $-K$ (because $\gamma^* > \gamma_c \equiv K/\mu$). Along the line CD, as γ is decreased, the created dislocations annihilate, and at the point D all dislocations disappear. Finally, as γ increases from $-\gamma_c$ to zero, the crystal behaves elastically with $\beta = 0$. In this close cycle OABCDO dissipation occurs only on the lines AB and CD. It is interesting that the lines DA and BC are parallel and have the same length. In phenomenological plasticity theory this property is modeled as the translational shift of the yield surface in the stress space, the so-called linear kinematic hardening.

5. Conclusion

In this paper we have shown that the anti-plane constrained shear problem for single crystals placed in a soft device can be analytically solved within the continuum dislocation theory. If the resistance to the dislocation motion is negligible, then there is a threshold stress for dislocation nucleation. The dependence of the nucleation stress on the specimen size is slightly different from that of Hall–Petch. If the resistance to dislocation motion is taken into account, then the stress–strain curve is nearly the same as that of crystals in a hard device.

Acknowledgements

The paper is written when K.C. Le visited LMS, Ecole Polytechnique, Palaiseau (France). The financial support of that Institute is gratefully acknowledged.

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