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Higher-Order Stress and Size Effects Due to Self Energy of Geometrically Necessary Dislocations

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Summary

The self energy of geometrically necessary dislocations (GNDs) is considered to inevitably introduce the higher-order stress work-conjugate to slip gradient in single crystals. It is pointed out that this higher-order stress stepwise changes in response to in-plane slip gradient and thus directly influences the onset of initial yielding in polycrystals. The self energy of GNDs is then incorporated into the strain gradient theory of Gurtin (2002). The resulting theory is applied to model crystal grains of size D, leading to a D^{-1}-dependent term with a coefficient determined by grain shape and orientation. It is thus shown that the self energy of GNDs induced by slip gradient accounts for the grain size dependence of initial yield stress and also the dislocation cell size dependence of flow stress in the submicron to several micron range of grain and cell sizes.

Introduction

As is well known, polycrystals exhibit the dependence of yield stress on grain size. The Hall-Petch relation is said to be an established one for this dependence in the conventional range of grain size. The Hall-Petch plot, however, usually has nonlinearity, as grain size is reduced from the conventional range. It is noted that the nonlinearity can occur around one to several microns of grain size, leading to the stronger, grain size dependence of yield stress than that by the Hall-Petch relation, as was observed in [1-3]. It is also noted that such fine grained polycrystals tend to clearly show initial yield points at stresses markedly depending on grain size [e.g., 1-3]. It is thus worthwhile to analyze the grain size dependence of yield stress in the submicron to several micron range of grain size.

The size effects mentioned above are targeted by the strain gradient theories of plasticity, which have been proposed in several studies so far, as was summarized in [4]. The theories are classified into two groups, i.e., higher-order and lower-order theories. Gurtin [5] developed a higher-order theory, in which a higher-order stress was introduced as the work-conjugate to slip gradient in single crystals. His theory seems promising for analyzing the size dependence of yield stress, because the constraint of slip on grain boundaries is explicitly represented using the additional boundary condition on slip. Okumura et al. [6] thus implemented his theory in a homogenization method to analyze the yield behavior of a 2D model polycrystal; however, no marked dependence on grain size was obtained with respect to initial yield stress.

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In this study, the self energy of geometrically necessary dislocations (GNDs) is considered to analyze the grain size dependence of yield stress. First, by discussing the self energy of GNDs in single crystals, the higher-order stress work conjugate to slip gradient is inevitably introduced. The self energy of GNDs is then incorporated into the strain gradient theory of Gurtin [5]. The resulting theory is applied to model crystal grains, so that an analytical prediction is derived for the grain size dependence of yield stress. The prediction obtained is compared with published experimental data on the grain size dependence of initial yield stress and the dislocation cell size dependence of flow stress.

Theory

We assume small deformation and employ Cartesian coordinates x_i $(i = 1, 2, 3)$. Hereafter, $(\ )_{,i}$ will indicate the differentiation with respect to x_i.

GNDs occur, if the slip in slip system β, $\gamma^{(\beta)}$, has gradient [7]. GNDs are, in general, mixed dislocations, as illustrated in Fig. 1, where $m_i^{(\beta)}$ and $s_i^{(\beta)}$ are the unit vectors indicating the slip plane normal and slip direction on slip system β, respectively, and $t_i^{(\beta)}$ is defined as $t_i^{(\beta)} = e_{ijk} s_j^{(\beta)} m_k^{(\beta)}$. Here e_{ijk} denotes the permutation symbol. Since mixed GNDs are decomposed into edge and screw components, the density of GNDs, $\rho_G^{(\beta)}$, is expressed as [7, 8]

$$\rho_G^{(\beta)} = b^{-1} \left[(\gamma_{,i}^{(\beta)} s_i^{(\beta)})^2 + (\gamma_{,i}^{(\beta)} t_i^{(\beta)})^2 \right]^{1/2}, \tag{1}$$

where b denotes the magnitude of the Burgers vector. Let us define the in-plane component of $\gamma_{,k}^{(\beta)}$ to be $\gamma_{,k\_}^{(\beta)} = (\gamma_{,i}^{(\beta)} s_i^{(\beta)}) s_k^{(\beta)} + (\gamma_{,i}^{(\beta)} t_i^{(\beta)}) t_k^{(\beta)}$. Eq. (1) then becomes

$$\rho_G^{(\beta)} = b^{-1} \left(\gamma_{,k\_}^{(\beta)} \gamma_{,k\_}^{(\beta)} \right)^{1/2}. \tag{2}$$

A single dislocation in an infinitely large single crystal has the following self energy per unit length: $E_0 = \alpha \mu b^2$, where α is a coefficient, and μ indicates the modulus of rigidity. Then, if the interaction among GNDs is negligible, and if α is assumed to be constant, the self-energy density of GNDs, $\psi^{(\beta)}$, is written as

$$\psi^{(\beta)} = \alpha \mu b^2 \rho_G^{(\beta)} \tag{3}$$

The above equation can be valid especially just after initial yielding, where $\rho_G^{(\beta)}$ is supposed to be low. Using Eqs. (2) and (3), the increment of $\psi^{(\beta)}$ is expressed as $d\psi^{(\beta)} = \xi_i^{(\beta)} d\gamma_{,i}^{(\beta)}$, where $\xi_i^{(\beta)}$ is the higher-order stress defined as

$$\xi_i^{(\beta)} = \alpha \mu b \nu_i^{(\beta)}, \tag{4}$$

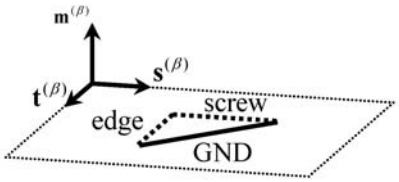


Figure 1: Mixed GND on slip system β.

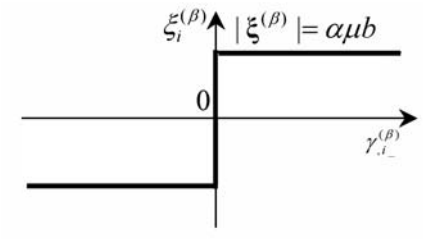


Figure 2: Step change of higher-order stress $\xi^{(\beta)}$ in response to in-plane slip gradient $\underline{\nabla}\gamma^{(\beta)}$.

and $v_i^{(\beta)}$ signifies the direction of in-plane slip gradient $\gamma_{,i\_}^{(\beta)}$, i.e.,

$$v_i^{(\beta)} = \gamma_{,i\_}^{(\beta)} \Big/ \left(\gamma_{,k\_}^{(\beta)}\gamma_{,k\_}^{(\beta)}\right)^{1/2}. \tag{5}$$

It is emphasized that $\xi_i^{(\beta)}$ is interpreted as the work-conjugate to slip gradient $\gamma_{,i}^{(\beta)}$. As seen from Eqs. (4) and (5), $\xi_i^{(\beta)}$ has the magnitude equal to $\alpha\mu b$ and stepwise changes in response to in-plane slip gradient $\gamma_{,i\_}^{(\beta)}$, as shown in Fig. 2. This stepwise variation in $\xi_i^{(\beta)}$, which is a consequence of the self energy of GNDs expressed as Eq. (3), brings about explicitly influencing the initial yielding of polycrystals.

The high-order stress $\xi_i^{(\beta)}$ derived above is now incorporated into the Gurtin theory [5]. He generally introduced the work-conjugate to slip gradient for the purpose of establishing a framework of strain gradient plasticity of single crystals. He proposed a variational principle in which displacement u_i and slip $\gamma^{(\beta)}$ independently have their variations δu_i and $\delta\gamma^{(\beta)}$. If only $\delta\gamma^{(\beta)}$ is considered in a region V, and if $\gamma^{(\beta)}$ is assumed to be either constrained or free on its boundary ∂V, his variational principle takes a form

$$\int_V \sigma_{ij}\delta\varepsilon_{ij}^p dV = \sum_\beta \int_V \left(k^{(\beta)}\delta\gamma^{(\beta)} + \xi_i^{(\beta)}\delta\gamma_{,i}^{(\beta)}\right) dV \tag{6}$$

where σ_{ij} and ε_{ij}^p indicate stress and plastic strain, respectively, and $k^{(\beta)}$ is the work-conjugate to slip $\gamma^{(\beta)}$ and is interpreted as slip resistance. Here, it is noted that $\varepsilon_{kl}^p = \sum_\beta \gamma^{(\beta)}\mu_{kl}^{(\beta)}$, where $\mu_{kl}^{(\beta)} = \frac{1}{2}(s_k^{(\beta)}m_l^{(\beta)} + m_k^{(\beta)}s_l^{(\beta)})$. The above equation then provides the following yield condition that needs to be satisfied in V [5]:

$$\tau^{(\beta)} - k^{(\beta)} + \xi_{i,i}^{(\beta)} = 0, \tag{7}$$

where $\tau^{(\beta)}$ denotes the resolved shear stress on slip system β, i.e., $\tau^{(\beta)} = \mu_{ij}^{(\beta)}\sigma_{ij}$.

Substitution of Eq. (4) into Eq. (6) gives

$$\int_V \sigma_{ij}\delta\varepsilon_{ij}^p dV = \sum_\beta \int_V \left(k^{(\beta)}\delta\gamma^{(\beta)} + \alpha\mu b\nu_i^{(\beta)}\delta\gamma_{,i}^{(\beta)}\right) dV \tag{8}$$

The above equation means that plastic work consists of the energy dissipation due to slip and the change in the self energy of GNDs.

Analysis of Model Grains

In this section, using the theory described in the preceding section, 2D and 3D model grains are analyzed by assuming a constant slip resistance (i.e., $k^{(\beta)} = k_0$) and no slip on grain boundaries (i.e., $\gamma^{(\beta)} = 0$ on ∂V).

Let us consider a circular grain of diameter D, for which Cartesian coordinates x, y and z are taken as shown in Fig. 3. Let us suppose that the grain has $s^{(\beta)}$ and $m^{(\beta)}$ oriented in the x- and z-directions, respectively. Then, the constraint of slip on ∂V causes in-plane slip gradient $\nabla\gamma^{(\beta)}$ to occur in the vicinity of ∂V. According to Eqs. (4) and (5), thus, $\xi^{(\beta)}$ develops so as to be directed from ∂V to the grain center; $\xi^{(\beta)}$has the magnitude equal to $\alpha\mu b$ in the vicinity of ∂V. Consequently, we have $\xi^{(\beta)} = -\alpha\mu bn$ on ∂V, where n indicates the outward unit normal to ∂V. Hence, using Eq. (7) and the divergence theorem, the average of $\tau^{(\beta)}$ in the grain, $\langle\tau^{(\beta)}\rangle$, is evaluated as

$$\left\langle \tau^{(\beta)} \right\rangle = k_0 + 4\frac{\alpha\mu b}{D}. \tag{9}$$

Let us apply Eqs. (4) and (7) to a spherical grain of diameter D (Fig. 4), in which $s^{(\beta)}$ and $m^{(\beta)}$ are oriented in the x- and z-directions, respectively. Let us suppose that slip $\gamma^{(\beta)}$ is about to occur in the whole grain. The constraint of slip on ∂V, then, causes $\nabla\gamma^{(\beta)}$ in the vicinity of ∂Von each cross-section perpendicular to the z-direction, as illustrated in Fig. 4. This results in $\xi^{(\beta)} = -\alpha\mu b\tilde{n}$ on ∂V, where $\tilde{n}$ denotes the outward unit normal to ∂V defined on each cross-section perpendicular to the z-direction. Then, using Eq. (7) and the divergence theorem, we derive

$$\int_V \xi_{i,i}^{(\beta)} dV = -\alpha\mu b \int_{\partial V} n_i\tilde{n}_i dA, \tag{10}$$

$$\left\langle \tau^{(\beta)} \right\rangle = k_0 + \frac{3\pi}{2}\frac{\alpha\mu b}{D} \tag{11}$$

Let us consider a tetrakaidecahedron grain of side length l, in which $m^{(\beta)}$ is oriented in either the [001] or [111] direction (Figs. 5(a), (b)). This grain has the volume equal to $8\sqrt{2}l^3$, so that the grain is supposed to have a diameter D satisfying $8\sqrt{2}l^3 = (\pi/6)D^3$. Then, applying Eqs. (7) and (10) to the grain gives

$$\left\langle \tau^{(\beta)} \right\rangle = k_0 + 5.16\frac{\alpha\mu b}{D}, \text{ if } m^{(\beta)} \text{ oriented in } [001], \tag{12}$$

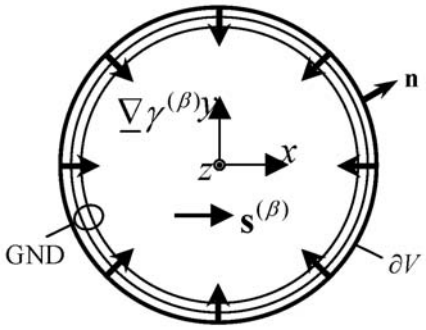


Figure 3: Circular grain.

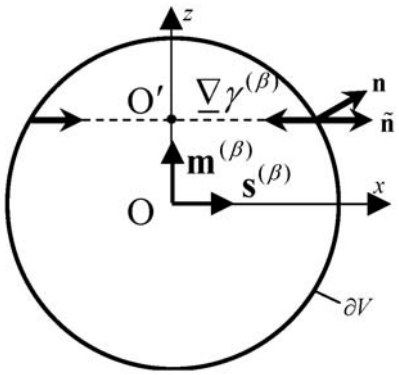
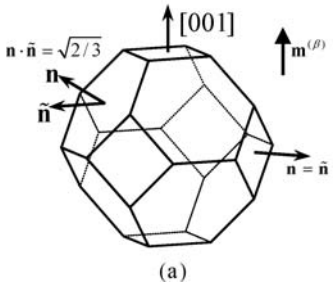


Figure 4: Spherical grain.



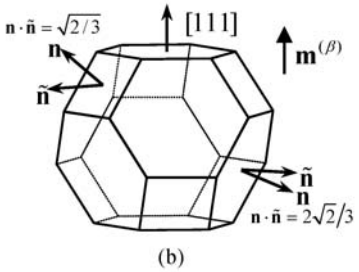


Figure 5: Tetrakaidecahedron grain; (a) $\mathbf{m}^{(\beta)}$ // [0 0 1], and (b) $\mathbf{m}^{(\beta)}$ // [1 1 1].

$$\left\langle \tau^{(\beta)} \right\rangle = k_0 + 4.82\frac{\alpha\mu b}{D}, \text{ if } m^{(\beta)} \text{ oriented in } [111]. \tag{13}$$

Comparison with Experiments

The second terms on the right-hand sides in Eqs. (9), (11), (12) and (13) are regarded as expressing the grain size dependence of critical resolved shear stress. Therefore, by introducing the Taylor factor M, the uniaxial tensile yield stress of polycrystals, σ_Y, is evaluated to be

$$\sigma_Y = \sigma_0 + M\Theta\frac{\alpha\mu b}{D}, \tag{14}$$

where $\sigma_0 = Mk_0$, and $\Theta \simeq 5$ according to Eqs. (12) and (13).

Fig. 6 compares the prediction by Eq. (14) and the published experimental data on the grain size dependence of σ_Y. For the prediction by Eq. (14), we have assumed that $M = 3$, and that α has the following expression based on dislocation loops of diameter D [9]:

$$\alpha = \frac{2-\nu}{8\pi(1-\nu)}\ln\left(\frac{4D}{r_0}-2\right), \tag{15}$$

which reduces to $\alpha = 0.10\ln(6.5\times10^3 D)$ by taking ν =0.33 and $r_0 \approx b/3$ with $b \simeq 2.5\times10^{-4}\mu$m: it is noted that the dislocation core energy has been taken into account by taking $r_0 \approx b/3$ [9]. For the experimental data, stresses at low offset strains 0.2% and 0.5% , $\sigma_{0.2}$ and $\sigma_{0.5}$, have been plotted as σ_Y, because no interaction among GNDs has been taken into account in deriving Eq. (14). It is seen from Fig. 6 that the prediction by Eq. (14), which has the D^{-1}-dependence of σ_Y, agrees considerably well with the experimental data in the submicron to several micron range of D. We therefore can say that the self energy of GNDs is responsible for the initial yielding of fine-grained polycrystals. Fig. 7 compares

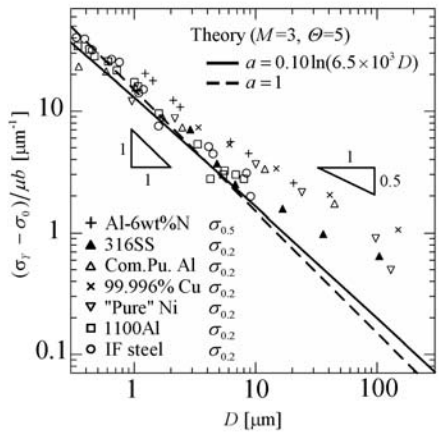


Figure 6: Prediction by Eq. (14) and experimental data on the dependence of initial yield stress on grain diameter **D**.

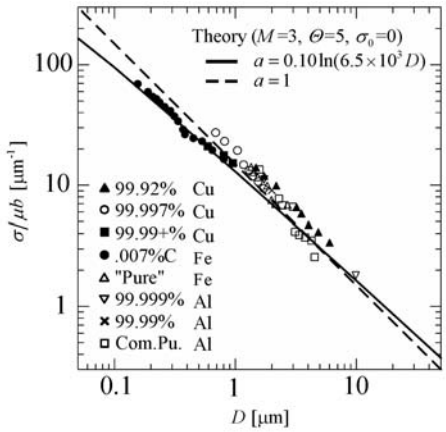


Figure 7: Prediction by Eq. (14) and experimental data on the dependence of flow stress on dislocation cell diameter **D**.

the prediction by Eq. (14) and the experimental data on the dependence of flow stress on the dislocation cell diameter D in the stage II. The experimental data in the figure were plotted by Stacker and Holt [10]. As seen from the figure, Eq. (14) is successful in predicting the experimental data. This allows us to say that the self energy of GNDs nicely accounts for the dislocation cell size dependence of flow stress in the stage II.

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