Numerical Modeling of Scale Dependent Mechanical Properties of Metal Polycrystals

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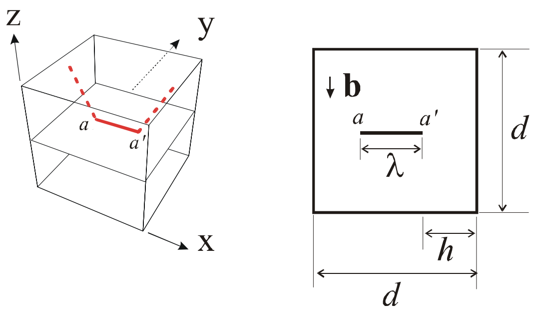
Abstract. Movement of dislocations and their interaction with grain boundaries during yielding process of metal polycrystals are numerically simulated . Simulation results show that when the size of FR source is close to grain diameter, the resolved shear stress needed to emit a dislocation loop increases sharply with decreasing grain size. This effect is introduced into the critical resolved shear stress, which is used in the continuum mechanics-based crystal plasticity analysis. Results of the analyses of polycrystal models show distinct increases of yield stress for specimens with smaller mean grain diameter. Evolution of GN dislocations in fine- and coarse-grained polycrystals are discussed.

Introduction

Scale dependent characteristics of mechanical properties of metal polycrystals are well known. In recent years, there have been many research efforts to model such effects into the theory of continuum mechanics (for example, Ohashi [(1)]). However, scale dependent characteristics of the yield stress are not yet fully understood in terms of mechanics and there are a lot of points to be studied. In this paper, we consider the first step of slip deformation in a crystal grain where dislocations are emitted from a Frank-Read type dislocation source. The dislocation source length cannot be larger than the grain size and this fact brings about a strong size effect of yield stress in single crystals [(2)]. Similar and even more complex phenomena take place in grains of polycrystals [(3)]. In this paper, we first consider the initial movement of a dislocation arc that expands from a FR source and its interaction with grain boundaries. To simulate such a process, we use a three-dimensional dislocation dynamics simulation package MDDP [(4)] and find the minimum resolved shear stress for the FR source to emit at least one closed loop. Results of the dislocation dynamics simulations are then modeled into the expression of critical resolved shear stress of slip systems, which is used in the continuum mechanics-based crystal plasticity analyses of a six-grained polycrystal model under tensile load.

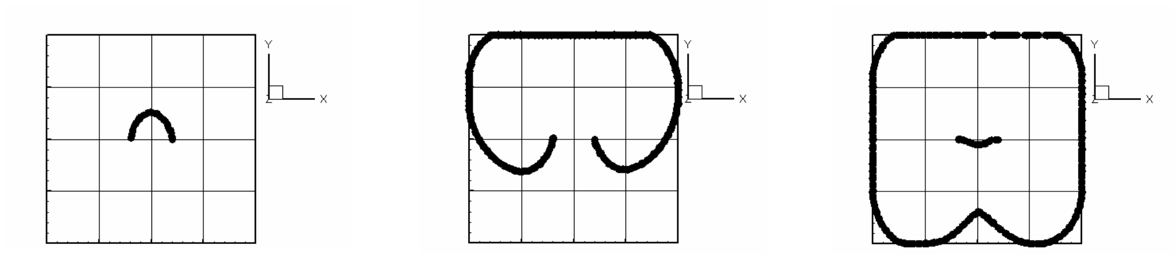
Dislocation dynamics simulation

Let us assume a cuboidal-shaped single crystal specimen of copper (Fig. 1). Six surfaces of the specimen correspond to grain boundaries, and movement of dislocations is confined to the interior of the specimen. The dimension of the slip plane which is trimmed by four grain boundary planes is $d \times d$ and a dislocation segment of length λ is placed on it. Both ends of the dislocation segment are assumed to be pinned and cannot move.



(a) (b)

Fig.1 (a) Cuboidal-shaped crystal grain employed for the dislocation dynamics simulation. A dislocation segment *aa*' lies on the slip plane and operates as a Frank-Read source. (b) Geometry of the slip plane, Frank-Read source and Burgers vector.



(a) (b) (c)

Fig. 2 Formation of a closed dislocation loop in a crystal grain surrounded by rigid walls. Sizes for the grain and the FR source are d=1 and λ=0.2 μm, respectively. At this condition, $\tau_{\infty} = 60.375 MPa$ and the applied shear stress is $\tau = 1.027\tau_{\infty}$.

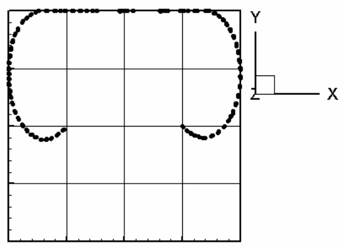


Fig. 3 Expansion of a dislocation arc when d=1 and λ=0.5 μm. $\tau = 1.9\tau_{\infty}$ is applied.

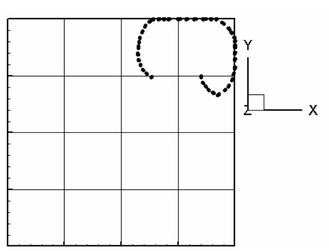


Fig. 4 Growth of dislocation arc that is generated from a FR source near the grain boundary. d=1 and λ=0.2 μm. $\tau = 1.027\tau_{\infty}$ is applied.

We simulate the movement of dislocations when a constant shear stress τ is applied to the specimen. Fig. 2(a)-(c) show snap shots of dislocation movement for the case when $\lambda = 0.2\mu m$, $d = 1\mu m$ and $\tau = 1.027\tau_{\infty}$, where $\tau_{\infty} = \mu\tilde{b}/\lambda$. Some parts of the dislocation line hit grain boundary planes (Fig. 2(b)), but the dislocation continues to expand and makes up a closed loop (Fig. 2(c)). Fig. 3 shows the results when $\lambda = 0.5\mu m$, $d = 1\mu m$ and $\tau = 1.9\tau_{\infty}$. In contrast to the results shown in Fig. 2, growth of the dislocation arc stopped after it hit grain boundaries and makes the shape shown in Fig. 3. Larger stress is needed to form a closed dislocation loop.

Let us assume a crystal grain with a certain grain size and assume that there can be FR sources with any size smaller than the grain. Applied stress gradually increases from zero. On one hand, the FR source with the largest size will become activated before the smaller ones, because τ_{∞} is inversely proportional to the size λ of the FR source. On the other hand, a *large* FR source with a size as large as the grain diameter cannot fully operate to form a closed loop at an initial stage of yield, since some parts of the dislocation arc may hit the grain boundaries at an early stage of its growth and it cannot fully grow until shear stress much larger than τ_∞ is applied and, subsequently, smaller FR sources may be activated. The stress needed to form a closed loop is also dependent on the position of the FR source. Fig. 4 shows the result when sizes for the FR source and the grain and the applied stress are the same to the ones used in Fig. 2. When the FR source is positioned close to the grain boundary, the minimum stress to emit a closed loop is larger.

This discussion indicates that there is an optimal size of FR source between zero and the grain size, from which a fully developed dislocation loop can be formed at the minimum stress level. Such a FR source should be placed somewhere near the center of the grain. We simulate dislocation emission from a FR source that is placed at the center of the grain. Various combinations of sizes for FR source and grain are chosen. The minimum shear stress τ_{thresh} (critical stress) at which the FR source emits only one closed loop is searched by DD simulation for various conditions of grain and FR source sizes. Details of the simulations are described in Ohashi *et al.* [5].

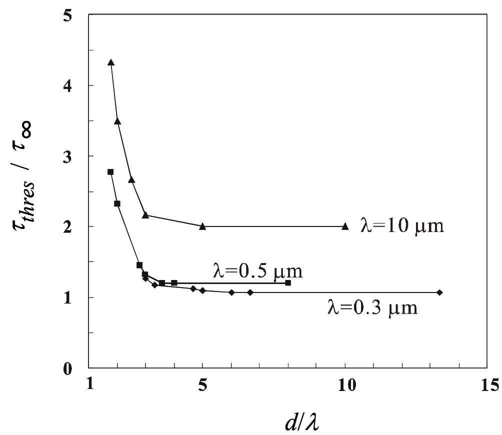


Fig. 5 Dislocation dynamics simulation results for $\tau_{thres} / \tau_\infty$ as a function of d / λ.

The results obtained are shown in Fig. 5. When the ratio of the grain size to FR source length is sufficiently large ($d / \lambda \gg 3$), the stress needed for a FR source to emit a dislocation loop does not depend on the grain size, while in the region $d / \lambda < 3$, the ratio $\tau_{thresh} / \tau_\infty$ rapidly increases with reduction of grain size. This fact, in turn, indicates that when shear stress is gradually applied to a crystal grain with a certain grain diameter, a FR source with length nearly equal to 1/3 of the grain diameter and positioned near the center of the grain emits the first dislocation loop. The minimum shear stress needed to emit a dislocation loop is then given as a function of grain size *d* by

$$\tau = \beta \frac{\mu \tilde{b}}{(d/3)} = 3\beta \frac{\mu \tilde{b}}{d}, \qquad (1)$$

when there are no obstacles to the expansion of a dislocation arc other than grain boundaries. Coefficient β, which is defined by the ratio of the level-off stress and τ_∞, is dependent on the FR source length λ and other factors, but its dependence on λ is weak.

Extended Bailey-Hirsch model for the critical resolved shear stress

Let us implement the results of the dislocation dynamics simulations into the continuum mechanics-based crystal plasticity theory. Fig. 6 schematically illustrates the obstacle effects of grown-in dislocations and grain boundary plane. Dislocation arc emitted from a dislocation source has to intersect with grown-in dislocations and pile up at the grain boundary plane.

These process contribute to raise the critical resolved shear stress. If slip resistance by grown-in dislocations or other obstacles play as much of a role as the grain boundaries do, we can simply add this slip resistance to give the extended Bailey-Hirsch type model for the critical resolved shear stress (CRSS) [(5)]:

$$\theta^{(n)} = \theta_0(T) + \sum_{m=1}^{12} \Omega^{(nm)} a\mu\tilde{b}\sqrt{\rho_S^{(m)}} + 3\beta \frac{\mu\tilde{b}}{d} \tag{2}$$

where $\rho_S{}^{(m)}$ is initially the density of grown-in dislocations and then the density of SSDs on slip system *m*.

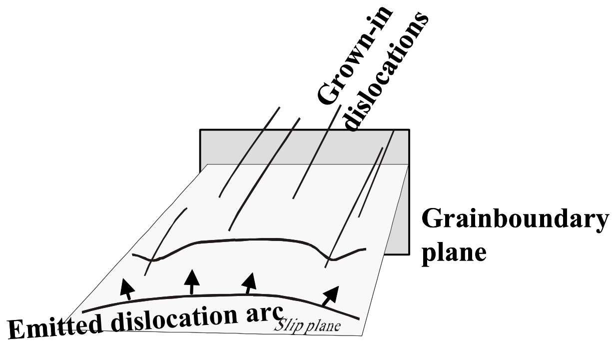


Fig. 6 Schematic illustration for the slip resistance of moving dislocation arc.

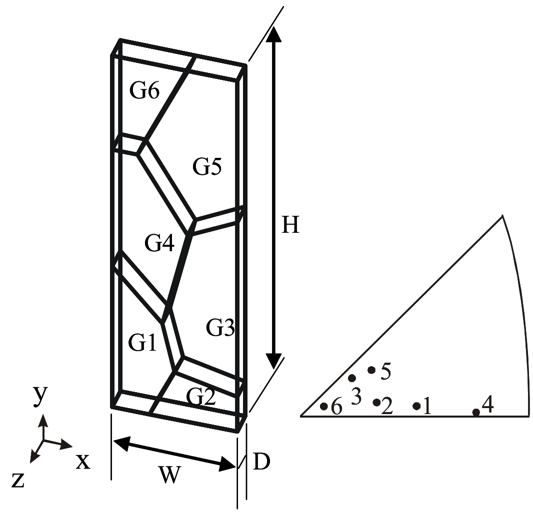


Fig.7 Six-grained polycrystal model employed in this study.

Continuum mechanics-based crystal plasticity analysis of yielding of polycrystals

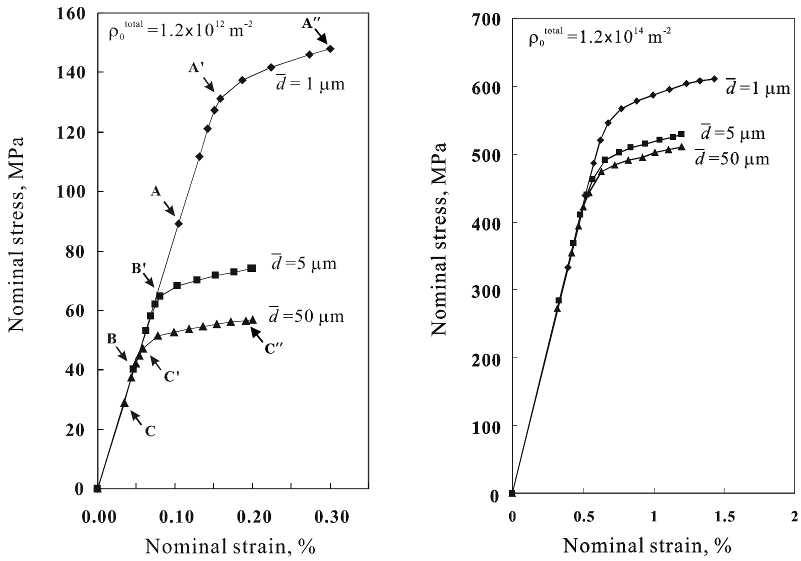
Fig. 7 shows the polycrystal model employed in this study. There are six crystal grains of polygonal shaped plate. The proportion of the specimen is *W*:*H*:*D*=5:15:1 and we use three similar specimens of *W*=1, 5 or 15 μm. The material is assumed to be pure copper and there are twelve {111}<110> slip systems. Tensile load is applied to the specimen and slip deformation is analyzed by a crystal plasticity software code with the CRSS given by eq. (2). $\beta = 1$ is used. Representative length scale *d* of each crystal grain in the model is calculated by the following equation,

$$\pi\left(\frac{d}{2}\right)^2 = (area\,of\;\;polygon)\ . \tag{3}$$

Mean grain diameter $\bar{d}$ is close to the width of the specimen *W* and we suppose $\bar{d} = W$. Grown-in dislocations are distributed uniformly on twelve slip systems. We analyze three cases for the initial dislocation density where the total of the initial dislocation densities on slip systems are $1.2\text{x}10^{12}$, $1.2\text{x}10^{13}$ or $1.2\text{x}10^{14}$ m^{-2}.

Fig. 8(a) and (b) show stress-strain curves obtained when the total initial dislocation densities are 1.2×10^{12} and $1.2 \times 10^{14}\,m^{-2}$, respectively. Points A, B, and C in Fig. 8(a) indicate the onset of plastic slip deformation in the specimen, which we call microscopic yield points, while points A', B' and C' are macroscopic yield points where we observe distinct deviations from linear elastic line in the deformation curve. The smaller the mean grain diameter is the larger are the macroscopic and microscopic yield points. Scale dependent character of yield stress becomes less prominent when the initial dislocation density is larger (Fig. 8(b)). The reason for this effect is that the second term in the right hand side of Eq. (2) plays major role when the initial dislocation density is large.

Scale dependent characteristics of the macroscopic yield stresses σ_y are summarized in Fig. 9. The macroscopic yield stresses increase approximately linearly with the inverse of the mean grain diameter.



(a) (b)

Fig. 8 Stress-strain curves of six-grained polycrystal models when mean grain diameter $\bar{d}$ is 1, 5 or 50 μm and when the initial dislocation density is (a) 1.2×10^{12}, and (b) 1.2×10^{14} m^{-2}.

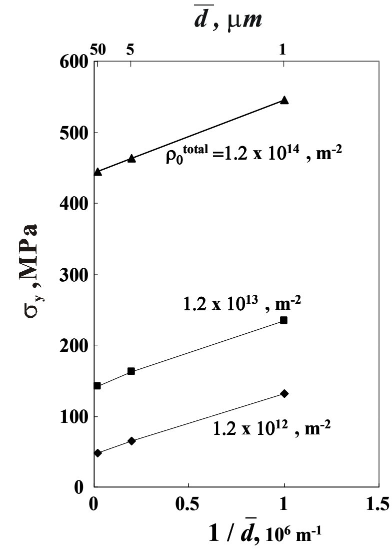


Fig. 9 Macroscopic yield stress plotted as against the inverse of the mean grain diameter.

Fig. 10(a) shows the density histogram of the geometrically necessary (GN) dislocations on the primary slip system $(11\bar{1})[101]$ in the specimens with the mean grain diameter $\bar{d}$ =1 and 50 μm at the deformation stage of macroscopic yielding (points A' and C' in Fig. 8(a)). The total initial density of SS dislocations on twelve slip systems is 1.2×10^{12} m^{-2}. Histogram of the GN dislocation density has its peak between 10^{12} and 10^{13} m^{-2} in the specimen with $\bar{d}$ =1 μm, while the peak in the specimen with $\bar{d}$ =50 μm is at about 10^{11} m^{-2}. The smaller the mean grain diameter is the larger is the GN dislocation density, even when the plastic deformation is very small.

Fig. 10(b) shows the density histogram of the two specimens when the plastic part of the nominal strain is about 0.125% (points A'' and C'' in Fig. 8(a)). The peak of the density in the specimen with $\bar{d}$ =1 μm largely shifts to a higher value, showing that plastic strain gradient inside crystal grains developed significantly. On the other hand, position of the peak in the histogram for the specimen with $\bar{d}$ =50 μm does not change largely. Accumulation of GN dislocations in polycrystal with large grains is moderate.

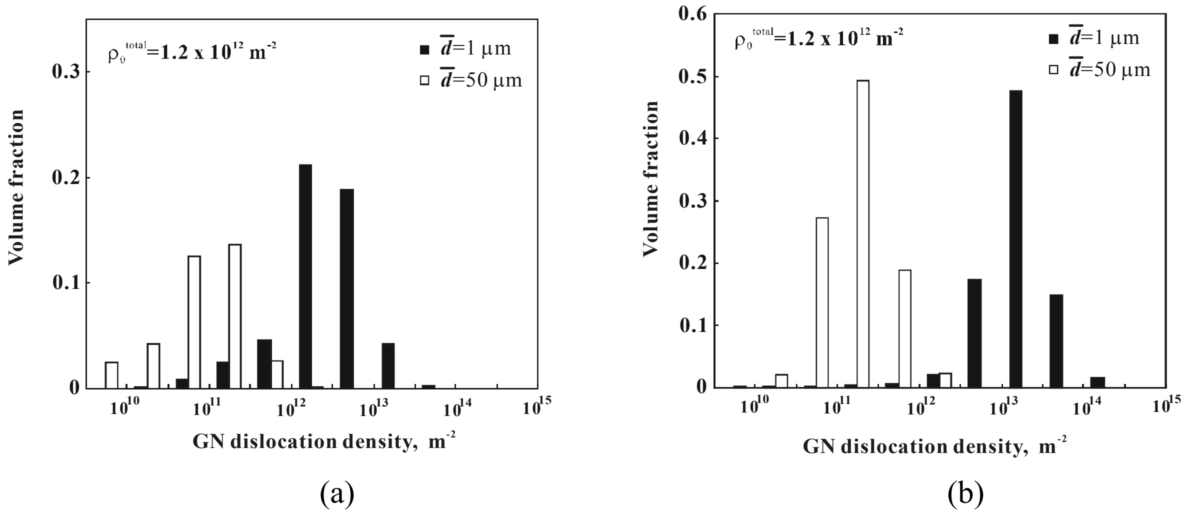


Fig. 10 Histograms of the GN dislocation density on the primary slip system. (a) Histograms at the macroscopic yield points A' and C' and (b) Histograms when the plastic part of the nominal strain is about 0.125%.

Summary

Expansion of dislocation arcs emitted from a Frank-Read type dislocation source inside a crystal grain were simulated by three dimensional dislocation dynamics technique and effects of grain boundaries on the movement of dislocations were introduced into a continuum mechanics based crystal plasticity models. Results of the continuum mechanics analysis of six-grained polycrystal models under uniaxial tensile load showed scale dependent yield stresses. Evolution of the geometrically necessary dislocations in coarse- and fine-grained polycrystal models were discussed.

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