DEFECTS INTERACTION CONDITIONS IN NEAR-FIELD OF GRAIN BOUNDARIES

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Summary A new condition of dislocation-grain boundary interaction was proposed to describe the experimental results of nanoindentation to the inhomogeneous near-field of GB. The conventional conditions proposed so far were also calculated using ideal bicrystal model with <110> symmetric tilt GB. It was found that the already proposed *M*-value was much sensitive to misorientation angle and newly defined *L*- or *L'*-values could be applied for the indentation problem subjected to uniform compression.

INTRODUCTION

The Hall-Petch (H-P) relationship is the well-established strengthening of materials by the interaction between dislocation and grain boundary (GB). Even when the yield stress is defined as a *x*%-offset yield strength, such as 0.2% (normal proof), 5%, or 10%, the H-P law of $\sigma_{x\%} \propto d^{-1/2}$ still holds, where *d* is the average grain diameter [1]. However, microscopic mechanisms of dislocation-GB, -dislocation, and -the other defects interactions might be dependent to each plastic deformation state. Above all, the dislocation-GB interaction has many crystallographic and mechanical aspects, because the GB stability (energy) and fracture stress significantly change according to the misorientation angle [2]. In general, the yielding of polycrystals is microscopically resolved into the slip transfer across GB, or the nucleation of dislocations in the near-field of GB due to the internal stress. Although the H-P effect is a stochastic consequence of such fundamental mechanisms, there is no way to detect such an individual one. Nanoindentation is a potential tool for the measurement of incipient plasticity [3], and therefore it can be applied to detect the inhomogeneous dislocation-GB interactions directly [4].

In the present paper, a new boundary interaction condition is proposed calling *L*- or *L'*-value which considers both slip transfer and dislocation nucleation under uniform compression normal to surface to understand the experimental results obtained by nanoindentation. These defined values are compared with the already proposed criteria of *N*-value with respect to a stress tensor transformation between two grains [5], *M*-value to shear force vector transformation [6] and *LRB*-condition which takes in a Burgers vector of the residual dislocation [7]. The properties of these values are numerically investigated using the ideal bicrystal model with <110> symmetric tilt GB of copper.

BOUNDARY INTERACTION CONDITIONS

Criteria of slip transfer model

Simple criteria to express the boundary interactions have been proposed from crystallographic and mechanical perspectives. Imagine that two grains A and B with an intermediary GB are subjected to uniform compression σ_{33} normal to the surface. A stress tensor transformation between two grains can be used to evaluate a ratio between the resolved shear stresses (RSSs) of two grains, which is called *N*-value [5]. Thus, the *N*-value can be determined by using only slip systems of two grains.

$$N = \max_{\alpha=1,12}\{\tau_{\mathrm{B}}^{\alpha} / \tau_{\mathrm{A}}^{\mathrm{P}}\} = \max_{\alpha=1,12}\{(\boldsymbol{n}^{\mathrm{P}} \cdot \boldsymbol{g}^{\alpha})(\boldsymbol{g}^{\mathrm{P}} \cdot \boldsymbol{n}^{\alpha}) + (\boldsymbol{g}^{\mathrm{P}} \cdot \boldsymbol{g}^{\alpha})(\boldsymbol{n}^{\mathrm{P}} \cdot \boldsymbol{n}^{\alpha})\}, \tag{1}$$

where ($\boldsymbol{n}^{\mathrm{P}}$, $\boldsymbol{g}^{\mathrm{P}}$) are the slip system (normal unit vector of the slip plane and glide unit vector, respectively) of grain A with a preferentially emitted dislocation, and ($\boldsymbol{n}^{\alpha}$, $\boldsymbol{g}^{\alpha}$) represent the α-slip system of adjacent grain B. A higher *N*-value suggests a larger transformed stress for dislocation emission in the adjacent grain. However, this value doesn't consider the geometric information of intersection of slip plane and GB.

Considering the slip transfer across GB plane, the following *M*-value was proposed and successfully applied to experimental results [6].

$$M = \max_{\alpha=1,12}\{\tau_{\mathrm{B}}^{\alpha} / \tau_{\mathrm{A}}^{\mathrm{P}}\} = \max_{\alpha=1,12}\{(\boldsymbol{L}^{\mathrm{P}} \cdot \boldsymbol{L}^{\alpha})(\boldsymbol{g}^{\mathrm{P}} \cdot \boldsymbol{g}^{\alpha})\}, \tag{2}$$

where ($\boldsymbol{L}^{\mathrm{P}}$, $\boldsymbol{L}^{\alpha}$) are line unit vectors of intersections between the slip planes of two grains and the GB. This value is based on the vector transformation of shear force on the slip plane of grain A to grain B. Consequently, the maximum *M*-value of 1 when $\boldsymbol{g}^{\mathrm{P}} = \boldsymbol{g}^{\alpha}$ and $\boldsymbol{L}^{\mathrm{P}} = \boldsymbol{L}^{\alpha}$ implies that it behaves as a single crystal. *LRB*-condition supplements the consideration of a Burgers vector $\boldsymbol{b}_r$ ($=\boldsymbol{b}_A - \boldsymbol{R}\boldsymbol{b}_B$, where $\boldsymbol{R}$ is rotational tensor of crystal coordinate system between two grains) of the residual dislocation between incoming and outgoing Burgers vectors of $\boldsymbol{b}_A$ and $\boldsymbol{b}_B$ for GB [7].

In order to investigate the properties of *N*- and *M*-values for various GBs, Eqs. (1) and (2) were calculated for the <110> symmetric tilt GB of copper, which GB energies are obtained by molecular dynamics, as shown in Fig. 1. After

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all of the slip systems (α =1,12 for face-centered cubic (fcc) materials) of grain B were calculated for any slip system of grain A, the maximum M-value and the square of magnitude of $\boldsymbol{b}_r$ are plotted in Fig. 2. The case of that either slip plane is parallel to GB is excluded from the calculation. The M-value is more sensitive ranging from 0.7 to 1.0 for change of misorientation angle Φ than N-value (not shown here). When the M-value is equal to 1, the dislocation passes freely across the GB, and thus no pile-up effect could be expected for Σ3B{112} (Φ=109.4 deg.). It is also reasonable that the higher M-value corresponds to the smaller residual Burgers vector, which means the less strain energy storage on GB.

Criteria of slip transfer and dislocation nucleation model for indentation

In the present paper, a new parameter is proposed, which considers the superposition of the applied compressive stress contribution by indentation to the slip transfer contribution of N- and M-values. For the N-value, the slip system P with the maximum Schmid factor (SF) to σ_{33} is first chosen in either grain A or B. RSS on slip system P can be expressed as

$$\tau^{\mathrm{P}} = (\mathrm{SF})^{\mathrm{P}}_{\max}\,\sigma_{33}\,. \tag{3}$$

This RSS is transformed by Eq. (1) as follows.

$$\tau^{\mathrm{M}} = \max_{\alpha=1,12}\{N^{\alpha}\tau^{\mathrm{P}}\} = \tau^{\mathrm{P}} \times \max_{\alpha=1,12}\{N^{\alpha}\}\,, \tag{4}$$

where the superscript M is α when N^{α} is maximum. Therefore, RSS in the adjacent grain τ^{S} can be described as

$$\tau^{\mathrm{S}} = \tau^{\mathrm{M}} + (\mathrm{SF})^{\mathrm{M}}\sigma_{33}\,. \tag{5}$$

Substituting Eqs. (3) and (4) into Eq. (5), we define the following L-value as the ratio of τ^{S} to σ_{33}, which appears similar to the SF in Eq. (3).

$$L = \tau^{\mathrm{S}} / \sigma_{33} = (\boldsymbol{e}_3\cdot\boldsymbol{n}^{\mathrm{P}})(\boldsymbol{e}_3\cdot\boldsymbol{g}^{\mathrm{P}}) \times \max_{\alpha=1,12}\{(\boldsymbol{n}^{\mathrm{P}}\cdot\boldsymbol{g}^{\alpha})(\boldsymbol{g}^{\mathrm{P}}\cdot\boldsymbol{n}^{\alpha}) + (\boldsymbol{g}^{\mathrm{P}}\cdot\boldsymbol{g}^{\alpha})(\boldsymbol{n}^{\mathrm{P}}\cdot\boldsymbol{n}^{\alpha})\} + (\boldsymbol{e}_3\cdot\boldsymbol{n}^{\mathrm{M}})(\boldsymbol{e}_3\cdot\boldsymbol{g}^{\mathrm{M}})\,, \tag{6}$$

where the subscript 3 denotes the compressive direction normal to the surface. Similarly, considering the M-value of Eq. (2) instead of the N-value, the L'-value is defined as

$$L' = (\boldsymbol{e}_3\cdot\boldsymbol{n}^{\mathrm{P}})(\boldsymbol{e}_3\cdot\boldsymbol{g}^{\mathrm{P}}) \times \max_{\alpha=1,12}\{(\boldsymbol{L}^{\mathrm{P}}\cdot\boldsymbol{L}^{\alpha})(\boldsymbol{g}^{\mathrm{P}}\cdot\boldsymbol{g}^{\alpha})\} + (\boldsymbol{e}_3\cdot\boldsymbol{n}^{\mathrm{M}})(\boldsymbol{e}_3\cdot\boldsymbol{g}^{\mathrm{M}})\,. \tag{7}$$

The change of L'-value is obtained for the previous bicrystal model under uniform compression on (110) surface, as shown in Fig. 3. The result suggests that Σ3A{111} (Φ=70.52 deg.) is easiest for nucleation of plasticity in the near-field of GB.

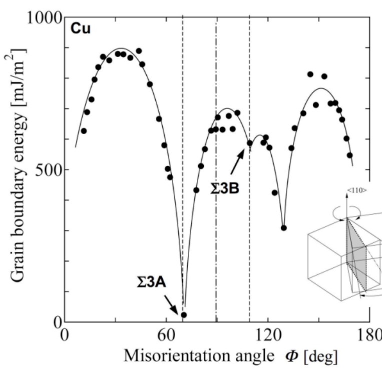

Fig. 1 GB energy distribution by MD.

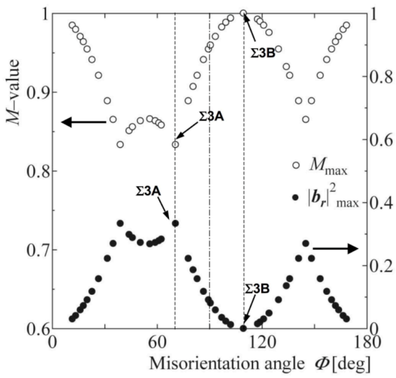

Fig. 2 Change of M-value and $|\boldsymbol{b}_r|^2$ to Φ.

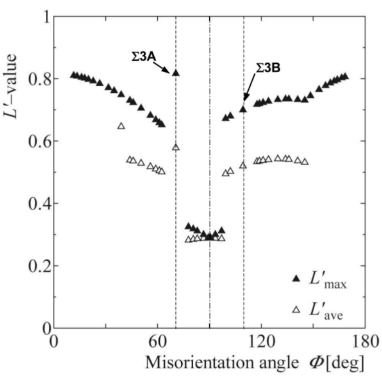

Fig. 3 Change of L'-value to Φ.

CONCLUSIONS

A new condition of dislocation-boundary interaction was proposed to describe the experimental results of nanoindentation in the inhomogeneous near-field of GB. The conventional values proposed so far were also calculated for ideal bicrystal model with <110> symmetric tilt GB and found that M-value is much sensitive to misorientation angle and L- or L'-values could be applied for the indentation problem subjected to uniform compression. The author (YS) gratefully acknowledges financial support from the JSPS, Grants-in-Aid for Scientific Research (S) (20226004).

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