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# MESO-MECHANICS APPROACH TO THE ANALYSIS OF DISLOCATION ACCUMULATION IN METAL MICROSTRUCTURES

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The plastic slip process in face centered cubic metals is analysed by finite element continuum mechanics using models for behavior of dislocations. Density evolution and accumulation of dislocations during slip deformation in metal microstructures are described to evaluate strain hardening of slip systems. Some essential features of the system are described and analysis results of dislocation accumulation and stress-strain response of some model crystals are shown.

## 1. INTRODUCTION

Movement and accumulation of dislocations in metal microstructures are points of crucial importance in the study of deformation and fracture of metal crystals. We have two typical length scales for dislocations: one is the magnitude of Burgers vector, which is at the same order as lattice constants, and the other is mean slip distance of dislocations in microstructures, which is not defined by dislocations themselves but dependent on deformation history, temperature, grain size or mean distance of strengthening particles. To study behaviors of dislocations in such a longer length scale, presumably in micrometer order, a technique has been developed [1,2] where finite element analysis for slip deformation in continuum but non-uniform media is combined with models of movement and accumulation of dislocations. We have to introduce basically two kinds of models for dislocations: one is the statistically stored dislocations and their mean slip distance before they stop moving; the other is the geometrically necessary dislocations, density of which is proportional to gradient of plastic slip strain [3]. To describe interaction between dislocations on different slip systems and to account for rapid hardening by multiple slip, we utilize an interaction table between slip systems where magnitudes of the interaction are described in terms of dislocation reaction.

In this report, we briefly describe the whole structure of the simulation system which includes governing equations for slip deformation of f.c.c. crystals, dislocation models and correlation between them. Some results of slip deformation analysis are shown and calculated density distributions of dislocations are compared with experimental or theoretical ones.

## 2. CRYSTAL PLASTICITY ANALYSIS WITH DISLOCATION MODELING

### 2.1 Mathematical framework

Fig. 1 shows elements used in our crystal plasticity analysis system and related topics. Elements in the upper left corner give a framework for the crystal plasticity analysis; geometry of the metal microstructure is described by finite elements and their deformation is analyzed with the constitutive equation.

The plastic slip is assumed to occur on {111} slip plane and in <110> slip direction (Fig.2). Due to the symmetric character of the lattice of the face centered cubic type crystal, there are twelve slip systems. Activation condition of these slip systems is given by Schmid law; When the critical resolved shear stress for the slip system n is written as $\theta^{(n)}$,

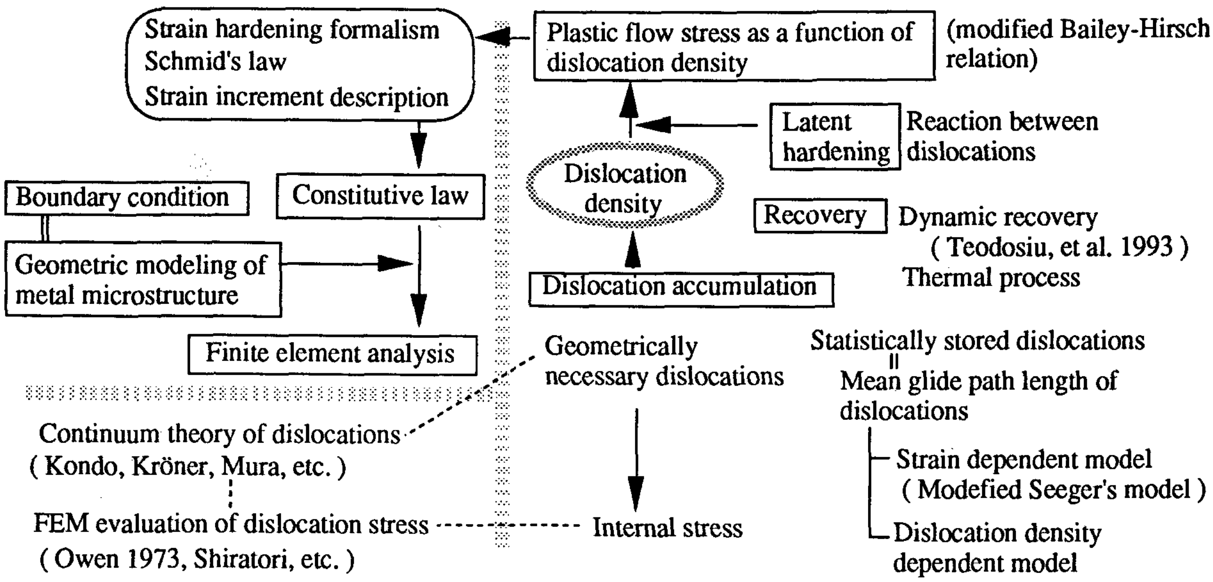


Fig. 1 Crystal plasticity analysis system based on the finite element method and models for behavior of dislocations.

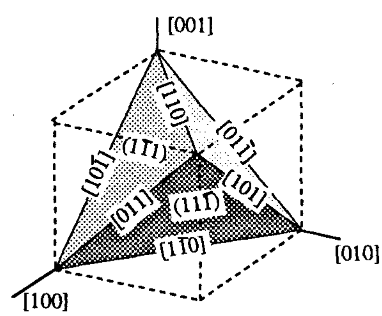


Fig. 2 Thompson's tetrahedron. Its surfaces and edges correspond to slip planes and slip directions of f.c.c. crystals.

the Schmid condition is given by the following equations.

$$P_{ij}^{(n)}\sigma_{ij}=\theta^{(n)}, \qquad (1)$$

$$P_{ij}^{(n)}\dot\sigma_{ij}=\dot\theta^{(n)}, \quad (n=1,..,12), \qquad (2)$$

where

$$P_{ij}^{(n)}=\frac{1}{2}\{v_i^{(n)}b_j^{(n)}+v_j^{(n)}b_i^{(n)}\}, \quad (n=1,..,12). \qquad (3)$$

$\sigma_{ij}$ denotes stress in the global coordinate system and dotted symbols denote their increments. $v_i$ and $b_i$ (i=1-3) are unit vectors normal to the slip plane and parallel to the slip direction, respectively. Superscripts in parentheses denote the slip system number. $P_{ij}^{(n)}$ is the outward normal of the yield hyperplane for the slip system n in the stress space [4].

Increment of the critical resolved shear stress is comprised of contributions from temperature change and strain hardening.

$$\dot\theta^{(n)} = -q\dot T+\sum_m h^{(nm)}\dot\gamma^{(m)}. \qquad (4)$$

The parameter $h^{(nm)}$ defines the strain hardening coefficient. If rotation of the crystal orientation during deformation is neglected, which is acceptable while the deformation is small, the constitutive equation for slip deformation is written as follows [5-7].

$$\dot{\sigma}_{ij}=[S^{e}_{ijkl}+\sum_{n}\sum_{m}\{h^{(nm)}\}^{-1}P^{(n)}_{ij}P^{(m)}_{kl}]^{-1}(\dot{\varepsilon}_{kl}-\alpha^{*}_{kl}\dot{T}) \;, \quad (5)$$

$$\alpha^{*}_{kl}=\delta_{kl}\alpha+q\sum_{n}\sum_{m}\{h^{(nm)}\}^{-1}P^{(n)}_{kl} \;. \quad (6)$$

2.2 Models for dislocations' behavior

The critical resolved shear stress is defined as a function of temperature and density of accumulated dislocations [1];

$$\theta^{(n)}=\theta_0(T)+\sum_{m=1}^{12}\Omega^{(nm)}a\mu\tilde{b}\sqrt{\rho_a^{(m)}}. \quad (7)$$

The first term $\theta_0(T)$ gives the lattice friction for movement of dislocations, which is a function of temperature and is defined by experimental data for the temperature dependence of the yield stress. The second term represents the forest effect of accumulated dislocations on moving dislocations. $\rho_a^{(m)}$ denotes the density of dislocations which have accumulated on the slip system m. Constants $\tilde{b}$, $\mu$ and a denote magnitude of the Burgers vector, the elastic shear modulus and a numerical factor of order 0.1, respectively. The matrix $\Omega^{(nm)}$ is named the interaction matrix of the slip systems. The interaction of two dislocations is categorized into six types [8,9] by geometrical arrangement of Burgers vectors of the two dislocations. Since the interaction of slip systems originates from interactions between the moving and the accumulated dislocations, each component of the interaction matrix must be defined in accordance with the category of the dislocation interaction [1].

Let us write the contribution to $\rho_a^{(m)}$ from the statistically stored and geometrically necessary dislocations as [10],

$$\rho_a^{(m)}=\rho_S^{(m)}+C_e\rho^{(m)}_{G,edge}+C_s\rho^{(m)}_{G,screw} \;, \quad (8)$$

where $\rho_S^{(m)}$ denotes the density of the statistically stored dislocations on the slip system m, while $\rho^{(m)}_{G,edge}$ and $\rho^{(m)}_{G,screw}$ denote the density of the geometrically necessary dislocations.

Density evolution of the statistically stored dislocations due to plastic slip is evaluated by the following model.

$$\dot{\rho}_S^{(n)}=c\,\dot{\gamma}^{(n)}\,/\,\tilde{b}\,L_S^{(n)}. \quad (9)$$

Here, c is a numerical factor of order 1 and $L_S^{(n)}$ denotes the slip distance for statistical storage [3] of dislocations on slip system n. We have introduced some models for the statistical slip distance as a function of shear strain [6] or density of accumulated dislocations[1]. The strain hardening characteristics of pure metal single crystals is largely influenced by the models for $L_S^{(n)}$; model for $L_S^{(n)}$ is the most important factor to reproduce realistic strain hardening characteristics of pure metal single crystals.

The geometrically necessary dislocations accompanies to gradient of plastic shear strain. The edge and screw components of the geometrically necessary dislocations on slip system n are [11],

$$\rho^{(n)}_{G,edge}=-\frac{1}{\tilde{b}}\frac{\partial\gamma^{(n)}}{\partial x_i}b_i^{(n)} \;, \quad (10)$$

$$\rho^{(n)}_{G,screw}=\varepsilon_{ijk}\frac{1}{\tilde{b}}\frac{\partial\gamma^{(n)}}{\partial x_i}b_j^{(n)}\nu_k^{(n)} \;, \quad (11)$$

which are evaluated by numerical differentiation of the shear strain distribution.

If we suppose that $\rho_a^{(m)}$ is a time independent internal state variable, q and $h^{(nm)}$ are calculated from eqs (4), (7) and (8) as follows.

$$q=-\frac{\partial}{\partial T}\theta_0(T) \;, \quad (12)$$

$$h^{(nm)}=\frac{\partial\theta^{(n)}}{\partial\rho_a^{(m)}}\times\left[\frac{\partial\rho_S^{(m)}}{\partial\gamma^{(m)}}+c_e\frac{\partial\rho^{(m)}_{G,edge}}{\partial\gamma^{(m)}}+c_s\frac{\partial\rho^{(m)}_{G,screw}}{\partial\gamma^{(m)}}\right]. \quad (13)$$

Eq. (13) may be written simply ,

$$h^{(nm)}=\frac{a\mu\Omega^{(nm)}}{2\sqrt{\rho_a^{(m)}}}\left[\frac{c}{L_S^{(m)}}+\frac{c_e}{L^{(m)}_{G,edge}}+\frac{c_s}{L^{(m)}_{G,screw}}\right], \quad (14)$$

where $L^{(m)}_{G,edge}$ and $L^{(m)}_{G,screw}$ correspond to geometric

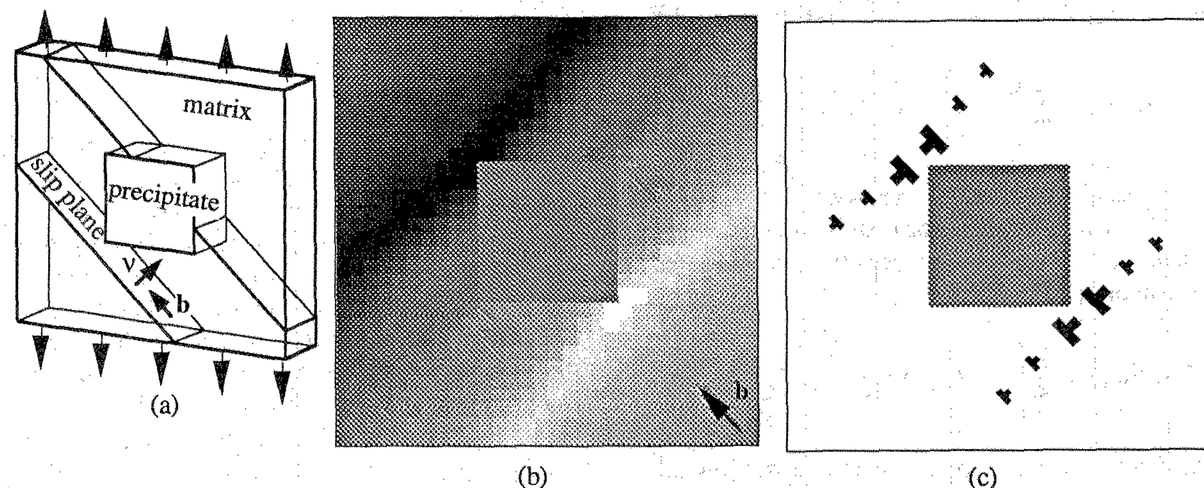


Fig. 3 (a) Simplified model of precipitate-matrix system. On the upper and bottom surfaces of the specimen, pulling force is uniformly applied. Crystal orientation is chosen so that the slip plane normal and slip direction of the primary slip system lie parallel to the specimen surface. (b) Simulation result for the distribution of the edge component of geometrically necessary dislocations on the primary slip system. Gray level used in the area of precipitate corresponds to the zero dislocation density. (c) Schematic illustration of the geometrically necessary dislocations obtained in (b).

slip distances of dislocations [3].

## 3. NUMERICAL EXAMPLE

Let us simulate the dislocation accumulation arround a predipitate. Fig. 3(a) illustrates the employed model; the model is a rectangular shaped plate with dimension 30 x 30 x 1 microns. The plate includes a rectangular shaped precipitate whose latetral dimension is 10 microns. Lattice friction of the precipitate is chosen to be hard enough compared to that for the matrix. Then the plastic slip occurs only in thematrix region. The yield stress of the matrix is 22.32 MPa. Fig. 3(b) shows the density distribution of the edge component of the geometrically necessary dislocations on the primary slip system when the average tensile stress is 22.57 MPa. The maximum of the shearing strain on the primary slip system at this deformation stage is about 0.38 %. Lighter the gray level, larger the dislocation density. The gray color in the precipitate region corresponds to zero density. In the upper left area the density is negative and in the lower right area the density is positive. The minumum and the maximum density near the upper left and lower right edges of the precipitate are -1.67 and 1.70 x $10^{12}$ $m^{-2}$, respectively. Fig. 3(c) shcematically shows the dislocation distribution. Positive and negative dislocations are punched out from the precipitate.

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