ANALYSIS OF KINK-FOLD DEFORMATION BASED ON DISCLINATION THEORY

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Summary Microscopic computational approaches for deformable body mechanics are discussed. It is shown that disclination model has potential to be developed to a coarse-grained model in a multiscale analysis which is promising to reveal the mechanism of kink deformation. As an example of application of discrete defect model based on disclination theory, the dislocation-grain boundary interaction is studied.

INTRODUCTION

The mechanical properties of magnesium alloy containing long-period stacking order phase have attracted a great deal of attention. The both high strength and high ductility of this alloy are thought to be related to the formation of kink deformation band. The detailed investigations, however, have only just started. The kink band consists of a unique arrangement of microscopic lattice defects. Collective behavior of dislocations on basal slip planes is important for the formation of kink band. Disclination is a higher-order lattice defect which is equivalent a special arrangement of dislocations. By using the disclination model, expression of deformation can be simplified. In this article, the boundary value problem based on disclination theory is formulated to study the kink deformation.

BOUNDARY VALUE PROBLEM BASED ON DISCLINATION THEORY

The discrete dislocation plasticity [1], which is one of promising method to investigate the deformation and fracture (e.g., Ref.[2]) from a microscopic viewpoint, is extended to deal with disclinations.
In the formulation, the velocity, $\dot{u}_i$, strain rate, $\dot{\varepsilon}_{ij}$, and stress rate, $\dot{\sigma}_{ij}$ are described, respectively, by the superposition of analytical solution[3] of $(\tilde{\ })$-field and numerical solution of $(\hat{\ })$-field as shown in Fig. 1.

$$\dot{u}_i = \dot{\tilde{u}}_i + \dot{\hat{u}}_i, \quad \dot{\varepsilon}_{ij} = \dot{\tilde{\varepsilon}}_{ij} + \dot{\hat{\varepsilon}}_{ij}, \quad \dot{\sigma}_{ij} = \dot{\tilde{\sigma}}_{ij} + \dot{\hat{\sigma}}_{ij} \tag{1}$$

where the $(\hat{\ })$-field is the complementary field of $(\tilde{\ })$-field. The surface traction and the displacement constraint is determined appropriately on the surface S.

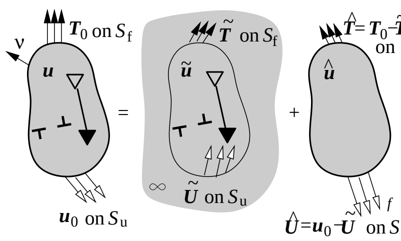

Figure 1. Decomposition of boundary value problem

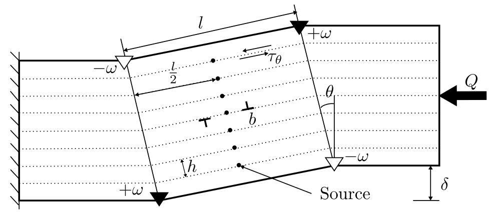

Figure 2. Disclination model for kink band

The fundamental equations of $(\hat{\ })$-field are as follows.

$$\frac{\partial \dot{\hat{\sigma}}_{ij}}{\partial x_j} = 0, \tag{2}$$

where,

$$\dot{\hat{\sigma}}_{ij} = L_{ijkl}\dot{\hat{\varepsilon}}_{kl}, \quad \dot{\hat{\varepsilon}}_{ij} = \frac{1}{2}\left(\frac{\partial \dot{\hat{u}}_i}{\partial x_j} + \frac{\partial \dot{\hat{u}}_j}{\partial x_i}\right). \tag{3}$$

The boundary condition on S_f on which the traction rate $\dot{T}_i^0$ is specified is given by

$$\dot{\hat{\sigma}}_{ij} n_j = \dot{T}_i^0 - \dot{\tilde{T}}_i. \tag{4}$$

The boundary condition on S_u on which the velocity $\dot{U}_i^0$ is specified is given by

$$\dot{\hat{u}}_i = \dot{U}_i^0 - \dot{\tilde{U}}_i. \tag{5}$$

Another method based on the extended finite element method (X-FEM) can be chosen to deal with the discontinuity due to the lattice defects [4].

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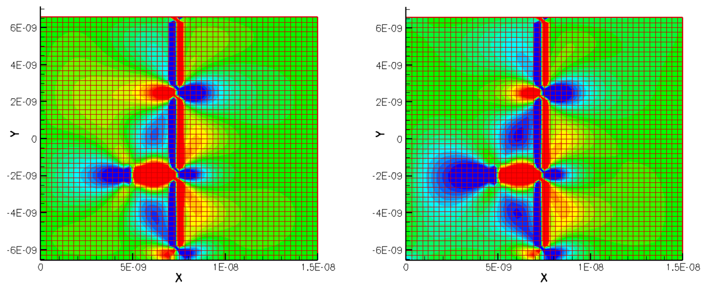
A kink band can be described by two disclination dipoles. The disclination dipole is equivalent to a continuum description of dislocation wall. Therefore, this kink band formation is realized by dislocation motion on different slip planes. In this modeling, the kink band consists of four disclinations and the development of kink deformation can be expressed by the intensity ω of each disclination (Fig.2). The driving force is obtained by the release rate of the potential energy with respect to the intensity of disclination. This energy release process occurs with dislocation-kink boundary interaction and climb of dislocation on the kink boundary. The establishment of multiscale model of this stress relaxation process should be important.

ANALYSIS EXAMPLE: DISLOCATION - GRAIN BOUNDARY INTERACTION

The extended finite element method (X-FEM)[4] is modified to deal with the discontinuity of disclination field. While small angle grain boundaries are modeled by dislocation array, large angle boundaries are modeled by disclination dipoles. Then, the interaction between dislocation and grain boundary is analyzed (The detail of analysis is in Ref.[5]) . Figure 3 shows the result of a problem of dislocation grain boundary interaction. The color shows the contour of shear stress.

Figure 4.(a) shows the relationship between strain energy and position of dislocation measured from the free surface. The slope of these curve corresponds to the Peach-Koehler force. When the dislocation is located near the free surface, attractive force from the image dislocation. The force between dislocation and GB depends on the position of slip plane and the sign of Burgers' vector as well as boundary constraints.

It is very essential to take into account the appropriate boundary conditions for the study of development of misorientation angle of grain boundary as well as kink boundary.



(a) (b)

Figure 3. Dislocation - GB interaction (A large angle GB): (a) case2(+) Traction-free boundary; (b) case2(+) Fixed boundary

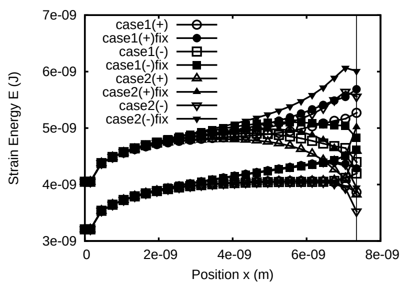


Figure 4. Strain energy due to the interaction of dislocation and GB

CONCLUSIONS

Disclination model can be formulated in a context of a multiscale defect dynamics model. It is extended from a discrete dislocation model to deal with kink deformation. That is, the development of kink deformation can be expressed simply by the intensity ω of each disclination.

The dislocation - grain boundary interaction was studied by the lattice defect model. The result shows the important information to construct the variational formulation of development of kink band. So, this model based on disclination theory can be regarded as a coarse-grained model in a multiscale analysis which is promising to reveal the kink deformation mechanism.

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