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Quantitative investigations on dislocation based discrete-continuous model of crystal plasticity at submicron scale

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ABSTRACT

Although the multi-scale discrete-continuous model (DCM) which couples discrete dislocation dynamics (DDD) and finite element method (FEM) to study crystal plasticity at submicron scale has been proposed for many years, some key issues are still not well addressed yet. First, a new regularization method with slip plane dependent regularization parameter is proposed in this paper to localize the discrete plastic strain to continuum material points and shows excellent accuracy compared with previous studies. Second, it is often thought of that DCM cannot accurately calculate the so called 'image force' acting on the dislocation near free surface. This study argues that the image force can be calculated accurately in the hybrid DCM in which the interpolated stress is used in the computation. The reproduction of deformed crystal configuration during finite deformation is another critical issue in DCM, especially for considering the rotation of slip system. The deformation field transfer between DDD and FEM, and the corresponding treatment of surface dislocations and slip system rotation are proposed to well capture the localized deformation. As an application, the dislocation behavior and stress field in heteroepitaxial films with thin/thick substrates are successfully investigated by the improved DCM.

1. Introduction

The mechanical behaviors of crystal material at submicron-to-nanometer scales have recently received a great deal of attention, due to the urgent demands in reliable fabrication and functioning service of micro/nano-electronic-mechanical systems (MEMS/NEMS). The experimental investigations have discovered lots of atypical phenomena of crystal plastic deformation at these length scales, such as size effect (Dunstan and Bushby, 2013) and strain burst (Uchic et al., 2004; Hu et al., 2014), etc. However, current experiments alone still cannot provide sufficient insight into the physical process. In the recent decades, discrete dislocation dynamics (DDD) has been becoming a rigorous tool to capture the dislocation evolution detail during plastic deformation at submicron scales (Espinosa et al., 2006; Csikor et al., 2007; Devincre et al., 2011; Zhou et al., 2011; Zhou and LeSar, 2012; Cui et al., 2014) and successfully fill the gap between atomistic simulations and theoretical analysis of continuum plasticity. Nevertheless, DDD modeling alone cannot consider the finite deformation of the computational cell. In addition, it is difficult to deal with complex boundary conditions and surface effect (Gao et al., 2010), since it is based on the theoretical solution of stress field for a dislocation in an infinite crystal. To overcome these problems, DDD is usually coupled with finite element methods (FEM) (Van der Giessen and Needleman, 1995; Zbib et al., 2002; Liu et al.,

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2009) or boundary element methods (El-Awady et al., 2008; Zhou et al., 2010), respectively. These coupling procedures can be mainly divided into two categories: one is superposition method (SPM), and the other is so called discrete-continuous model (DCM). In the following, only the streamlined presentations of the framework for these two methods are described for completeness. Details of the methods are described elsewhere (Van der Giessen and Needleman, 1995; Lemarchand et al., 2001; Zbib and Diaz de la Rubia, 2002; Zbib et al., 2002; El-Awady et al., 2008; Liu et al., 2009; Gao et al., 2010; Vattré et al., 2013).

SPM is first proposed by Van der Giessen and Needleman (1995). As schematically shown in Fig. 1(a), the total stress field $\boldsymbol{\sigma}$ in a finite crystal medium is the sum of analytical stress field of dislocations in an infinite media $\boldsymbol{\sigma}^{\infty}$ and a complementary elastic solution $\widehat{\boldsymbol{\sigma}}$ (El-Awady et al., 2008; Gao et al., 2010), which is calculated by subtracting the surface traction $\widetilde{\mathbf{T}} = \boldsymbol{\sigma}^{\infty} \cdot \mathbf{n}_s$ and correcting from the displacement boundary conditions. Here, $\mathbf{n}_s$ is the normal direction of surface. The short range interaction can be relatively well captured by SPM (Vattré et al., 2013). However, the analytical stress fields of all dislocations must be recalculated at each time step, which requires extensive computing time. Besides, it is relative complicated to deal with anisotropic media (Chen and Biner, 2006) and bimaterial (O'day and Curtin, 2005). More importantly, the concept of 'plastic strain' is not explicitly introduced.

DCM is based on the concept of 'eigenstrain' in micromechanics, which can directly calculate the plastic strain and solve the boundary value problem under a unified framework (Lemarchand et al., 2001; Zbib and Diaz de la Rubia, 2002). In previous work (Liu et al., 2009; Gao et al., 2010), it mainly contains the following three information-transfer procedures as shown in Fig. 1(b): (i) Calculating the plastic strain $\boldsymbol{\varepsilon}^{p}$ induced by the glide of dislocations using DDD simulation. Then, the plastic strain is localized to the continuum material point, which is crucial in the whole calculation procedure and will be studied in detail in Section 2. This replaces the conventional phenomenological constitutive law to calculate the total stress,

$$\overset{\triangledown}{\boldsymbol{\sigma}^{e}} = \mathbf{C}^{e} : (\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}^{p}) \tag{1}$$

where $\overset{\triangledown}{\boldsymbol{\sigma}^{e}}$ is the Jaumann rate of Cauchy stress $\boldsymbol{\sigma}$, $\mathbf{C}^{e}$ is the tensor of elastic modulus, $\dot{\boldsymbol{\varepsilon}}$ is the total strain rate. (ii) The equilibrium stress field associated with the homogenized plastic strain is calculated by FEM under a specific boundary condition in a unified continuum mechanics framework. It is expressed as follows (Liu et al., 2009; Gao et al., 2010),

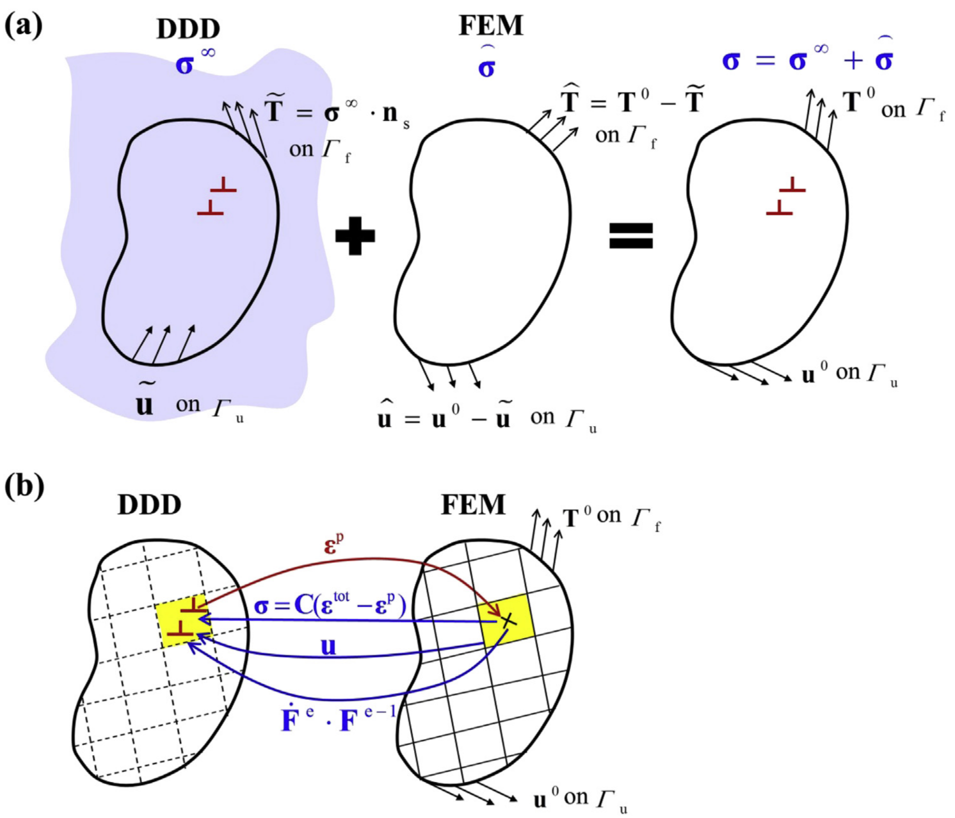

Fig. 1. (a) Schematic diagram of SPM (Van der Giessen and Needleman, 1995); (b) Schematic of variable-transferring procedures in improved DCM.