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Developing micro-scale crystal plasticity model based on phase field theory for modeling dislocations in heteroepitaxial structures

Liyuan Wang, Zhanli Liu*, Zhuo Zhuang**

Applied Mechanics Lab., School of Aerospace Engineering, Tsinghua University, Beijing 100084, China

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ABSTRACT

The capability of conventional crystal plasticity theory is extended in this paper to model a single dislocation behavior in heteroepitaxial structures. The plastic slip associated with each slip system is described by a continuous smooth field independently, which is the phase field interpolating between a slipped and an unslipped region. A dislocation is identified with location where the phase field value changes smoothly, to represent a smeared dislocation. Under a thermodynamically consistent framework that distinguishes between stored energy and dissipated energy during plastic deformation, the coupled balance equations of plastic slip evolution and quasi-static stress equilibrium are derived by using the principle of virtual power. With numerical implementation by finite element method, it is flexible to deal with material anisotropy and elastic modulus mismatch in heteroepitaxial structures at micro-scale, which are advantages of the proposed model compared to Khachaturyan-type phase field model of dislocations. Another advantage is that it is straightforward to handle the interaction and co-evolution of several types of material microstructures, such as dislocations and interfaces, within a unified continuum mechanics framework. Several examples are presented to illustrate the applicability and accuracy of the new method in modeling dislocations in complex heteroepitaxial structures.

1. Introduction

Heteroepitaxial structures, e.g. epitaxial films or core–shell nanopillars, have recently received much attention because of their important applications in engineering, such as electronics, optoelectronics and solar cells (Freund, 2000; Fu et al., 2004; Panda and Tseng, 2013). However, dislocation-free heteroepitaxial structures cannot be grown with arbitrary thickness and misfit dislocation will form above a critical thickness. The dislocation and its strong interaction with material interface not only influence the mechanical properties such as fracture toughness and strength, but also change the electrical or optical properties of heteroepitaxial crystalline materials (Bennett, 2010; Zbib et al., 2011; Liu et al., 2013; Abdolrahim et al., 2014). Understanding the underlying dynamics of dislocations in heteroepitaxial structures is crucial to provide a better insight into

* Corresponding author. Tel./fax: +86 10 62783014.
** Corresponding author. Tel./fax: +86 10 62783014.
E-mail addresses: liuzhanli@tsinghua.edu.cn (Z. Liu), zhuangz@tsinghua.edu.cn (Z. Zhuang).

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the material design and property prediction. However, there is still lacking of an effective tool to study the dislocation behaviors in complex heteroepitaxial structures.

In the past decades, discrete dislocation dynamics (DDD) that explicitly tracks dislocation lines has proven to be a useful simulation method in modeling dislocations in homogeneous bulk crystals (Amodeo and Ghoniem, 1990; Zbib et al., 1998). However, it is difficult to deal with the dislocations in heteroepitaxial structures due to the image force produced by the interfaces. Currently, most DDD methods are based on the superposition of analytical solutions of stress fields for dislocations in infinite domain. However, the existence of multi-material Green's functions is limited (Han and Ghoniem, 2005). The solution on a finite domain is the sum of infinite domain dislocation solutions and the image field corrections from the model boundary, which is usually calculated by boundary element method (El-Awady et al., 2008; Takahashi and Ghoniem, 2008) or finite element method (FEM) (Giessen and Needleman, 1995; Fivel and Canova, 1999; Weygand et al., 2001). The superposition DDD method cannot reflect the basic concept of plastic strain and is limited by relying on the existed analytical solutions.

As an alternative, the coupled discrete-continuum model (DCM) was proposed, in which dislocations are associated with eigenstrain and the equilibrium field is determined directly by FEM (Lemarchand et al., 2001; Zbib and de la Rubia, 2002; Liu et al., 2009; Gao et al., 2010; Cui et al., 2014; Vattré et al., 2014). The critical thickness of epitaxial films for plastic relaxation (Groh et al., 2003) and the dislocation behaviors in heteroepitaxial films (Cui et al., 2015a) have been studied by this method. However, the DCM still needs the analytical solution to modify the stress field when the dislocation is close to the interface (Cui et al., 2015b). In addition, how to handle the finite deformation is still a challenging issue that all the discrete based models are facing.

Recently, several dislocation modeling methods completely based on continuum mechanics framework are developed. The most advantage of these methods is that the equilibrium field is solved directly. Based on field dislocation mechanics, a general crystal plasticity model was developed by Acharya (2001). The dislocation density serves as the primary internal variable and a finite element discretization of the model was presented (Roy and Acharya, 2005). It has been used to study the mechanical response of multi-layer thin films (Puri et al., 2011). Inspired by crack modeling using extended finite element method (XFEM), the displacement fields of dislocation are approximated by the sum of standard finite element part and discontinuous enriched part (Belytschko and Gracie, 2007; Gracie et al., 2007). However, the enrichment for the dislocation core is not available for anisotropic materials (Gracie et al., 2008; Oswald et al., 2009).

Among all the dislocation modeling methods, the phase field method (PFM) which represents the discontinuities associated with dislocations by regularization, is receiving more and more attentions (Khachaturyan, 1983; Hu and Chen, 2001; Wang et al., 2001; Rodney et al., 2003; Koslowski et al., 2004). The advantage is that it can automatically take into account the interaction and co-evolution of dislocations and interfaces within a unified continuum mechanics framework (Wang et al., 2003; Lei et al., 2013). Currently, most phase field models of dislocations are based on the microelasticity theory of Khachaturyan and Shatalov (Khachaturyan, 1967; Khachaturyan and Shatalov, 1969; Khachaturyan, 1983). In the model, it takes 'stress-free' inelastic strain to represent dislocations. The elastic strain energy caused by dislocations is then expressed as a closed form function of the inelastic strain through the exact Green's function. While, the analytical Green's function solution is not available for complex structures or complex boundary conditions. For elastically inhomogeneous structures, the virtual misfit strain which is considered as additional phase fields has to be introduced and increases the number of equations to be solved (Wang et al., 2002). The dislocation behaviors in heteroepitaxial thin films have been studied by the phase field microelasticity model (Wang et al., 2003). The film and the substrate are assumed having the same elastic modulus to avoid dealing with the additional misfit strain (Wang et al., 2003). On the other hand, the equations are solved by the fast Fourier transform (FFT) method, which restricts the application to complex structures, like heteroepitaxial core–shell nanopillars. Besides, based on Ginzburg-Landau equation, the model does not distinguish between stored energy and dissipated energy during plastic deformation (Wang et al., 2001, 2003; Lei et al., 2013).

In this work, a micro-scale crystal plasticity model based on phase field theory is developed to overcome the difficulties in the Khachaturyan-type phase field model of dislocations. In contrast, the 'stress-free' inelastic strain is directly considered as the plastic strain based on crystal plasticity theory in the proposed model. The plastic slip associated with each slip system is described by an independent phase field variable to model a single dislocation. The elastic strain energy is expressed as a function of the elastic strain through the crystal plasticity constitutive model. Under a thermodynamically consistent framework that distinguishes between stored energy and dissipated energy during plastic deformation, the coupled balance equations of plastic slip evolution and quasi-static stress equilibrium are derived by using the principle of virtual power. Then the boundary value problem is solved directly by FEM. It can be used for complex structures or complex boundary conditions where the analytical Green's function solution is not available, which is one advantage of the proposed model. Another advantage is that the elastic modulus mismatch in heteroepitaxial structures is easy to be treated without additional complications. Besides, with numerical implementation by FEM, it is flexible to deal with finite deformation in heteroepitaxial structures at micro-scale.

An outline of this paper is given as follows. The theoretical model is developed in Section 2. Three computational demonstrations are presented in Section 3, which include a screw dislocation near a free surface, a screw dislocation in an anisotropic material and an edge dislocation near a bimaterial interface. Through these examples, the accuracy of the proposed model is studied by comparing with analytical solutions. Dislocations in heteroepitaxial structures are simulated in Section 4. The conclusions are provided in Section 5.