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A phase field study focuses on the transverse propagation of deformation twinning for hexagonal-closed packed crystals

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ABSTRACT

The thickening mechanism of the deformation twinning (DT) has been frequently studied in numerous researches and the transverse propagation of that is beginning to trigger the attention of scholars. Recently, some researchers report that the twin front of $\{10\bar{1}2\}$ mode of Magnesium is composed of a conjugate twin plane and prismatic/basal (PB) planes, and the combined mobility of these planes rule the overall kinetics of twin propagation. Focusing on that, a continuum phase field model is proposed to investigate the equilibrium shape of tensile twins and the kinetics of the twin front. A new form of surface free energy is introduced in this model for the purpose of describing the orientation-dependent properties of twin boundaries. The simulations well reproduce the PB interfaces and the results indicate that the anisotropic surface energy plays a dominant role in forming the irregular facets on the twin front. A generalized energy-momentum tensor is derived and analyzed for shear loading in order to investigate the equilibrium and mobility of twin boundaries, and the simulations show that the configurational forces distributed on the PB interfaces are smaller than that on the other twin planes, which implies that the growth of twin is beneficial for the formation of PB interfaces. The simulations also indicate that the anisotropic twin boundary energy is not responsible for the large aspect ratio nature of twins, which may be governed by the competition between thickening mechanism and transverse propagation mechanism of the DT.

1. Introduction

DT is a significant and general plastic deformation mechanism that is very helpful for increasing both the strength and ductility of the materials, therefore, a better understanding of the effects of the microstructure, energy competitive relationship and defects of crystals on the DT and their underlying mechanism is required for designing advanced materials or improving existing materials (Cahn, 1954; Christian and Mahajan, 1995; Youssef et al., 2005, 2006). In hexagonal-closed packed (HCP) crystals, DT plays a dominant role in plasticity mechanism because deformation by slip along some directions either is not possible or at least requires very high stresses (Capolungo et al., 2010, 2009; Yoo, 1981). There were many

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theories intensively presented and developed to study the DT in recent years as well as numerical computation (Abdolvand et al., 2011; Cheng and Ghosh, 2015; Choi et al., 2011; Popova et al., 2015).

Molecular dynamics (MD) method is the most commonly reported numerical method to study the DT and it has been extensively and successfully used to investigate the mechanical behaviors of crystals at the atomistic scale (Li and Ma, 2009b, 2009c; Zhou et al., 2011; Zhou et al., 2006, 2007; Zhu et al., 2009). The configuration of twinning dislocations and twin boundary interfacial structure are well observed and studied in the discrete approach. At the same time, DT is also reproduced in a continuum approach – phase field model (PFM), which is beneficial to understand the nature of the DT in a different point of view and to find the new mechanisms that the atomic simulations has ignored. It is convenient to compute the chemical and structural non-uniformities associated with the interface in the framework of Gibbs thermodynamics and Landau theory of phase transitions by using PFMs, which are widely used for the simulation of defects and deformation, liquid–solid and solid–solid transformations, especially for modeling martensitic transformation (Artemev et al., 2001; Falk, 1982; Finel et al., 2010; Jacobs et al., 2003; Jin et al., 2001; Levitas, 2013; Levitas and Lee, 2007; Levitas and Preston, 2002; Vedantam and Abeyaratne, 2005). The theory of stress-induced martensitic transformation is applicable to the DT system because of the relationship between the two theories and the twin nuclei can be described as a small coherent "martensitic phase" domains whose habit plane is the twinning plane (Christian and Mahajan, 1995; Wang and Li, 2010). Two hypothetical theories are proposed to investigate the twin nucleation since the twin nuclei's structure is unknown. One is that the twin nuclei is considered as an inhomogeneous inclusion subject to far-field stress which has been studied by the well-known Eshelby's equivalent inclusion theory (Eshelby, 1957), the other is introducing a dipole of partial dislocations in the perfect crystal which has been well studied in MD works (Wang et al., 2009b).

In parallel with the two hypotheses of twin nuclei, two kinds of strategies for describing the lattice mismatches of the DT are employed in PFMs, one regards the twin nuclei as a partial dislocation associated with the dislocation-type eigenstrain, and the other considers the twin nuclei as an inclusion with a simple shear eigenstrain embedded in the parent phase.

The advantage of the dislocation nuclei PFM is that the convenience of reproducing the twin microstructures at grain boundaries, twin–twin interaction and the thickening mechanism of the DT. For example, the representative model proposed by Hu et al. successfully described the stress-induced twinning and de-twinning in face-centered-cubic crystals (Hu et al., 2010). Their simulation results demonstrated that the model was able to predict the twin nucleation and twinning dislocations, as well as the morphology of the twin growth and interaction. Later, within this numerical framework, Heo et al. studied the DT and predicted the twinning plane orientation and microstructure evolution (Heo et al., 2011). Gu et al. studied the DT in tantalum and their results shown remarkably similarity with the MD (Gu et al., 2013). On the basis of Eshelby's equivalent inclusion theory, Clayton and Knap proposed a inclusion nuclei PFM describing the DT in defect-free magnesium single crystals (Clayton and Knap, 2011). The anisotropy of interfacial energy on the twin was set in a stationary Ginzburg–Landau equation, in which the kinetic parameter associated with the twin boundary mobility was removed. Then, based on their model Kondo et al. proposed their PFM coupled with the dislocation-base crystal plasticity for HCP crystals (Kondo et al., 2014). The advantage of the second approach is that researchers can examine their PFM by comparing their simulation results with the Eshelby's inclusion theory because of the close relationship. This approach is employed in our model, and the resulting simulations show the dependency of twin nucleation on the critical resolved shear stress.

It is well known that the DT is highly affected by the temperature, strain rate and stacking faults (Armstrong and Zerilli, 1999; El-Danaf et al., 1999; Song and Gray, 1995). A strong relationship has been observed between the critical twinning stress and grain size (Barnett, 2008; El-Danaf et al., 1999; Ghaderi and Barnett, 2011; Zhu et al., 2013). Experimental results indicate that critical twinning stress shows a Hall-Petch type behavior of coarse-grained crystals both in HCP and FCC crystals (Barnett et al., 2004; Jain et al., 2008). So far, a solid physic understanding for grain size effects in twinning has not been well developed.

Very recently, the experimental observations on Co and Mg using transmission electron microscopy showed that the twinning boundaries of the $\{10\bar{1}2\}\langle\bar{1}011\rangle$ twin model have a very larger derivation from the $\{10\bar{1}2\}$ plane (Zhang et al., 2014, 2012). The discovery cannot be explained by the traditional point that the twinning dislocations are strictly bounded in the twinning plane. The atomic shuffling mechanism seems plausible to explain this phenomenon as it permits the twinning dislocations to migrate from the twinning plane (Li and Ma, 2009a; Wang et al., 2013c; Zhang et al., 2012). However, the controversies are far from over as the shuffling-dominated mechanism is opposed to the well-established concept of conservative twin boundary migration. There were several MD works published to explain this phenomenon in a different point of view. For instance, Wang et al.'s work directly pointed out that the twinning dislocations glide in the $\{10\bar{1}2\}$ plane can climb along the PB interfaces, and the motion of PB interfaces is still governed by the twinning dislocations (Wang et al., 2013b). Ostapovets and Gröger asserted that the glide of twinning disconnections is a primary mechanism of the twin boundary migration (Ostapovets and Gröger, 2014).

Several MD simulations reproduced the PB interfaces of a twin on the atomic scale (Ghazisaeidi and Curtin, 2013; Ostapovets and Gröger, 2014; Xu et al., 2013). Xu et al.'s work shows that the twin front was formed by the PB planes and the $\{\bar{1}012\}$ plane. They believe that the serrated $\{10\bar{1}2\}$ twin boundaries observed by Zhang et al. is accommodated by a succession of PB interfaces in both of their equivalent perpendicular orientations (Xu et al., 2013). It is worth noting that the Ostapovets et al.'s simulations show that the conjugate plane of twin front is unstable and it transforms to the PB interface along with the twin growth, which is inconsistent with Xu et al.'s work as their simulations show that the plane is quite stable in twinning. This contradiction is relate to the formation energy of these twin planes and will be carefully discussed later. The PB formation energy computed by density functional theory and Liu potential both proved the PB energy is higher than