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Micromechanics of tensile twinning in magnesium gleaned from molecular dynamics simulations

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Abstract

This work discusses coarse-grained micromechanics of tensile twinning in magnesium (Mg) extracted from molecular dynamics (MD) simulations. We perform MD simulations on Mg single crystal orientations with initial idealized defect structures at temperatures $T = 5$ K and 300 K. A detailed atomistic analysis reveals that tensile loading along the c-axis of a defective crystal causes an initial incomplete slip ahead of the defect on the first-order pyramidal $\langle c + a \rangle$ planes, followed by the formation of a $\{11\bar{2}1\}$ twin embryo and basal dislocation. These mechanisms aid the formation of $\{10\bar{1}2\}$ twins, which evolve rapidly while $\{11\bar{2}1\}$ twins disappear. We present a micromechanics picture of the deformation-induced twin structure evolution that is tracked by incorporating a twin orientation analysis (TOA) scheme within Open Visualization Tool. The functional dependencies of the volume fraction (v.f.) and number of twins on the overall plastic strain extracted from this analysis provide a basis to construct kinetic laws for twin evolution in terms of nucleation, growth and coalescence. Preliminary results indicate that $\{10\bar{1}2\}$ v.f. evolution is dominated by twin growth in the presence of defects at room temperature, and it may not be strongly rate dependent.

Keywords: Deformation twinning; Magnesium; MD simulations; Micromechanics; Continuum plasticity

1. Introduction

Deformation twinning (DT) is an important mode of plasticity in a variety of crystalline materials. Low-symmetry crystalline structures ubiquitously exhibit this mechanism owing to an insufficient number of independent slip systems to accommodate applied deformation. Materials with hexagonal close packed (hcp) crystal structure fall in this class, some of them deemed highly desirable as structural materials. Among them, magnesium is of significant interest because of its low mass density and impressive attributes such as excellent biodegradability and high damping capacity. The deformation modes in Mg are characterized by two important crystallographic vectors: the basal direction (the a direction) and the c-axis (the [0001] direction) perpendicular to the basal plane, and the materials are canonically described using the ratio $\kappa = c/a$. Based on this, the plastic deformation modes are broadly categorized into (i) basal slip, (ii) non-basal (out-of-(basal) plane) slip and (iii) DT [1]. Non-basal slip modes are usually plastically hard modes of deformation and may not necessarily be the preferred carriers of plasticity, especially if DT provides an easier alternative. Further, unlike DT in high-symmetry crystal structures, where the slip and twinning planes are identical (e.g. face-centered cubic metals), the twinning systems in hcp structures are distinct from their slip systems. Again, Mg is an excellent example of this in that the basal slip ($(0001)\langle 11\bar{2}0\rangle$) is the most profuse slip mode characterized by the lowest critical resolved shear stress (CRSS) amongst all the possible slip and twin modes. However, when the applied loading is such that it results in tension along the

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c-axis, the plastic deformation is accommodated by twinning on the $\{10\bar{1}2\}\langle\bar{1}011\rangle$ system, referred to as tension twinning. Under c-axis compression, $\{10\bar{1}1\}\langle\bar{1}012\rangle$ compression twinning systems and non-basal slip prevail [2]. Moreover, DT has strong implications on the macroscopic strengthening, hardening and stability of deformation.

Pioneering theoretical work and reviews provide detailed accounts of the topological underpinnings of the different DT modes at the atomic scale in a wide range of hcp materials [1–3]. With recent developments in molecular dynamics (MD) modeling and simulations, detailed atomistic insight on the incipient features of the DT and slip modes in Mg is possible, together with sophisticated topological and kinetic analysis [4–7]. MD simulations reveal novel deformation characteristics not accessible or reported in coarse-grained experiments [7–9]. For instance, they provide insight into TB core structures [10,11] and likely twin nucleation mechanisms in Mg single crystals [4]. While the current emphasis using MD simulations has been on elucidating the atomistic underpinnings of the slip and twin processes, explorations on to coarse-grained descriptions of twinning amenable to continuum modeling are scarce. From a continuum perspective, it is important to ask: how does the twin volume fraction (v.f.) evolve under applied loading? What are the roles played by the nucleation and growth processes? Are they co-operative or competitive in nature? How do initial defect structures mediate these characteristics in comparison with pristine structures (i.e. without any initial defects)? How does the evolution of one type of twin affect the other twin types? These and allied questions are important as they provide a way to connect the atomic scale information to their corresponding coarse-grained description in continuum frameworks. The primary interest in tracking twin v.f. within MD simulations is because it is also tractable in experiments and characterization techniques at similar length-scales (e.g. nanoscale testing/transmission electron microscopy) [12], and is therefore amenable to direct comparison. Further, this could potentially help discern the contributions to the overall twin v.f. from nucleation and growth of individual twins, which is important in formulating physically based continuum models [13–15]. Therefore, along with the twin v.f. evolution, it is important to understand the evolution of number of twins in a given crystal volume.

Motivated by these questions, we focus here on extracting coarse-grained information of the DT evolution in the form of the twin v.f. and the number of twins in a given crystal volume. We also highlight key underlying atomistic details and compare them with those in the literature where applicable. It is known that the evolution characteristics of the tensile and compressive twins in Mg are distinctly different [16–18]. Their atomistic underpinnings are also distinct and complex [1,19] and, as such, they merit separate discussions. Therefore, attention is restricted here only to the tensile twinning characteristics in Mg; we will discuss compressive twinning in a future work. We investigate the evolution of twinning in single crystal pure Mg under uniaxial tensile loading parallel to the [0001] direction (also referred to as the basal pole or c-axis). To elucidate the role of defects on the evolution of plasticity in general and twinning in particular, we consider three model problems: (i) a pristine crystal; (ii) a crystal with an initial spherical nanovoid; and (ii) a crystal with an initial square-shaped nanocrack parallel to the basal plane. These defect structures are surrogates for real defects, such as initial dislocation density, pre-existing twins and vacancies.

2. Simulation details

The following information is common to the three canonical cases considered in this work. The initial configuration comprises a single crystal Mg cube of size 20 nm ($\sim 360,000$ atoms). The MD simulations are performed using the embedded atom method (EAM) interatomic potential developed by Sun et al. [20], as it has been shown to corroborate well with the ab initio results in terms of the dislocation core structure and the stacking fault parameters [21]. To begin with, a simulation cell is equilibrated under an isothermal–isobaric (NPT) ensemble at a zero pressure for 20 ps with a time step of 2 fs. In all cases, the applied tensile strain rate along the c-axis is $\dot{\varepsilon} = 1 \times 10^9\ \mathrm{s}^{-1}$. The faces of the cube are subjected to periodic boundary conditions. The simulations are performed at two temperatures, $T = 5$ K and $T = 300$ K, to explore its role in the evolution of twin v.f.

For a crystal with an initial void as a defect, atoms in a spherical volume of 2 nm diameter at the center of the crystal are removed and this configuration is subjected to conjugate gradient energy minimization (Fig. 1a). Likewise, a nanocrack is introduced by removing atoms within a square region of size 2 nm × 2 nm that is one atomic layer thick (Fig. 1b). In the following sections, we first discuss the twinning characteristics at $T = 5$ K, at which the influence of thermal vibrations is expected to be negligibly small. Later (Section 7), we discuss the twin v.f. evolution characteristics near room temperature.

To enable extracting coarse-grained information on the spatial and temporal evolution of different twin structures, a twin orientation analysis (TOA) scheme is incorporated within the Open Visualization Tool (OVITO) [22]. This facilitates automatic rendering of the twinned volumes based on the reorientation of the c-axis in those regions with reference to the c-axis in the undeformed configuration. This is obtained by calculating the current orientation of the basal pole (i.e. the [0001] direction) for individual hcp atoms using the elastic deformation gradient tensor $\mathbf{F}^e$ within OVITO [23]

$$\theta = \arccos\left(\mathbf{F}^e \boldsymbol{e}_c \cdot \boldsymbol{e}_z\right)$$

where $\boldsymbol{e}_c$ and $\boldsymbol{e}_z$ are the unit vectors normal to the basal plane in the local lattice coordinate before deformation and along the loading direction, respectively. The individual atoms are colored based on the angle θ. Recently, Barrett et al. [7] presented a somewhat different approach