Effect of multiaxial loading on evolution of {10Ī2} twinning in magnesium single crystals

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ABSTRACT

We employ molecular dynamics (MD) simulations to investigate the evolution of {10Ī2} twinning in magnesium single crystals with an initial crack. The focus is on discerning the effect of multi-axial loading (resulting in c-axis extension) on the evolution of variant twin volume fraction and number of twins. Both these quantities fully describe the evolution of the overall twin volume fraction. In all the five loading conditions considered here, the evolution of variant volume fraction clearly shows the signature of twin coalescence through discrete jumps, which coincide with decrease in the number of twins that belong to the variant pair. Interestingly, coalescence occurs between twins that belong to conjugate variants, in addition to coalescence between twins of the same variant. The activation of twin variants is consistent with the Schmid factor. However, variants with identical Schmid factors do not necessarily activate simultaneously. Further, active twin variants with identical Schmid factors do not evolve at the same rate and as a result they do not contribute equally to the overall twin volume fraction. The evolution of N_T occurs a discontinuous manner through the competition of nucleation, coalescence and detwinning processes. Each of these processes is strongly influenced by the details of the loading states. A general rule is – the fewer the nucleation events of twins belonging to different variants, larger the overall volume fraction attained leading up to saturation (f_{sat}). Incipient non-basal slip precedes twinning ahead of the crack tip. Significant dislocation plasticity evolves during and after twinning and it occurs on basal and prismatic ⟨a⟩ slip systems. Prior to the dominance of twin coalescence, f exhibits an exponentially decaying distribution with respect to N_T at a given strain. We present expressions for the evolution of volume fraction and number of twins that qualitatively reproduce the observed features observed for the loading conditions investigated in this work. These should serve as a starting point for constructing improved models for modeling twinning evolution at continuum length scales.

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1. Introduction

Twinning is an important plasticity mechanism in hexagonal close packed (HCP) metals. It plays an important role in defining their strength, hardening and ductility. In some HCP metals, e.g. magnesium (Mg), profuse twinning occurs on one or more of the six {10Ī2}⟨Ī011⟩ twin systems at very low stresses under c-axis extension, commonly known as tension or *extension* twinning. It contributes significantly to texture evolution, which affects the plastic flow at large deformations [1–6]. Recent experiments on notched geometries indicate that extension twinning has important implications on the damage tolerance of Mg alloys under triaxial stress states [7–11].

Crystal plasticity serves as a useful resolution to interrogate strength and damage characteristics of single crystal and polycrystal microstructures. Finite element based crystal plasticity simulations are commonly used to study the twinning-induced plastic deformation in HCP metals [12–14]. In such frameworks, a common approach to model twinning is to track twin volume fraction on each twin system (e.g. [14,15]) at each Gauss point (Fig. 1). The evolution of flow hardening due to twinning is usually captured through constitutive laws that do not worry about the intricacies of twin–twin interactions, or do so in a phenomenological way. In other words, they may not faithfully account for physical effects arising from the discreteness of twinning events pertaining to nucleation, growth and coalescence. While recent continuum modeling efforts have focused on energetic and statistical aspects of twinning [16–20], there are several aspects that need to be addressed. For instance, it is important to determine the interactions between different twin variants in their individual evolution characteristics. Models for twin volume fraction evolution that embed interacting effects through twin nucleation, growth, coalescence and detwinning phenomena would be of
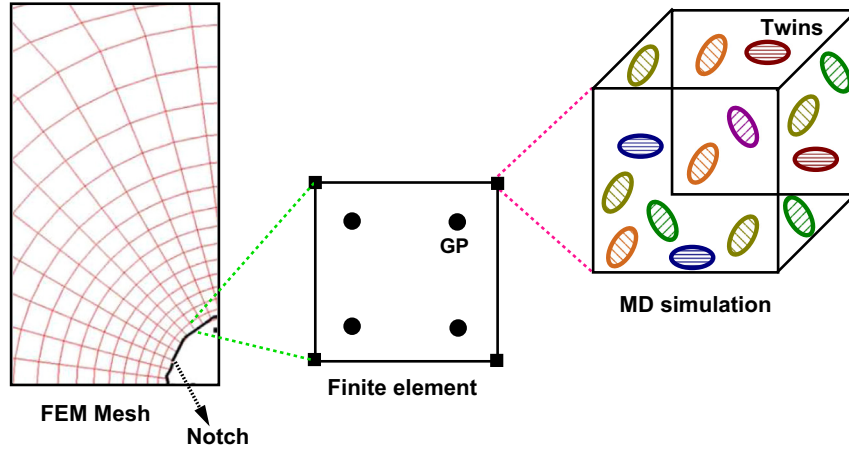
Fig. 1. Schematic illustration showing the hierarchy of length scales involved in a typical finite element based crystal plasticity simulation. At each Gauss point twin volume fraction is a result of the evolution of twin variants. This variant level information may be obtained from atomistic simulations. In the rightmost figure, twins belonging to all six possible $\{10\bar{1}2\}$ twin variants are shown with different colors. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

strong interest in complex phenomena such as damage.

The twin volume fraction serves as a bridge between continuum and atomistic length scales, both computationally and experimentally. In an atomistic simulation, the overall twin volume fraction (f) at a given strain ε can be expressed as

$$f(\varepsilon) = \frac{\mathcal{N}_{tw}}{\mathcal{N}} = \sum_{\beta=1}^{6} f_\beta(\varepsilon) \tag{1}$$

written in terms of the total number of twinned atoms ($\mathcal{N}_{tw}$) and the total number of atoms ($\mathcal{N}$) in the simulation domain. This is equivalent to the summation of the variant twin volume fraction (f_β) over all the six twin variants. Now, if $n_\beta(\varepsilon)$ is the total number of twins for the variant β at ε, then

$$f_\beta(\varepsilon) = \sum_{k=1}^{n_\beta} \psi_k(\varepsilon) \tag{2}$$

where ψ_k is the volume fraction of the kth twin belonging to twin variant β and n_β is the total number of twins for variant β.

One may seek to develop improved twin volume fraction evolution laws by quantifying the evolution of n_β and ψ_k. Recently, Aghababaei and Joshi [21] discussed nucleation, growth and coalescence contributions in the evolution of the overall twin volume fraction using molecular dynamics (MD) simulations. However, that work did not probe the evolution of individual twin variants and their interaction. Moreover, it focused on describing twinning evolution under uniaxial stress state. In this work, we take that initial effort much further. Using MD simulations, we present a coarse-grained analysis of the evolution of extension twinning under different loading conditions. Our results demonstrate how macroscopic loading conditions affect the evolution of the number of twins and twin volume fraction for each variant, which in turn influences the overall twin volume fraction. The paper is organized as follows: Section 2 describes the MD simulation geometry and the details of the loading cases considered in this work. Section 3 discusses how twinning evolution occurs in the form of the number of twins and their volume fractions with a focus on the nucleation, growth, coalescence and de-twinning processes. We briefly present some ideas on how such information could be described as evolution laws for continuum modeling. Finally, Section 4 summarizes our findings.

2. Simulation details

We simulate the deformation of single crystal Mg with a pre-existing square crack in the basal plane using LAMMPS [22]. The crack serves as an idealized heterogeneity that triggers defect (dislocation, twin) nucleation [23]. The simulation domain is identical to the one adopted by Aghababaei and Joshi [21] comprising a cube of 20 nm hosting 363 636 atoms. The crack is simulated by removing atoms at the center of the domain, which reduces the actual number of atoms in the system to 363 609. The crystal orientation is as follows: the global x-axis is along the crystal $\langle 2\bar{1}\bar{1}0 \rangle$, the global y-axis is along $\langle 01\bar{1}0 \rangle$ and the global z-axis corresponds to $\langle 0001 \rangle$ (Fig. 2). We adopt the modified embedded-atom method (MEAM) potential with parameters obtained by Kim et al. [24]. A time step of 2 femtoseconds (fs) is used to integrate the equations of motion using the velocity Verlet algorithm. Periodic boundary conditions (PBCs) are applied in the three directions. The system is first equilibrated at zero bar
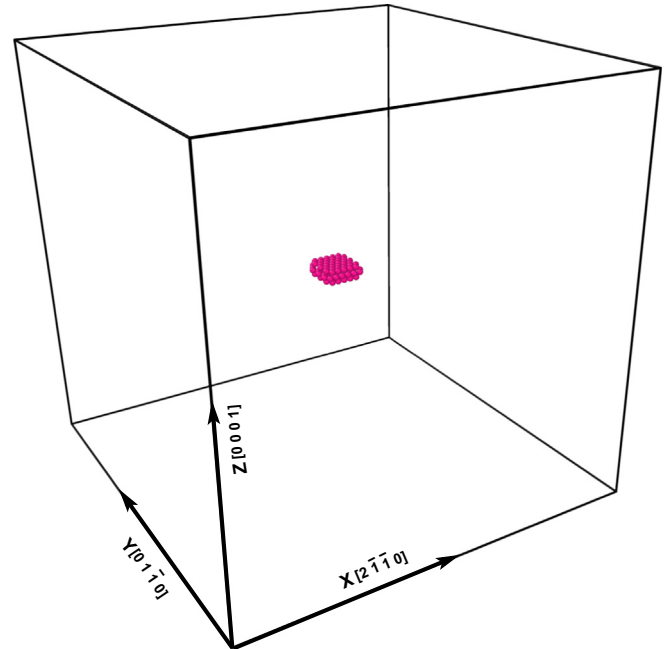

Fig. 2. MD simulation domain with a pre-existing crack. HCP atoms are suppressed to indicate the crack.