Influence of Crystallographic Orientation on Twin Nucleation in Single Crystal Magnesium

C.D. Barrett[1], M.A. Tschopp[1], H. El Kadiri[1], B. Li[1]

[1]Center for Advanced Vehicular Systems
Mississippi State University, Starkville, MS USA

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Abstract

Experimental plasticity on single crystals has found substantial non-Schmid effects in both twinning and non-basal slip in pure magnesium. The deviation from Schmid's law has been attributed to the strong sensitivity of both twinning and slip to small lattice heterogeneities [1] and the effect of pre-slip and non-planar dislocation dissociation [2]. However, most molecular dynamics simulations use heterogeneities so the effect of slip on twin nucleation and vice-versa has been shrouded. This has motivated us to investigate the influence of crystal loading orientation on *homogeneous* slip and twin nucleation using molecular dynamics. These simulations allowed us to appreciate the propensity and nature of twin nucleation when pre-existing defects are absent. Analyses of deformation mechanisms and stress-strain responses shows that homogeneous dislocation nucleation on the basal slip system is correlated with the highest Schmid resolved shear stress, while homogeneous nucleation of tensile twins did not always correlate with the highest Schmid resolved shear stress.

Introduction

Twinning readily occurs in double lattice structures such as hexagonal-close-packed (HCP) structures primarily because the close-packed directions contained within the basal planes cannot accommodate c-axis deformation. Other slip modes having a Burgers' vector with a non-zero component along the c-axis, such as pyramidal $\langle c+a \rangle$ slip are at least five times harder than basal slip in polycrystals. Although twinning is believed to be athermal, the critical stress to activate prismatic and pyramidal slip decreases with increasing temperature, thereby minimizing the contribution of twinning at higher temperatures unless the strain rate is increased. Twinning sharply reorients the parent crystal, transmutes parent dislocations [3], and introduces substantial interfaces, thereby causing strong crystallographic anisotropy and a rapidly increasing hardening rate behavior, particularly when twinning is able to consume the entire parent grain in sharply textured materials. As high-strength wrought magnesium alloys are systemically textured, twinning is highly sought to be prohibited or mitigated so to promote forming at cost-effective rates without risking distortion of components. In part, these have motivated renewed efforts towards a fundamental understanding of the mechanisms underlying twin nucleation in HCP lattices.

While some insight into twin nucleation behavior may be able to be obtained via in situ high resolution transmission electron microscopy (TEM) experiments, these experiments are often very difficult to perform and are not without complications. The use of molecular dynamics (MD) simulations to probe plasticity in HCP structures has received much interest in the last decade. The primary objective of these simulations has been to elucidate the mechanisms of twin nucleation as well as some interest dedicated to non-basal slip activities. In these simulations, the twin nucleation problem tends to be a highly-debated subject. The influence of the interatomic potentials for HCP metals on twinning is important in the results of MD simulations. Also, the use of constrained free surfaces introduces a planar defect into the system that influences twinning in many MD simulations. Planar defects, such as grain boundaries, and line defects, such as dislocations, play an important role in twin nucleation. Twins systemically nucleate at low angle grain boundaries in polycrystals [4]. Furthermore, recent experiments have shown that even under profuse twinning conditions, twins nucleate only after 1.3% plastic strain. These studies show that prior slip plays a key role in twin nucleation and have actually substantiated the theories developed earlier by Mendelson [2] on the role of prior slip in twin nucleation. This slip-twin interaction may have also an important influence on the non-Schmid behavior observed when single crystals have been experimentally tested. For instance, Kelley and Hosford [1] showed a surprising behavior of non-basal slip and twins nucleating in samples designed to favor only one single deformation mode based on assumptions from the Schmid law classically used in single lattice structures such as FCC and BCC. This had

led to considerably conflicting values of threshold stresses of non-basal slip and twinning systems.

So, how can the influence of resolved stress components *and* heterogeneities be addressed using molecular dynamics simulations? Molecular dynamics simulations that use pre-existing defects in a crystal lattice make it difficult to distinguish what is the effect of resolved stress components and what is the effect of the introduced heterogeneities. However, previous simulations on homogeneous and heterogeneous dislocation nucleation in FCC crystals may provide the framework for answering this question. Tschopp, Spearot, and McDowell [5] approached this problem in FCC Cu by: 1) analyzing the influence of resolved stresses on *homogeneous* dislocation nucleation in single crystal Cu, 2) formulating a phenomenological nucleation that accounted for resolved stress components, 3) analyzing the influence of added defects on *heterogeneous* dislocation nucleation, and 4) inserting a damage-like parameter to capture the resulting influence due to lattice hetereogeneities. While twin and dislocation nucleation in HCP metals is considerably different from dislocation nucleation in FCC crystals, the methodology can be applied to HCP metals. The key first step in this methodology is understanding how resolved stresses impact homogeneous nucleation in single crystals and developing a fundamental phenomenological model that can capture this. In this paper, we have used MD simulations to explore *homogeneous* dislocation and twin nucleation in single crystal Mg under uniaxial loading conditions as a function of crystallographic orientation. The crystallographic orientation of loading will impact the resolved shear stresses on various dislocation and twin systems within Mg. This will enable us to explore the relationships between the actual mechanisms, multiple potential slip/twin systems, and the corresponding Schmid and non-Schmid resolved shear stresses to try to develop better phenomenological models for twin nucleation as a function of crystallographic orientation.

Simulation Methodology

A parallel molecular dynamics code (LAMMPS, [6]) that incorporates domain decomposition is used to deform the single crystal atomistic models. A similar methodology to that previously used to examine homogeneous dislocation nucleation in single crystal FCC crystals is used here [7; 8; 9]. First, the configuration is equilibrated using MD in the isobaric-isothermal (NPT) ensemble at a pressure of 0 bar and a temperature of 100 K for 10 ps. Next, the configuration is deformed in uniaxial tension at a constant strain rate of 10^9 s^{-1} with a stress-free condition

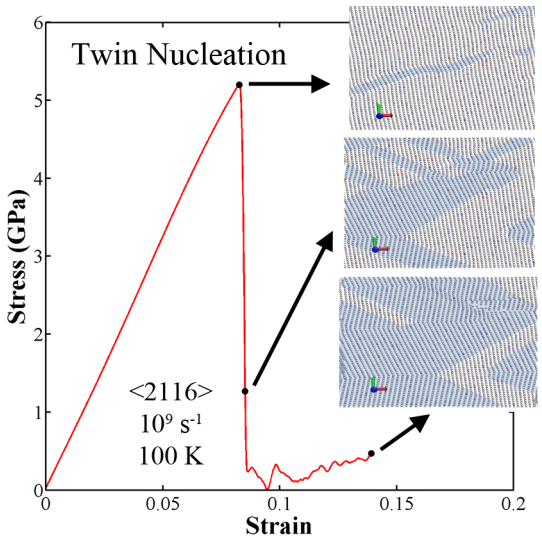

Figure 1: An example stress-strain curve showing twin nucleation at the maximum tensile stress.

for the other two boundaries. For mechanical properties, the system stress is calculated using the virial definition. The stress required for twin or dislocation nucleation is defined as the maximum uniaxial tensile stress. Figure 1 shows a stress-strain curve for the ⟨2116⟩ loading orientation at a strain rate of 10^9 s^{-1} and a temperature of 100 K. As shown in Fig. 1, visualization of selected tensile axis orientations along the appropriate planes showed that twins/dislocation are nucleated at a displacement very close to the maximum tensile stress for all single crystal models. In most cases, twins appeared to nucleate slightly before the maximum tensile stress is reached (<1.0% below the maximum tensile stress). However, in light of the difficulty of visually ascertaining exactly when the twin nucleates (i.e., how many spatially clustered, distorted atoms on the twinning plane constitute a single twin embryo), the maximum tensile stress provides an accurate indication of the stress required to homogeneously nucleate a twin in each single crystal model.

The Sun et al. [10] embedded-atom method potential for Mg is employed in this study. The Sun et al. potential was fit to crystal, liquid, and melting properties of Mg and dislocation core structures compare well compared to ab initio and experimental values [11]. Furthermore, Yasi and colleagues [11] found that the Sun et al. potential better captured the splitting distance of dissociated edge and screw partial dislocations on the basal plane than the Liu et al. [12] potential when compared to ab initio

results. Additionally, the Peierls stresses for basal (0.3 and 3.6 MPa for edge and screw) and prismatic slip (13 and 44 MPa for edge and screw) are in agreement with experiments. For all these reasons, the aforementioned potential is deemed sufficient to characterize homogeneous twin nucleation in single crystal Mg.

A 3D periodic computational cell is used to investigate homogeneous twin nucleation in single crystal Mg under uniaxial tension at a constant strain rate. Cell dimensions are chosen to properly enforce the 3D periodic boundary conditions for each orientation, with a minimum length of 20 nm in all directions. This length is chosen to minimize both the effect of periodic boundaries on twin nucleation and the number of atoms in the system for computational efficiency. The non-integer nature of the c/a ratio for the interatomic potential complicates the generation of a 3D periodic cell in HCP metals. Although not explicitly shown in this work, simulations investigating the effect of the periodic length validate that the stress required for twin nucleation is essentially unaffected by further increases in the size of the simulation cell. This minimum periodic length results in cells with sizes on the order of 10^5-10^6 atoms. Therefore, the minimum length of 20 nm is deemed sufficient to avoid significant effects of periodic boundaries on the 3D dislocation nucleation dynamics.

Figure 2 shows the tensile axis for the 13 crystallographic orientations examined in this work, within the basic stereographic triangle with $\langle 0001 \rangle$, $\langle 10\bar{1}0 \rangle$, and $\langle 1\bar{2}10 \rangle$ vertices. Each single crystal model is deformed under uniaxial tension at a temperature of 100 K. The expected twinning system is the $\{10\bar{1}2\}$ $\langle 10\bar{1}\bar{1} \rangle$ twin system for all tensile axis orientations in the $\langle 0001 \rangle$-$\langle 10\bar{1}0 \rangle$-$\langle 1\bar{2}10 \rangle$ triangle.

The computational methodology used to investigate twin nucleation in this work differs from MD simulations for HCP metals described in previous literature. First, we have chosen to use a larger number of orientations to explore the anisotropy in twin nucleation throughout the stereographic triangle. Second, the simulation boundary conditions are different than previous simulations. Many previous simulations have used a fixed boundary to apply tension or simple shear, thereby admitting heterogeneous twin nucleation at the free surface and fixed regions. The present simulations incorporate a 3D periodic computational cell with no free surfaces or fixed regions and twin nucleation occurs homogeneously as a function of the local stress state. The current uniaxial deformation simulations of twin nucleation take into account the resolved shear stress, the resolved normal stress, and natural couplings that exist between resolved stresses on the twinning and slip planes.

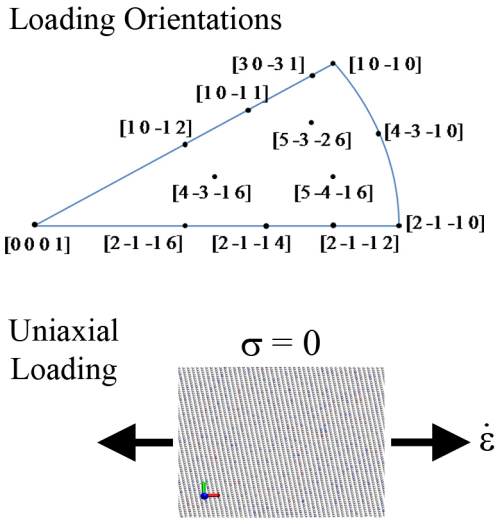

Figure 2: Uniaxial loading orientations and conditions for single crystal deformation simulations.

Simulation Results

The stress-strain curves for the 13 crystallographic loading orientations are shown in Figure 3. As in Fig. 2, the single crystals are loaded in tension and the stress increases until a peak stress, at which either a dislocation, twin, or void/crack nucleates within the single crystal. For each loading orientation, the deformation mechanism was characterized by examining the relevant slip/twin planes and directions to ascertain what defect corresponded to the peak nucleation stress. The stress-strain curves are colored according to deformation type. In many loading orientations, the stress required to nucleate dislocations tended to be lower than that for twins. In the curve with the highest nucleation stress, neither dislocations or twins were observed to nucleate. It should be noted that these stresses are the uniaxial tensile stresses required for the nucleation events; the resolved stresses are lower.

Of the 13 crystallographic orientations studied, five orientations nucleated twins and seven orientations deformed via slip. The final orientation was loaded in the basal $\langle 0001 \rangle$ direction and showed no evidence of twinning or slip. Interestingly, this orientation has the highest likelihood of twinning under tensile stress, yet no twinning is observed. Again, recall that the single crystal models used here are absent of point defects, pre-existing dislocations, or free surfaces. Perhaps the lack of twin nucleation

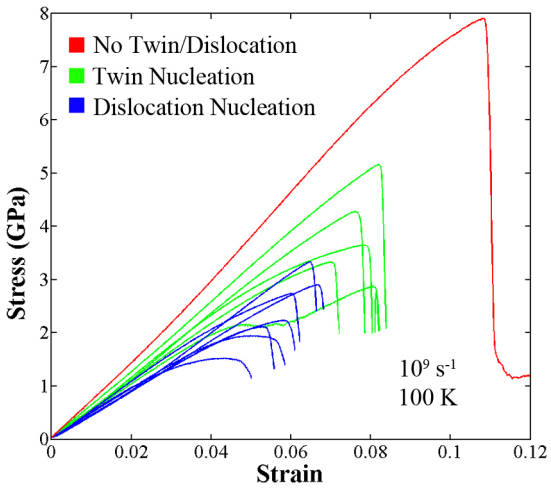

Figure 3: Stress-strain curves for all single crystal models.

suggests that other point, line, or planar defects need to be present in the lattice in order to spur the twin nucleation process. Additionally, analysis of resolved stress components may shed light on this phenomenon.

The crystallographic loading orientations which nucleated dislocations by slip were all characterized as basal slip, as would be expected from the Schmid resolved shear stress. The twins were easily identified, but further classification of twinning plane and directions is still ongoing work. It appears that a number of twin modes were observed in these simulations.

The influence of temperature (100 K, 200 K, 300 K, 400 K) and strain rate (10^8-10^{10} s^{-1}) was examined for a few loading orientations. In the loading orientations examined, the temperature range examined affected the nucleation stress and strain, but the mechanism tended to be unaffected. Higher temperature simulations at 400 K showed a lower elastic modulus, nucleation stress, and strain at nucleation. Interestingly, the rate of propagation of the twinned structure appeared more rapid in simulations run at higher temperatures. Simulations at strain rates from 10^8 s^{-1} to 10^{10} s^{-1} showed very little variation in results. These conditions nucleated the same deformation mechanism, at near the same stress, with the nucleating stress decreasing slightly as strain rate decreases. The choice of a strain rate of 10^9 s^{-1} appears valid. Interestingly, in many of the loading orientations which nucleated twins, one variant was observed to nucleate with multiple twin variants observed thereafter as the strain was increased. In only one loading orientation, the $\langle 10\bar{1}0\rangle$ orientation, were multiple twin variants nucleated at the peak stress.

The resolved stress components may shed light on why each loading orientation nucleated either twins or dislocations. Figure 4 shows the resolved shear stresses calculated from the nucleation stress and the Schmid factor for various twinning/slip systems. Here, we calculated the resolved shear stresses for $\{10\bar{1}2\}\ \langle 10\bar{1}1\rangle$ twins, $\{0001\}\ \langle 11\bar{2}0\rangle$ basal dislocations, $\{10\bar{1}0\}\ \langle 11\bar{2}0\rangle$ prismatic dislocations, $\{10\bar{1}1\}\ \langle 11\bar{2}0\rangle$ pyramidal dislocations, and $\{11\bar{2}2\}\ \langle 11\bar{2}3\rangle$ pyramidal $\langle c+a\rangle$ dislocations. The resolved stress for all systems are plotted along with the observed twin/dislocation system (circled in black). The observed resolved shear stress varies with loading orientation, but in nearly all the loading orientations the observed mechanism had the highest Schmid factor and, therefore, the highest resolved shear stress. All of the loading orientations characterized as nucleating dislocations on the basal or prismatic slip systems predicted that that slip system had the highest resolved shear stress. The $\langle 10\bar{1}0\rangle$ loading orientation nucleated twins at a very low resolved shear stress, but the '2' indicated on the plot refers to the simultaneous nucleation of two twin variants. In this case, the low Schmid factor may be accommodated by the ability to simultaneously nucleate on two twin systems. Additionally, while the observed twinning system did not always have the highest resolved shear stress, the prismatic and pyramidal slip systems are known to have higher critical

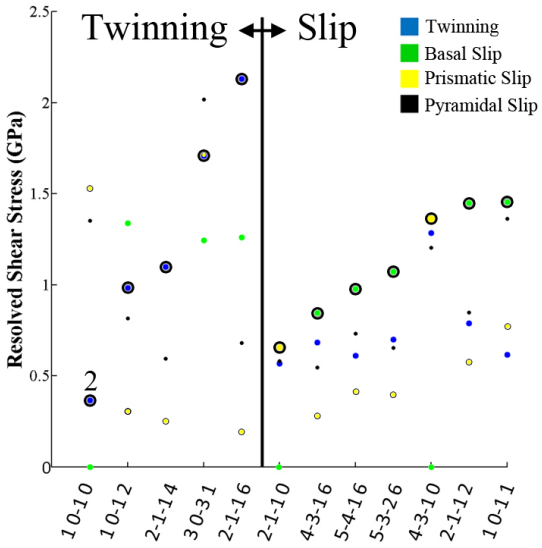

Figure 4: Resolved shear stresses on the twinning and slip systems for different loading orientations and the observed twin/dislocation system (circled in black).

resolved shear stresses, possibly explaining the nucleation of twins for these orientations. The $\langle 10\bar{1}2 \rangle$ loading orientation appeared to nucleate twins even though the basal slip mechanism has a higher resolved shear stress. It is not known why this occurs; future work will investigate the potential influence of non-Schmid resolved stresses on nucleation as well as the role of the interatomic potential. It is clear that only calculating resolved stresses via the Schmid factor may not be able to completely capture the complicated slip-twin nucleation event. Furthermore, examining in greater detail the atomic positions and crystallography corresponding to the twin nucleation event itself may shed light on whether dislocation nucleation plays a key initial role in the nucleation of twins on these systems.

Summary

The objective of this research is to elucidate the mechanisms of dislocation/twin nucleation in single crystals and grain boundaries for Mg. Here, we concentrate on single crystal calculations, where we used molecular dynamics simulations to study the influence of crystallographic orientation on dislocation/twin nucleation under uniaxial loading. Multiple crystallographic loading orientations from around the stereographic triangle were deformed under uniaxial tension to examine the role of resolved stresses on twin/dislocation nucleation. The results of this work detailed the influence of crystallographic loading orientation in single crystals on dislocation and twin nucleation mechanisms in magnesium. Here, we have shown that the Schmid resolved shear stress adequately predicts basal or prismatic slip in all orientations which were observed to nucleate dislocations on the basal and prismatic slip planes. However, in orientations where twins nucleated, the Schmid resolved stresses may not alone be able to completely capture the complicated slip-twin nucleation event.

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