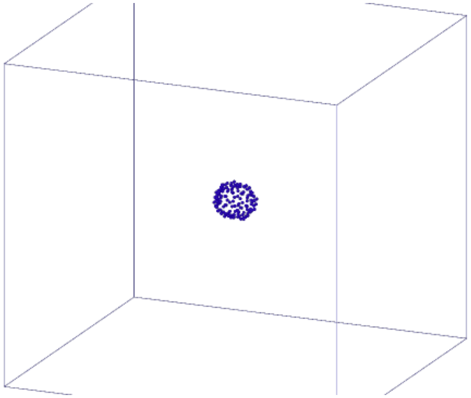
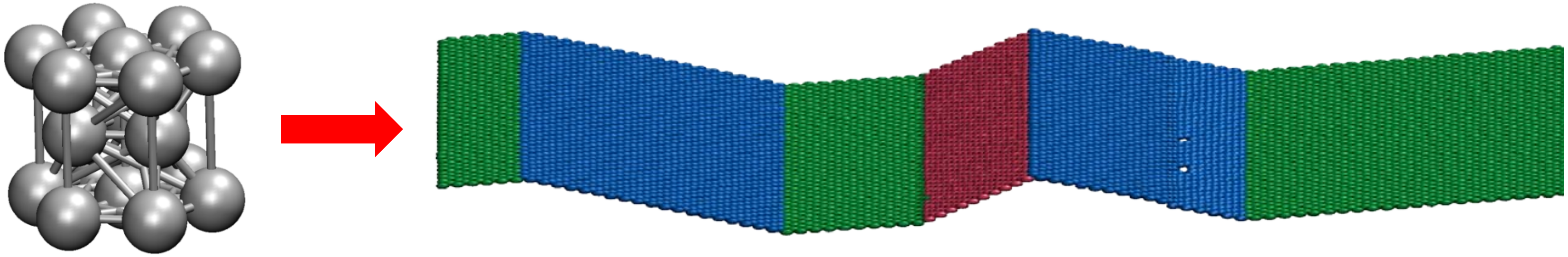
Influence of Crystallographic Orientation on Twin Nucleation in Single Crystal Magnesium





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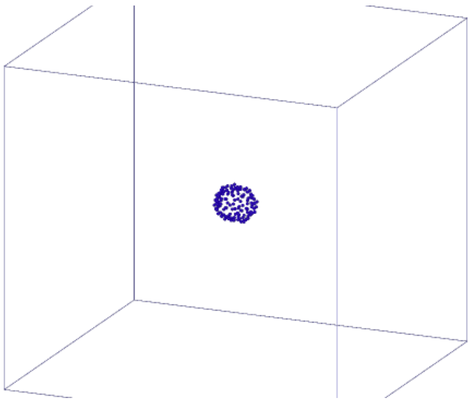
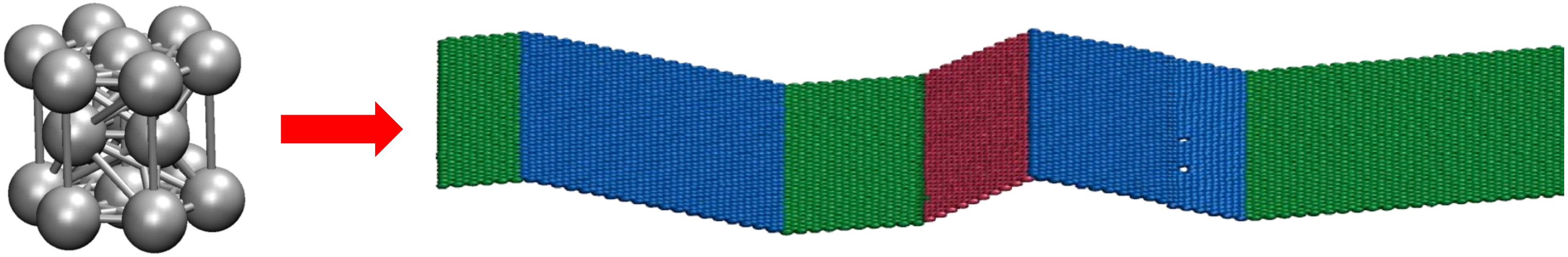
Introduction

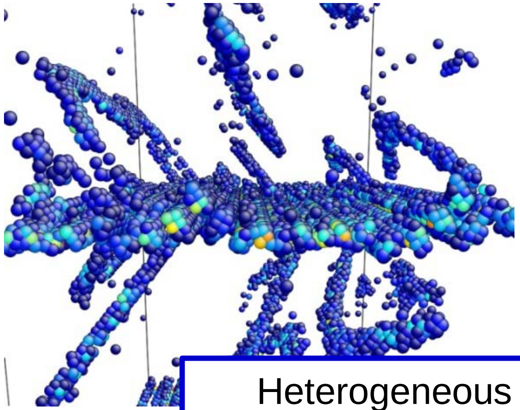
It is well known that plasticity in magnesium alloys is governed by twinning as well as dislocation motion. However, the nanoscale phenomena that govern ***twin nucleation*** are not as well understood.





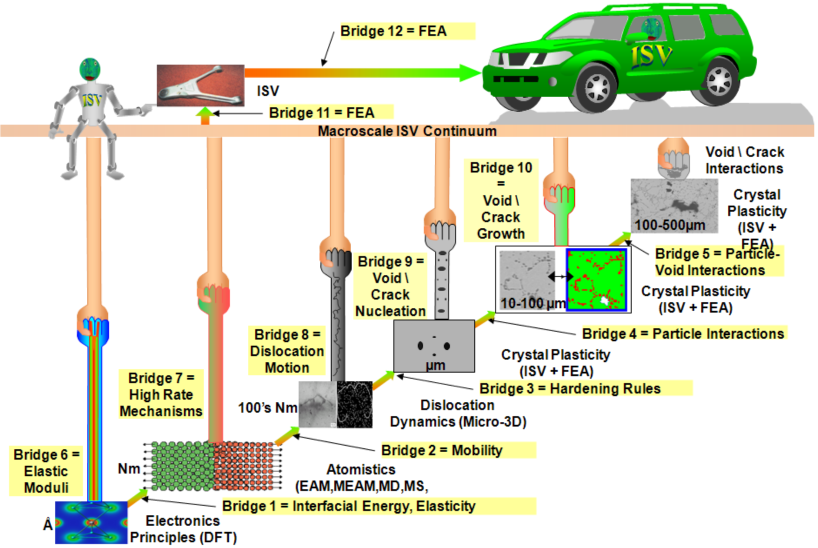
Introduction

Multiscale models that capture twinning in polycrystalline Mg can benefit from nanoscale information. Understanding ***both*** homogeneous and heterogeneous twin nucleation is relevant for these models.



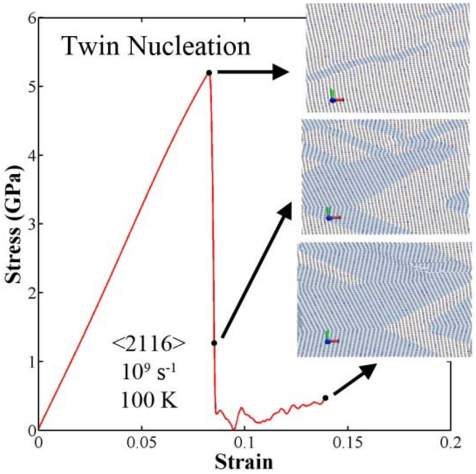
Heterogeneous Nucleation in Mg

Simulations & Experiments over Multiple Length Scales are Required



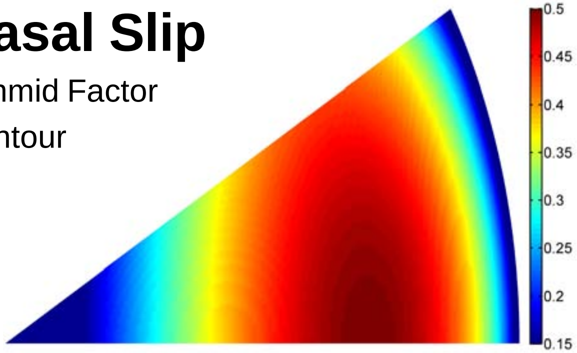
Introduction

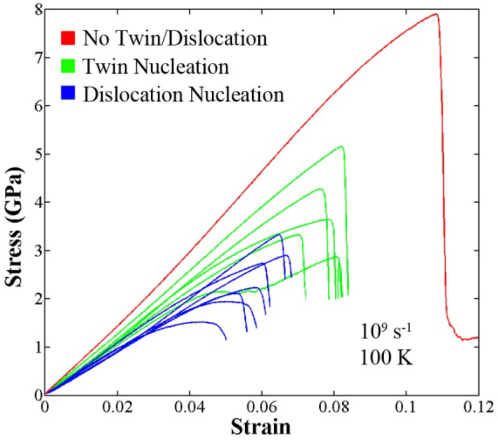
In this work, molecular dynamics simulations are used to investigate how tensile loading axis orientation (and the corresponding stress state) affect homogeneous twin and dislocation nucleation in Mg.

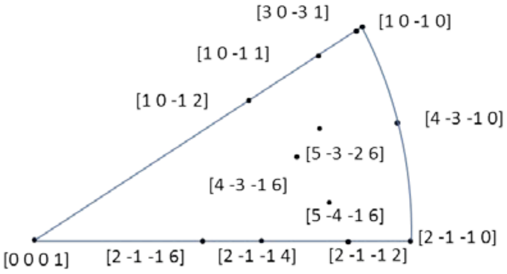


Basal Slip

Schmid Factor Contour





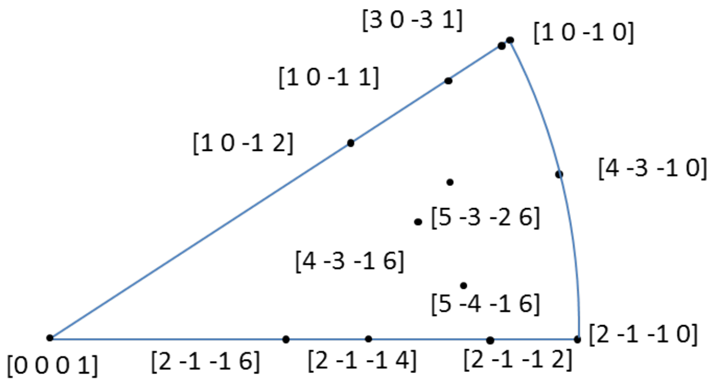


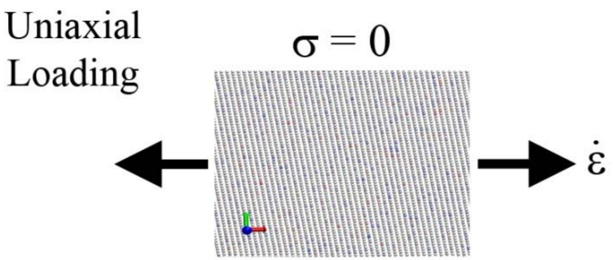
Simulation Methodology

- Molecular Dynamics Simulations
  - LAMMPS was used w/ VMD to visualize simulations
- Boundary conditions
  - 3D periodic simulation cell with a minimum 20 nm length at boundaries
  - Temperature of 100 K
  - Uniaxial tensile loading with zero stress condition at lateral boundaries
- Sun et al. (2006) Mg EAM potential
  - Yasi et al. (2009) found that this potential best captured (i) the splitting distance of dissociated screw and edge dislocations and (ii) the Peierls stresses for basal and prismatic slip in agreement with ab initio calculations and experiments.

Plimpton, S, J. Comp. Physics (1995).
D.Y. Sun et al. Phys Rev B (2006).
J.A. Yasi et al. MSMSE (2009).

13 Loading Axis Orientations

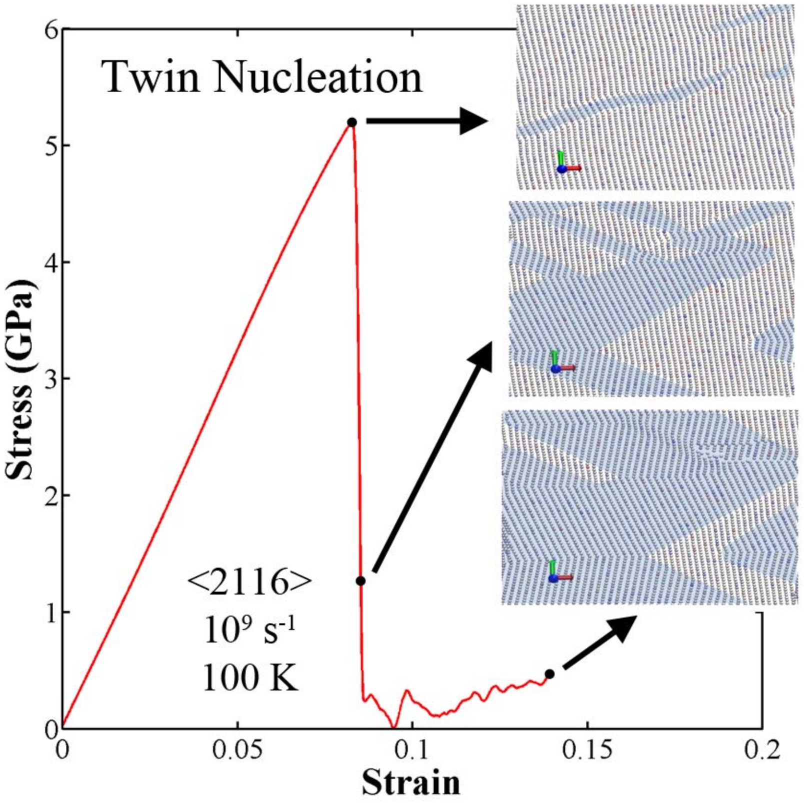


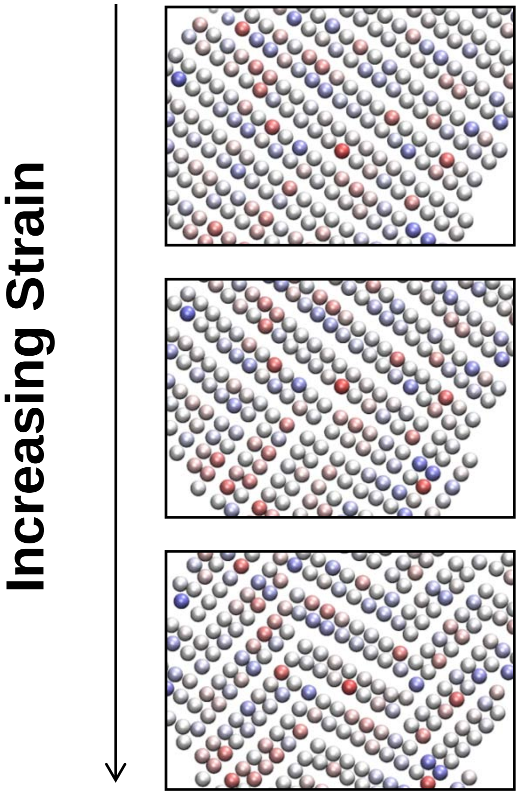


10^9 s^{-1} strain rate

Simulation Results

Stress-Strain Response: Twin Nucleation

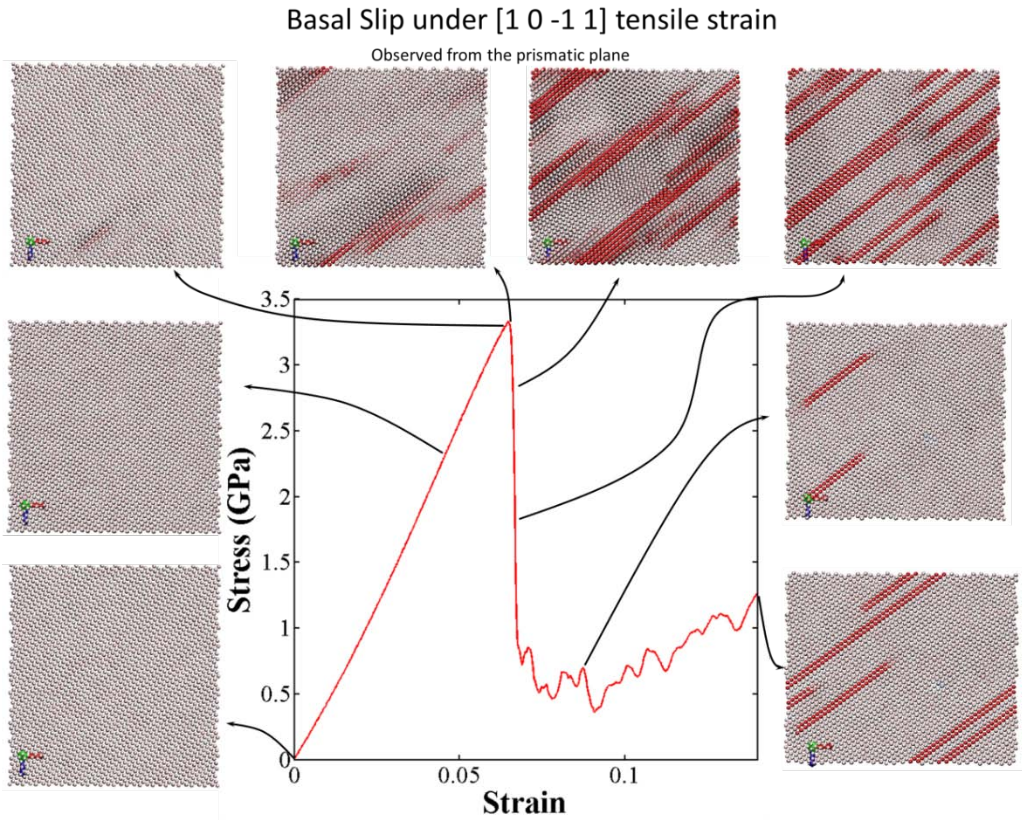




Analysis of the relation of twinning to the stress-strain curve showed twin nucleation occurs at the yield stress and propagates quickly through the simulation.

Simulation Results

Stress-Strain Response: Dislocation Nucleation



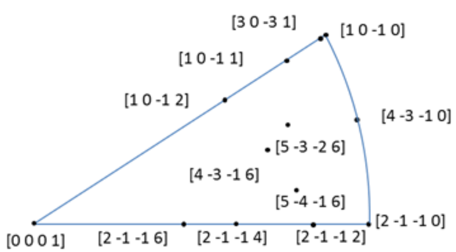
Colored by potential energy (dislocations are shown in red)

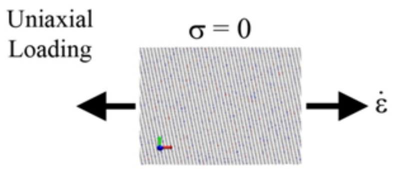
Analysis of the relation of slip to the stress-strain curve showed that dislocation nucleation occurs at the maximum stress and propagates quickly through the simulation.

Simulation Results

Stress-Strain Response for Twin and Dislocation Nucleation

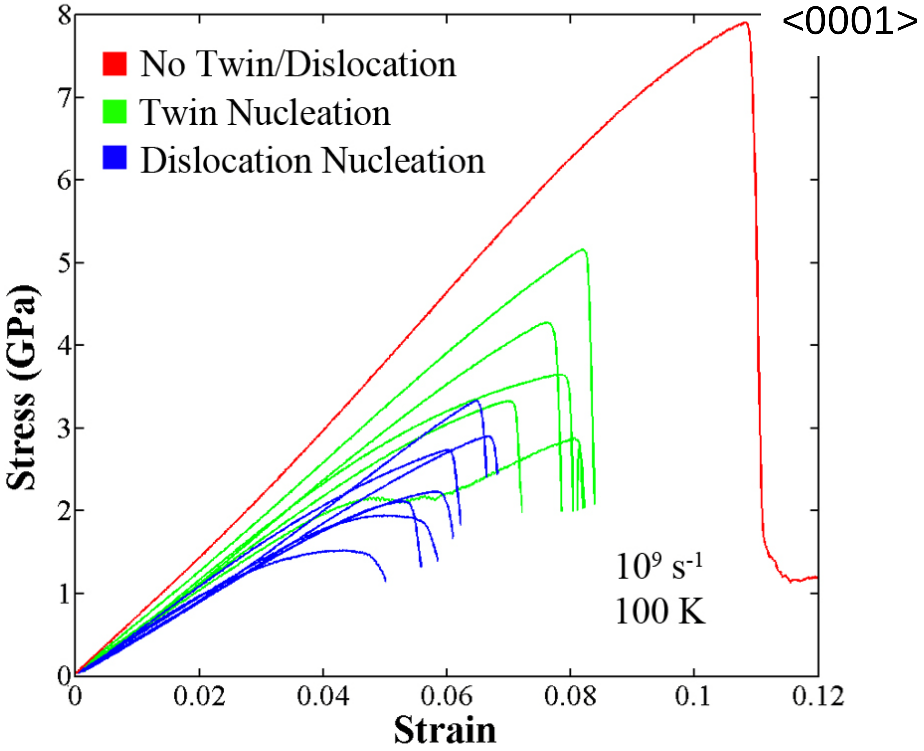
13 Loading Axis Orientations





10^9 s^{-1} strain rate

Stress-Strain curves for all orientations



In general, twins required higher stresses to nucleate. Note that this is the applied stress and not the resolved stress component.

Simulation Results

Identification of twin mode or slip system

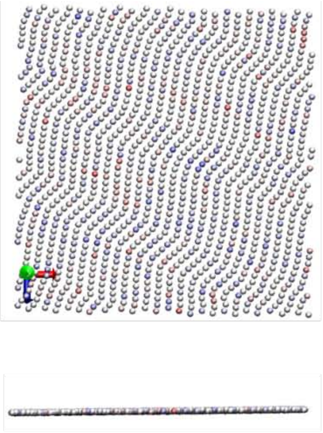


Figure 7: The Twin Plane Front and Side

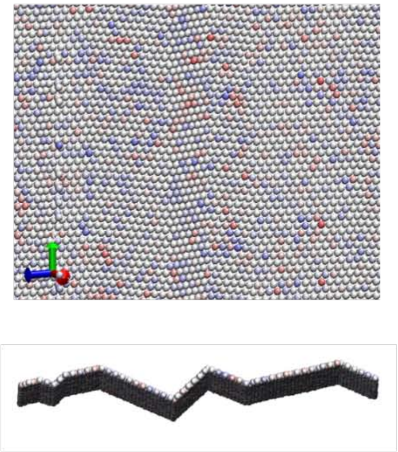


Figure 8: The Plane Orthogonal to the Twinning Direction

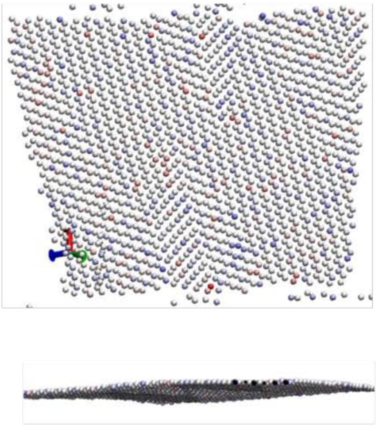


Figure 9: An Arbitrary Plane After Twinning

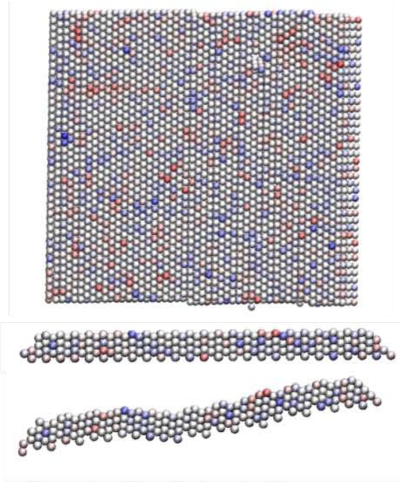


Figure 10: A Plane Undergoing Slip

The twinning system or dislocation slip system was characterized through a series of steps to identify:

(i) Twinning plane and twinning direction

(ii) Slip system and slip direction

* characterized as Basal, Prismatic or Pyramidal Dislocation OR Compression, Tension or Other Twin

Simulation Results

Classification of Homogeneous Twin/Dislocation Nucleation

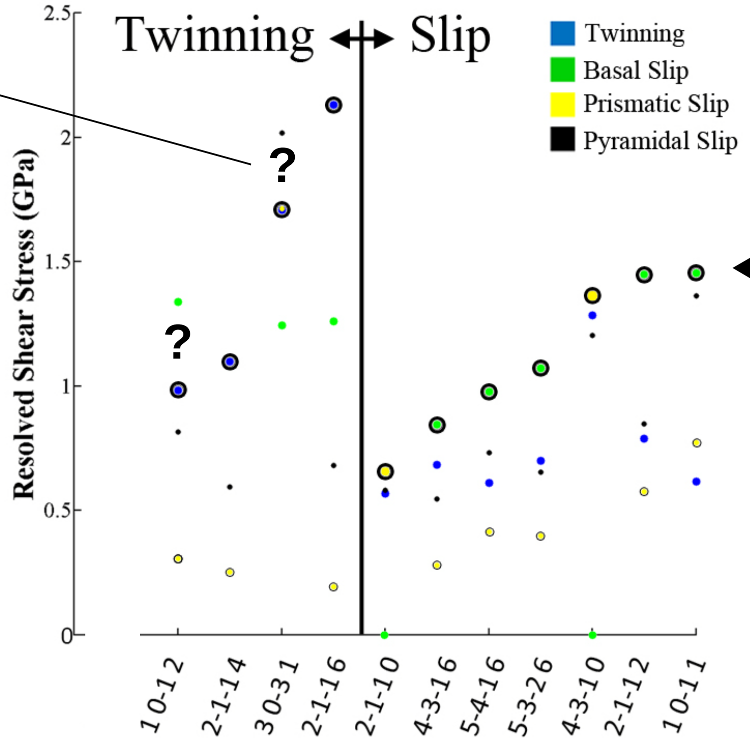
Orientation	Mechanism	System	Direction	Schmid Factor	Nucleation Stress (GPa)	
<3 0 -3 1>	Compression Twin	{1 0 -1 1}	<1 0 -1 2>	0.1791	4.35	Twins
<1 0 -1 2>	Compression Twin	{1 0 -1 1}	<1 0 -1 2>	0.4644	3.23	
<2 -1 -1 4>	Other Twin	{1 1 -2 1}	<1 1 -2 6>	0.4967	3.35	
<2 -1 -1 6>	Other Twin	{1 1 -2 1}	<1 1 -2 6>	0.4639	5.20	
<2 -1 -1 0>	Prismatic Slip	{1 -1 0 0}	<1 1 -2 0>	0.433	1.52	Dislocations
<4 -1 -3 6>	Basal Slip	{0 0 0 1}	<1 1 -2 0>	0.4355	1.94	
<5 -4 -1 6>	Basal Slip	{0 0 0 1}	<1 1 -2 0>	0.4622	2.11	
<5 -2 -3 6>	Basal Slip	{0 0 0 1}	<1 1 -2 0>	0.4803	2.23	
<4 -1 -3 0>	Prismatic Slip	{1 -1 0 0}	<1 1 -2 0>	0.4996	2.73	
<2 -1 -1 2>	Basal Slip	{0 0 0 1}	<1 1 -2 0>	0.4982	2.91	
<1 0 -1 1>	Basal Slip	{0 0 0 1}	<1 1 -2 0>	0.4323	3.37	
<0 0 0 1>	Vacancy Nucleation	N/A	N/A	N/A	8.99	Other
<1 0 -1 0>	Unknown	N/A	N/A	N/A	3.54	

Each loading orientation was analyzed to find the system and direction of the nucleated twin or dislocation. In general, basal/prismatic dislocations and compression twins were nucleated for most orientations. (No tension twins nucleated?)

Simulation Results

Resolved Shear Stresses

Nucleation of pyramidal dislocations may require higher CRSS.

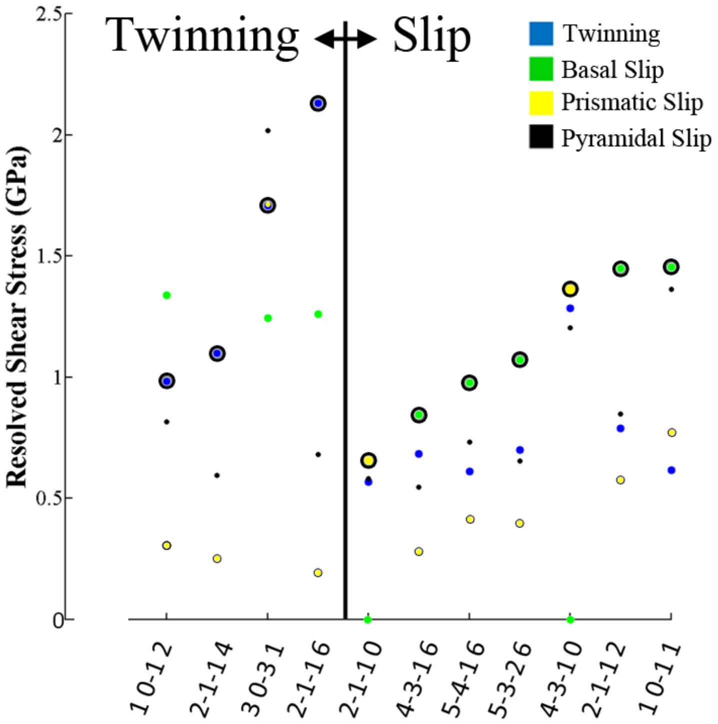


Bold circle denotes actual twin or slip system observed

The maximum resolved shear stress for each twin/slip system was plotted and the observed mechanism was compared. For most, the maximum shear stress correlated with the observed mechanism.

Simulation Results

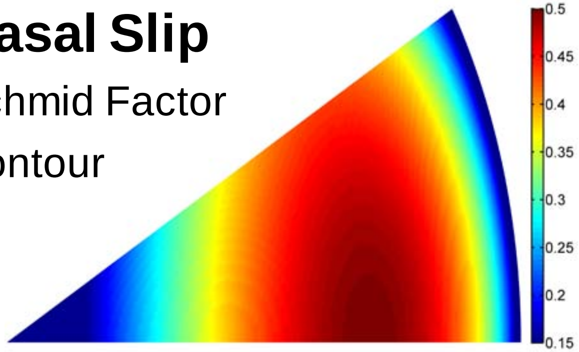
Resolved Shear Stresses



🟢 **Basal Slip**

Schmid Factor

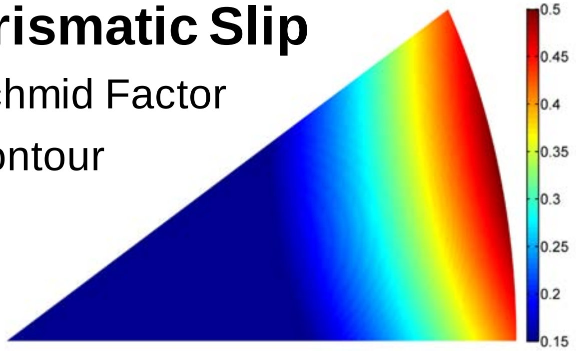
Contour



🟡 **Prismatic Slip**

Schmid Factor

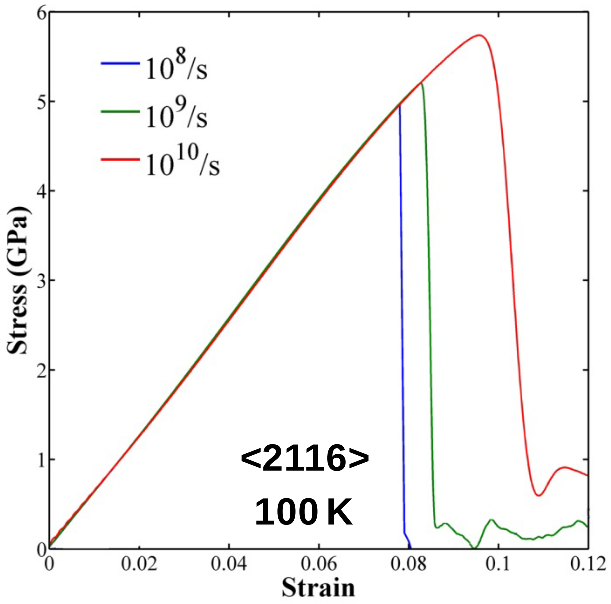
Contour

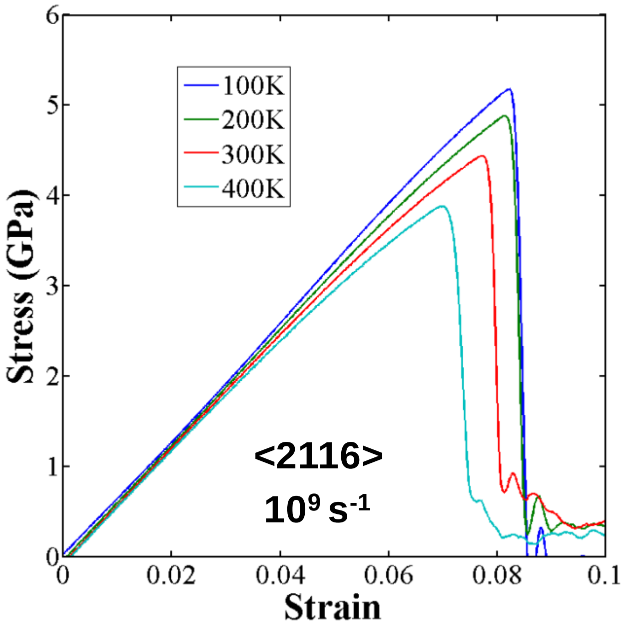


Why the difference in resolved shear stresses required for twin and dislocation nucleation? Future work will explore the potential role of non-Schmid stresses in nucleation phenomena in HCP metals.

Simulation Results

Strain Rate and Temperature Dependence





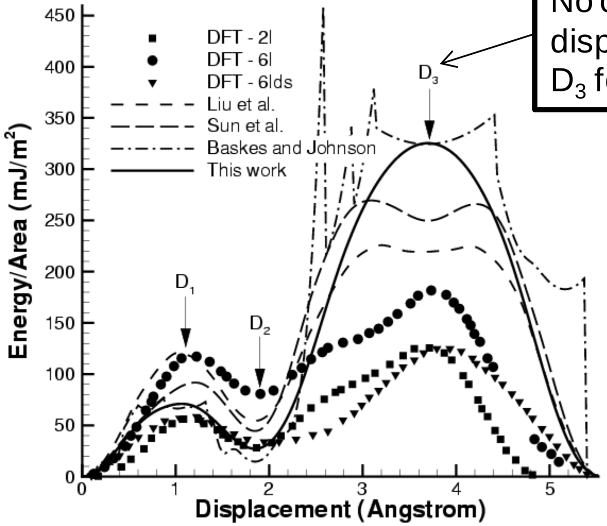
The stress required for twin nucleation decreases with decreasing strain rate. However, the strain rate of 10^9 s^{-1} shows similar mechanism to that at 10^8 s^{-1}.

The stress required for twin nucleation decreases as temperature is increased. Again, the nucleated defect is of the same type, though.

Simulation Results

Interatomic Potential Differences

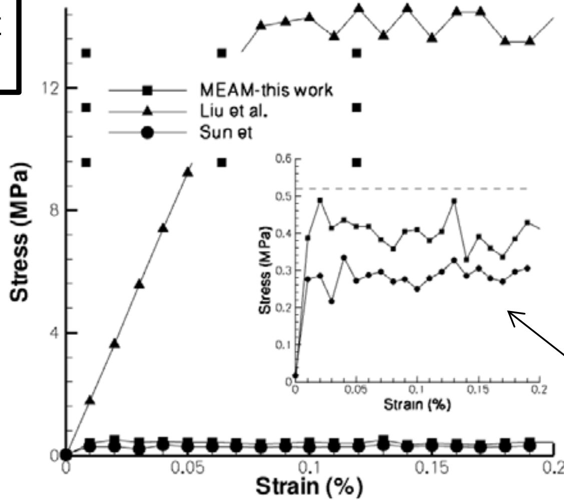
Generalized stacking fault energy curves for Mg



No cusp at displacement D_3 for MEAM

Peierls Stress Calculations

Basal Edge Dislocation Motion



Liu et al.

Expt

Groh et al.

Sun et al.

Better agreement with Expt

The interatomic potential for Mg deformation should capture the slip behavior correctly as well as the twinning behavior. A MEAM potential for Mg has been developed taking into account both stacking fault energy curves from *ab initio* calculations.

S Groh, MI Baskes, MF Horstemeyer, in preparation

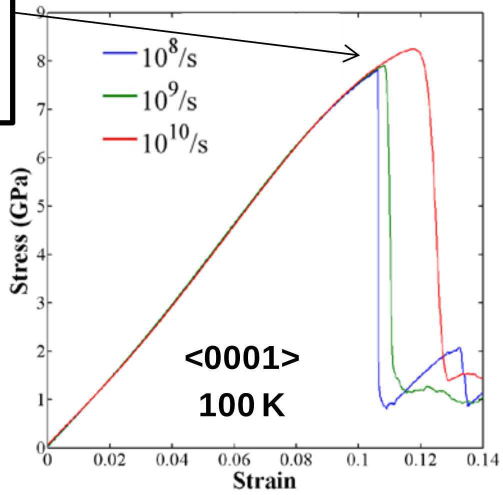
Simulation Results

Interatomic Potential Differences

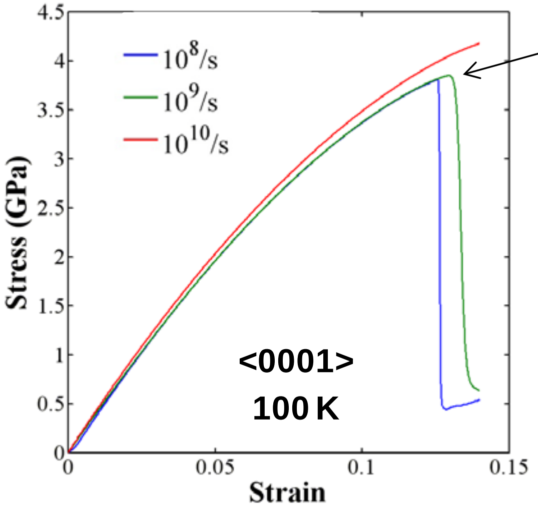
Vacancy nucleation and fracture

Questionable mechanism with Sun et al. potential…

Sun *et al.* (2006) Mg



MEAM Mg (Groh *et al.*)



Produced all six variants of tension twins

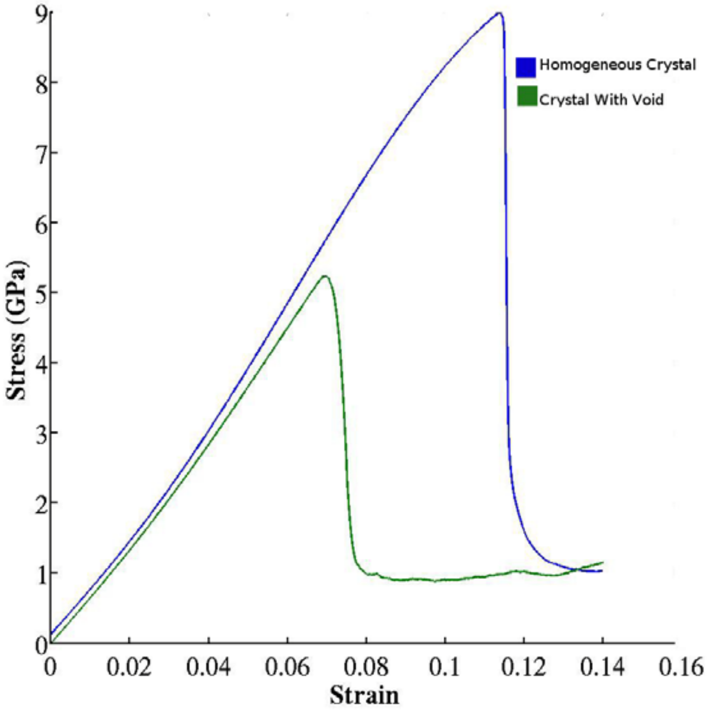
Better agreement w/ experimental mechanisms

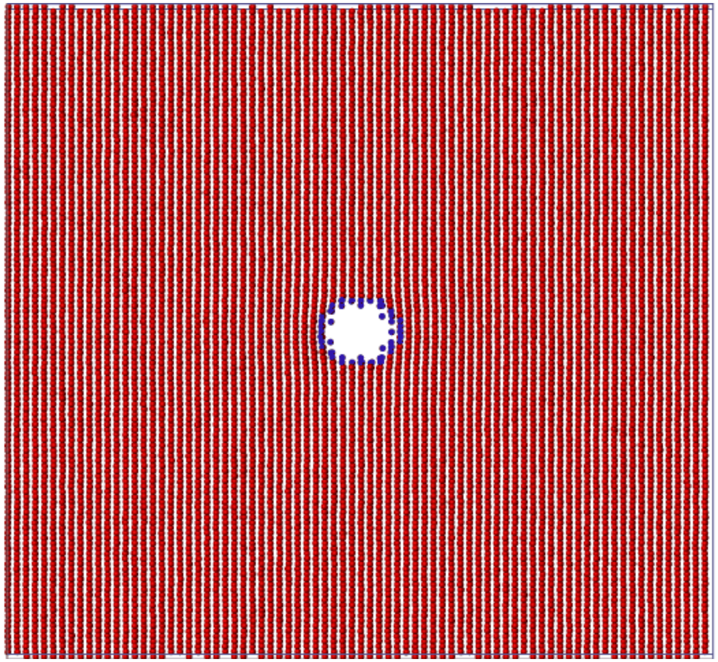
Additional work analyzes the differences between interatomic potentials for twin nucleation. For instance, a new MEAM interatomic potential for Mg (Groh *et al.*) has been formulated to agree with the stacking fault energy curves from *ab initio* results.

D.Y. Sun et al. Phys Rev B (2006).
S Groh, MI Baskes, MF Horstemeyer, in preparation

Simulation Results

Heterogeneous Nucleation from Voids

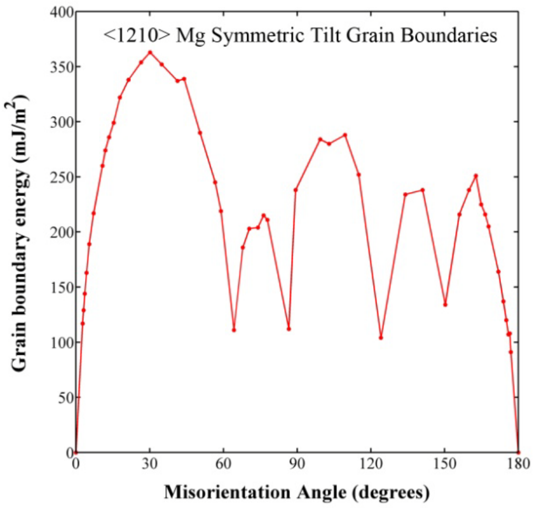




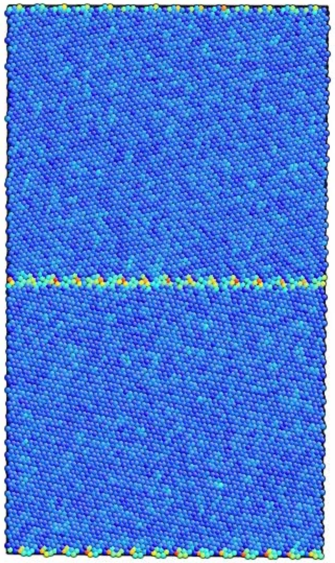
Adding a void to the simulation cell and then loading produces a prismatic dislocation loop and the characteristic tension twin. Further work investigating other loading orientations is underway (voids, boundary conditions, strain rate, cell size, free surfaces, etc).

Future Work

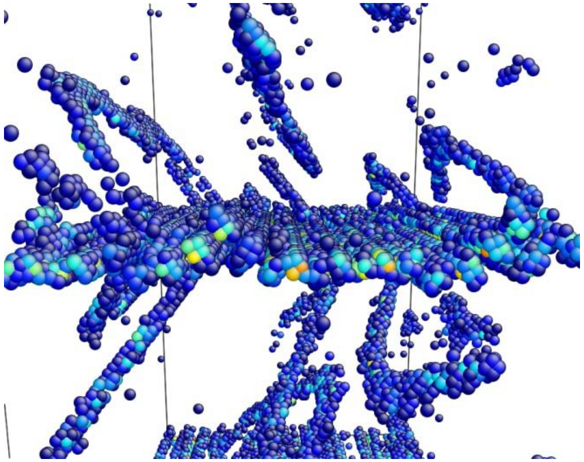
Grain Boundary Twin Nucleation



Generating grain boundary structures



Mg Bicrystal colored by potential energy

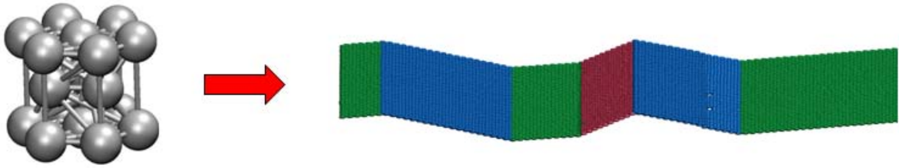


Twin and Dislocation nucleation from Mg Bicrystals

Thank you!

The presenters would like to acknowledge the support from Department of Energy, Southern Regional Center for Innovative Design (SRCLID) program, Contract No.: DE-FC26-06NT42755.

Questions?



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