Mesoscale Priority Research Direction

Atomistic to Mesoscale Modeling of Material Defects and Interfaces

Opportunity

The excitement and promise of nanostructured, multi-phase materials with superior damage tolerance are rapidly growing. One of the outstanding features of such materials is their unusually high density of interfaces. As such, it is the interface that controls their behavior and not the constituents that they join. An opportunity, thus, opens up for new materials discovery via tunable interfaces for target properties. However, understanding how interfaces control defects is still in its infancy.

Meso Challenge

Interfaces and their interactions with defects influence a wide range of behaviors from crystal reorientation, slip, twinning, boundary sliding, migration, phase stability, etc. Little of this can be predicted by treating only one type of defect/interface interaction alone.

References: Z. Q. Wang and I. J. Beyerlein, "An atomistically-informed dislocation dynamics model for the plastic anisotropy and tension-compression asymmetry of BCC metals" *International Journal of Plasticity* **27**(10) (2011) 1471-1484.; I. J. Beyerlein, R. J. McCabe, and C. N. Tomé, "Effect of microstructure on the nucleation of deformation twins in polycrystalline high-purity magnesium: a multi-scale modeling study" *Journal of the Mechanics and Physics of Solids* **59** (2011) 988-1003.; I. J. Beyerlein, J. Wang, M. R. Barnett, and C. N. Tome, "Double twinning mechanisms in magnesium alloys via dissociation of lattice dislocations" *Proc. Royal Soc. A doi: 10.1098/rspa.2011.0731*

Approach

<u>Atomistic-informed meso-scale modeling</u>: Models are packed with information. For one model to 'inform' another means that the transfer of knowledge of dominant mechanisms, phenomena, or physical properties, at the lower scale measurably transforms the way in which the higher scale is modeled and/or performs. In this regard, scientific expertise has to be exercised to determine what atomic scale information is useful and applicable to the rate conditions applied at the meso-scale.

Impact

<u>Process-aware performance</u>: Defects and interfaces influence all stages in the life of a material, from those introduced during processing, to those that nucleate and grow in service and affect performance, and to those that eventually lead to instabilities and govern service life. Designing materials with the complete material life cycle requires advancing predictive capabilities that link defect/interface dynamics from the atomic to the meso scales.

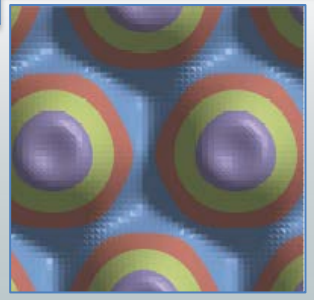
U.S. DEPARTMENT OF ENERGY | Office of Science

Contact: Irene J. Beyerlein

Mesoscale Priority Research Direction

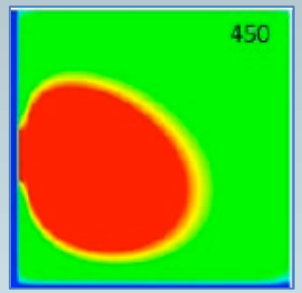
Atomistic to Mesoscale Modeling of Material Defects and Interfaces

ATOMISTIC | MESO-SCALE | MESO-SCALE



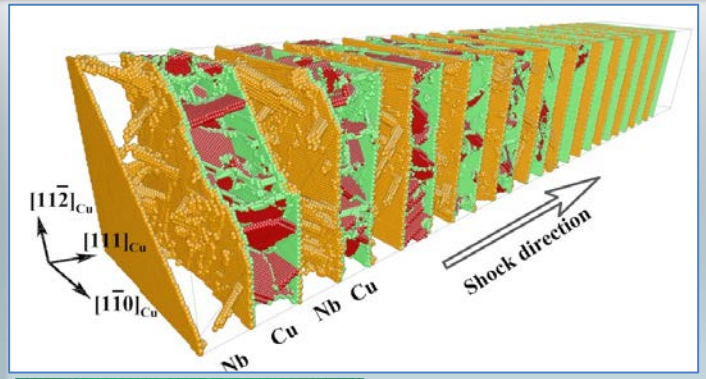
Density functional theory (DFT) of a gamma surface

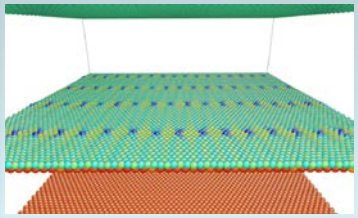
Courtesy of R. F. Zhang



DFT- or MD-informed phase field model of defect nucleation

Hunter et al. **84** (2011) Phys. Rev. B 144108



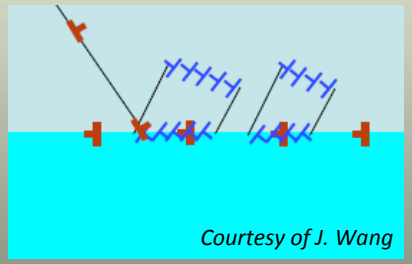


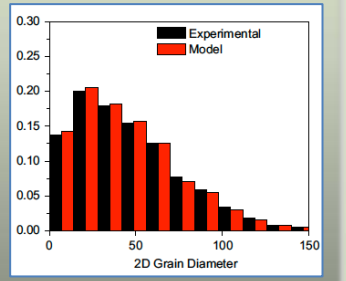
DFT-informed molecular dynamics (MD)

Zhang et al. **91** (2011) Phil Mag. Lett., 730-741

MD informed probability model for nucleation

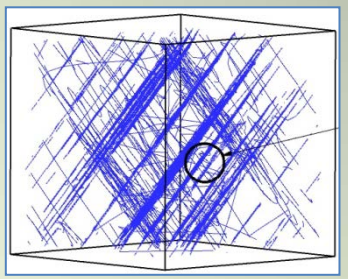
Beyerlein et al. **59** (2011) J. Mech. Phys. Solids 988-1003

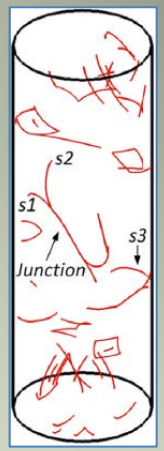




MD-informed dislocation dynamics (DD)

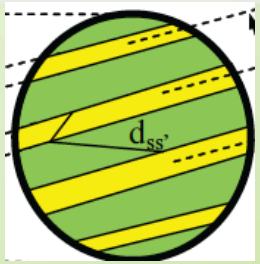
Wang et al. **27** (2011) Int. J. Plast., 1471-1484; C. Z. Zhou et al. 59 (2011) Acta Mater. 7673

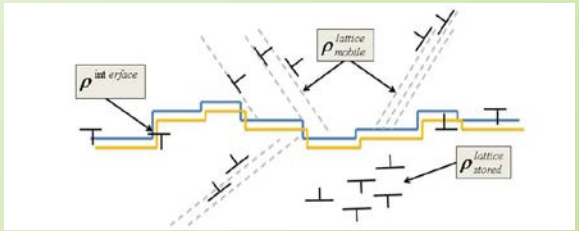




DD-informed model for single crystal response

Beyerlein et al. **9** (2011) J. Multi-scale Comp Engng, 459; Cao et al. 58 (2010) Acta Mater. 549





U.S. DEPARTMENT OF ENERGY | Office of Science

Contact: Irene J. Beyerlein