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April 2014

# Atomistically informed 3D phase field dislocation dynamics (PFDD) model for nanomaterials

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# Nanocrystalline Metals

We know:

- that plastic deformation is mediated by the motion and interaction of dislocations,….

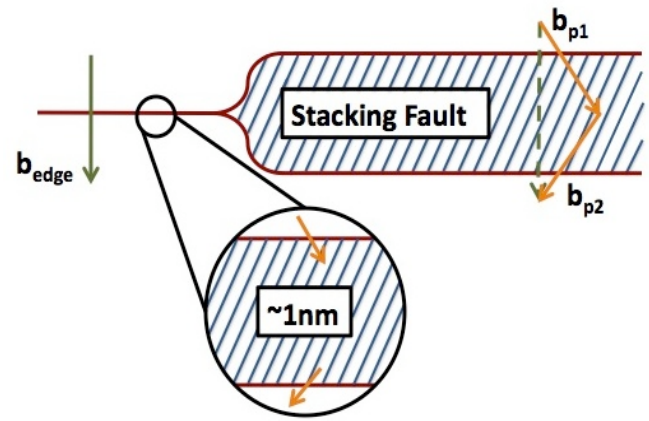
but, in nanocrystals, partial dislocations and stacking fault interactions become the primary driver of plasticity.

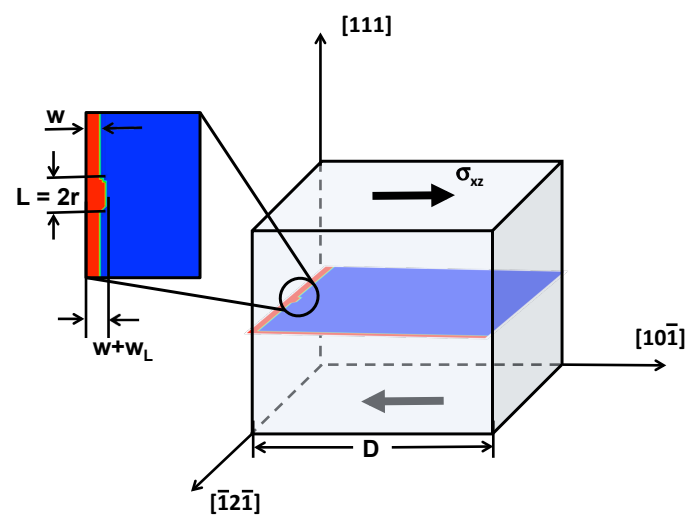
- that the extended core structure impacts elementary dislocation processes, such as cross-slip, nucleation, and lock formation,…

but we don't yet understand how.

- that partial dislocations are the basic defect responsible for alternative deformation mechanisms seen at the nanoscale, such as deformation twinning and emission and absorption at grain boundaries,…

but we still don't understand formation mechanisms and the impact on the overall mechanical response.



# Atomistically Informed PFDD

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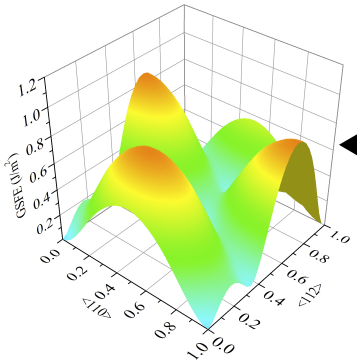
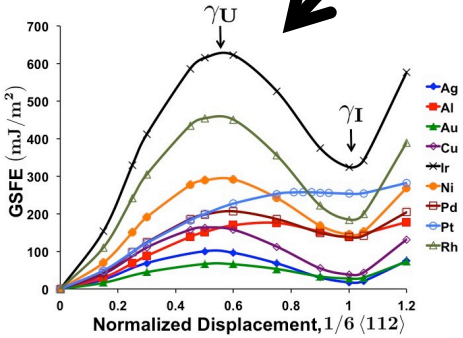
CMIME
Center for Materials at Irradiation and Mechanical Extremes

A. Hunter and I. J. Beyerlein, APL-Materials, **1** (2013) 032109.
A. Hunter *et. al.*, JAP, **115** (2014) 134314.

**Accurate expression of the dislocation core region.**

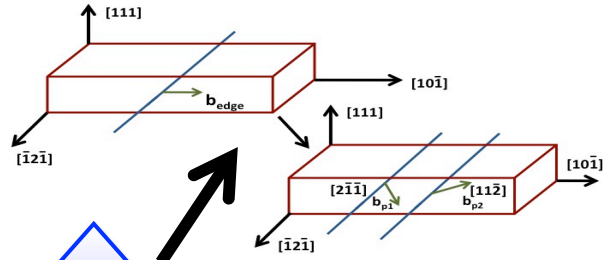
**Can describe the energetics at interfaces.**

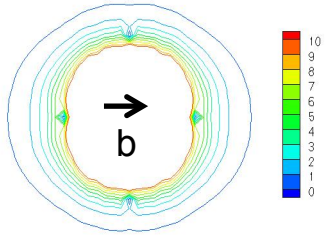


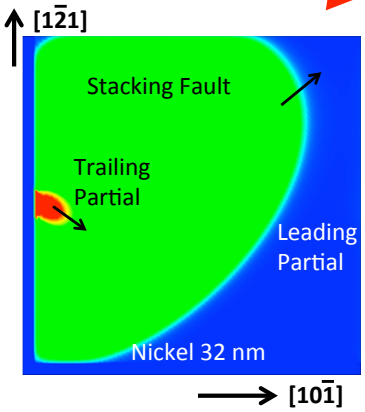




**MD/DFT**

**PFDD**




**Time and lengths scales similar to those used in experiment.**

**No empirical rules or ad hoc parameters**

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# Phase Field Dislocations

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**All physics are expressed in terms of the phase field variables, one for each active perfect dislocation slip system.**

Total System Energy

$$E = E^{elas} + E^{gsfe}$$

Internal: Dislocation-Dislocation Interactions

+

External: Dislocation Interactions with Applied Stress

+

Generalized Stacking Fault Energy

**Annihilation, Repulsion, etc.**

**Resolved Shear Stress**

**Core motion through crystal lattice**

**Extended (partial) dislocations**

**Connection to atomistic methods (DFT, MD)**

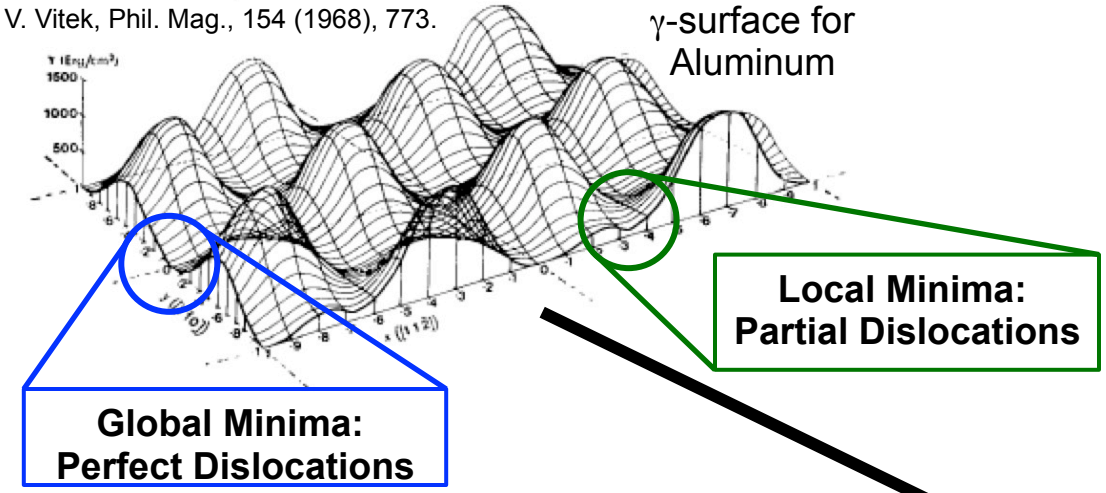
Evolve Kinetics with Ginzburg-Landau

$$\frac{\partial \zeta_n^\alpha(\mathbf{x},t)}{\partial t} = -L \frac{\delta E}{\delta \zeta_n^\alpha(\mathbf{x},t)}$$

A. Hunter and I. J. Beyerlein, MSEA, **600** (2014) 200-210.

# DFT-Informed PFDD

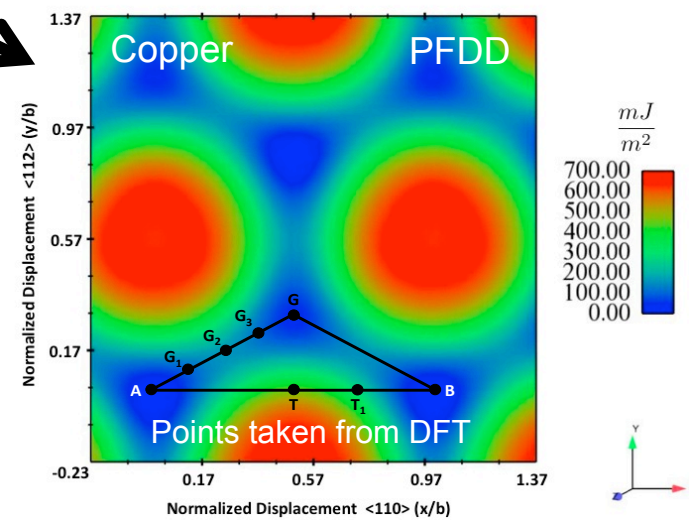
V. Vitek, Phil. Mag., 154 (1968), 773.




The <u>material γ-surface</u>:

Energy landscape that describes energetic maxima and minima atoms must overcome to shear passed one another.

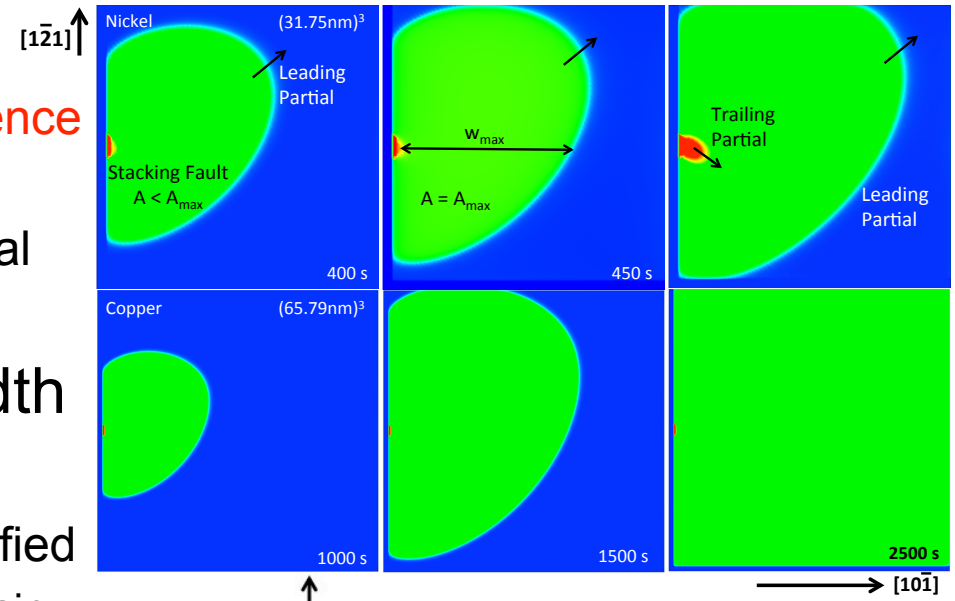
- Accounts for the additional energy required to create and expand a stacking fault.
  - Traditionally only one parameter is used.
- We use a <u>consistent</u> DFT approach for a wide range of metals.
  - Cu, Al, Ag, Au, Pd, Pt, Ni, Cu…

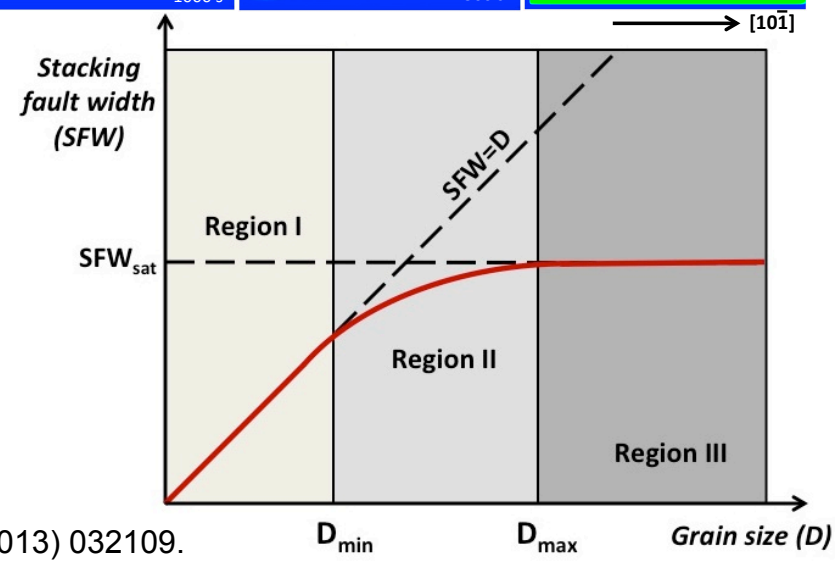



A. Hunter *et. al.*, MSMSE, **21** (2013) 025015.
A. Hunter *et. al.*, JAP, **115** (2014) 134314.

# Grain Size Effects

- Nucleation Stress
  - Essentially no grain size dependence
    - Converse to traditional thought.
  - Notable impact due to size of initial defect
- Size of the stacking fault width (SFW)
  - 3 key regions, previously unidentified
    - Region I: SFW is equal to the grain size
    - Region II: SFW increases with increasing grain size
      - Traditionally thought that SFW increases with decreasing grain size.
    - Region III: SFW has saturated at its largest value

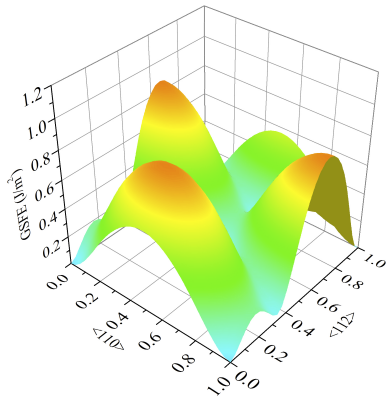


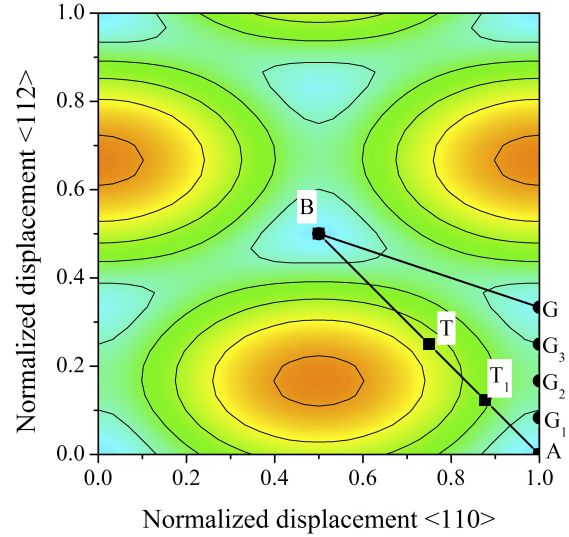

A. Hunter and I. J. Beyerlein, APL-Materials, **1** (2013) 032109.

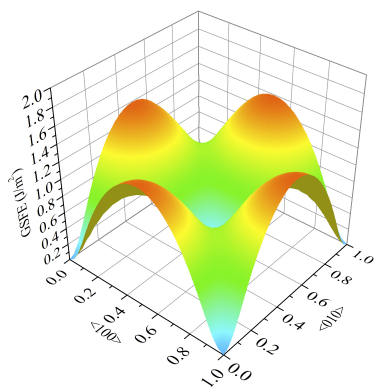
# Interface-driven Plasticity

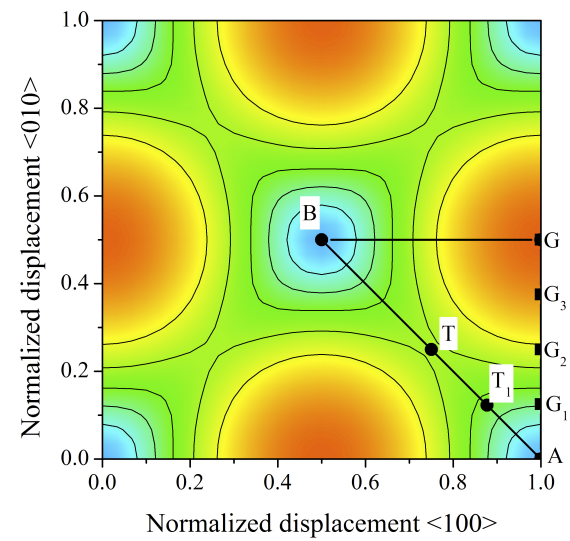
- In CMIME, this method will be used to study plasticity at bi-metallic interfaces.
  - Cu/Ni, Ag/Fe, Zr/Nb
- The direct connection to atomistics allows for an energetic description of the interface region.
- PFDD will quantitatively describe the natural evolution of dislocation interactions at heterophase interfaces by revealing the minimum energy pathway.




Cu/Ni {111}-type interface




Cu/Ni {001}-type interface