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Bridging Time and Length Scales using Atomic-Scale Modeling

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Challenges in Computational Multiscale Materials Modeling (CCMMM)
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Arlington, VA
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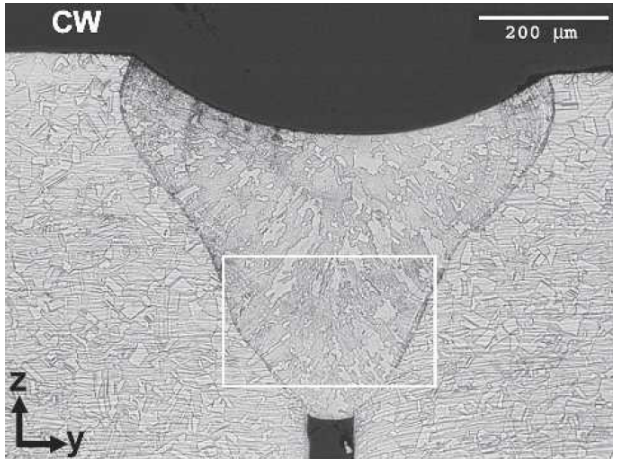
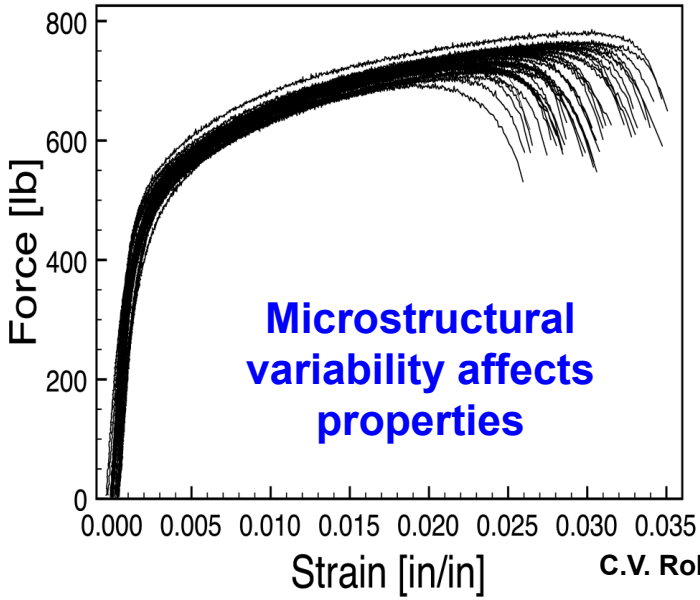
Microstructure influences material properties and their variation

- Materials are intrinsically inhomogeneous
  - Predicting microstructure's influence on properties is an ongoing challenge
  - Relationship between microstructural *variability* and *property statistics* is ***unknown***.





C.V. Robino, SNL

Science-based, probabilistic engineering models must include microstructural effects.

- **Butt weld two 304L stainless plates**
- **Cut out 40 equivalent tensile specimens**

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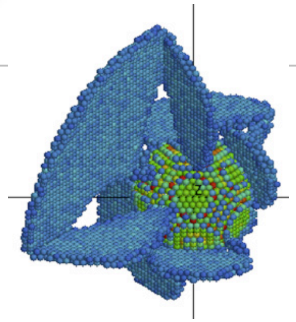
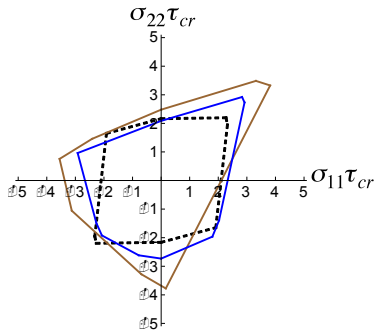
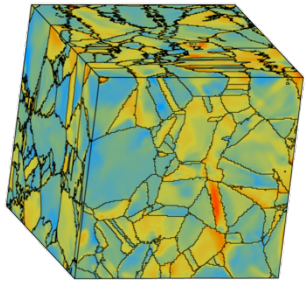
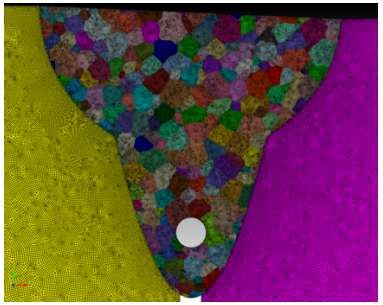
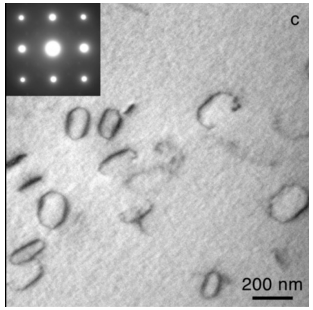
Microstructure is the critical link between atomic-scale processes and engineering applications

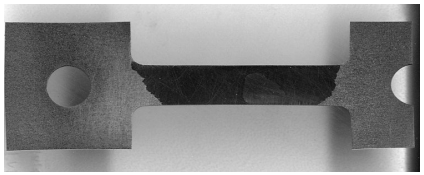


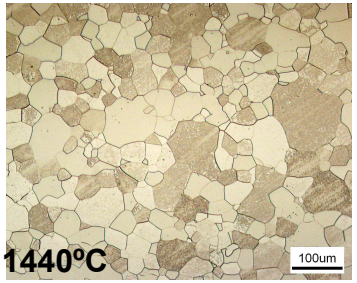


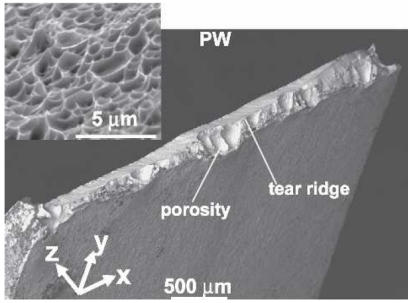








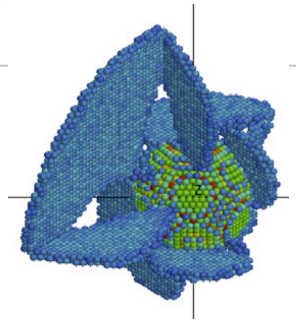


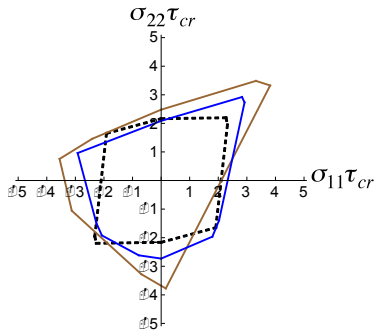


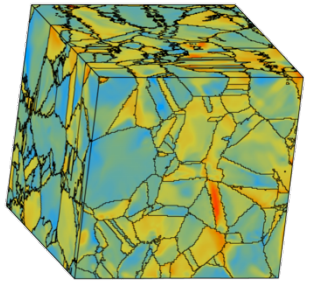
Atomic scale phenomena | **Single crystal behavior** | **Microstructural effects** | **Material performance**

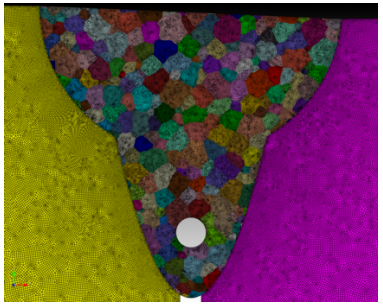
10^{-9} m, 10^{-9} s | 10^{-6} m, 10^{0} s | 10^{-3} m, 10^{3} s | 10^{0} m, 10^{6} s

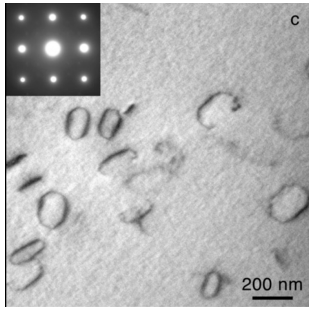
Microstructure is the critical link between atomic-scale processes and engineering applications

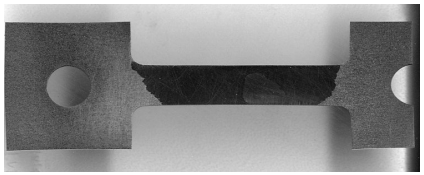


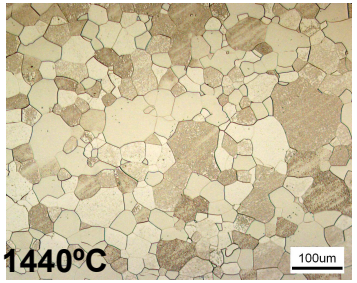


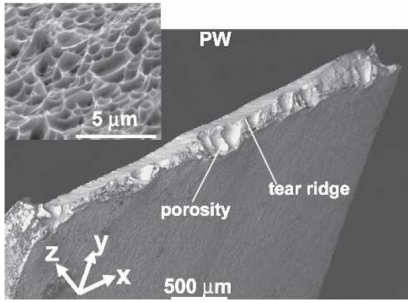












Atomic scale phenomena	**Single crystal behavior**	**Microstructural effects**	**Material performance**
DFT, MD, DD	crystal plasticity	kMC, PPFEM	FEM, QMU
TEM, APT, PAS	XRD, EBSD, µmachining, µtesting	EBSD, FIB, DIC, µmachining, µtesting	mechanical testing, microscopy

Atomic-level simulations can study small groups of the entities that comprise the microstructure

Classes of defects

- "0-dimensional" defects
  - Impurities, vacancies, interstitials, defect clusters…
- "1-dimensional" defects
  - Dislocations
- "2-dimensional" defects
  - Twins, fault planes, grain boundaries, interphase interfaces, surfaces, …

Properties of interest

- Thermodynamics
- Motion
- Interaction between defects
  - Energetics: e.g. binding
  - Dynamics: e.g. barriers
- Collective motion of defects

General challenges:

- **Can only explicitly treat a 'few' defects for a 'short' time**
- **Real materials are incredibly complex**

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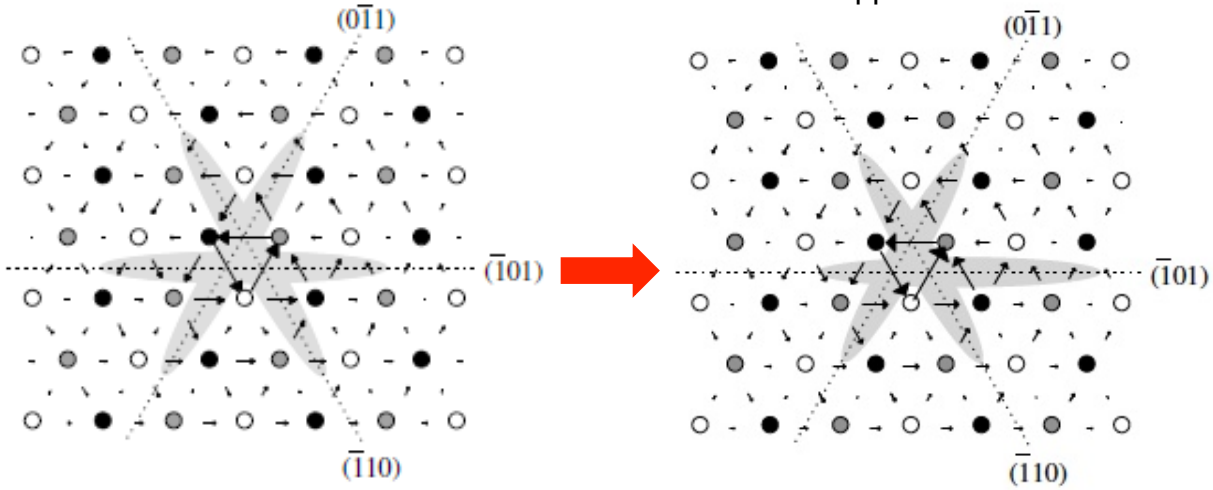
Atomic-scale to single crystal properties: Dislocation behavior in BCC metals

- Atomic scale simulations show dislocation core spreading onto adjacent (110) planes in BCC metals.
  - Core spreading creates a significant Peierls barrier to dislocation motion.
  - Because the dislocation spreads onto three planes, motion can be affected by stress components outside the preferred slip plane, i.e. non-Schmid stresses.

[111] zone depiction of a relaxed screw dislocation core in Mo

Distortion of the dislocation core under an applied shear stress



Groger, Vitek et al. *Acta Mat.* **56** (2008) 5412

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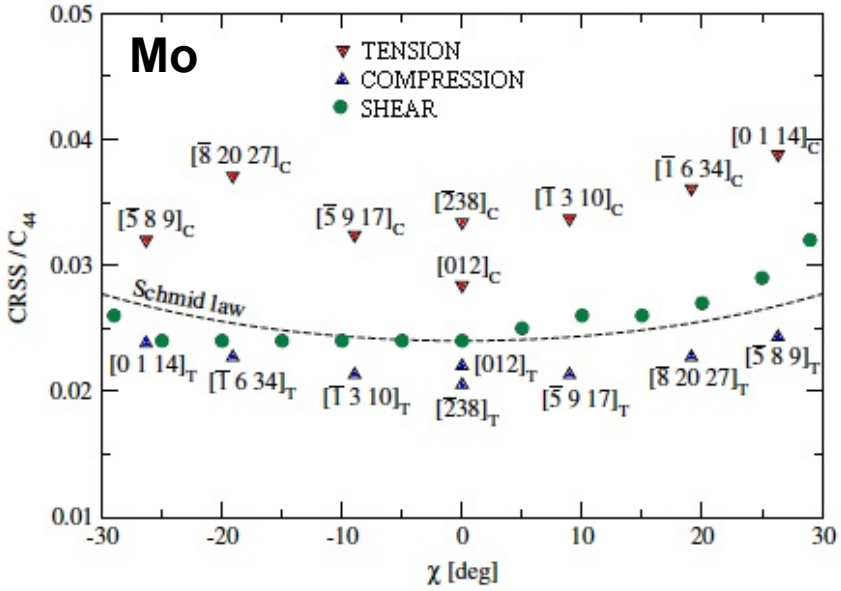
Implications of non-Schmid deformation

- The non-Schmid stress components arise from two causes:
  - Asymmetry within the slip plane (twinning/anti-twinning) is a minor effect.
  - Contributions by stress components outside the slip plane are significant.

"...glide of the 1/2[111] screw dislocation [on the (-101) plane] depends on shear stresses both parallel and perpendicular to the Burgers vector that act not only in the slip plane but also in other {110} planes of the [111] zone."

-Groger, Vitek et al. *Acta Mat.* **56** (2008) 5412.



The non-Schmid stress components cause the widely observed tension-compression asymmetry in BCC metals

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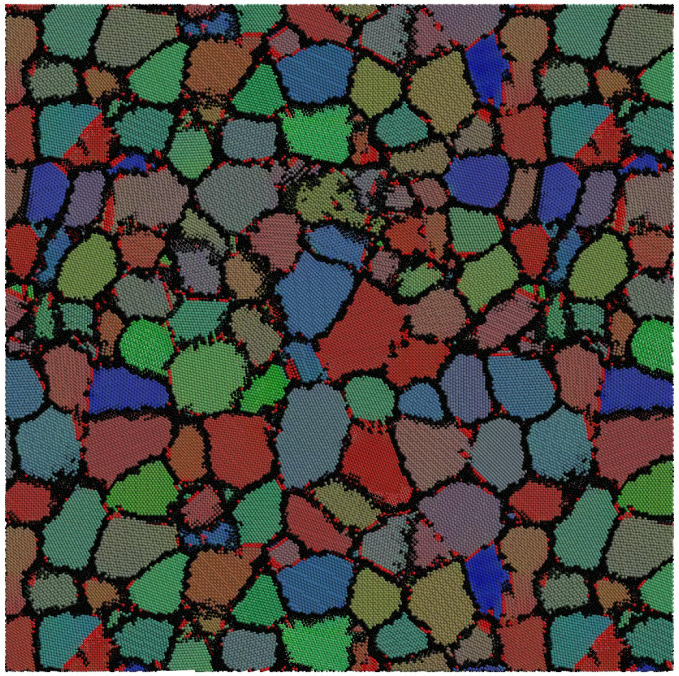
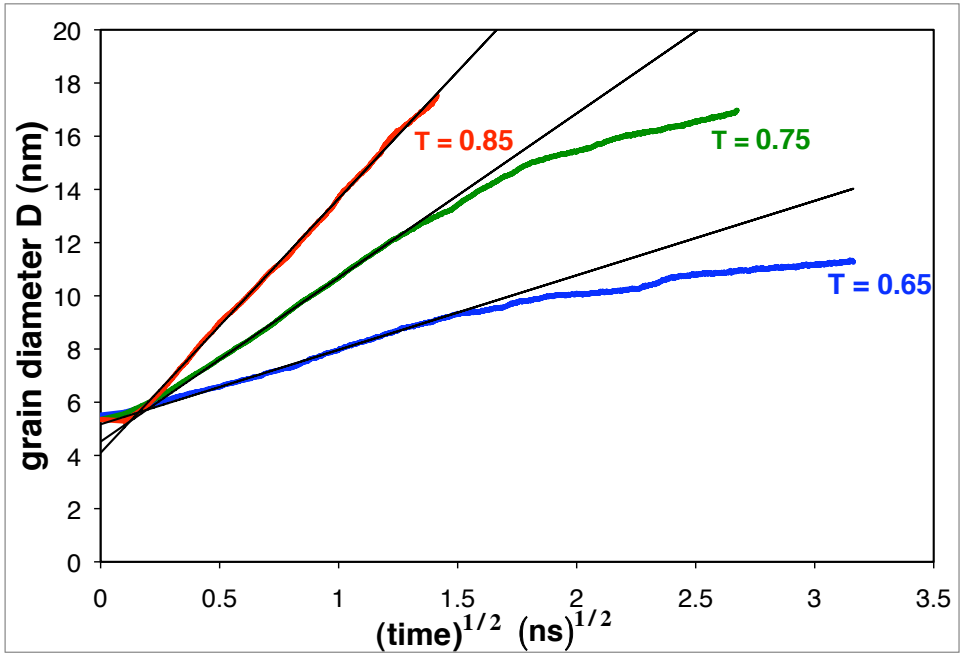
Brute Force MD can follow grain growth in nanocrystals What do we learn?



T = 0.75 T_M; 39 nm cube; 7.0 ns

- **Formation of twin boundaries**
- **Vacancies seen in grain interior**



- **Initial transient is not physical**
- **Conventional scaling of grain size with time$^{1/2}$ observed for significant period**
- **Why does the growth slow down?!?**

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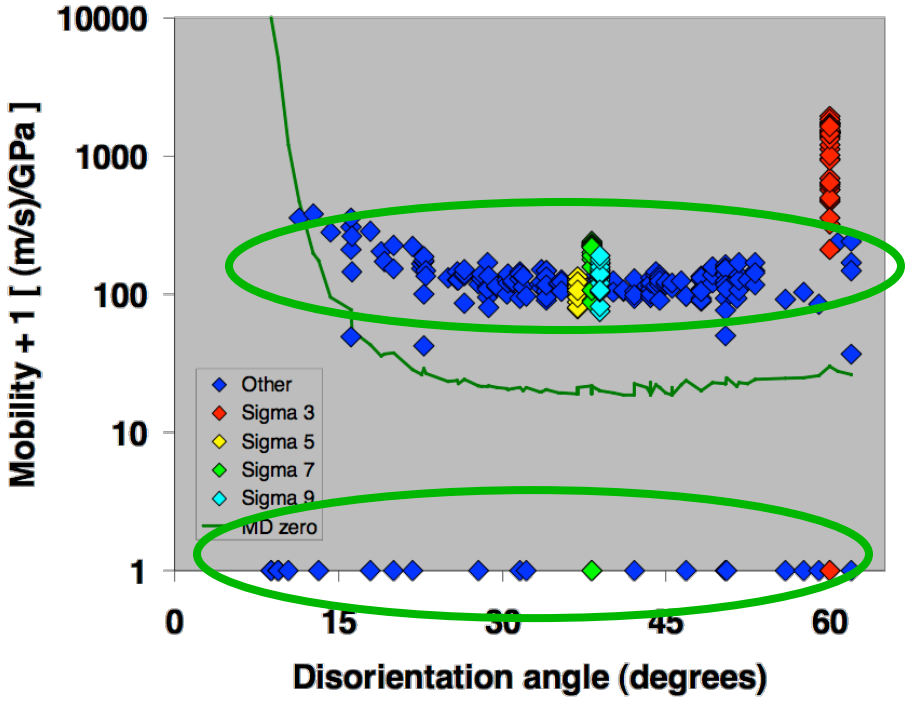
MD simulations can study individual boundaries: Catalog of mobility for 388 Ni grain boundaries

How could one use such data?

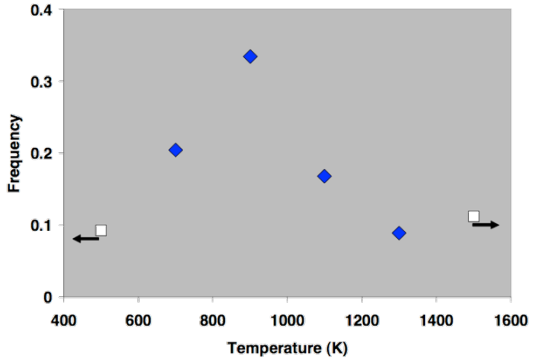


Could consider crystallographic dependence of mobility.
- ***But no trends in M found***
- ***But not enough data to interpolate***

Could look for groups of similar boundaries, regardless of crystallography
- ***High mobility boundaries***
- ***Low mobility boundaries***

- **Relative fraction of High and Low mobility boundaries is temperature dependent**
- **In many boundaries, associated with roughening**

Transition temperature between low/high mobility



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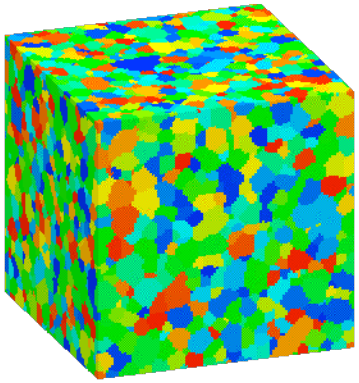
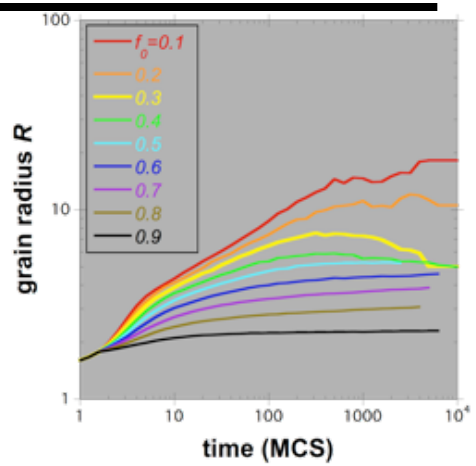
Mesoscale Microstructure Simulations reveal the consequences of temperature dependent population of High/Low mobility boundaries

- Monte Carlo Potts Model simulations
  - Low mobility: $M \sim 0$
  - High Mobility: $M \sim 1$
  - Fraction, f_0, of High/Low mobility
  - Allow system to evolve via normal grain growth physics

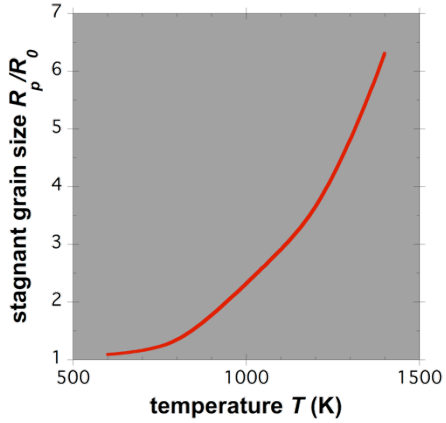


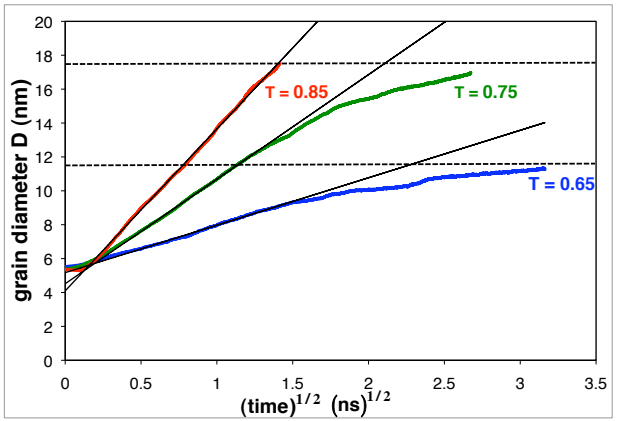


- Grain size stagnates
- f_0 determines final size

T (K)	f_0
600	0.9
800	0.7
1000	0.35
1200	0.2
1400	0.1

Convert temperature to fraction of low mobility boundaries





Explanation of grain growth stagnation in pure metals?
Holm, Foiles, Science 328, 1138 (2010)

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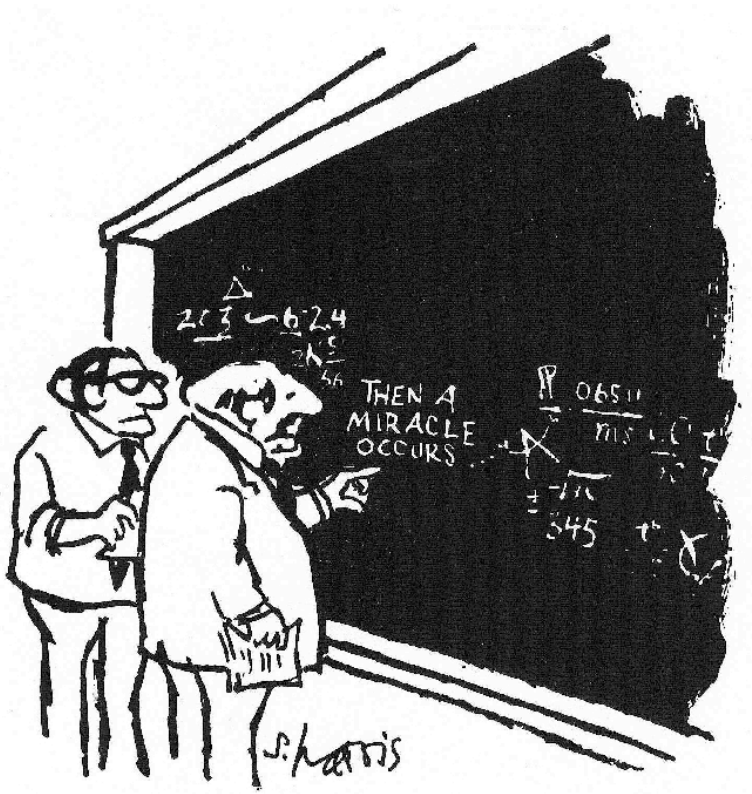
Availability of appropriate interatomic potentials is the Achilles Heal of molecular dynamics

- Quality of interatomic potentials determines the quality of the results
  - **No GIGO!!**
- Keep the goal of the simulations in mind
  - Quantitative vs Illustrative
- Typical potential development process
  - Assume functional forms (ad hoc or physically based)
  - Adjust functions/parameters to fit a set of training data
  - Publish it and watch it get used for problems it was *not intended for*!
  - Highly time and labor intensive
    - » "Will the potential be ready in time?"
- Potentials for multiple materials classes are rare and often suspect



"I think you should be more explicit here in step two."

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Interatomic Potential Wish List

- A full spectrum of approximations for computing the energy/forces in simulations
  - Highly accurate quantum techniques for specific critical quantities
    - » Will naturally be computationally expensive and only able to treat a small number of atoms
  - Highly efficient techniques that get the essential features
    - » Will allow for the treatment of complex processes with the goal of qualitative insight
  - Spectrum of intermediate methods
    - » This is not a “one size fits all” problem!!
- Ability to develop potentials ‘quickly’
  - Currently potentials often available too late to contribute

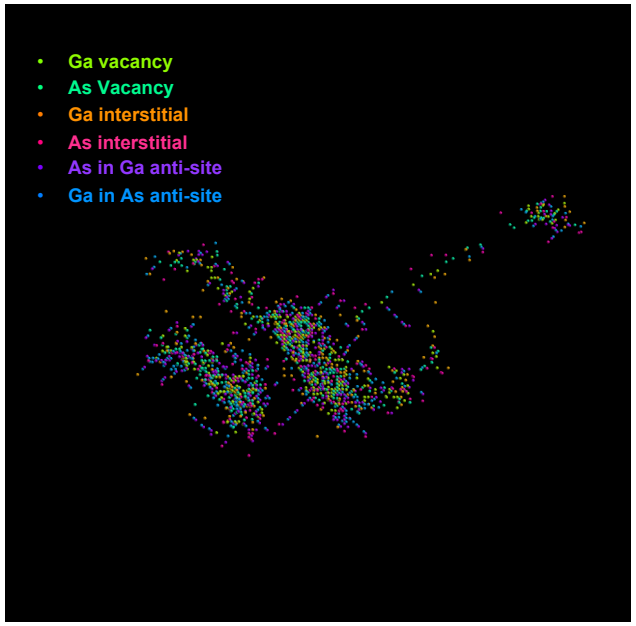
Need New Ideas!

PRL **104,** 136403 (2010) PHYSICAL REVIEW LETTERS week ending 2 APRIL 2010

Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons

Analysis/Visualization of Atomic-level simulation data is often an ad hoc, inefficient process

- Large-scale molecular dynamics simulation
  - Raw Output: Time evolution of 10^{6+} coordinates
  - Desired Output: Behavior/properties of higher-length-scale objects
    - » Examples: dislocations, grain boundaries
- Substantial effort has been made to create efficient, massively-parallel codes for MD simulations such as LAMMPS
- Analysis and visualization has received substantially less effort
  - Analysis of MD data can require compute resources that are a substantial fraction of basic MD run
  - Methods and code are home-grown and highly problem specific
    - » Choice of analysis often dictated by availability of codes rather than most useful approach



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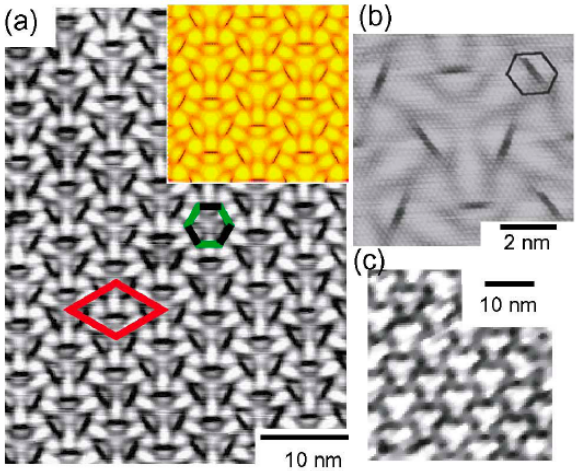
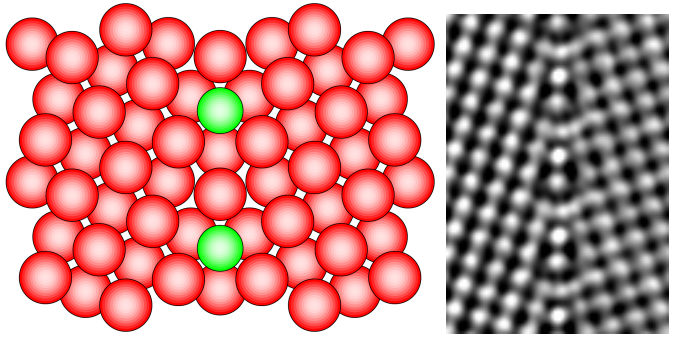
Determination of Defect Structure is often very difficult and frequently given insufficient care

- One typically knows the bulk structure, but must guess/compute the actual structure of defect
  - Nota Bene! Incorrect structure means wrong results!
- Typical approaches use local minimum searches (e.g. conjugate gradient) plus, in good cases, multiple initial states
  - Major effort in grain boundary work discussed earlier
- Global optimization problem involving both continuous and discrete variables
  - "Relaxation" of atomic coordinates
  - Optimize species at each site in alloys
  - "Add/Remove" atoms
  - Interstitial atoms – where and how many



Ag(111)/Ru(0001)
Ling, et al., PRL 92 116102 (2004)



Cu/Al Σ5(310)
Campbell, et al., Interface Science 12, 165 (2004)

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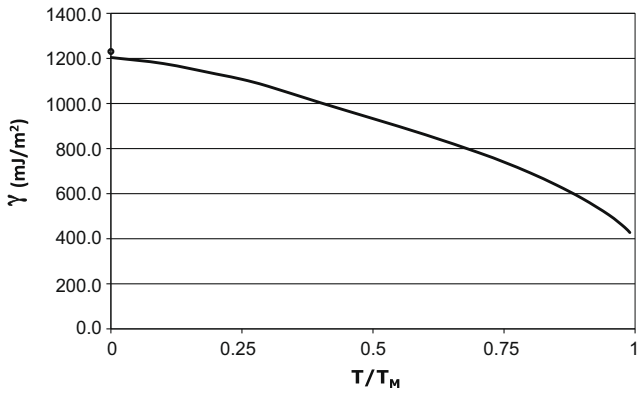
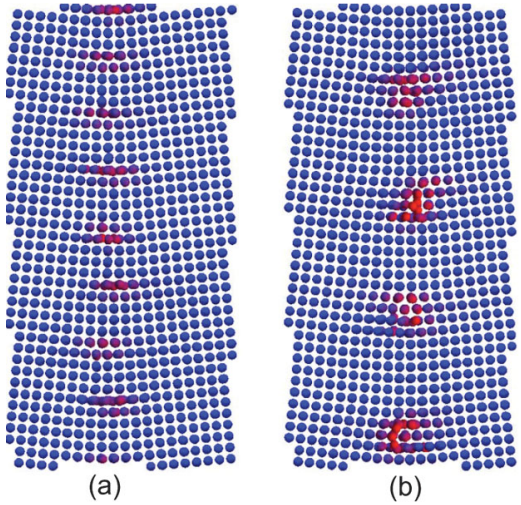
Finite-temperature effects are often underexplored



Ni Σ79 free energy
Foiles, Scripta Mater. 62, 231 (2010)



T-dependent grain boundary in Fe
Olmsted, et al., PRL 106, 046101 (2011)

- Connection to higher length scales is often through thermodynamic quantities such as interfacial *free*-energy
  - Clearly temperature dependent
  - Often calculated at T = 0
- Structures and properties may change with temperatures
  - Elastic constants are temperature dependent
    - » Leads to gb structure change on left
  - Variations of dynamic properties with temperature may not be what one expects
    - » Currently exploring this for the case of grain boundary motion

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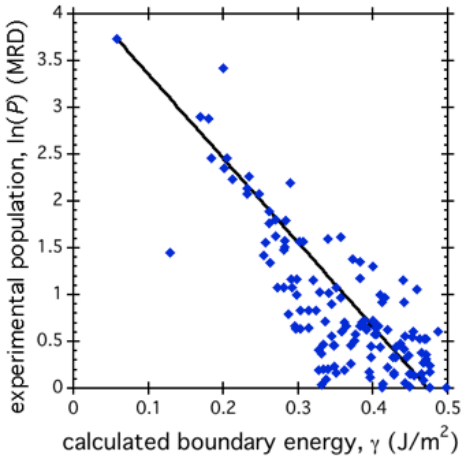
Opportunities/Future

- Increased validation and discovery from the detailed comparison of computations and experiments at the nanoscale
  - Advances in experimental methodology that permit examination at smaller scales
  - Advances in computation that permit simulations at larger scales



Comparison of calculated and experimental gb energy
Holm, et al., Acta Mater, in press.

- Understand the *variability* of materials properties
  - "Paradigm shift, from the idealistic view that all parts are created equal, to the realistic view that structure, properties, and performance are probabilistic"
    - » Corbette Battaile, SNL
  - This variability originates at the atomic/mesoscale
  - Increasingly important as structures move to ever smaller sizes

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