

Theory of Microstructures

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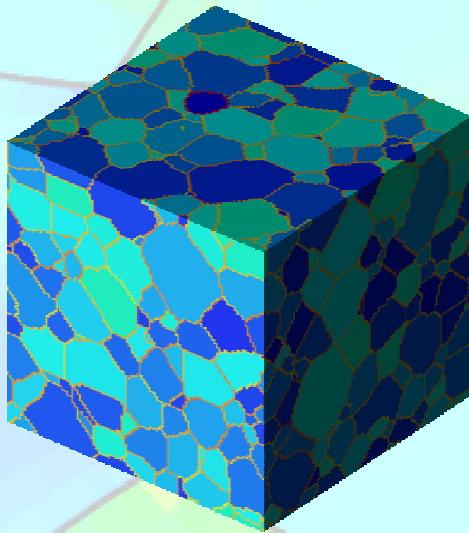
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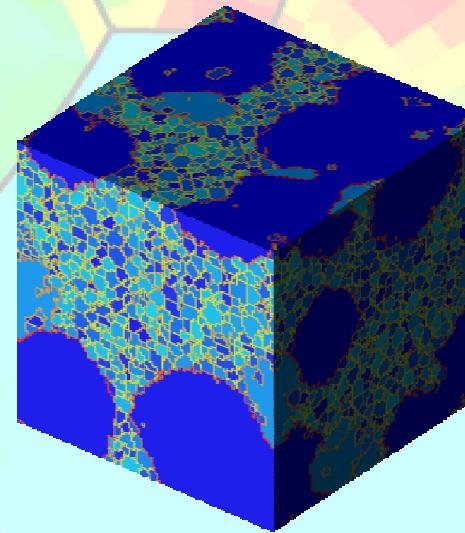
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How do atomic processes affect mesoscale structures?

- **Motivation:** Variations in grain boundary mobility (atomic scale) can have dramatic effects on microstructure (mesoscale).



Normal grain growth occurs in systems with uniform boundary mobilities.



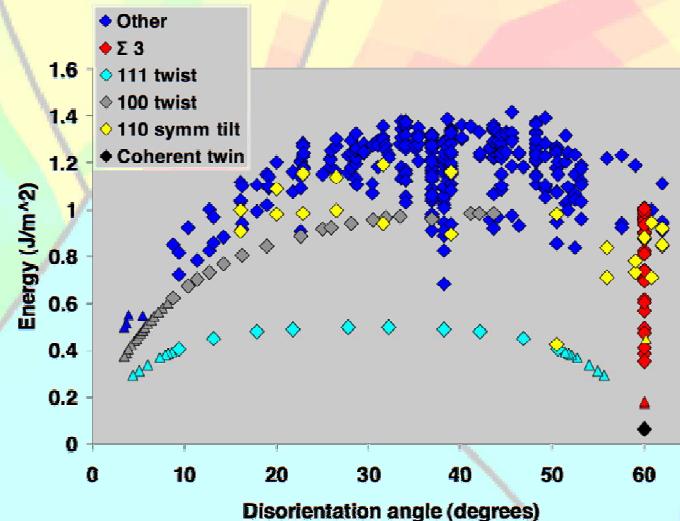
Abnormal grain growth occurs in systems with varying grain boundary mobilities.

Determining atomic scale properties: Grain boundary mobility

(1) Build and minimize a catalog of 388 flat grain boundaries

- Includes all boundaries that can fit inside a box of size $15a_0/2$.
- For each boundary, we minimize hundreds or thousands of configurations.
- By far the largest computational survey of grain boundary energies.

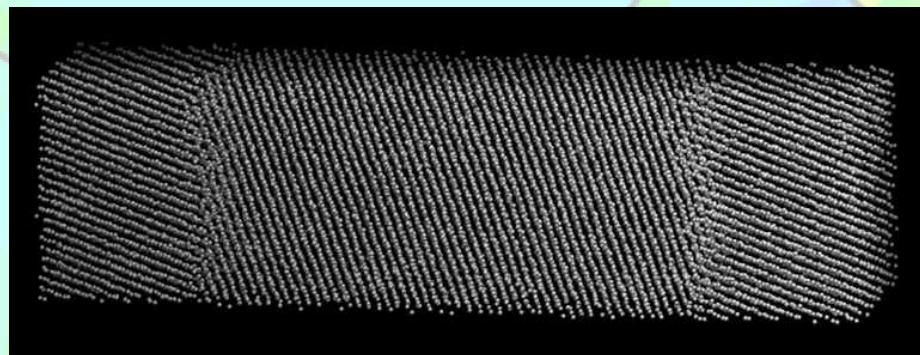
[Olmsted, Foiles, Holm, *Acta Mater.* 57 3694 (2009)]



(2) Apply a synthetic driving force method to determine mobility

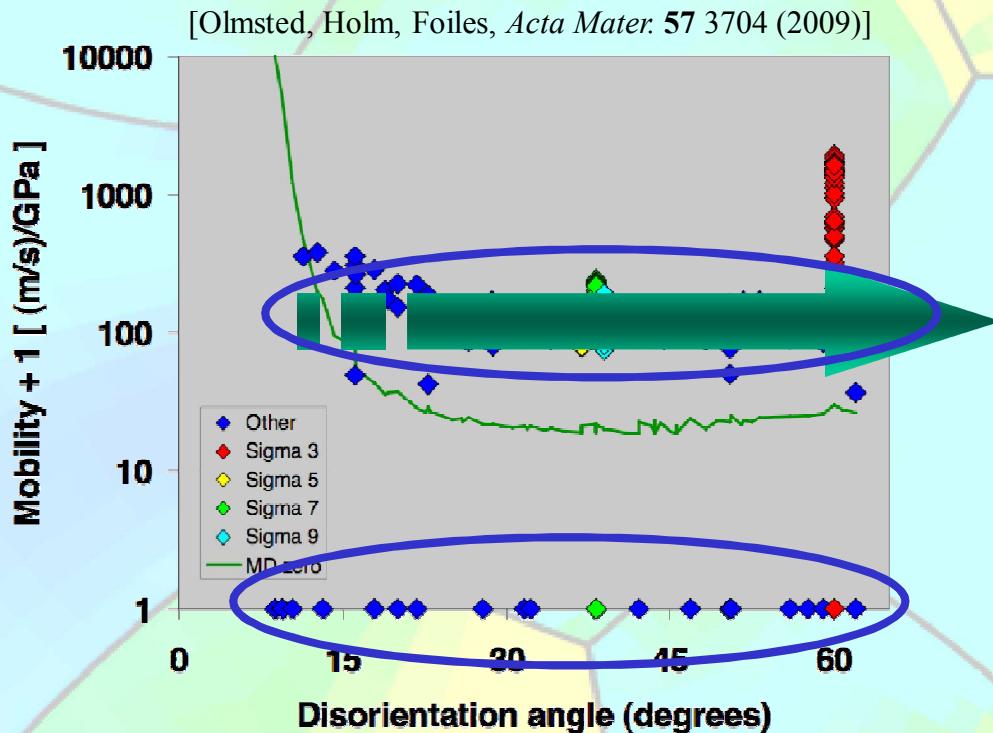
- The first method to calculate mobility of arbitrary, flat grain boundaries.
- Implemented in Sandia's LLAMPS code for MP MD.

[Janssens, Olmsted, Holm, Foiles, Plimpton and Derlet, *Nature Materials* 5[2] 124 (2006)]



Result: First comprehensive survey of grain boundary mobilities

- How can we use this data to understand microstructural evolution in polycrystalline materials?



Could consider crystallographic dependence of mobility.

-No clear trends in M with scalar crystallographic parameters.

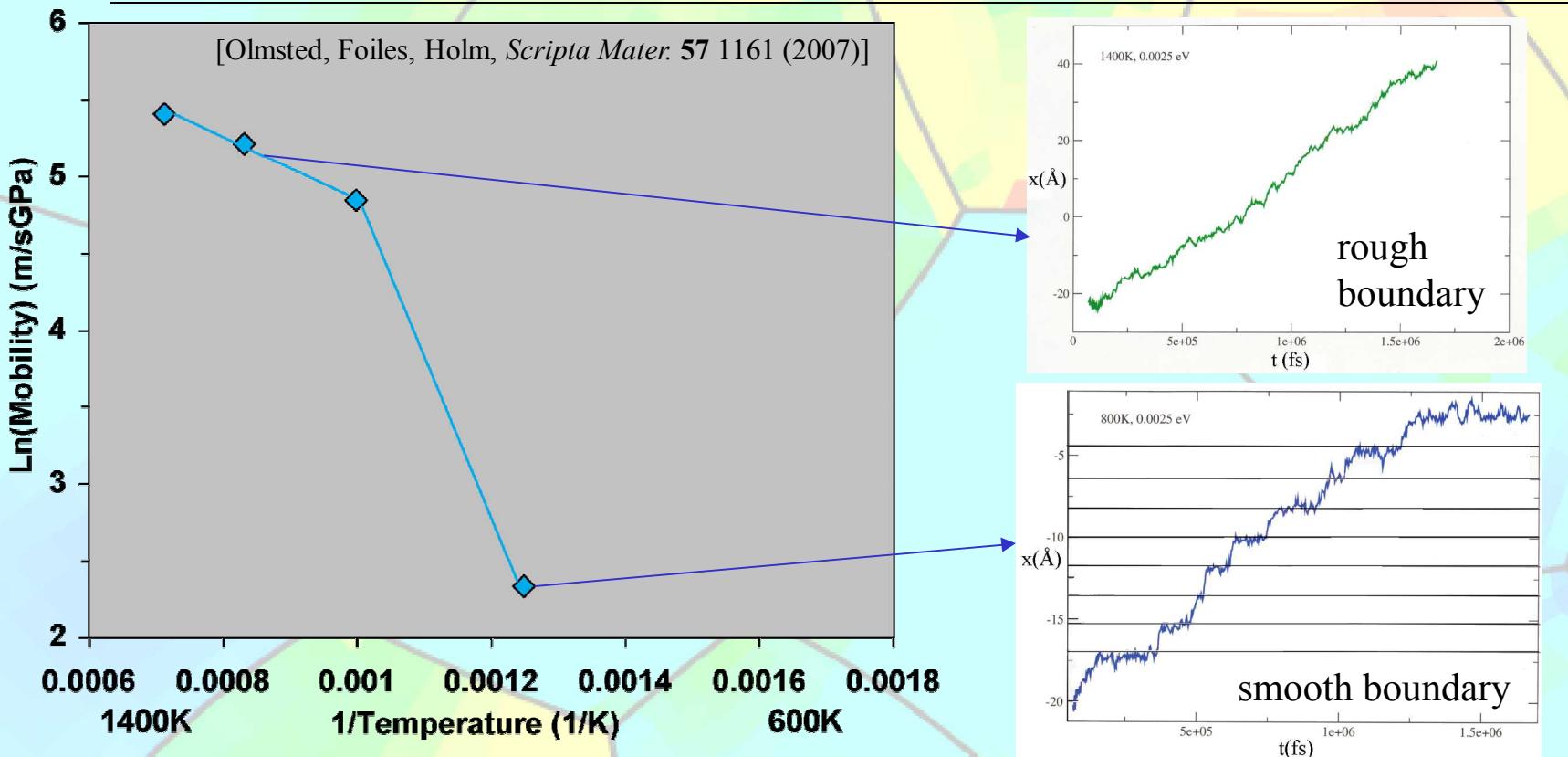
-Including boundary plane effects is challenging.

Could look for groups of similar boundaries, regardless of crystallography

-High mobility boundaries, with $M \sim 100 \text{ m/s}_\text{GPa}$

-Low mobility boundaries, with $M \sim 0 \text{ m/s}_\text{GPa}$

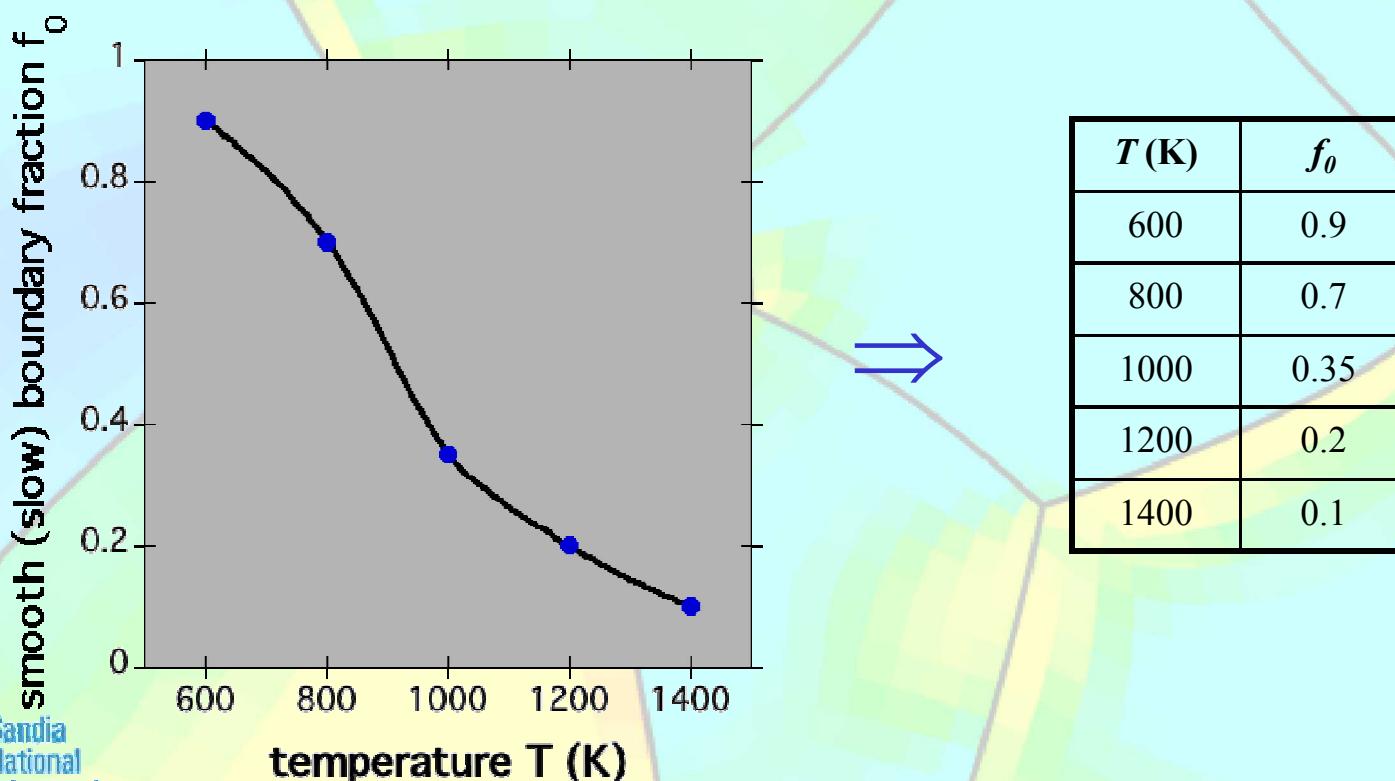
What do the mobility clusters represent?



- High T: high mobility, atomically rough, continuous motion
- Low T: low mobility, atomically smooth, stepwise motion
- Each boundary has a characteristic roughening temperature T_r

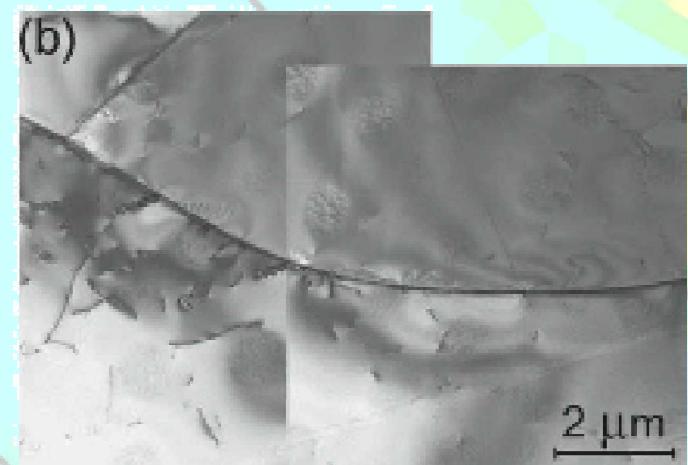
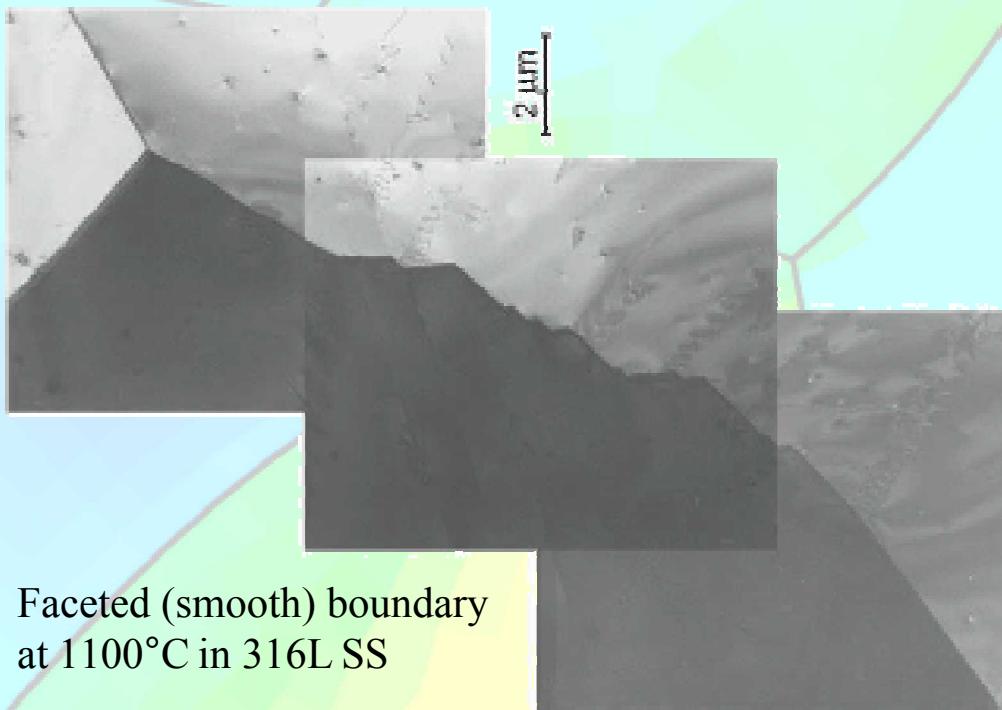
Atomic-scale simulations provide phenomenology of the roughening transition

- Grain boundaries undergo roughening transitions at widely varying temperatures.
- Smooth boundaries are almost immobile; rough boundaries are mobile.
- At a given T , both boundary types occur over the range of misorientations.



Experiments suggest further study

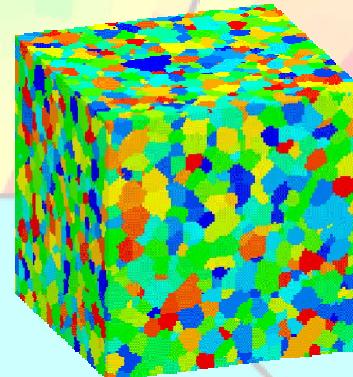
- Yoon and Cho [*J. Mater. Sci.* **40** (2005) 861] surveyed boundary roughening:
“In many metals and oxides, abnormal and normal grain growth behaviors were observed to be correlated with grain boundary roughening.”



⇒ How does grain boundary roughening affect grain growth in polycrystals?

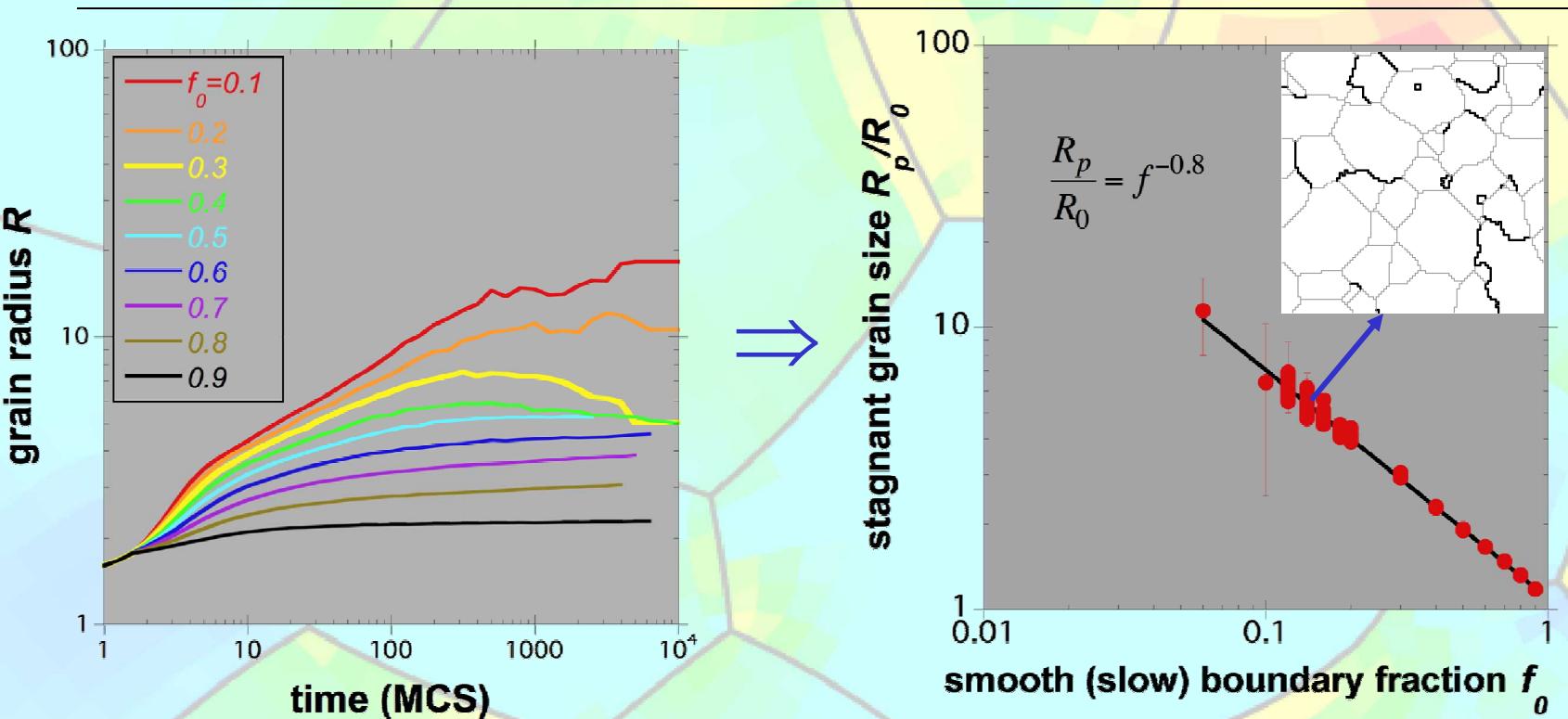
Incorporate boundary roughening data into microstructural evolution simulations

- Begin with an equiaxed polycrystalline microstructure
 - uniform boundary energies
 - slightly pre-coarsened
 - 100x100x100 lattice
- Assign boundary mobilities at random
 - smooth boundaries $M \sim 0$
 - rough boundaries $M \sim 1$
 - fraction of smooth boundaries f_0 depends on T
- Allow system to evolve via normal grain growth physics
 - Monte Carlo Potts model
 - 16 independent runs for each f_0
 - SPPARKS parallel code package
<http://www.sandia.gov/~sjplimp/spparks.html>



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

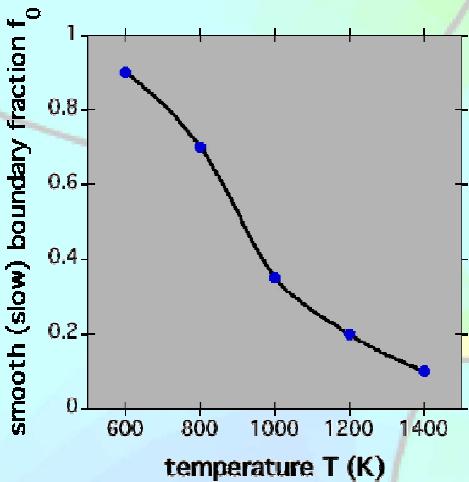
Grain growth kinetics



- Grain growth stagnates in the presence of smooth boundaries
- The stagnant grain size has a power law dependence on smooth boundary fraction f_0
- Not all boundaries must be immobile for the structure to be stagnant

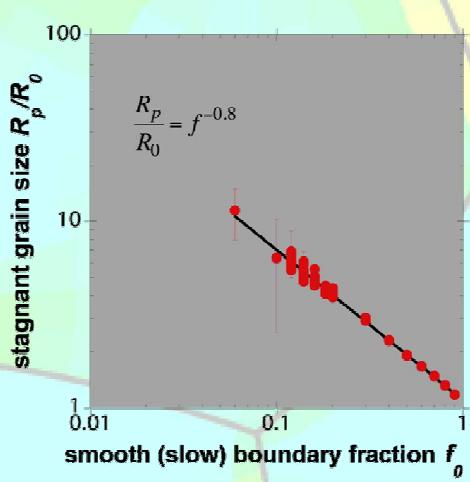
Mesoscale simulations connect atomic-scale phenomena to microstructure

Atomistic results



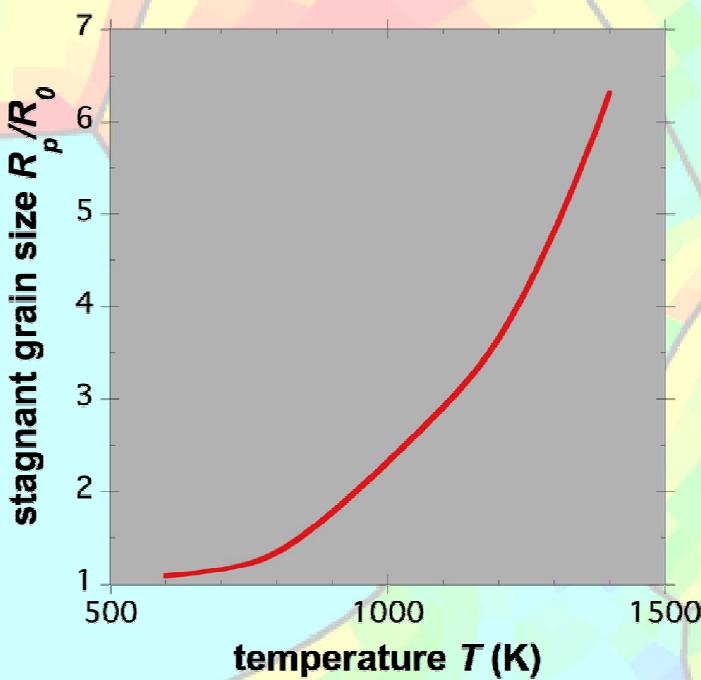
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Mesoscale simulations



⇒

Microstructural insights



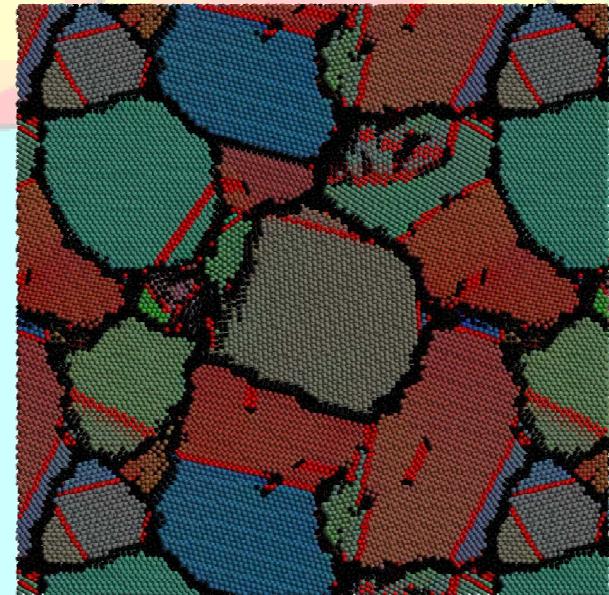
- Grain growth does not proceed to completion at any temperature
- The stagnant grain size increases with T

⇒ *Boundary roughening may play a critical role in microstructural evolution.*

Coupling back to atomistic simulations provides physical validation

Direct MD simulation of annealing of nanograined Ni

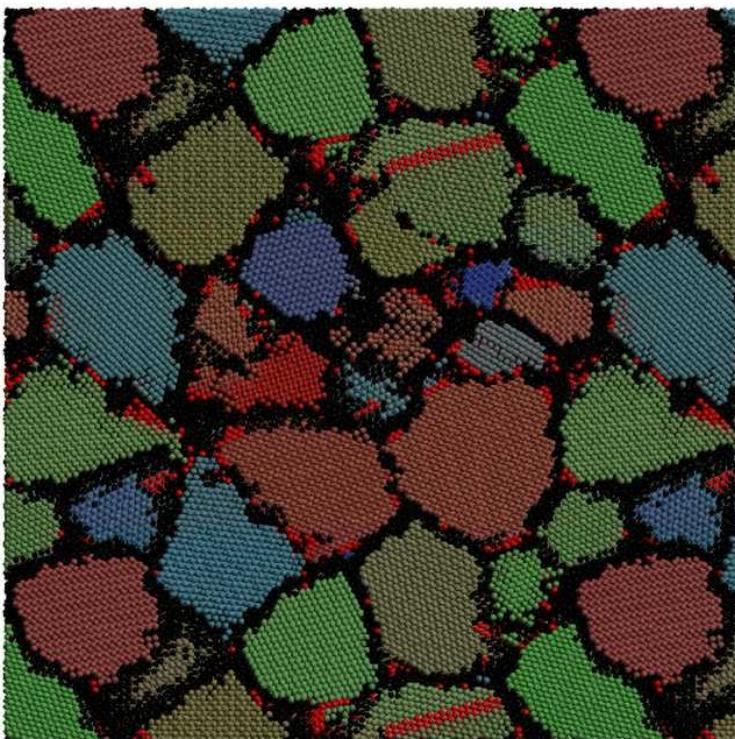
- 3-D Cubic cell with periodic boundary conditions
 - 55 or 110 a_0 (~ 20 or 40 nm) on a side
- Initial structure
 - 100 or 800 randomly centered and oriented Voronoi grains
 - Initial average grain diameter: ~ 5 nm
 - 650k or 5.2M atoms
- Foiles-Hoyt EAM Potential for Ni
- Temperatures: $0.85 T_M$, $0.75 T_M$, $0.65 T_M$
 - $T_M = 1565$ K for this potential



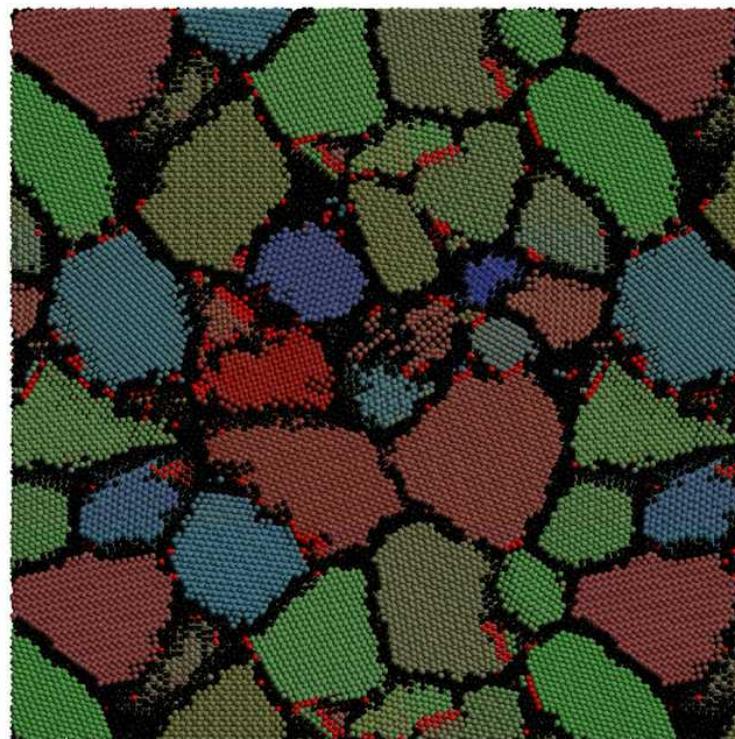
Visualization key:

- Color reflects local orientation of fcc neighbor shell
- Red: HCP configuration of nearest neighbors
- Black: Unidentified neighbor structure

Time evolution of microstructure differs with temperature

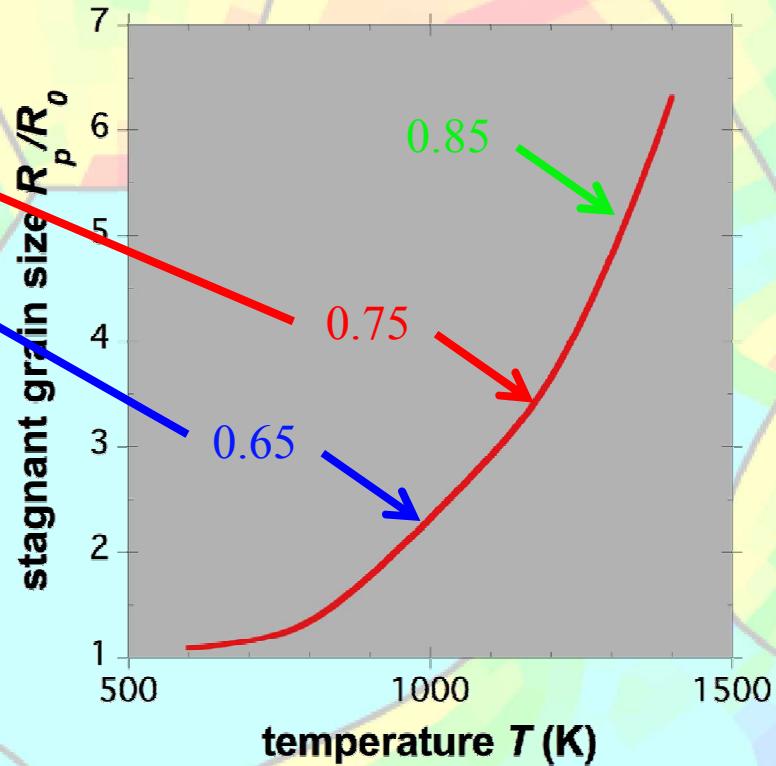
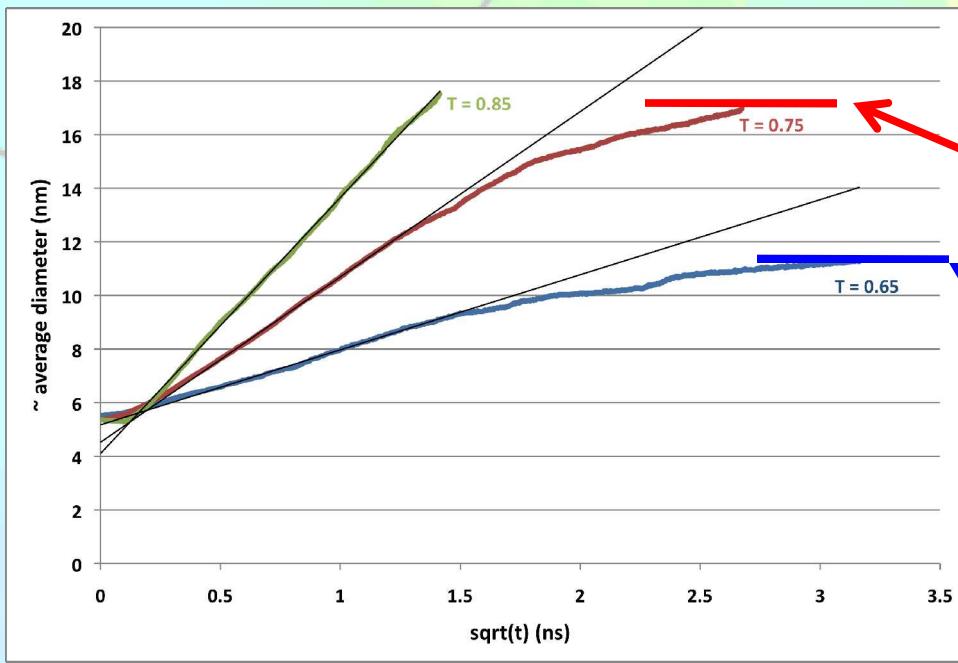


$T = 0.85 T_M$
0.6 ns



$T = 0.65 T_M$
10.0 ns

Atomic-scale results support mesoscale model for roughening stagnation



- 0.65 and 0.75 T_M samples stagnate at grain sizes consistent with the predictions of the microstructural simulation.
- Sample size is too small to reach stagnant size predicted for 0.85 T_M sample.

\Rightarrow Atomistic simulations quantitatively validate microstructural results and support the roughening stagnation model.

The longstanding problem of grain growth stagnation

- The equilibrium state of crystalline materials is a single crystal.
- However, grain growth only rarely proceeds to the single crystal state.
 - Pervasively observed in experiments
 - Assumed – without physical justification – in most grain growth models
- Typically attributed to solute drag or particle pinning, but occurs even in high purity materials.



If grain growth did not stop, the cost of Si photovoltaics would decrease dramatically.

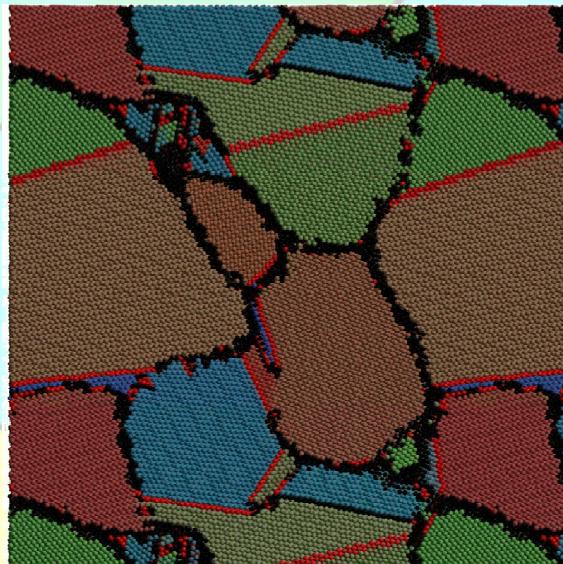
$$\frac{dR}{dt} = M\gamma \left(\frac{1}{R} - \frac{1}{R_c} \right)$$

Most grain growth models assume a maximum attainable grain size.

Integrating atomic and mesoscale simulations provides a new answer to an old question

Why does grain growth stop?

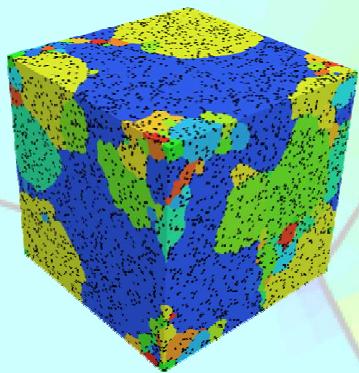
Smooth grain boundaries pin grain growth, even in high purity materials.



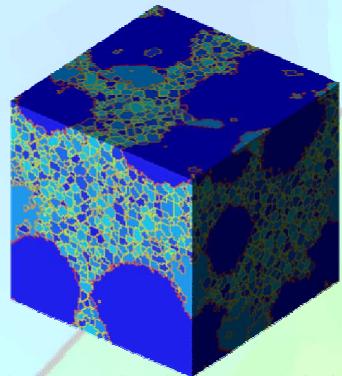
[Holm, Foiles, in technical review at *Science* (2010)]

- The first new stagnation mechanism proposed in half a century and the only one to explain how grain growth stops in perfectly pure materials.

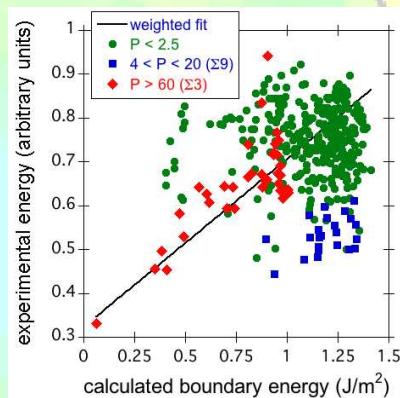
Other selected highlights: Computationally-enabled discovery



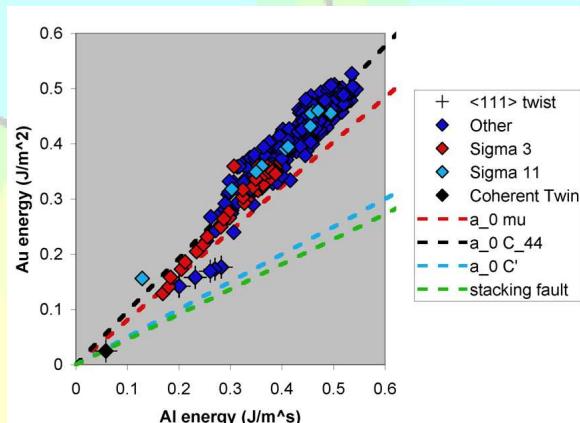
Discovery of
particle stimulated
abnormal grain growth



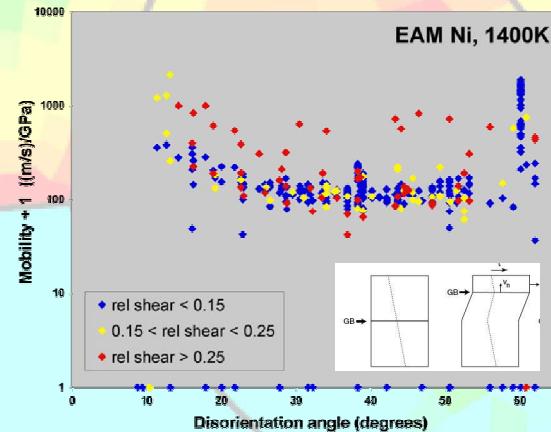
First predictive model for
texture mediated
abnormal grain growth



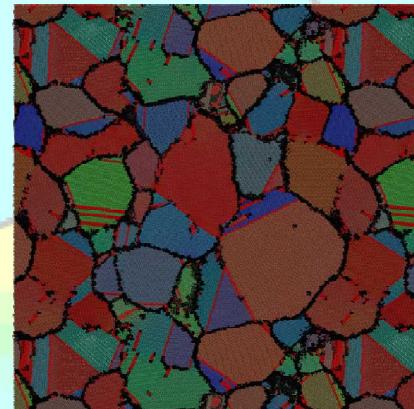
Most comprehensive comparison
between measured and computed
grain boundary energies



Established $a_0 C_{44}$ as the scaling factor
for fcc grain boundary energies



Discovery of pervasive shear-
coupled grain boundary motion



First observation of defect
generation during nanocrystalline
grain growth

Future Directions

- Create **high-throughput atomistic methods** for grain boundary / defect interactions.
 - Boundary interactions with solutes, bubbles, particles, dislocations.
 - Utilize results to inform models for microstructural evolution and response.
- Establish the first systematic and physically-based **understanding of abnormal grain growth (AGG)** as one phenomenon with many causes.
 - Construct a comprehensive catalog of AGG mechanisms and predictive models.
 - Include the range of AGG manifestations: single phase, multiphase, films, textured systems, strained systems, cryogenic temperatures, etc.
- Develop a microstructural-scale model for the evolution of grain structure in **elastically and plastically stressed systems**.
 - Inform experiments on systems where stress and microstructure interact (Tasks 1 and 3).
 - Employ results to understand the complex coupling between stress state, grain crystallography, and grain growth.

