Anisotropic EBSD Nickel data simulation and high temperature grain boundary migration study in 2D

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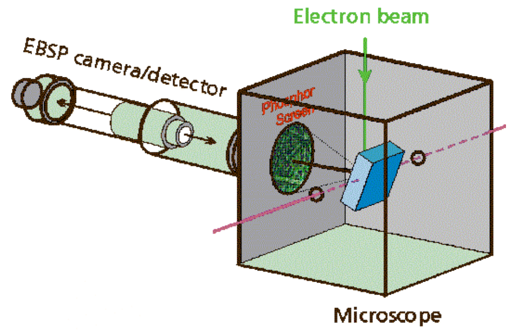
In this talk…

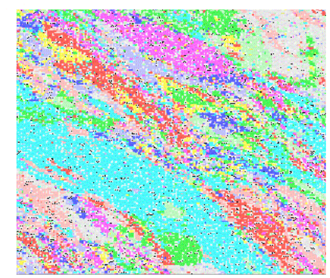
- Experimental Nickel data
  - 1941 orientation combinations
  - Refined by misorientation calculation
  - MPM simulation
- Grain boundary mobility
  - Srolovitz’s low temperature work review
  - High temperature study

EBSD summary:

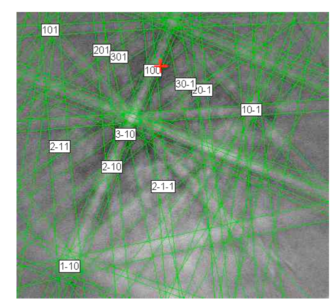
- EBSD is a commercially available tool for studying the crystallography and plastic strain state of crystalline materials.



- EBSD can be used to map grain orientation and to map grain boundaries.

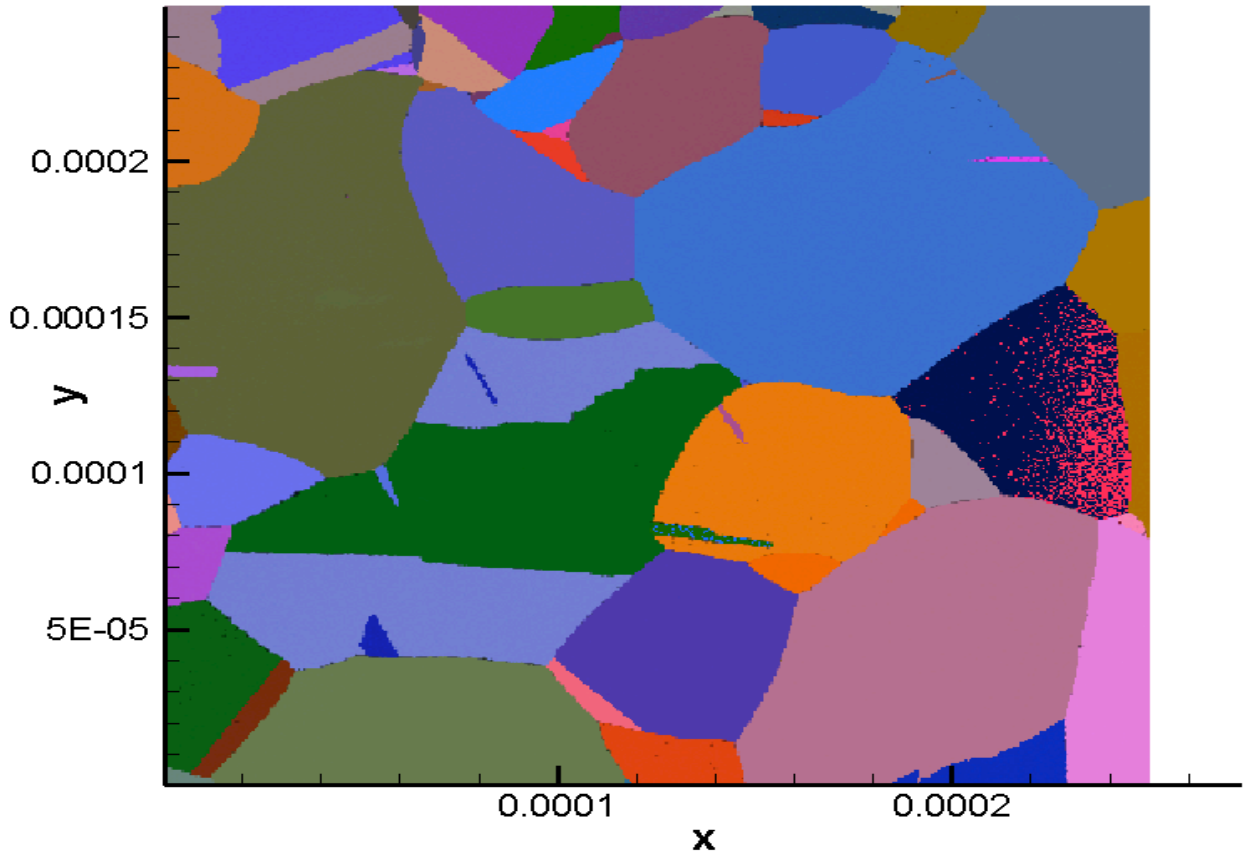


- EBSD can be used to identify unknown crystalline phases by matching patterns and in conjunction with X-ray microanalysis

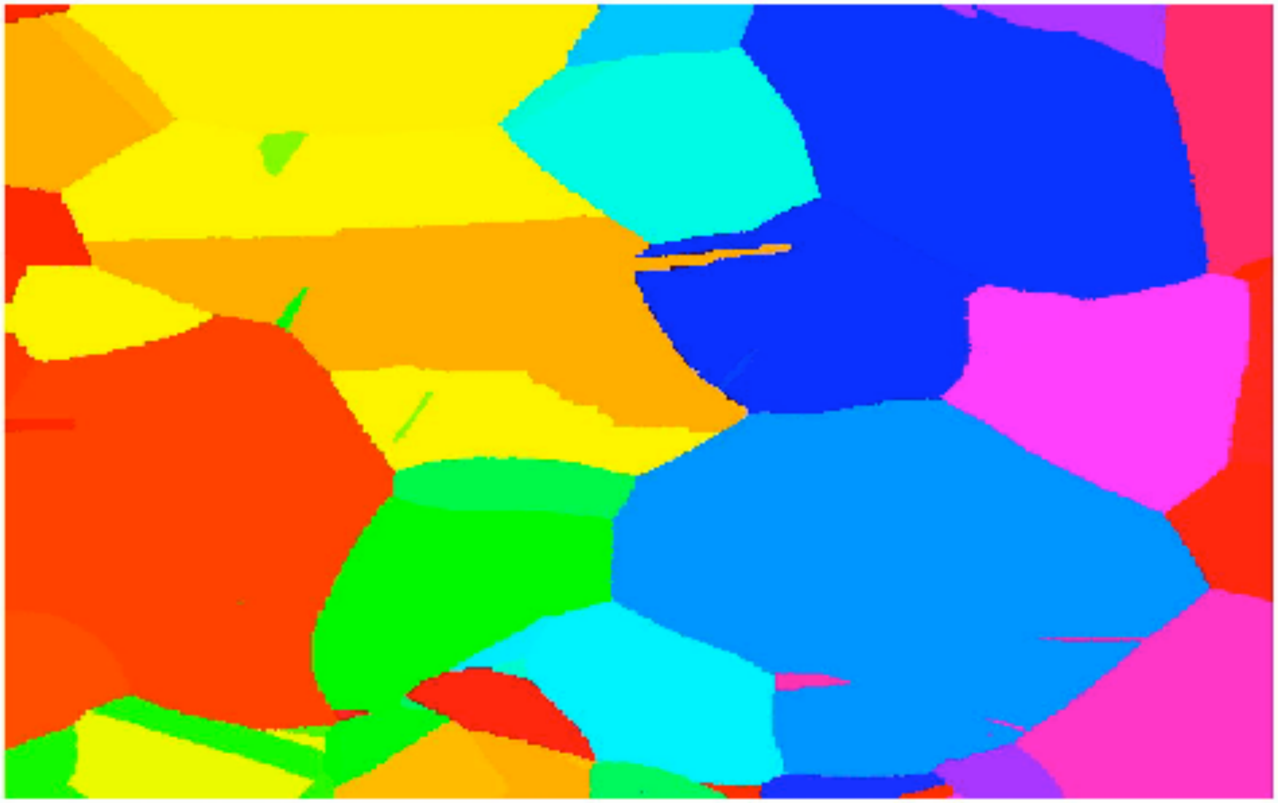


- EBSD techniques are being developed to map plastic deformation in metallic microstructures.

Raw Nickel data



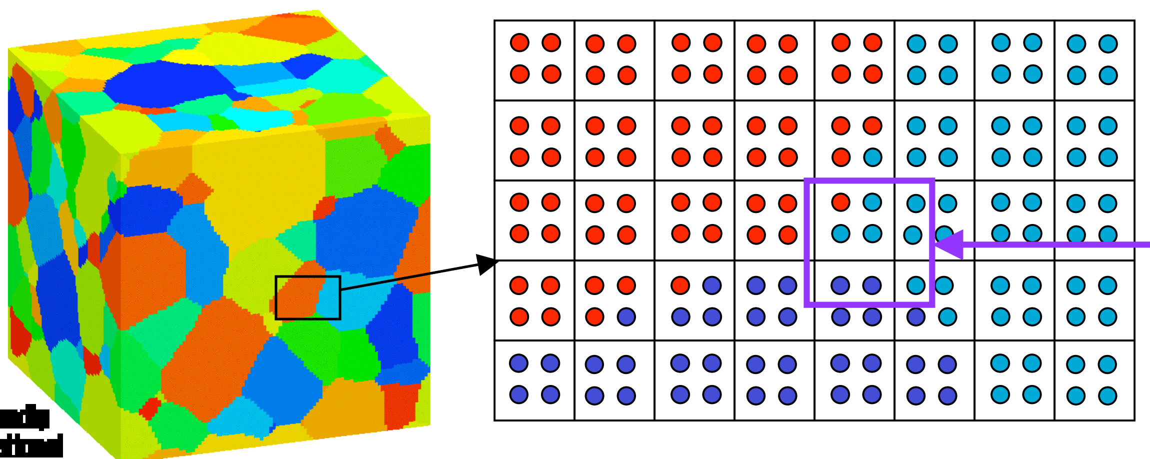
Refined Nickel data



MPM coupled with KMC

- **Material Point Method (MPM)**
  - lagrangian particle & cell method
    - continuum mechanics
    - 'solution' at material points (mass, momentum, energy, stress)
    - strain tensor enables use of traditional material response models
- **Lagrangian grid**
  - simplifies traction bc and HMC particle indexing
  - No particle cell crossing issues
- **Hybrid Monte Carlo (HMC) for grain growth**
  - Map microstructure onto particles*

* Particles contain information about crystallographic orientation, as well as mechanical state.

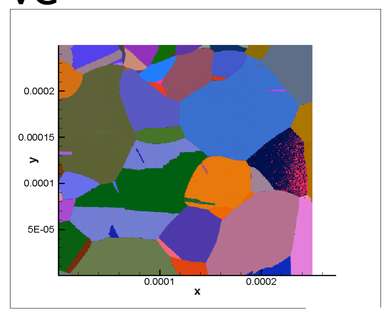


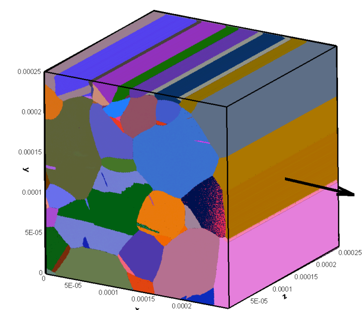
-Determine particle free energies based on elastic strain energy (at individual particle) and surface energy (from particle neighborhood)

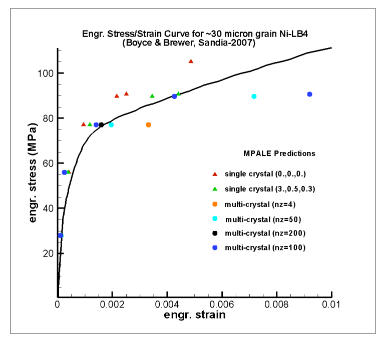
-MC decision algorithm

Comparison with Ni EBSD and uniaxial tension test

- **Problem:** Given 2D EBSD data for the crystal orientation of a nickel coupon, predict the engineering stress/strain curve
- **Data**
  - 250x250 micron
  - digital data set (500x500 points)
  - ~2000 different Euler angle combinations
- **Issues**
  - data is 2D, crystal slip planes are 3D
  - boundary conditions uncertain
- **Solution Strategy 1**
  - project 2D grains to 3D (columnar grains)
  - results indicate material is too ‘soft’ at higher stress
  - computational intensive
    - For nz=100 (aspect ratio=1),
    - 50M computational particles
    - 24hr with 1000p on Redstorm for load curve
      - AMD 2.4 Ghz Opteron processor

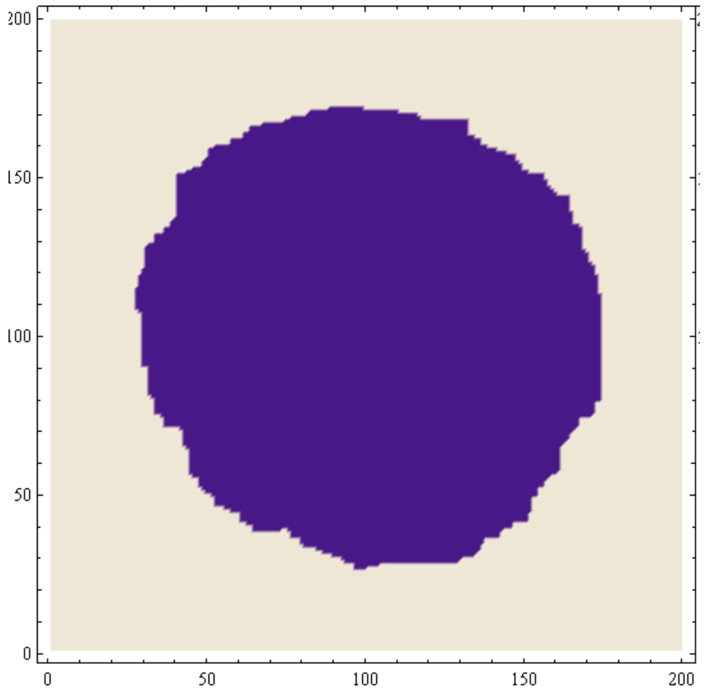




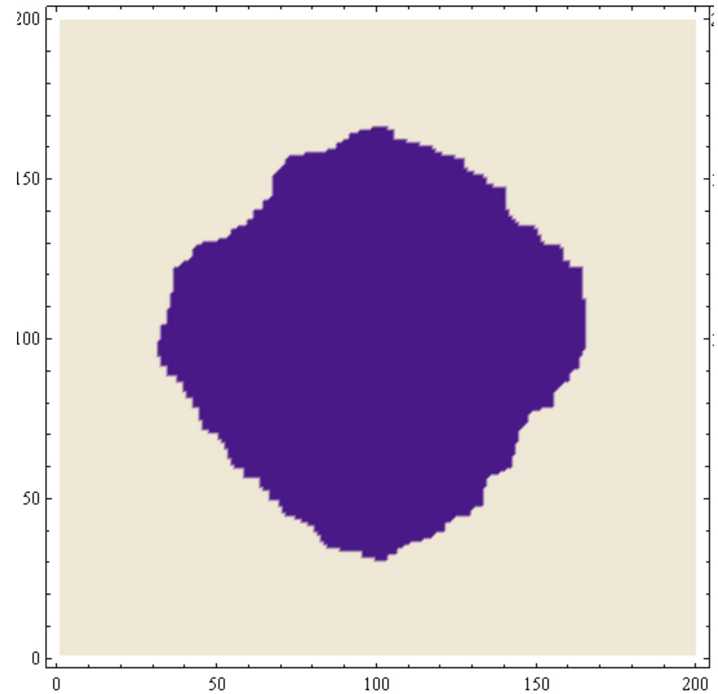


MC simulation result at T/Tc=0.3

No bulk energy

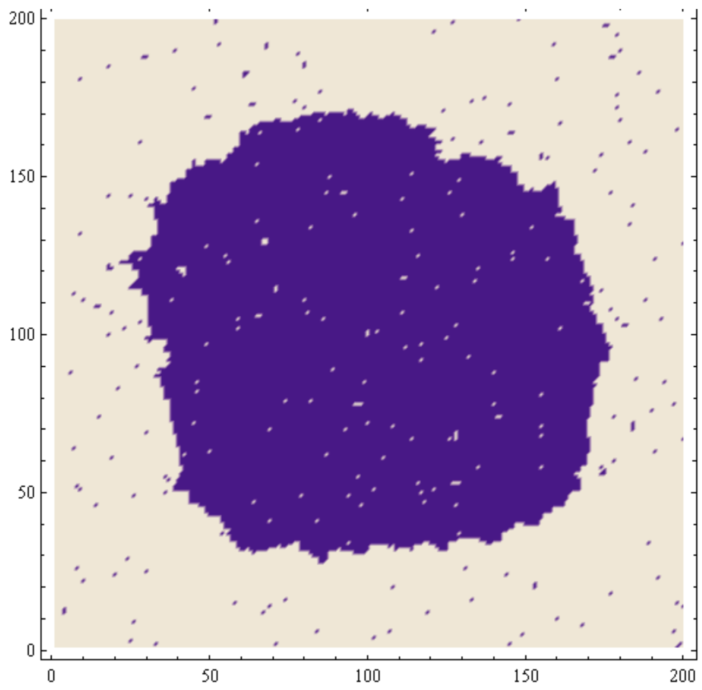


With bulk energy

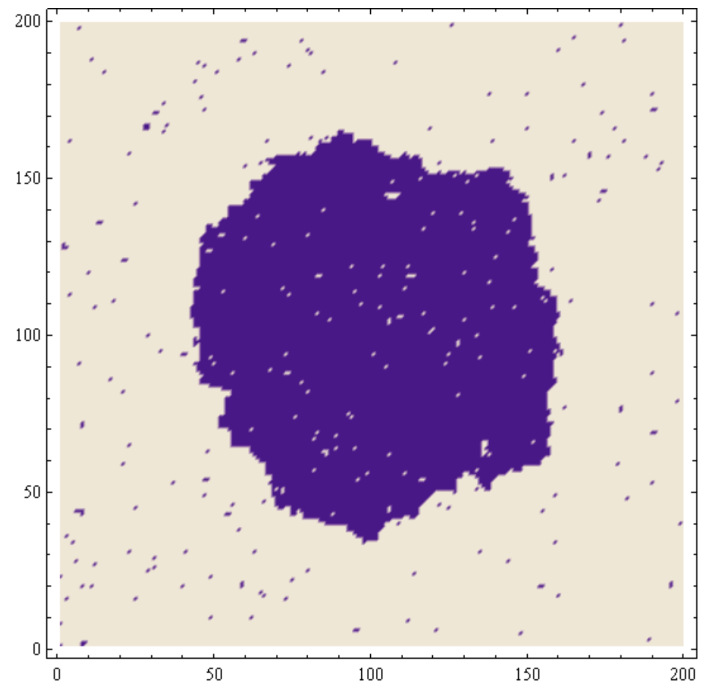


MC simulation result at T/Tc=0.7

No bulk energy

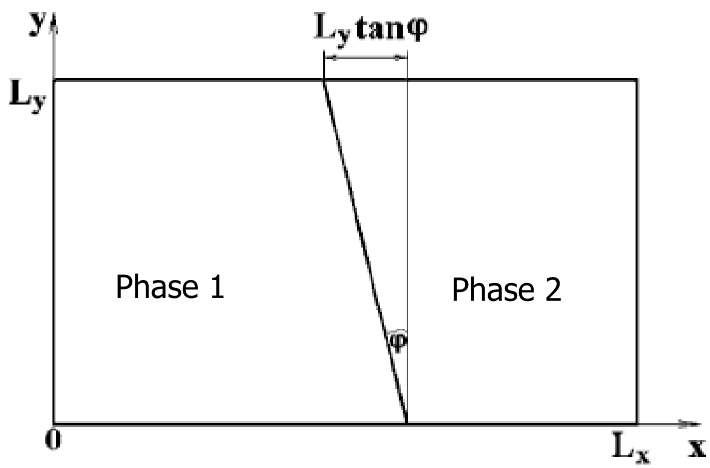


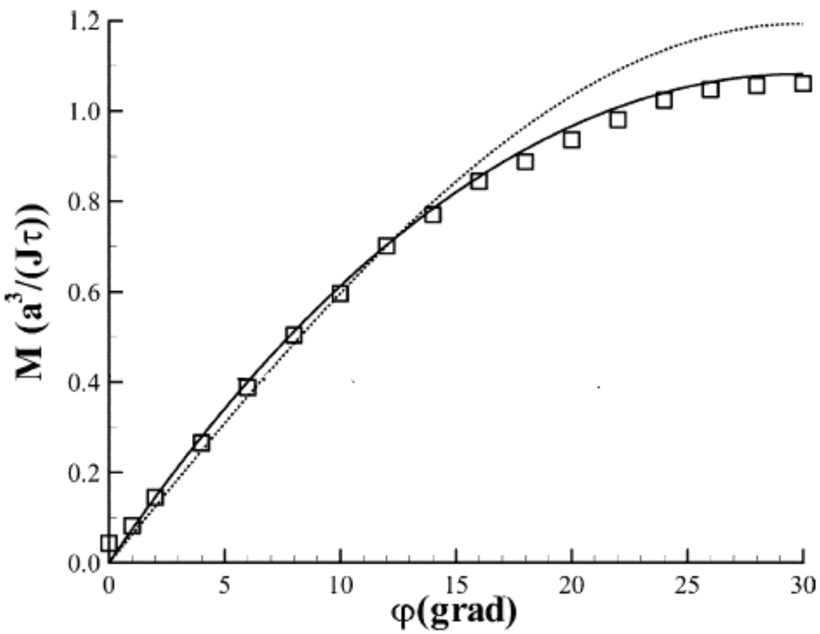
With bulk energy



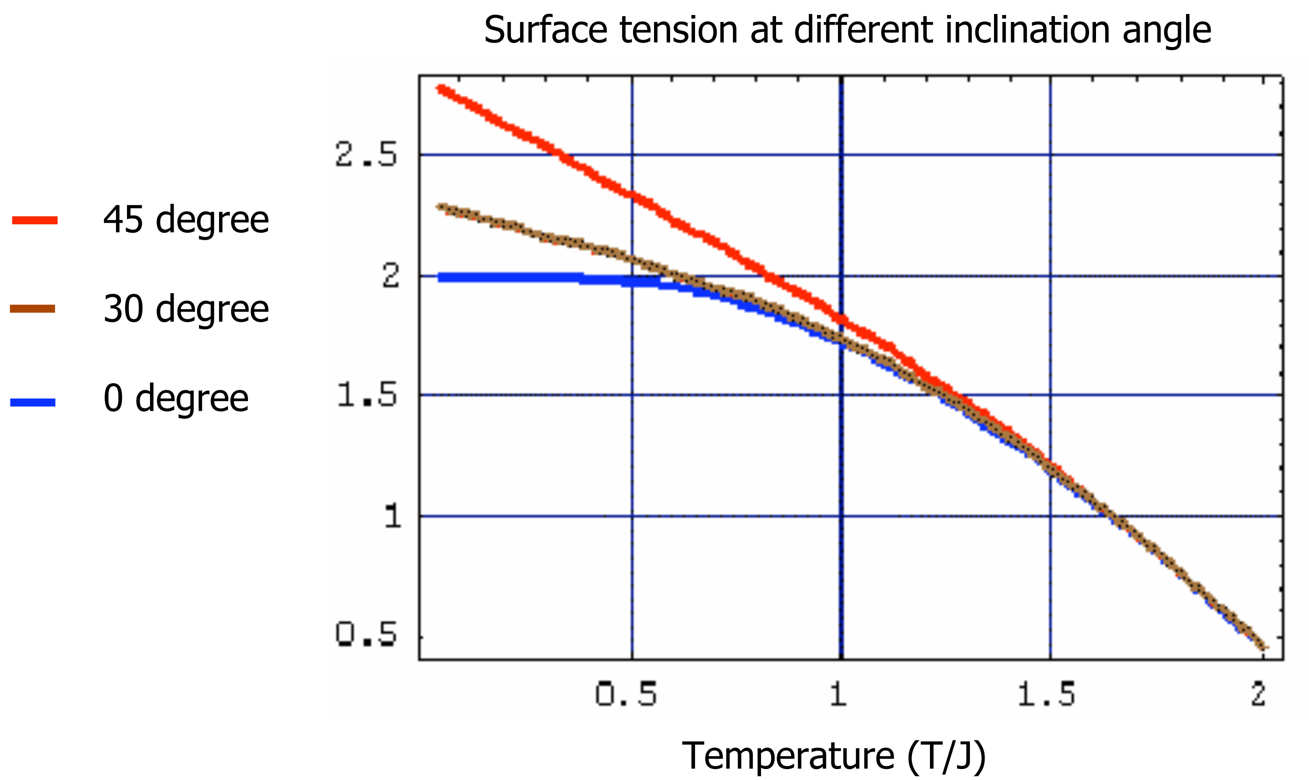
Grain boundary mobility via MC simulation

Geometry setting

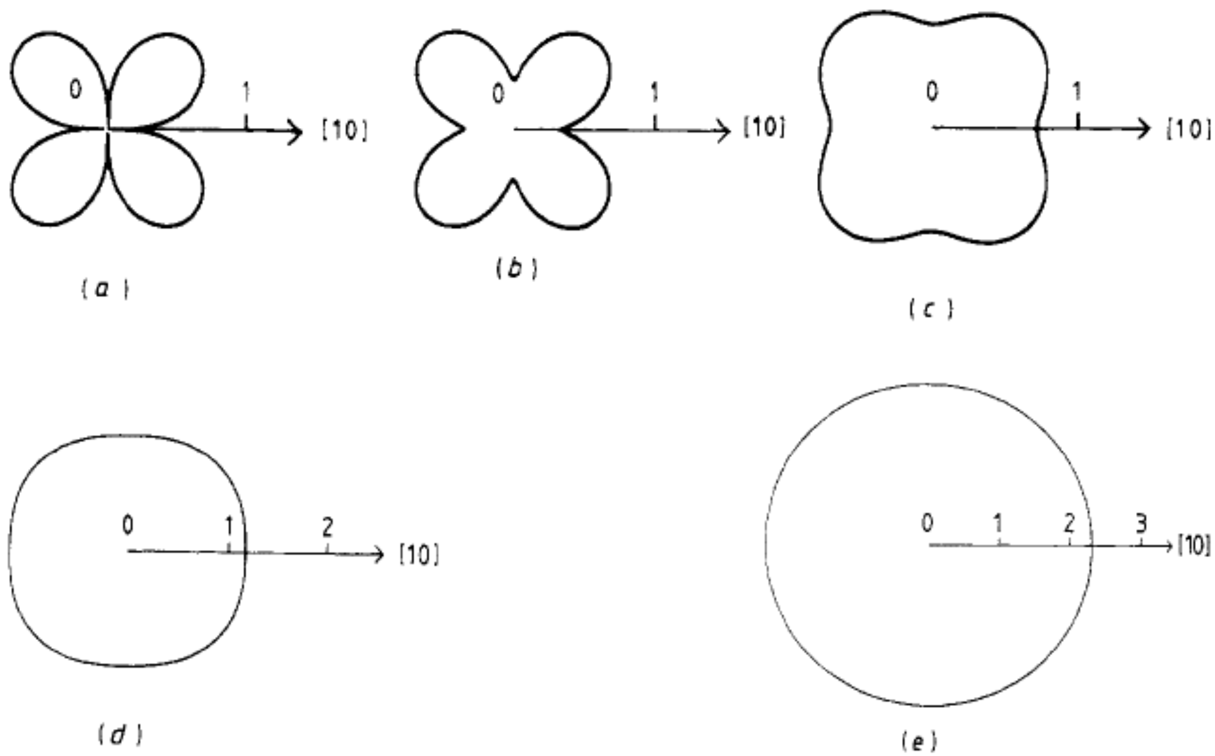




Anisotropic surface tension



Grain boundary stiffness at different T



Inverse square root of grain boundary stiffness. The temperatures are chosen as (a) T/Tc=0.1, (b) T/Tc=0.3, (c) T/Tc=0.5, (d) T/Tc=0.7, (e) T/Tc=0.9.

Conclusion and future research

- MPM result is consistent with experimental data
- At low temperature, both surface tension and grain boundary mobility are anisotropic
- At high temperature, both surface tension and grain boundary mobility are isotropic
- Grain boundary mobility is independent of driving force type
- KMC option will be turned on to see texture evolution
- Grain boundary mobility study will be extended to 3D

Thanks.

Any questions?