SAND2008-1987C

A Short Comment on the Temperature Variation of Grain Boundary Free Energy

Stephen Foiles
Computational Materials Science and Engineering Department
Sandia National Laboratories
Albuquerque, NM

Computational Materials Science Network Coordination Meeting
Northeastern University, Boston, MA
April 3-4, 2008

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Once upon a time: Direct Calculation of G.B. Free Energy versus T

- Method of calculation
  - Low temperature:
    - Quasi-harmonic calculations
  - High temperature
    - Thermodynamic Integration using MC based excess enthalpy
- High-symmetry boundary
  - Cu Σ5 (310)/[001] symmetric tilt boundary
- Dramatic reduction in grain boundary free energy

$$\frac{\gamma(T_M)}{\gamma(0)} \approx 0.4$$

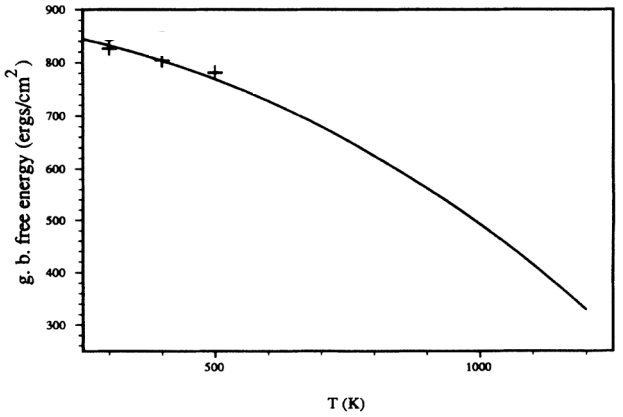
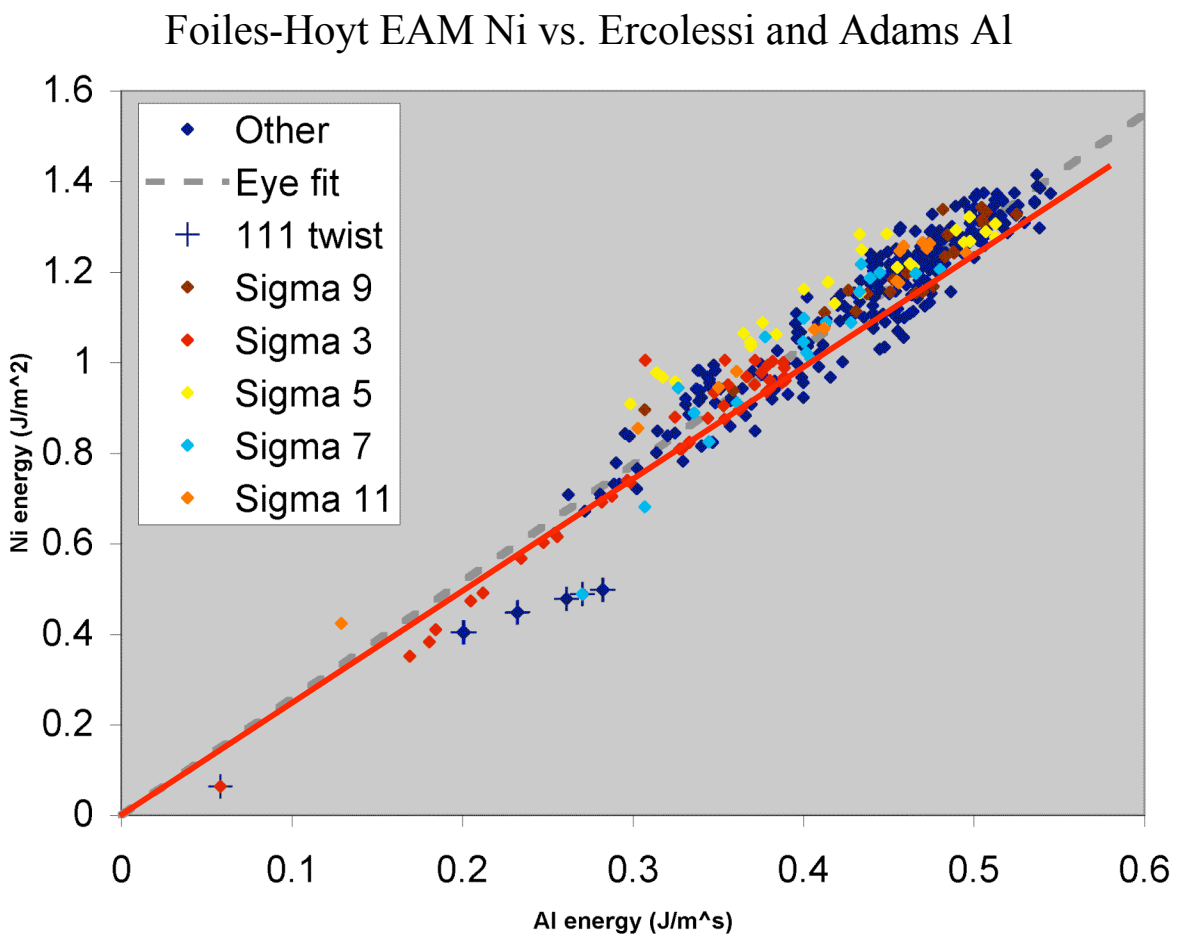


FIG. 9. The interfacial free energy of a Cu Σ5 (310)/[001] symmetric tilt boundary as computed from the MC simulations (solid line)

S.M. Foiles, "Evaluation of harmonic methods for calculating the free energy of defects in solids", Phys. Rev. B**49**, 14930 (1994).

Sandia National Laboratories

Comparison of Grain Boundary Energies in different metals: Ni vs. Al

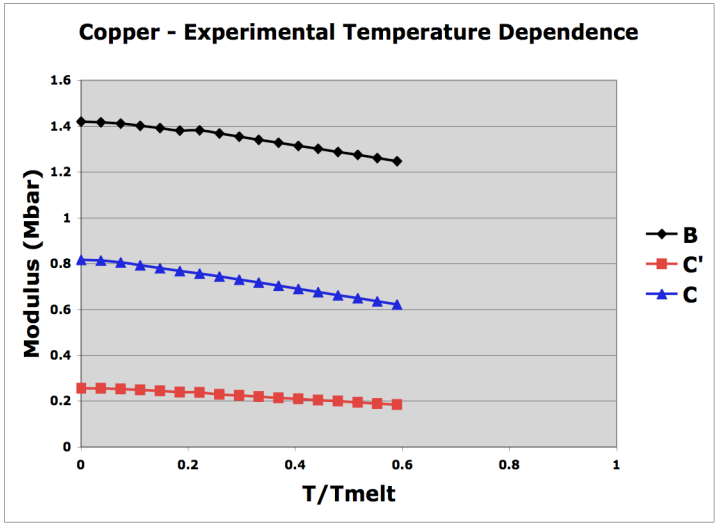


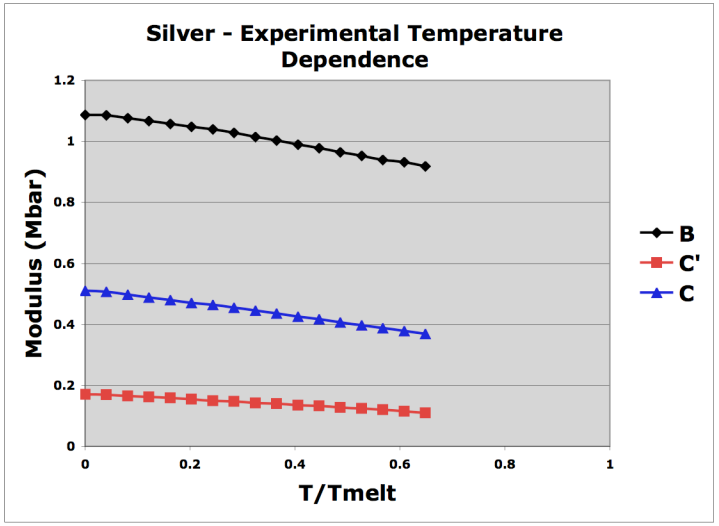
- Most of the variation in boundary energy is structural, not chemical.
- What scales boundary energy?
  - Shear modulus ratio: 2.4

  ⇒Supports a dislocation model for grain boundary structure
- <111> twist boundaries are relatively lower energy in Ni.
- The "special" Σ11 boundary is relatively lower energy in Al.

Sandia National Laboratories

Temperature Dependence of Elastic Constants: Noble Metals

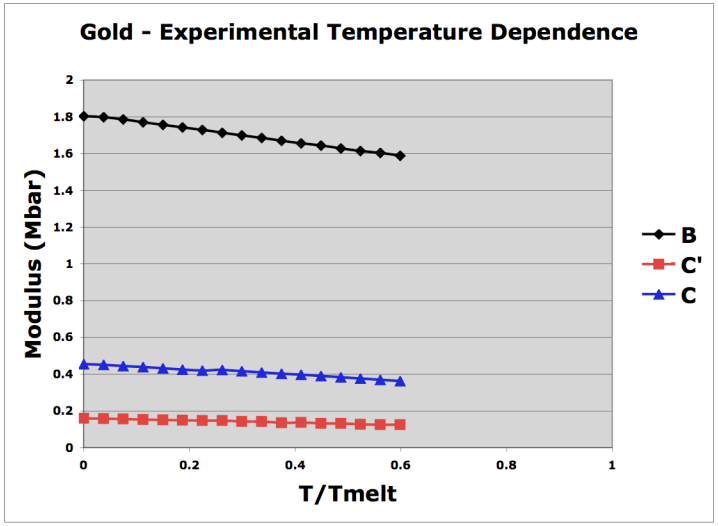




$$B = \frac{1}{3}(C_{11} + 2C_{12})$$

$$C = C_{44}$$

$$C' = \frac{1}{2}(C_{11} - C_{12})$$



Simmons & Wang, "Single Crystal Elastic Constants and Calculated Aggregate Properties" (MIT Press, 1971)

Sandia National Laboratories

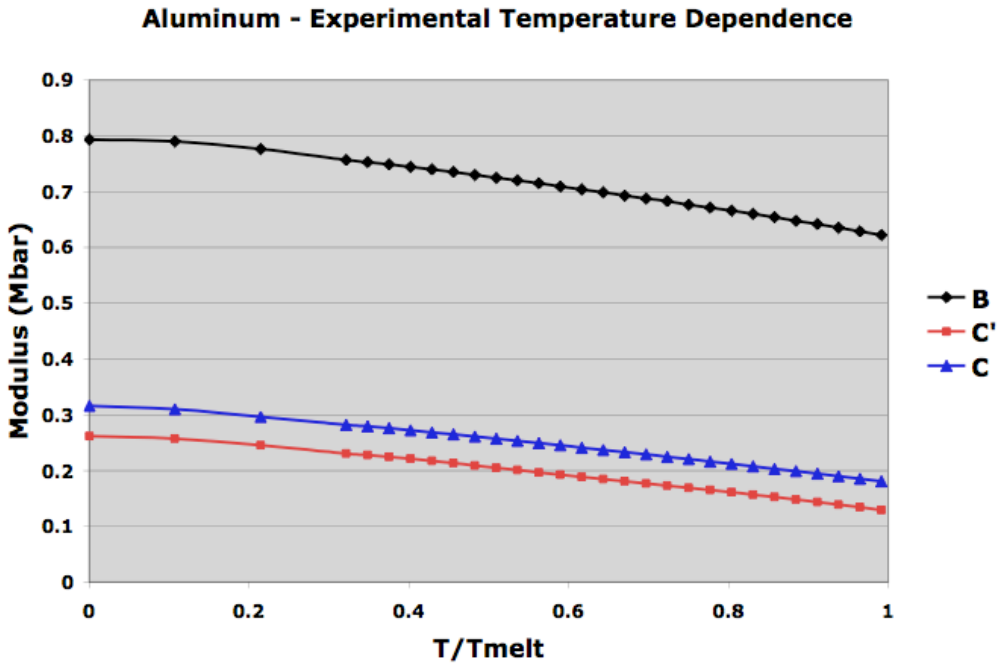
Temperature Dependence of Elastic Constants: Aluminum - Data up to T_M!

$$B = \frac{1}{3}(C_{11} + 2C_{12})$$

$$C = C_{44}$$

$$C' = \frac{1}{2}(C_{11} - C_{12})$$

Simmons & Wang, “Single Crystal Elastic Constants and Calculated Aggregate Properties” (MIT Press, 1971)



Sandia National Laboratories

Is elastic softening the main driver for reduction of grain boundary free energy with temperatue?

- Physically reasonable that grain boundary energy scales with shear modulus
  - Grain boundaries are arrays of dislocations
    - at least formally
  - Elastic strain energy of a dislocation scales with shear modulus
  - Consistent with comparison of grain boundary energies for different metals
- Magnitude of shear modulus softening is comparable to (though somewhat less than) the reduction in grain boundary free energy
  - **More data needed here!**

$$\frac{Modulus(T = T_M)}{Modulus(T = 0)}$$

	B	C	C'
Cu	0.77	0.58	0.50
Ag	0.75	0.56	0.45
Au	0.80	0.65	0.61
Al	0.78	0.57	0.49

Nobel metal data extrapolated to T_M

Sandia National Laboratories