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Update on Elastic Constants and Grain Boundary Energetics

Stephen Foiles, David Olmsted
Computational Materials Science and Engineering Department
Sandia National Laboratories
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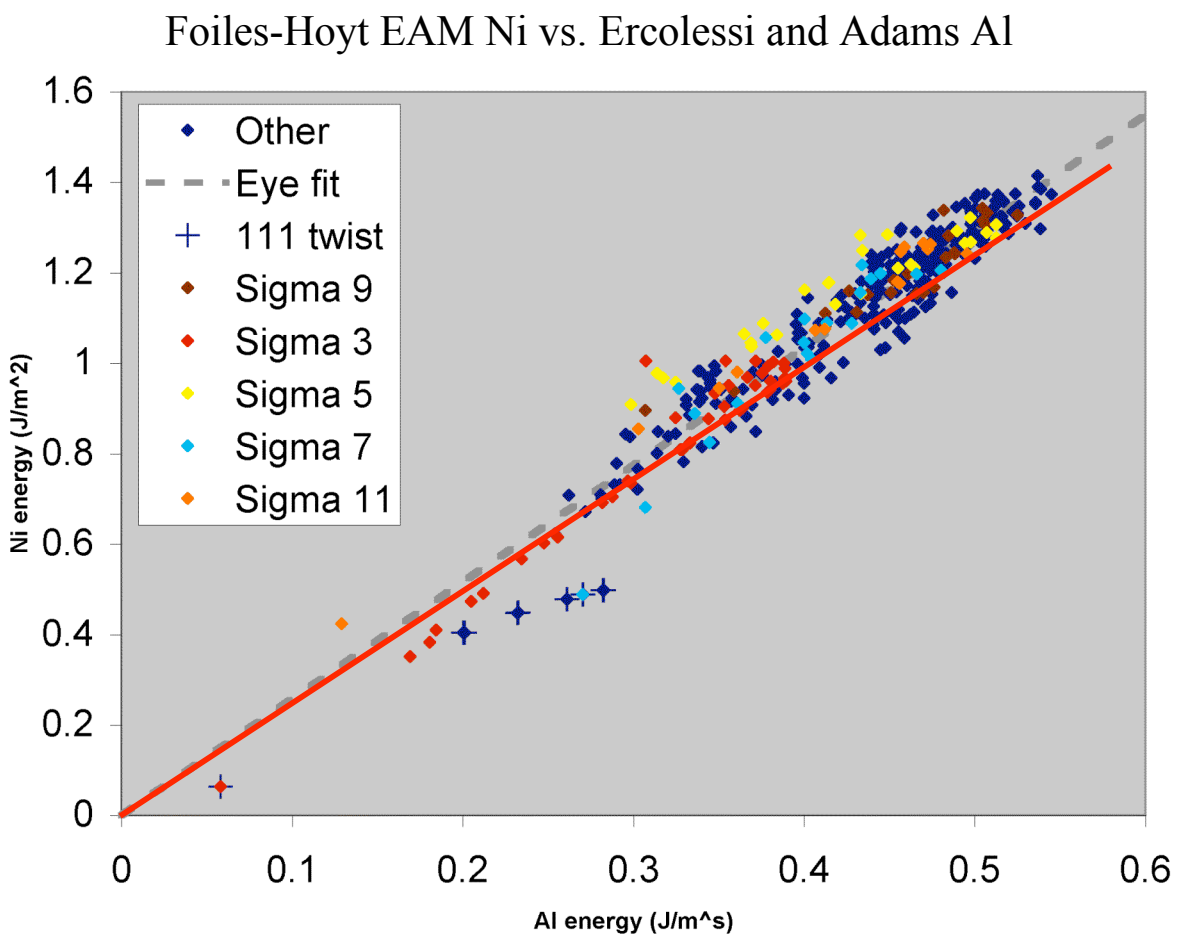
Last Time: Comparison of Grain Boundary Energies in different metals: Ni vs. Al



- 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.

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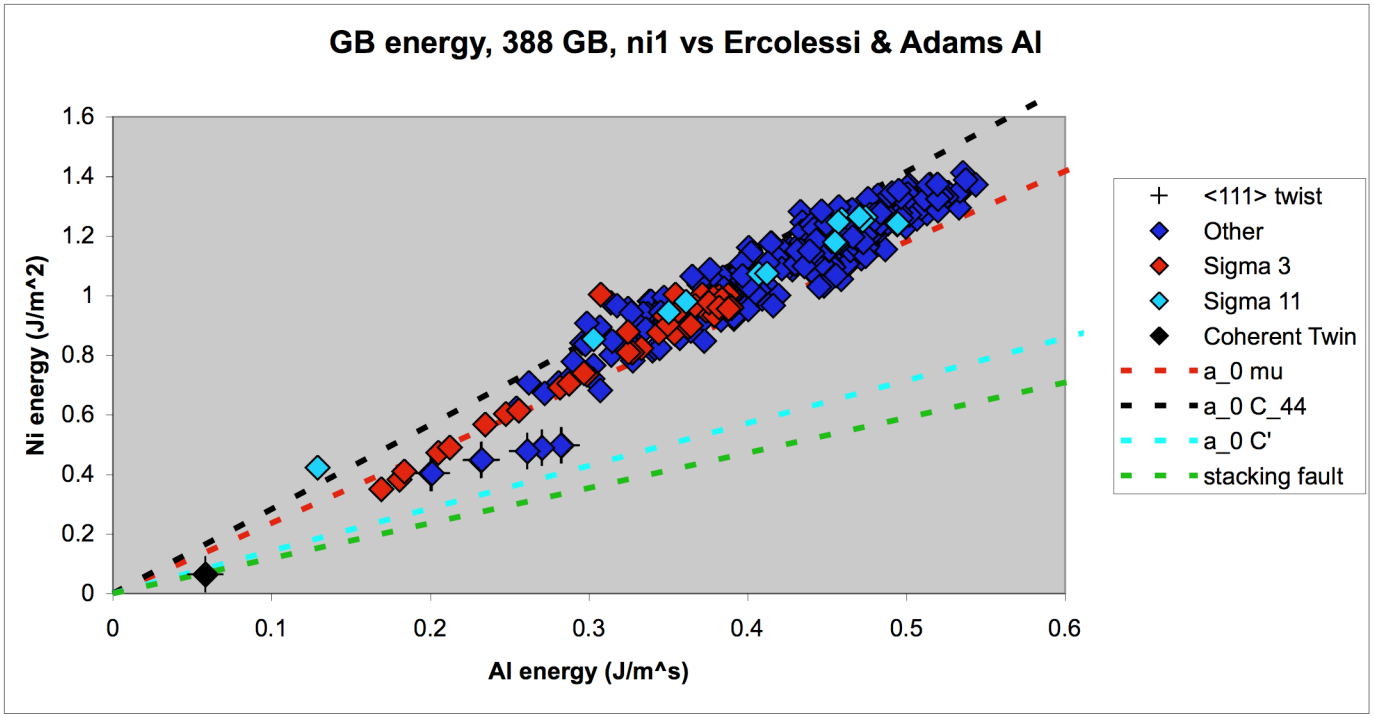
Which shear modulus is really the best?



- Actually Voight average shear (mu) and C_{44} are about equally good when comparing Ni and Al

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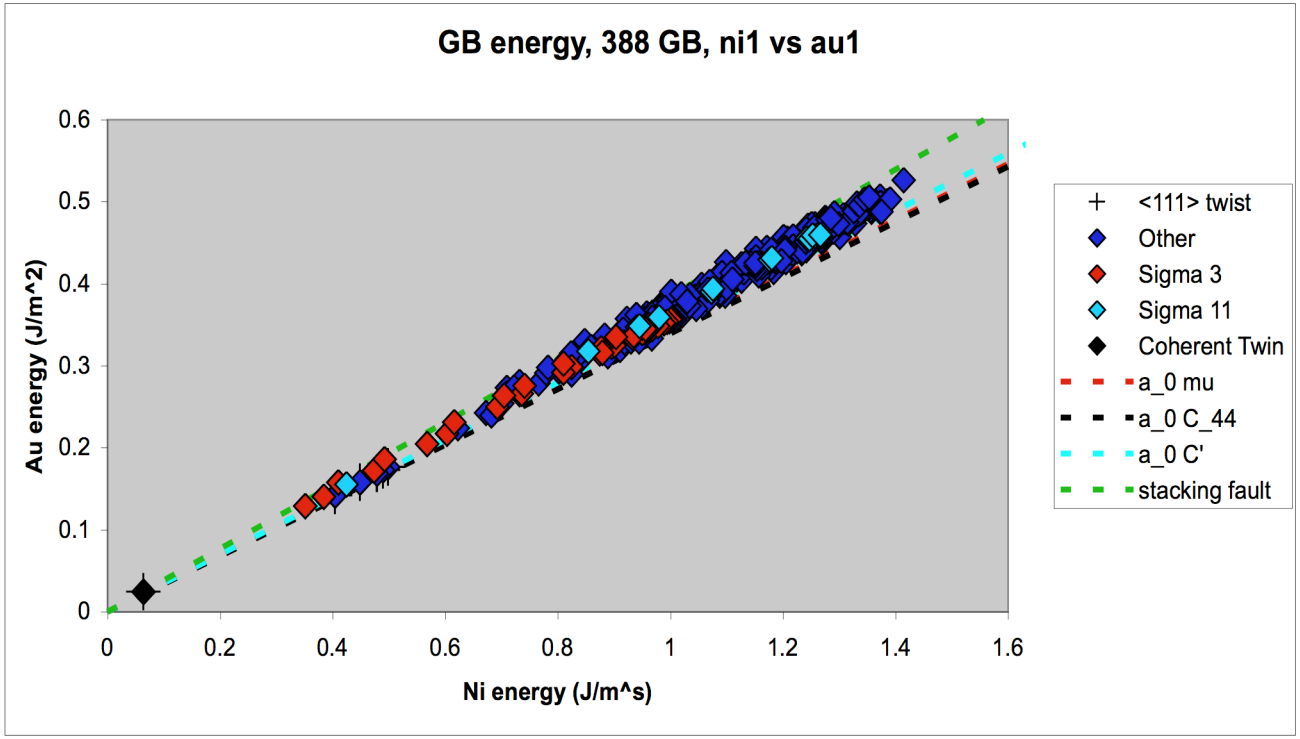
Let's compare Ni and Au



- Hmmgh! Just about anything works in this case!
- Note that there is much less scatter comparing the results for Ni and Au
  - Both potentials use similar functional forms

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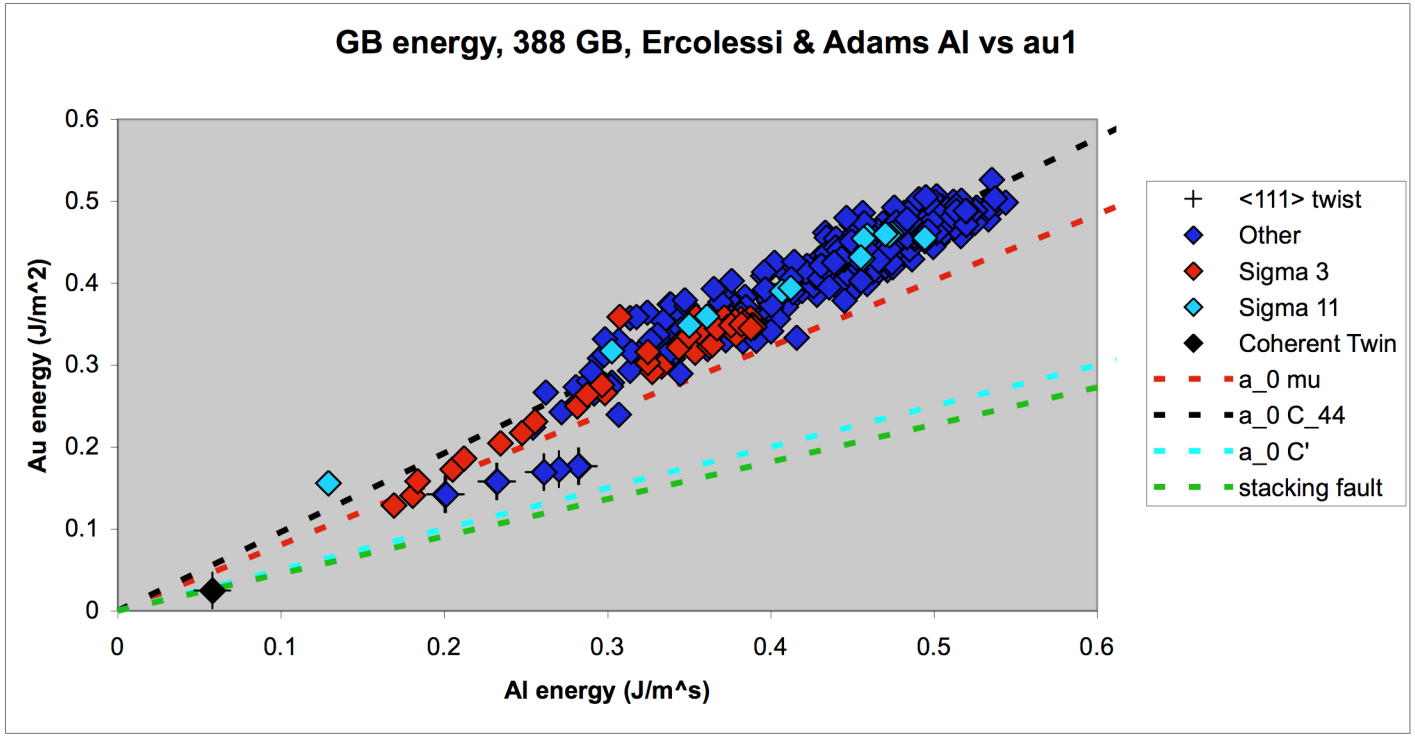
Comparison of Au and Al suggests a winner



- C_{44} appears the best modulus to use when comparing energies of different materials
  - David Seidman was right
    - D. Udler and D.N. Seidman, Phys. Rev. B54, 134 (1996)

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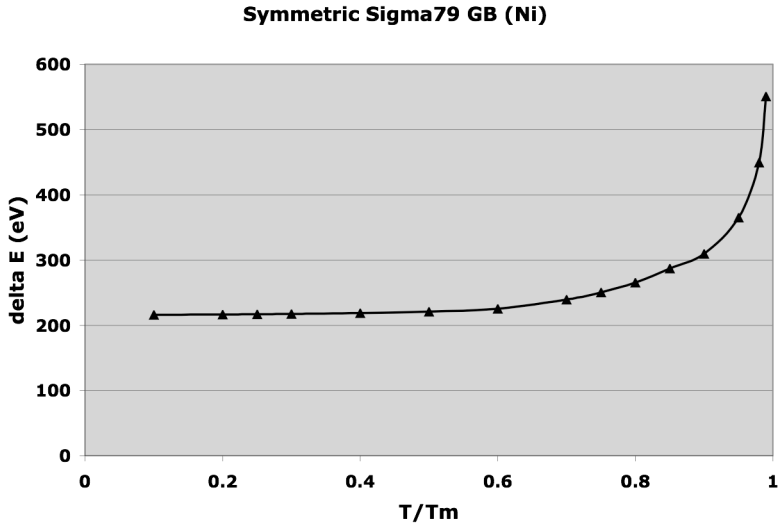
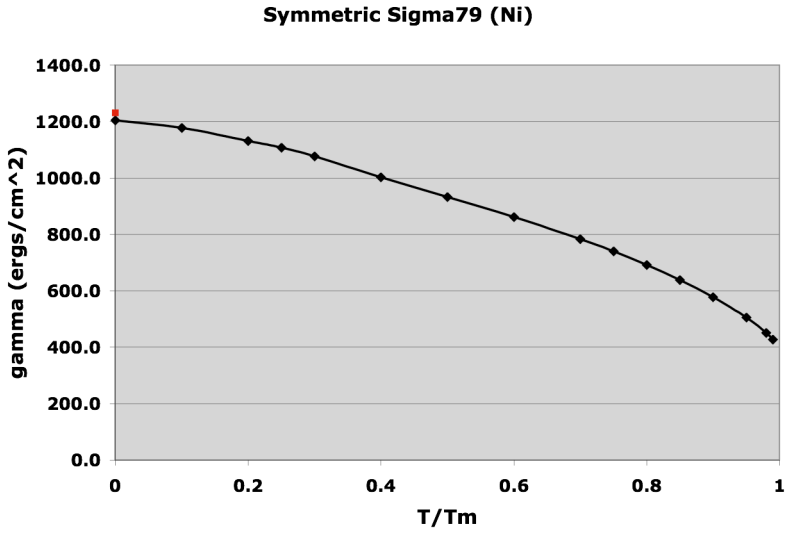
Last Time: Calculation of Temperature Dependence of γ
Σ79 [111] symmetric tilt boundary





- If know free energy at some T, can integrate to desired T
  - Need $\Delta E(T)$ and $\sigma(T)$ to perform integration
  - Both of these obtainable from MD simulation
- Use quasi-harmonic calculations to compute γ for $T \leq 0.25\ T_M$
- There is a significant drop in interface free energy with temperature
  - Question from last time: How does this compare with softening of elastic constants for the same interatomic potential?

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MD calculation of the *temperature dependent* elastic constants

- Generalize to EAM potentials the method of T. Cagin and J.R. Ray, Phys. Rev. B37, 699 (1988).
  - Fluctuation formulas are for microcanonical (NVE) ensemble
  - EAM generalization follows M.S. Daw and M.I. Baskes, Phys. Rev. B29, 6443 (1984)

$$\Omega C_{\alpha\beta\gamma\delta} = 2NT(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) + \left(\frac{\Omega^2}{T}\right)\left(\left\langle P_{\alpha\beta}\right\rangle\left\langle P_{\gamma\delta}\right\rangle - \left\langle P_{\alpha\beta}P_{\gamma\delta}\right\rangle\right) + \left\langle P_{\alpha\beta\gamma\delta}\right\rangle$$

$$N\Omega P_{\alpha\beta} = \frac{1}{2}\sum_{ij}\left(\phi'_{ij}\frac{r^{ij}_{\alpha}r^{ij}_{\beta}}{r^{ij}} + \left(F'(\rho_i) + F'(\rho_j)\right)\rho'_{ij}\frac{r^{ij}_{\alpha}r^{ij}_{\beta}}{r^{ij}}\right) - \sum_i m_i v^i_{\alpha} v^i_{\beta}$$

$$NP_{\alpha\beta\gamma\delta} = \frac{1}{2}\sum_{ij}\left[B^{ij}_{\alpha\beta\gamma\delta} + \left(F'(\rho_i) + F'(\rho_j)\right)W^{ij}_{\alpha\beta\gamma\delta} + \left(F''(\rho_i) + F''(\rho_j)\right)V^{ij}_{\alpha\beta}V^{ij}_{\gamma\delta}\right]$$

$$B^{ij}_{\alpha\beta\gamma\delta} = \left(\phi''_{ij} - \frac{\phi'_{ij}}{r^{ij}}\right)\frac{r^{ij}_{\alpha}r^{ij}_{\beta}r^{ij}_{\gamma}r^{ij}_{\delta}}{\left(r^{ij}\right)^2} \qquad W^{ij}_{\alpha\beta\gamma\delta} = \left(\rho''_{ij} - \frac{\rho'_{ij}}{r^{ij}}\right)\frac{r^{ij}_{\alpha}r^{ij}_{\beta}r^{ij}_{\gamma}r^{ij}_{\delta}}{\left(r^{ij}\right)^2} \qquad V^{ij}_{\alpha\beta} = \rho'_{ij}\frac{r^{ij}_{\alpha}r^{ij}_{\beta}}{r^{ij}}$$

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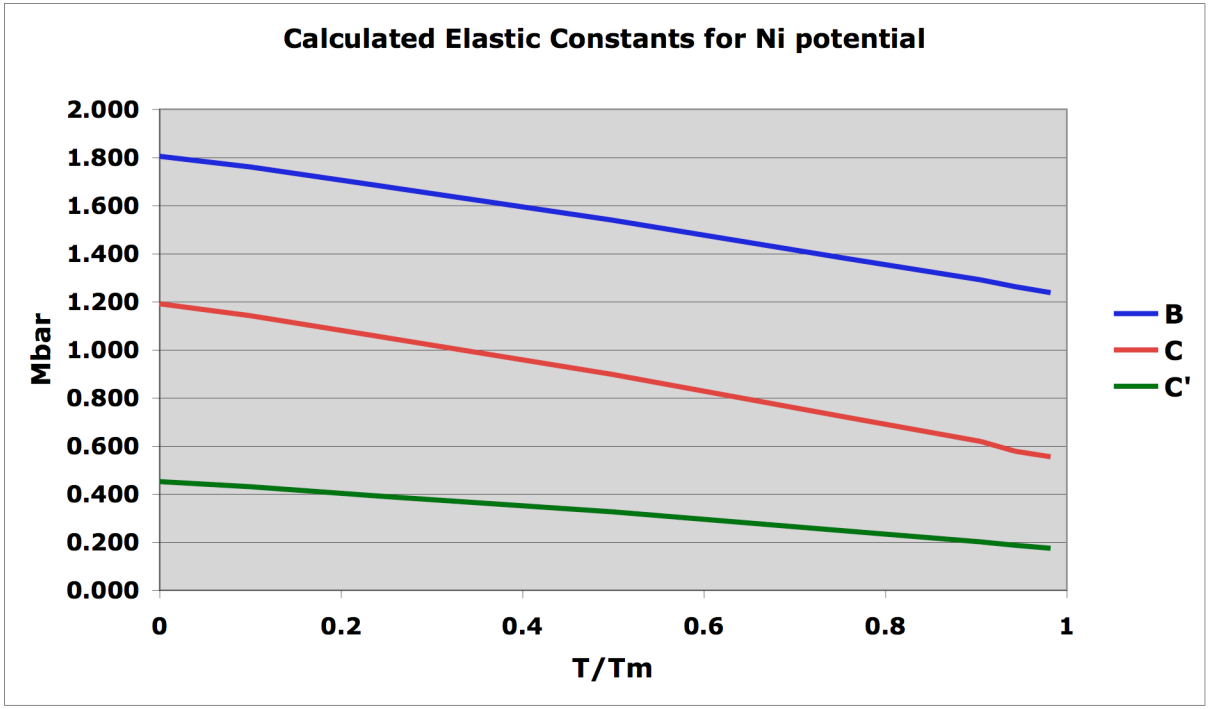
Computed temperature dependence for the Ni potential similar to experimental data for metals



- Have not found experimental data for Ni
- For Al where experimental data exists up to T_M
  - $B(T_M)/B(T=0) = 0.78$
  - $C(T_M)/C(T=0) = 0.57$
  - $C'(T_M)/C'(T=0) = 0.45$

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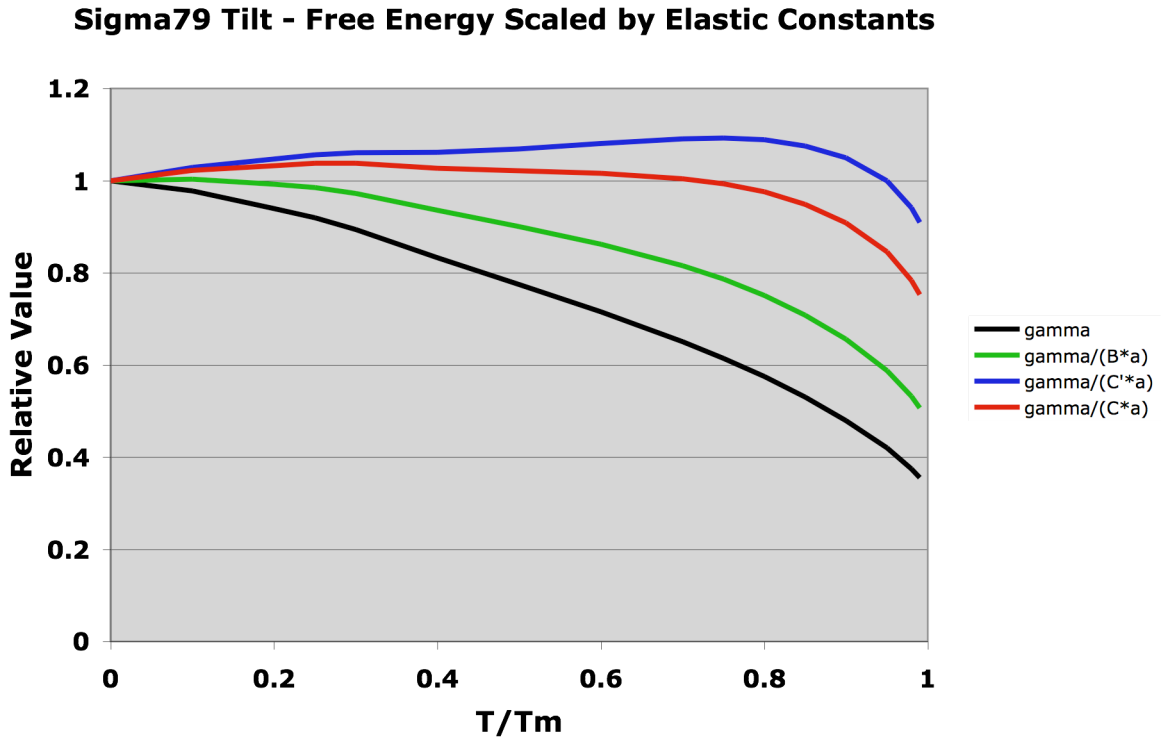
Grain Boundary Free Energy scales with C_{44} reasonably well up to $T \sim 0.75T_M$



- Results suggest that for moderate temperatures the variation of grain boundary free energy is dominated by elastic softening
- For high temperatures other mechanisms contribute

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