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Interaction of Grain Boundaries with Voids: A Correction to Zener-Smith?

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Zener-Smith assumption of the interaction energy

- **Interaction energy between a void (precipitate) is taken to be the energy of the grain boundary that is eliminated by the boundary intersecting the precipitate**

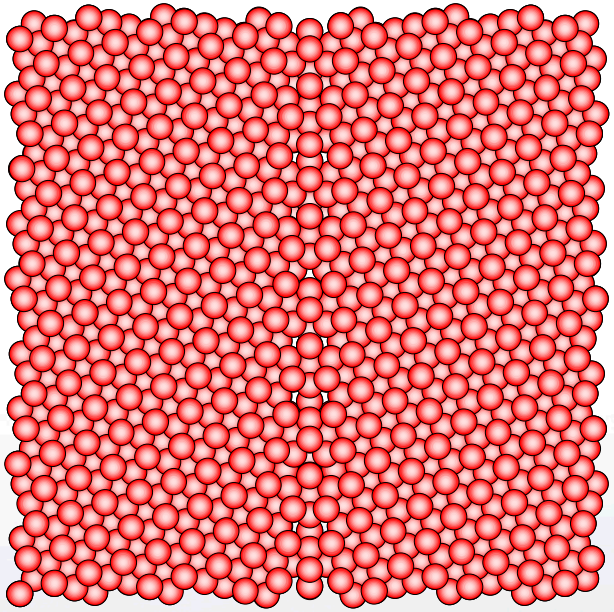
$$\Delta E = -\gamma_{gb}\pi(R^2 - d^2)$$

  - γ_{gb} *is the grain boundary energy*
  - R is the radius of the precipitate
  - d *is the distance of the center of the precipitate to the boundary*

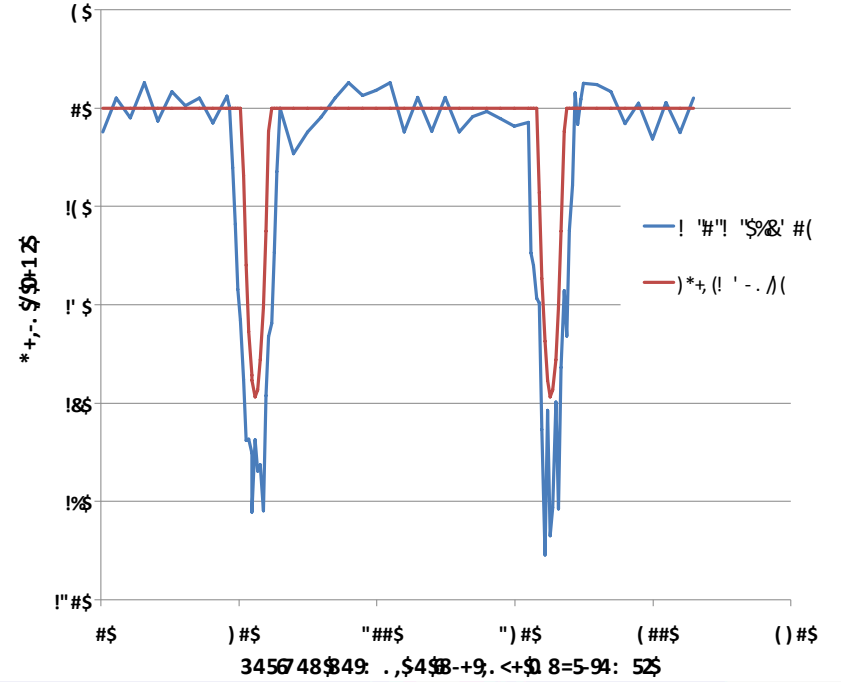
- ***Looks quite reasonable, but how quantitative is this?***

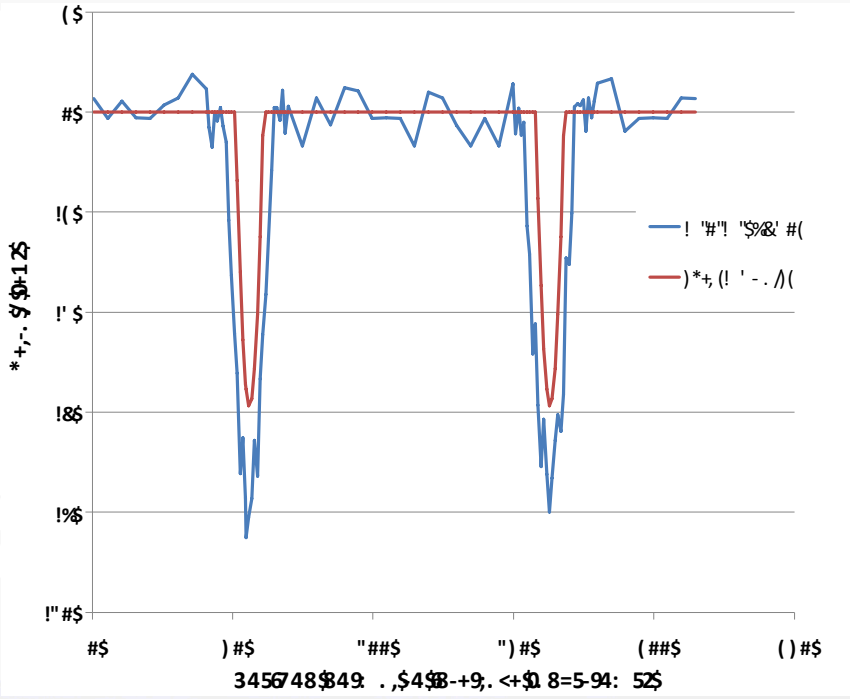
Model Calculation

- **Consider a Σ79 symmetric tilt boundary modeled with EAM potentials for Ni**
  - This boundary is fairly general
  - I have studied it before so that I already know the optimal structure and the grain boundary energy
- **Create spherical voids at different locations near the boundary and compute the minimized energy as a function of the distance of the void from the boundary**
  - Always remove the same number of atoms
  - Only local relaxation is performed so that macroscopic changes of shape of the void will not happen



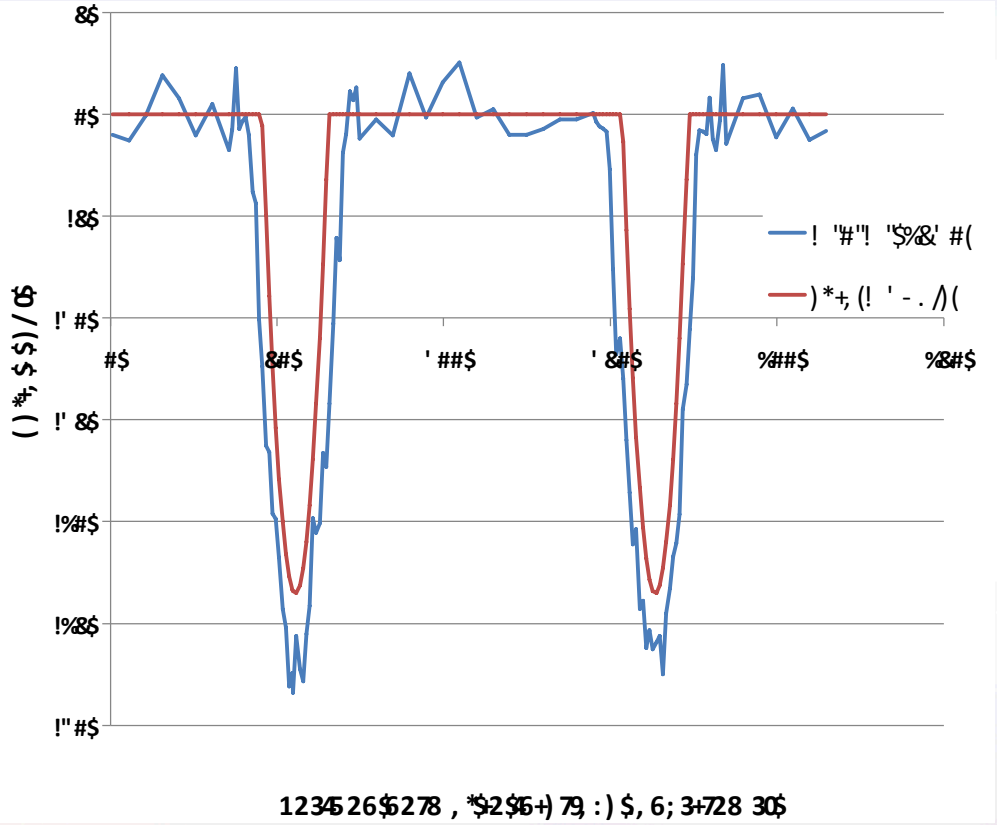
Zener-Smith appears to underestimate interaction





- 50 atom voids at 2 different positions in the plane of the boundary
- Atomistic interaction energy is larger than the simple estimate

Consider a larger void



- Note that the difference between the model and atomistic calculation seems to scale with the void radius!

Consider adding a junction line energy

- **Modified energy model**

$$r = \sqrt{\left(R^2 - d^2\right)}$$

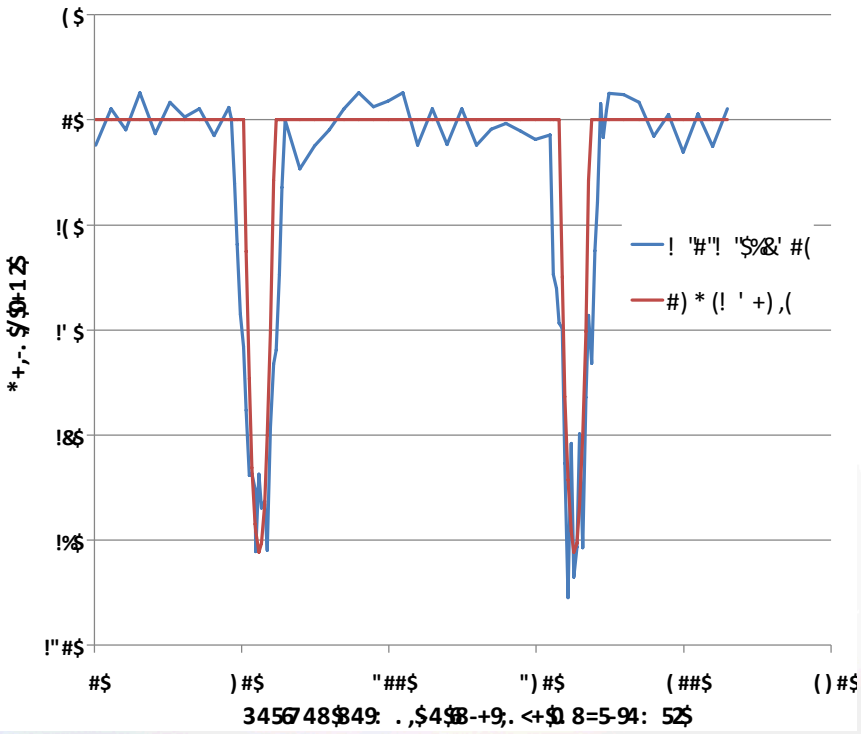
$$\Delta E = -\gamma_{gb}\pi r^2 + \varepsilon 2\pi r$$

- **The above results suggest a value of ε**

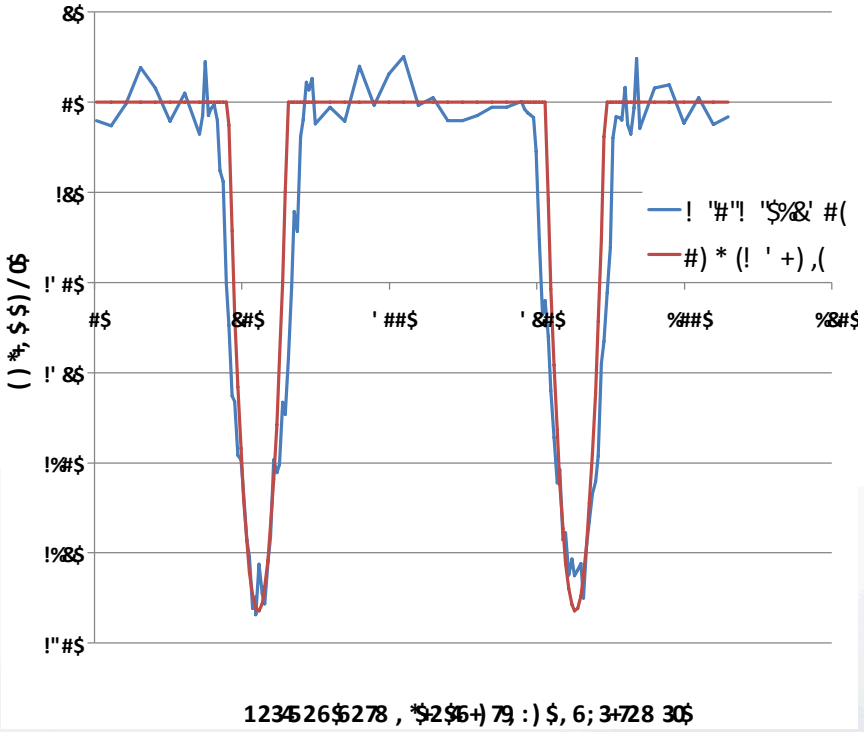
$$\varepsilon = -1.2x10^{-5}\frac{ergs}{cm} = -0.075\frac{eV}{\mathrm{A}}$$

Fits for the small and medium size voids

50 atom void



400 atom void



- **Of course this is expected**
  - new parameter was fit to this data

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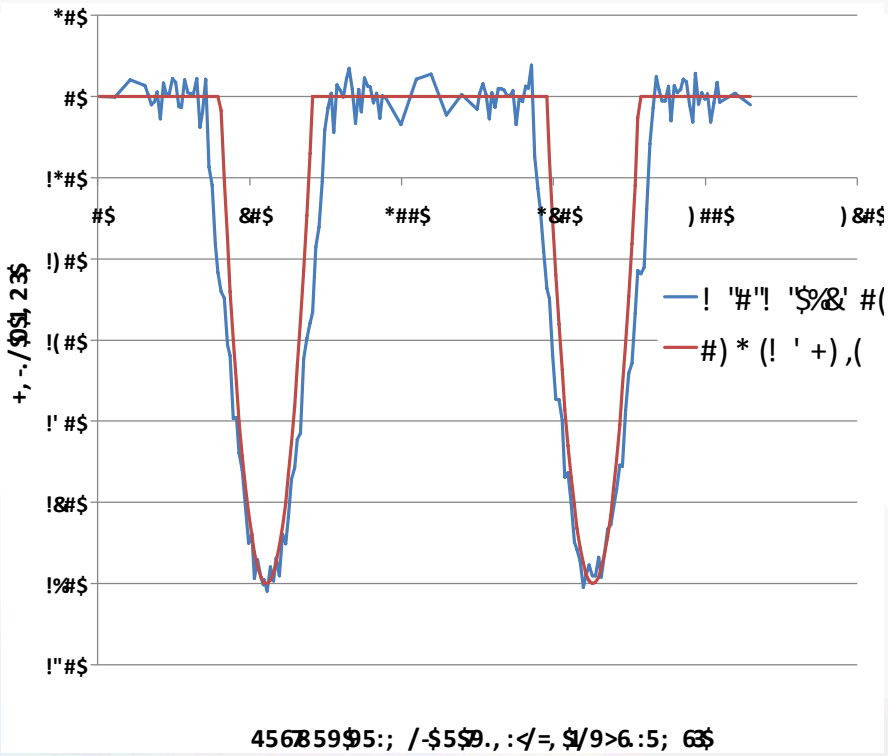
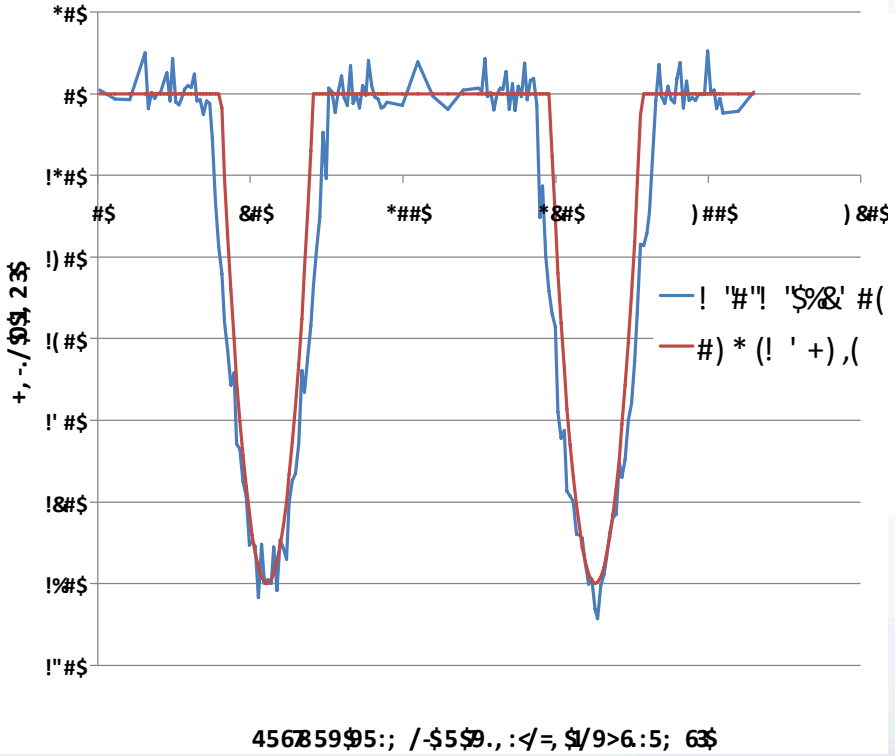
New model predicts larger voids





- 1350 atom voids
- Same parameters

Tantalizing, but many questions remain…

- **What is the equilibrium structure of the void at the boundary**
  - Driving force for creating a more pancake-like strucutre
  - Have not looked for optimum structure
  - Lower energy shape would increase binding of void to boundary
- **What about interactions with other precipitates**
  - Gas filled voids – role of bubble pressure?
  - Solid precipitates
- **Is this effect big enough to worry about?**
  - The grain boundary energies are not that well known
  - This is not a dominant contribution