Symmetric tilt boundary energy of Al and Cu

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  - EAM results
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- Conclusions

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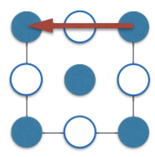
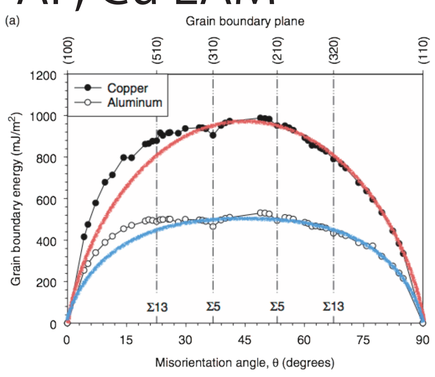
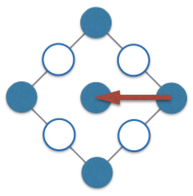
Al , Cu EAM







"Asymmetric tilt grain boundary structure and energy in copper and aluminium",
M. A. Tschopp and D. L. Mcdowell, Phil. Mag., Vol. 87 (2007), 3871–3892.
They used EAM potentials.

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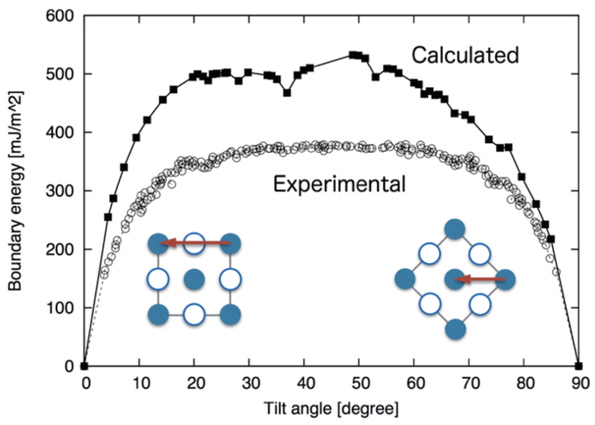
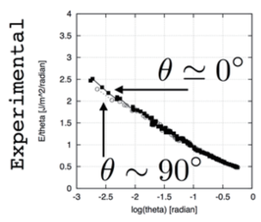
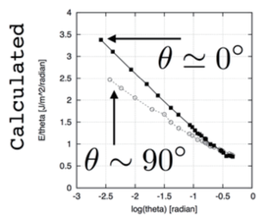
Al exp vs EAM



A. Otsuki,



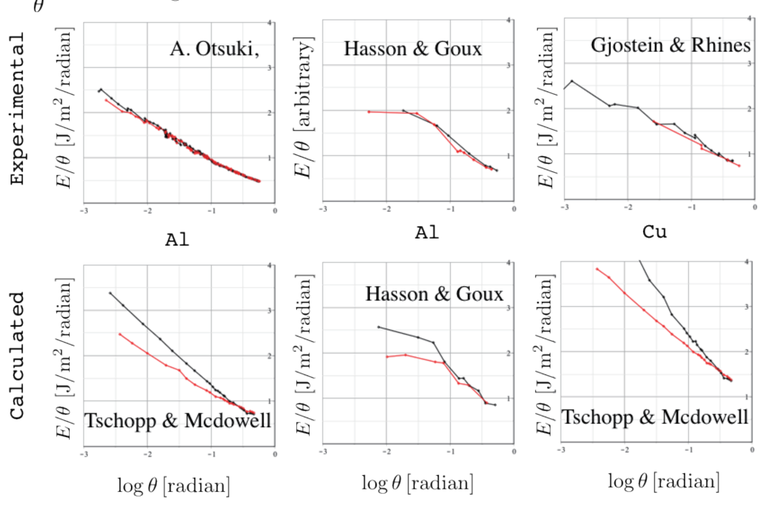
Tschopp & Mcdowell



Al , Cu whole

$$E = E_0\theta(A - \log\theta)$$

$$\frac{E}{\theta} = B - C\log\theta$$



VASP conditions & Boettger Mehod

- J. C. Boettger, "Nonconvergence of surface energies obtained from thin-film calculations," Physical Review B, vol. 49, pp. 16798–800, 1994.
- K. Doll and N. Harrison, "Chlorine adsorption on the cu (111) surface," Chemical Physics Letters, vol. 317, pp. 282–9, 2000.

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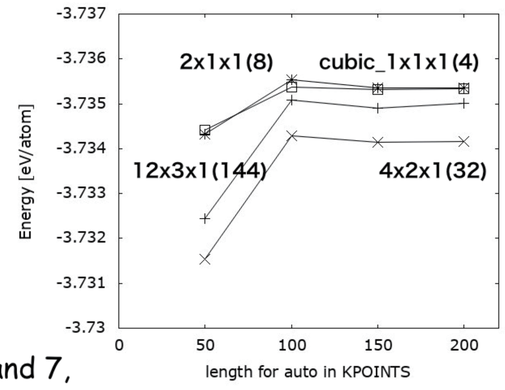
Energy convergence on k-points



VASP
Slab model: Σ 3, 5, and 7,
Al and Cu (100) symmetric tilt boundary.
Pseudopotential for Cu: PAW PBE
Energy cutoff: 273.214 eV
Energy: Tetrahedron method with Blöchl corrections.

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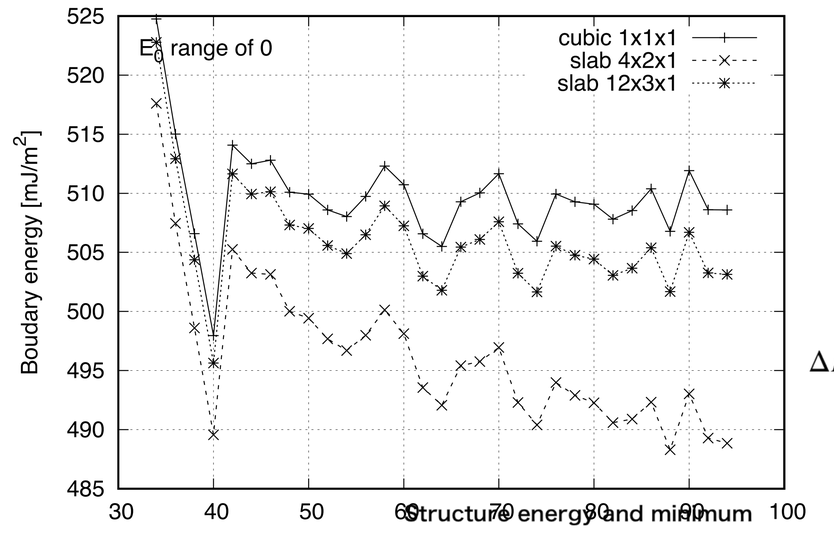
Al size dependency



Structure energy and minimum position by the first principles calculations

Boettger Mehod

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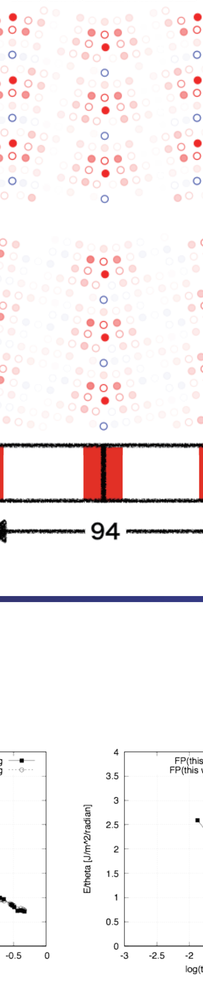
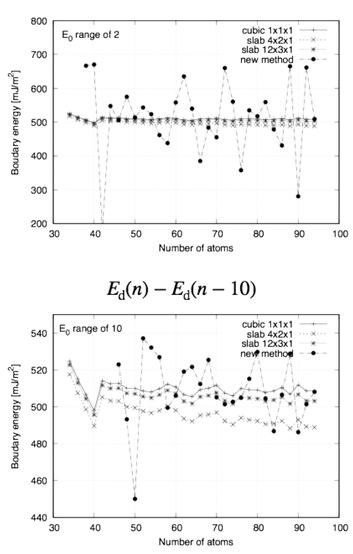
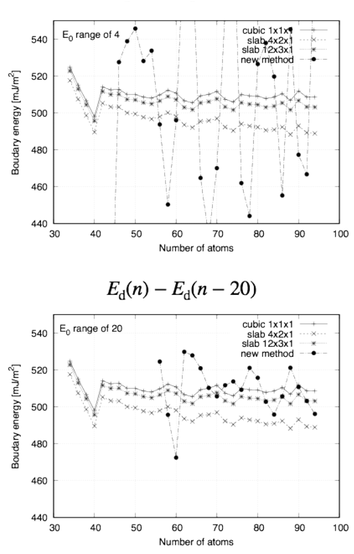


$$\Delta E = E_d(n) - nE_0$$
$$= E_d(n) -$$
$$\{E_d(n) - E_d(m)\}\frac{n}{n-m}$$

$E_d(n) - E_d(n-2)$



$E_d(n) - E_d(n-4)$



$E_d(n) - E_d(n-10)$

$E_d(n) - E_d(n-20)$

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EAM analysis

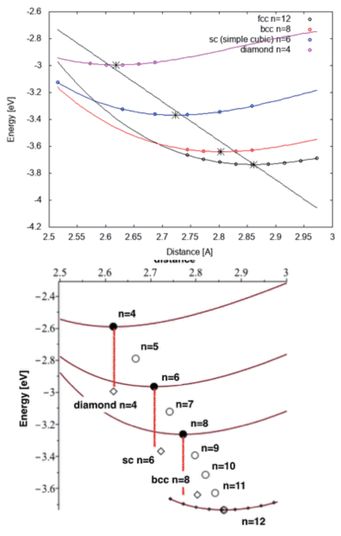
$$E_{\text{total}} = \sum \exp(-pr) - \sqrt{\sum \exp(-2qr)}$$
$$= n\exp(-pr) - \sqrt{n\exp(-2qr)}\,.$$

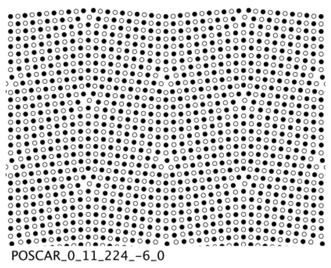
$$\frac{dE_{\text{total}}}{dr} = -np\exp(-pr) + q\sqrt{n\exp(-2qr)}$$

$$\frac{q}{p\sqrt{n}} = \left(\exp(q-p)\right)^{r_n}$$

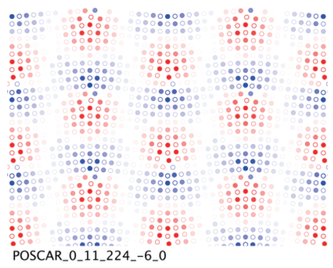
$$R = \frac{E_{\text{repulsive}}}{E_{\text{bond}}} = \frac{n\exp(-pr_n)}{\sqrt{n\exp(-2qr_n)}}$$
$$= \sqrt{n}\left(\frac{\exp(q)}{\exp(p)}\right)^{r_n}$$

$$R = \sqrt{n}\frac{q}{p\sqrt{n}} = \frac{q}{p}$$

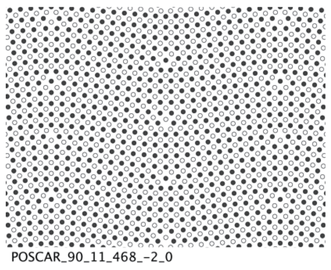




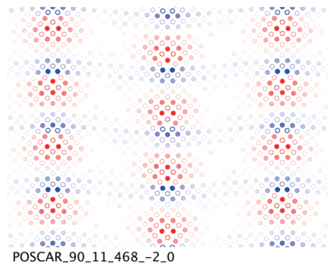
POSCAR_0_11_224_-6_0



POSCAR_0_11_224_-6_0

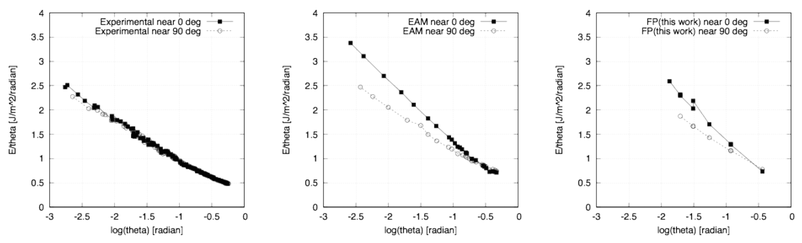


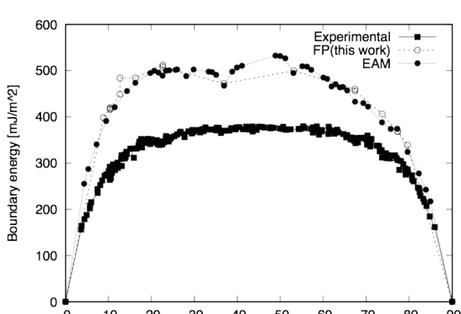
POSCAR_90_11_468_-2_0



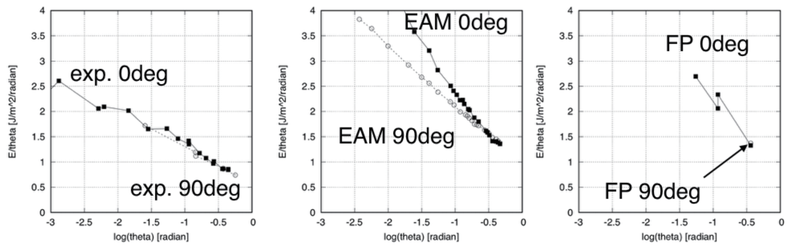
POSCAR_90_11_468_-2_0

Al results

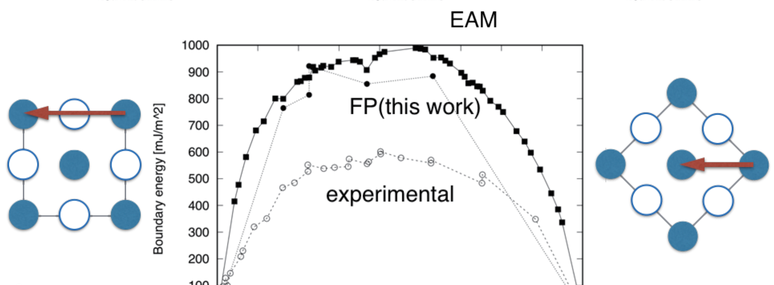




Cu results

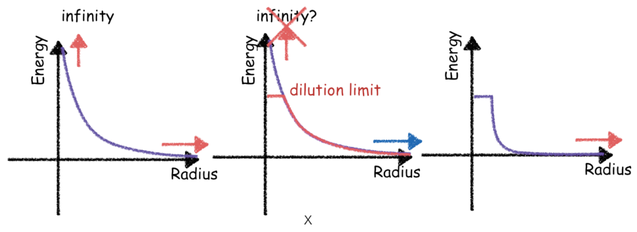


EAM



conclusions

- Small angle Al and Cu (100) tilt boundary shows small difference on the slopes at 0 and 90 degrees.
- Against the classical dislocation theory for small angle tilt boundary,
  - Small elastic field contribution (??)
  - Large core contribution (??)



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