Finite temperature first principles calculation of Al <100> twist boundary energy

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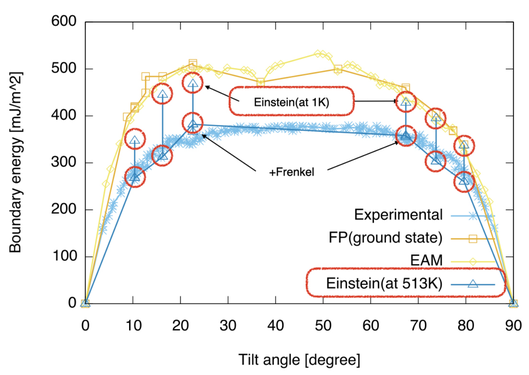
Background

- Last year, Nishitani published the finite temperature first principles calculations on Al <100> symmetric tilt boundary energy[1].
- The results are consistent with the experimental results of Otsuki.
- We will report the applications of his method on Al <100> twist boundary



S. R. Nishitani (2020) Finite-temperature first-principles calculations of Al ⟨100⟩ symmetric tilt grain-boundary energy, Philosophical Magazine, DOI: 10.1080/14786435 .2020.1855371.

Experimental results

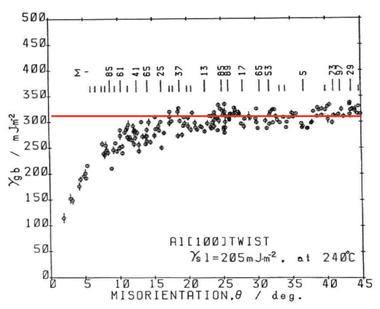


Fig.5-11 Grain boundary energy, γgb, as a function of θ for Al[100] twist boundary, where γsl =205mJ·m⁻².

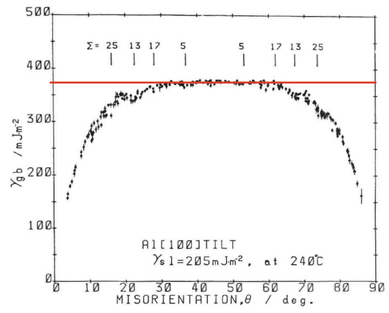


Fig.5-9 Grain boundary energy, γgb, as a function of θ for Al[100] tilt boundary, where γsl =205mJ·m⁻².

A. Otsuki, *Research on boundary energy of Al*, Ph.D. diss., Kyoto Univ., 1990, in Japanese.

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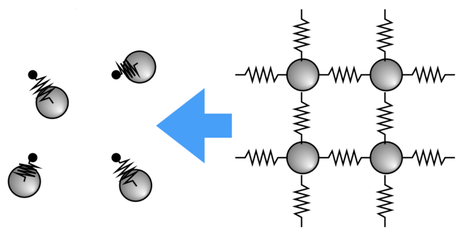
Method-I (Einstein)

Helmholtz Free Energy

$$F_i = E_i^0 - k_B T \ln Z_i$$
$$= E_i^0 - k_B T \sum_{j=x,y,z} \ln\left(\frac{\exp(-\hbar\omega_j/2k_BT)}{1-\exp(-\hbar\omega_j/k_BT)}\right)$$



Θ_{ij} Einstein temperature *j*-direction on the *i*-site

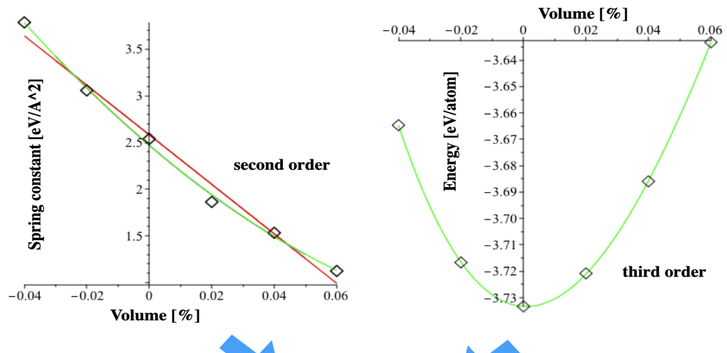
$$\Theta_{ij} = \frac{h\nu_{ij}(a)}{k_B}$$

$$\nu_{ij} = \frac{1}{2\pi}\sqrt{\frac{k_{ij}}{m}}$$

- nij : frequency
- kij : spring constant
- m : weight of oscillator, here equal to the atomic weight

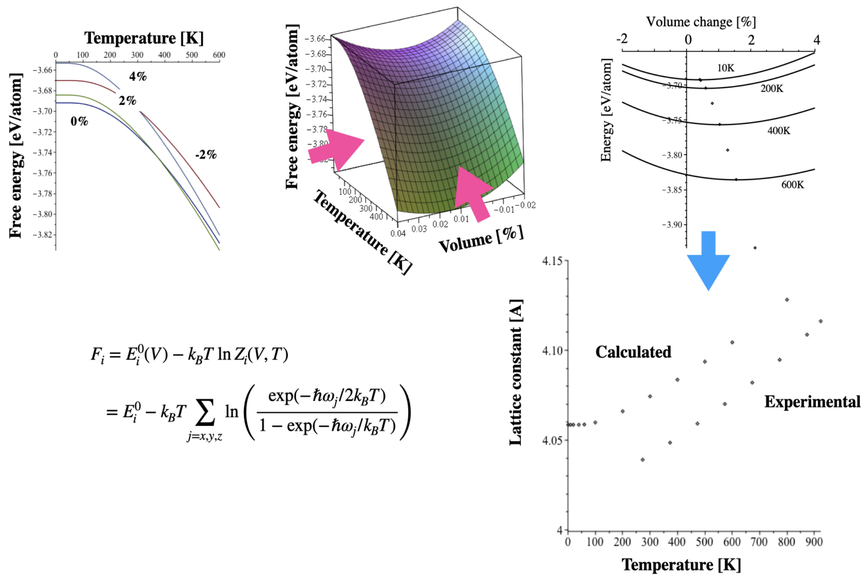
Perfect lattice

Spring constant:k **on-site energy:E_0**



Method-II (VASP)

- For the pseudopotentials of Al, we used the
  - projector-augmented wave (PAW) method and
  - generalised-gradient approximation (GGA).
- The cut-off energy of the plane wave was the default of the potential.
- The total energies were obtained by
  - the tetrahedron method, and
  - the relaxations were performed by the Methfessel-Paxton method with order 1.
- The k-point meshes,
  - which change with the unit cell's outer dimensions depending on the tilt angle θ,
  - were provided by the automatic generator implemented in VASP.
  - Ionic relaxations and finite-temperature calculations were performed using the length parameter of 50;



$$F_i = E_i^0(V) - k_B T \ln Z_i(V,T)$$
$$= E_i^0 - k_B T \sum_{j=x,y,z} \ln\left(\frac{\exp(-\hbar\omega_j/2k_BT)}{1-\exp(-\hbar\omega_j/k_BT)}\right)$$

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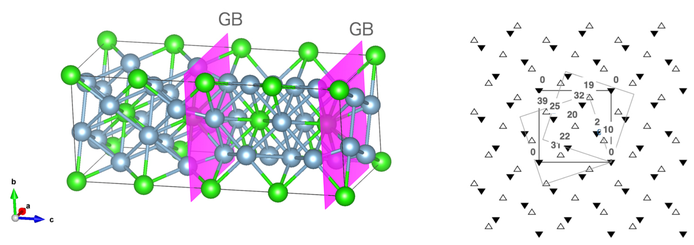
Result-I (boundary model)



perspective and horizontal view of atoms layout existing top and bottom of twist grain boundary plane of fcc lattice<100>

Summary

- We performed finite temperature first principles calculations on Al<100> twist boundary energy with the Einstein approximation.
- The temperature dependency is smaller than that of tilt boundary.
- The boundary energy at 500K is smaller than that of tilt boundary.
- The value at θ=36.87 degs is slightly smaller than that at 22.62 degs.

Result- II (boundary energies)

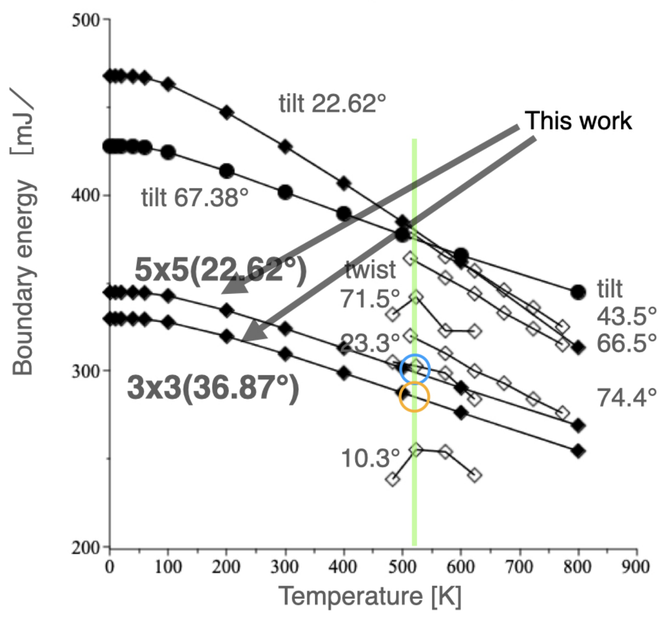
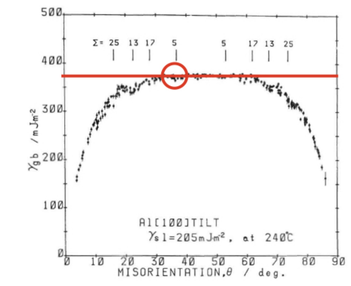


Figure 1 Comparison of Temperature dependency of the boundary energy predicted by the Einstein model and experimental



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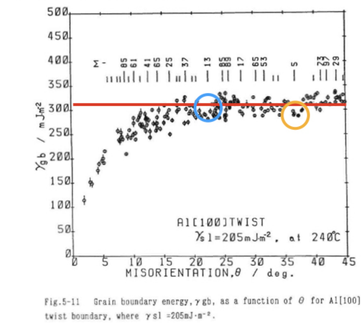

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