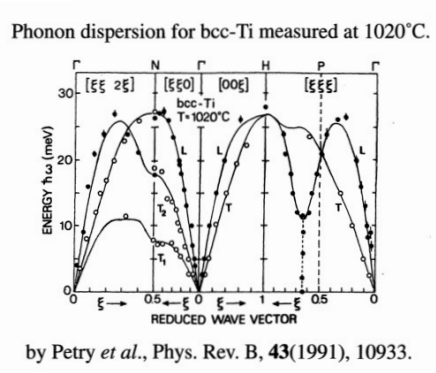
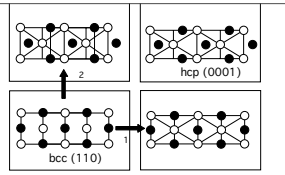
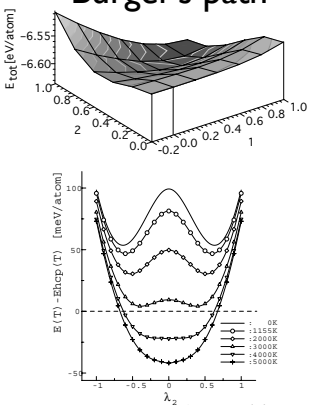
Ti case



adiabatic potentials of Burger's path

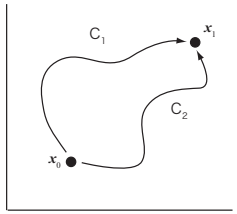


Burger's path



Free energy ...

Good news
state variables...



Bad news
Integrated value

$$F(T_{\mathrm{r}}) = F(T_0) - T_{\mathrm{r}} \int_{T_0}^{T_{\mathrm{r}}} \left(\frac{U}{T^2}\right)_V \mathrm{d}T$$

KWANSEI GAKUIN

Monte Carlo simulation for first principles free energy calculation

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Burger's path

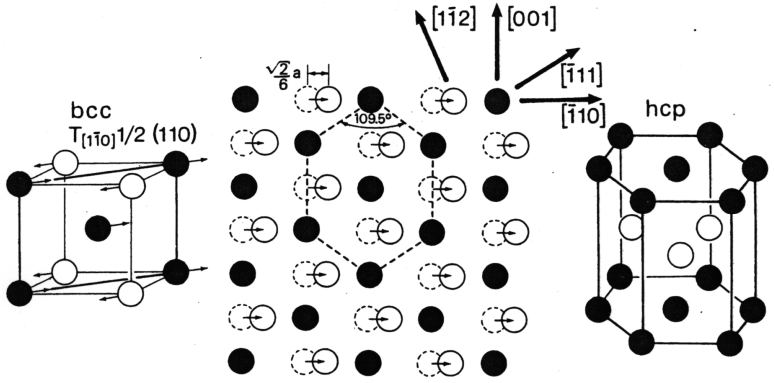
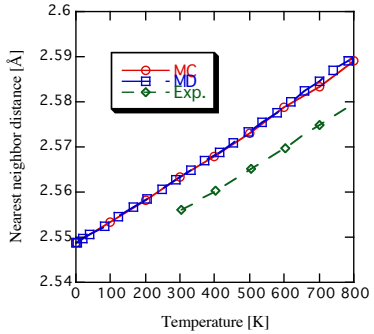
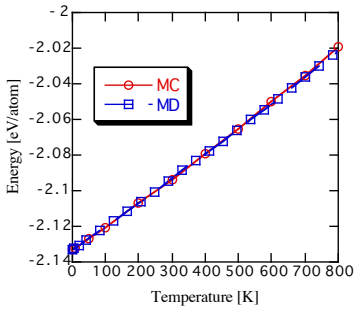


Fig.11 Scheme of the β-to-α transition

3

Results for L-J (I)
NPT-MC
lattice constants





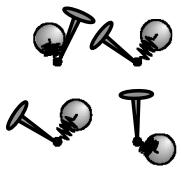
Lattice constants Internal energy U [eV/atom]

freeze specific free degrees

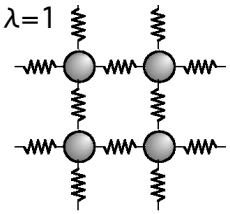
- moment freezing

Frenkel method

U_{virtual} :Einstein lattice
λ=0



U_{total}:VASP, LJ,...
λ=1



$$U(\lambda) = \lambda U_{\text{true}} + (1-\lambda) U_{\text{virtual}}$$

$$F(\lambda = 1) = F(\lambda = 0) + \int_0^1 \left\langle \frac{\partial U(\lambda)}{\partial \lambda} \right\rangle \mathrm{d}\lambda$$

$$\left\langle \frac{\partial U(\lambda)}{\partial \lambda} \right\rangle = \langle U_{\text{true}} - U_{\text{virtual}} \rangle$$

transition state