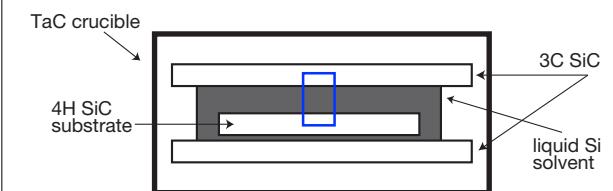
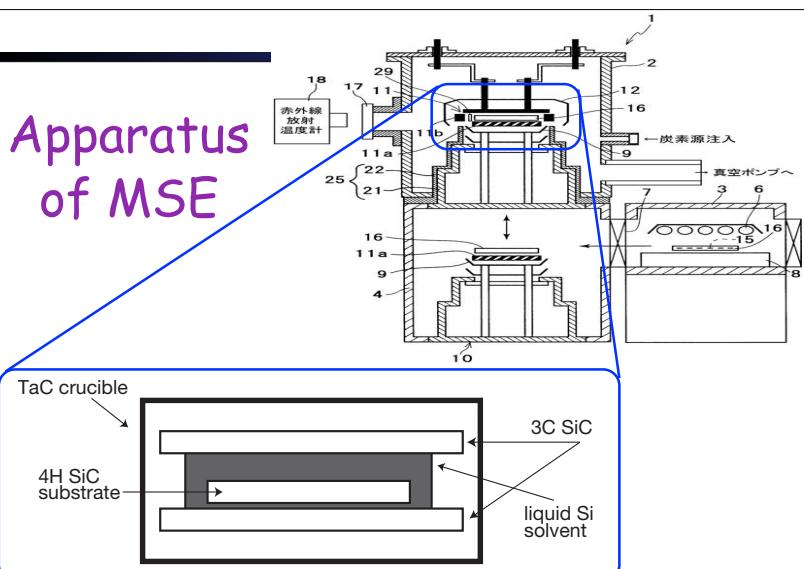


- SiCの液相成長
- 凝固, 準安定平衡, 振動効果の失敗例

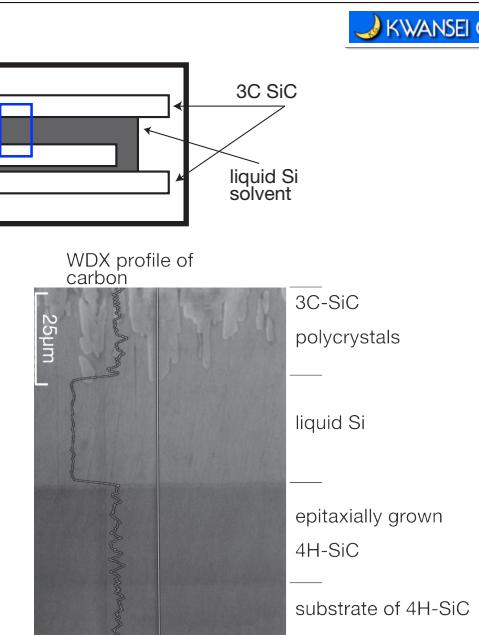
準安定溶媒エピタキシー法 (Metastable Solvent Epitaxy)



Apparatus
of MSE

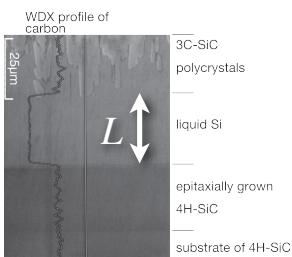
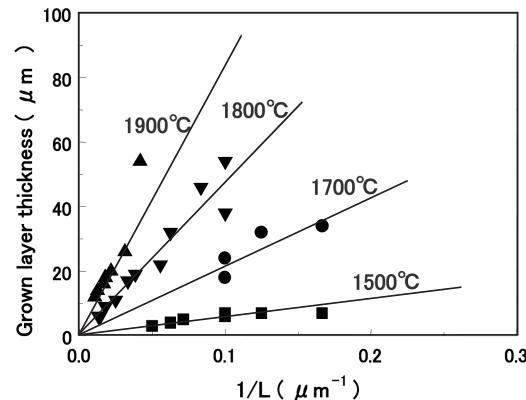


SEM image



Growth rate

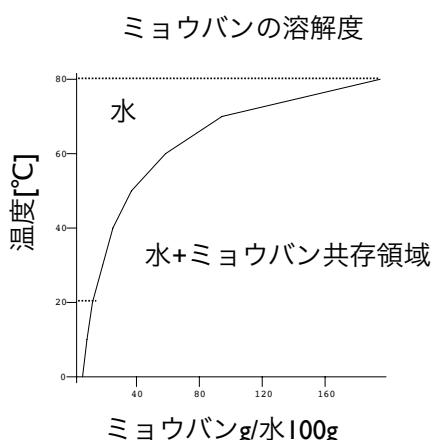
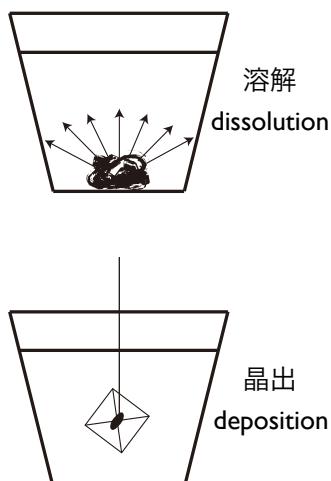
per 1/2 hour



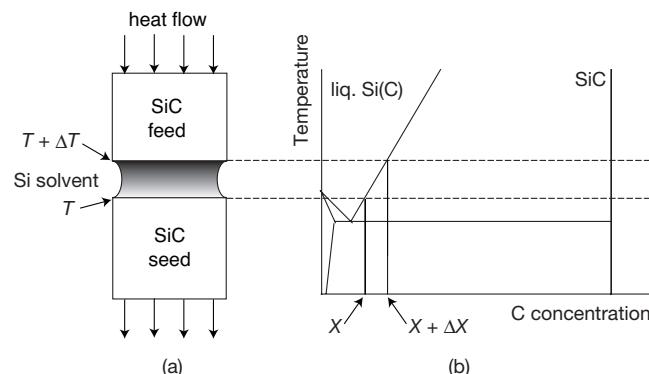
準安定溶媒エピタキシー法 (Metastable Solvent Epitaxy)

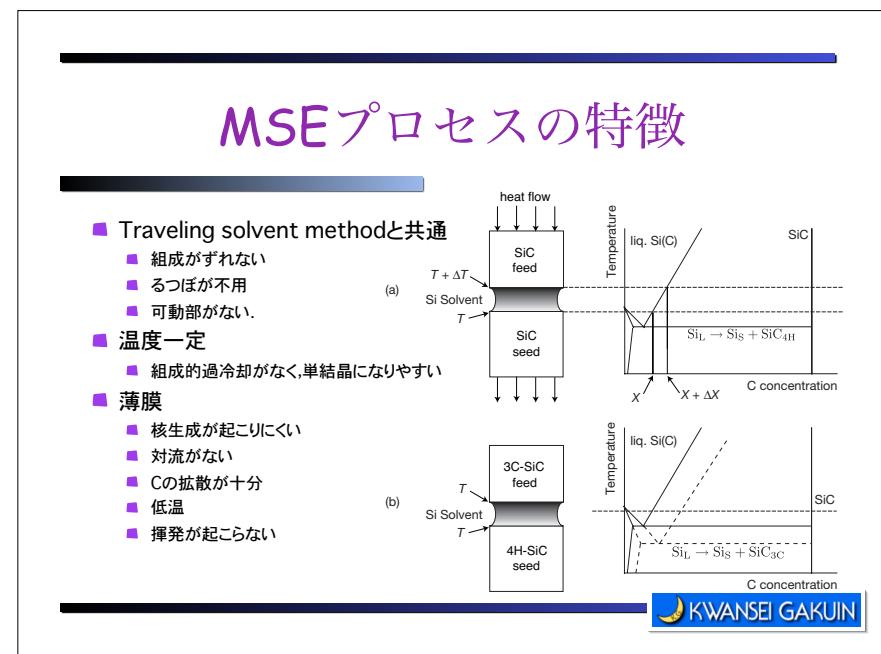
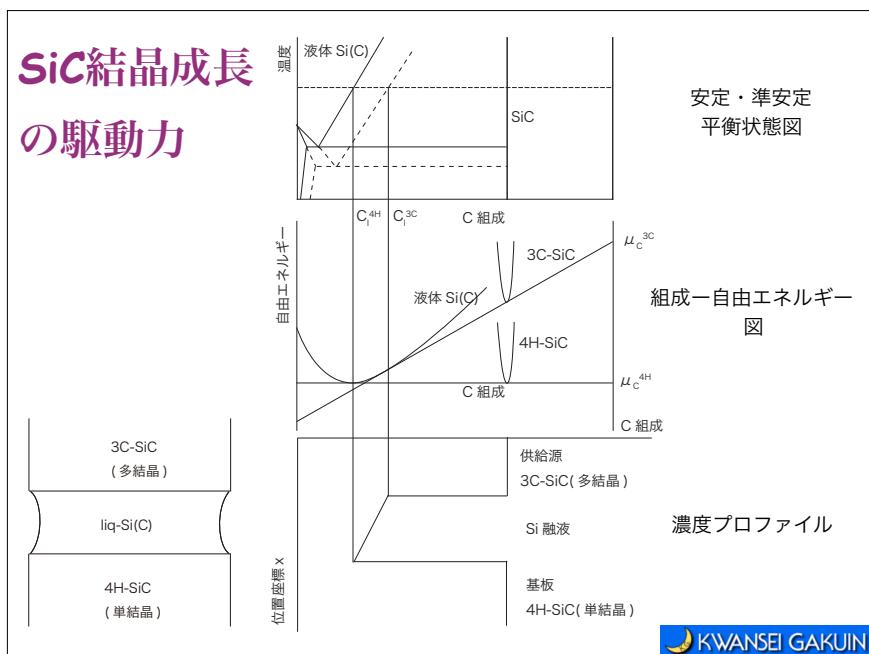
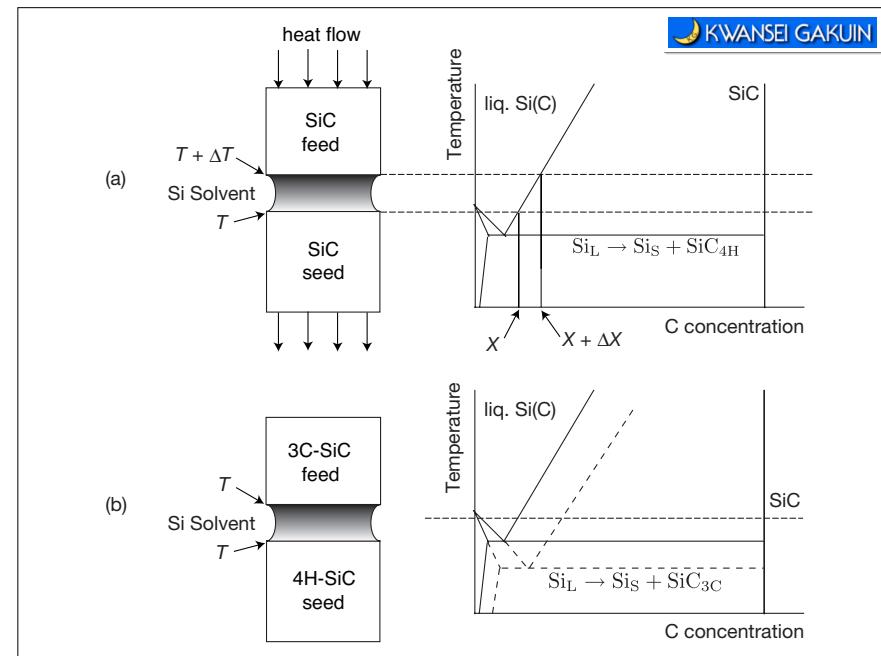
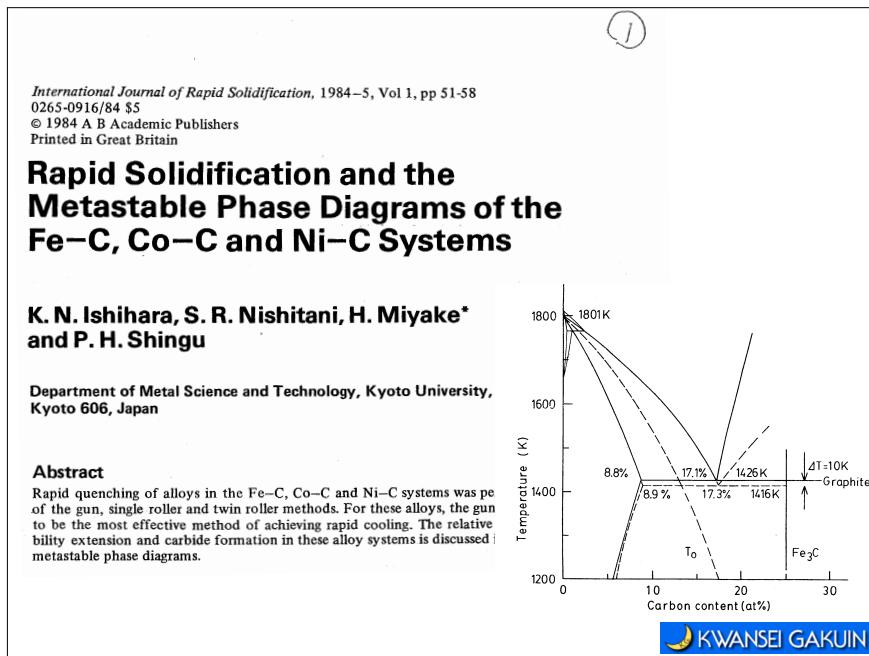
の準安定・安定平衡状態図
(double diagram)
による解釈

ミョウバンの単結晶作成



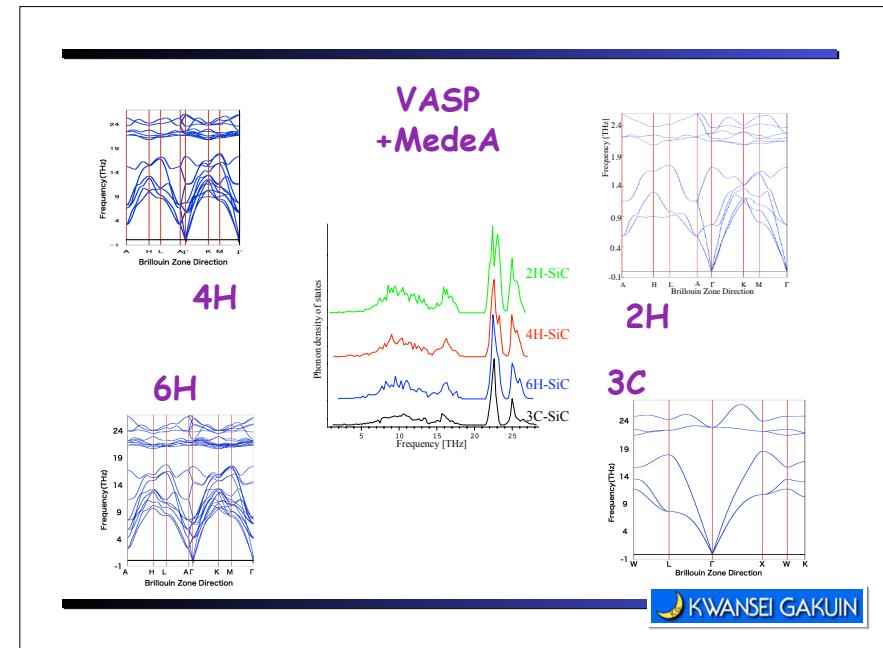
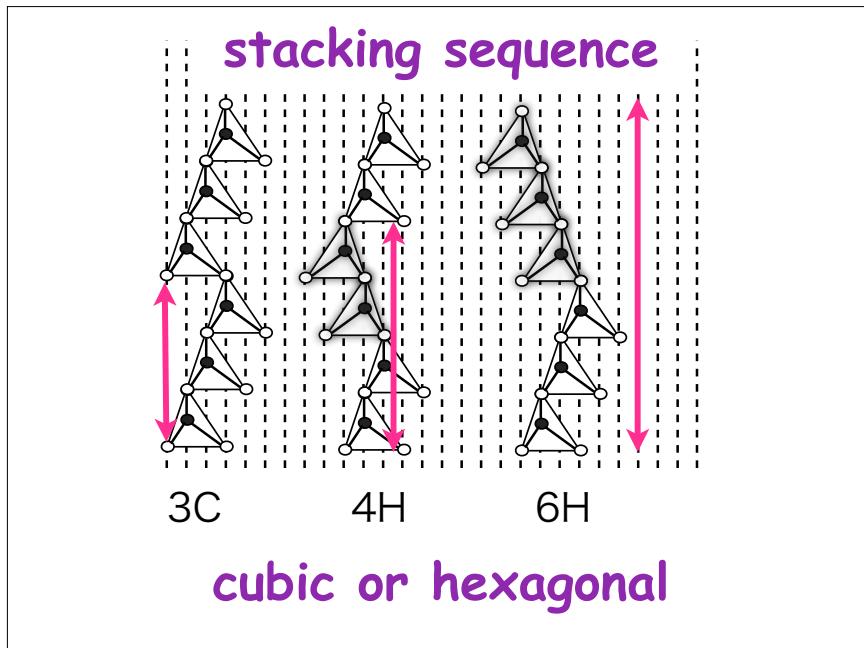
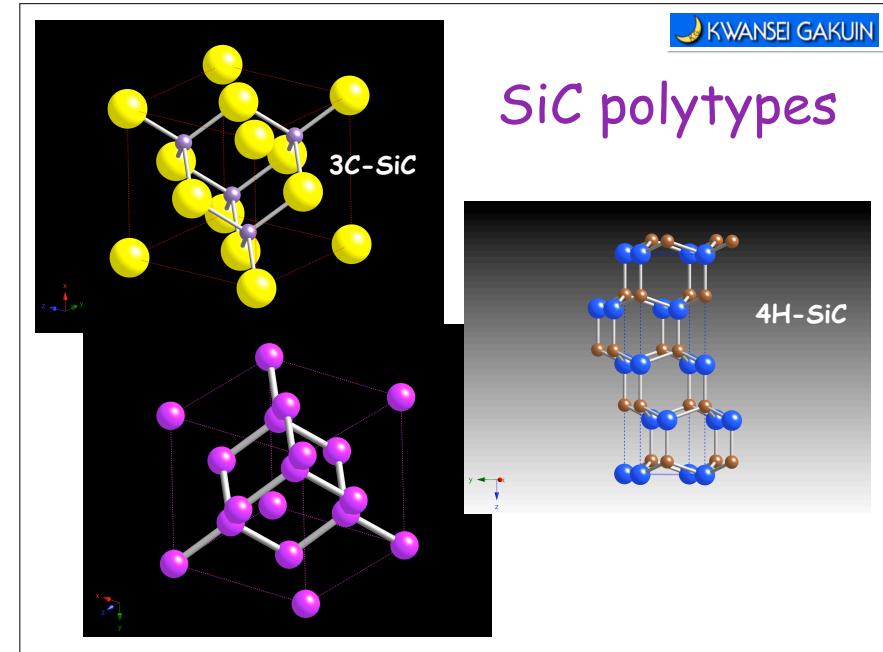
溶媒移動 (Traveling solvent) 法



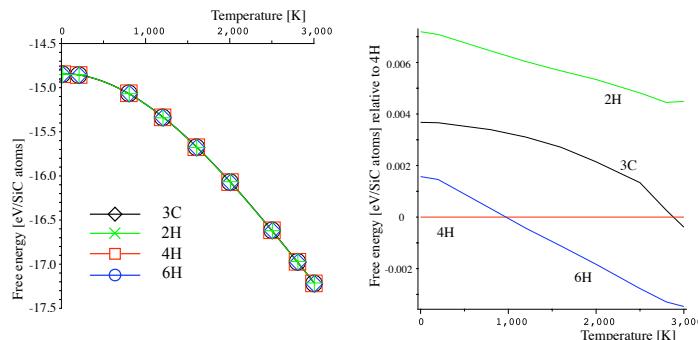


Stability of SiC polytypes

- Vibrational free energies
- phonon DOS
- VASP
- Quasi-harmonic approximation



Free energy with thermal expansion

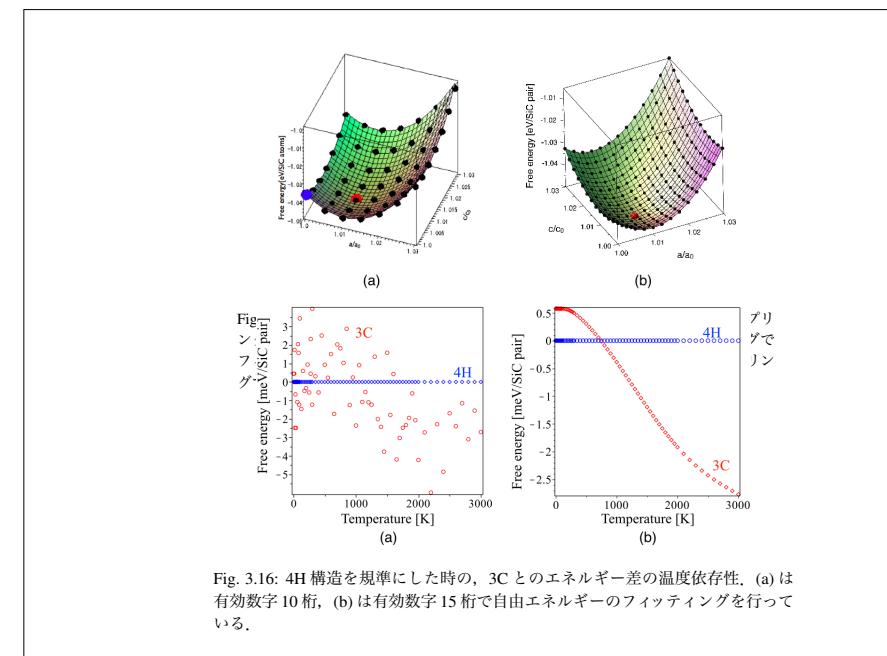
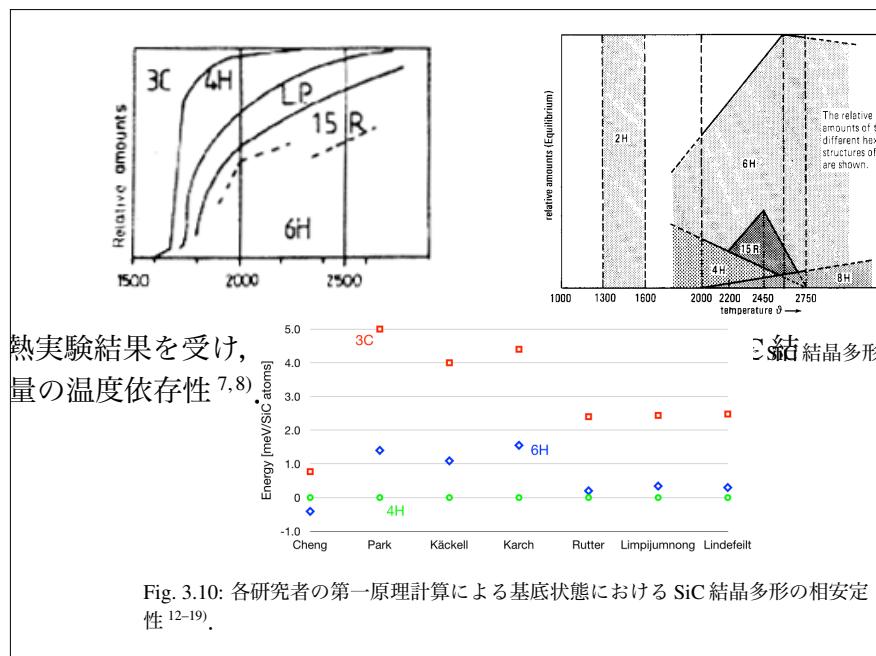


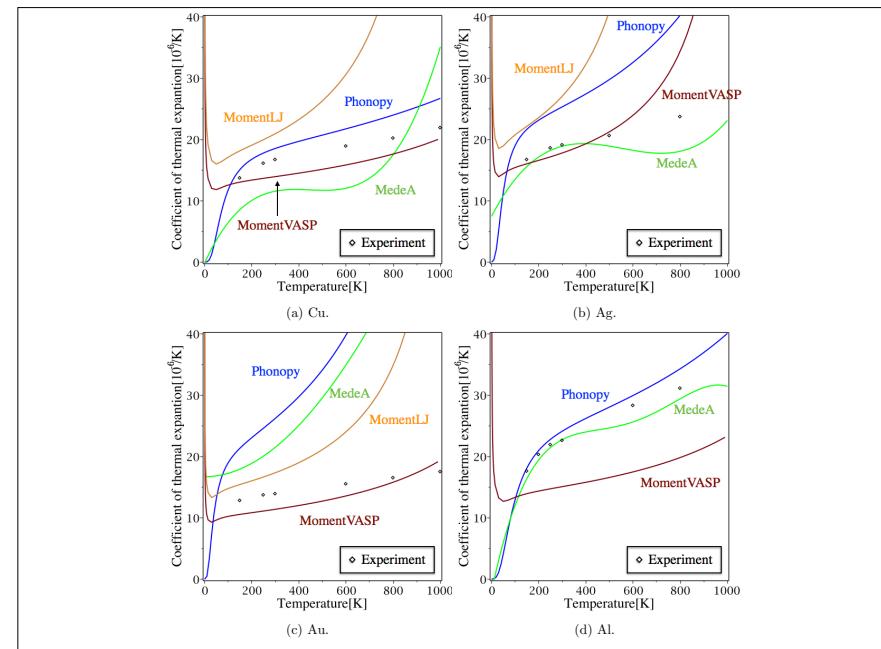
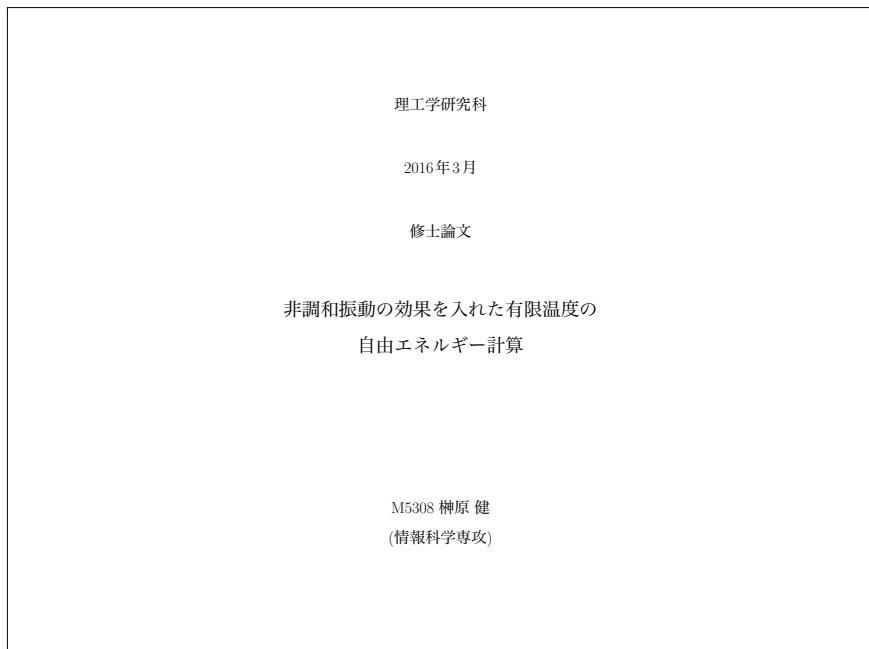
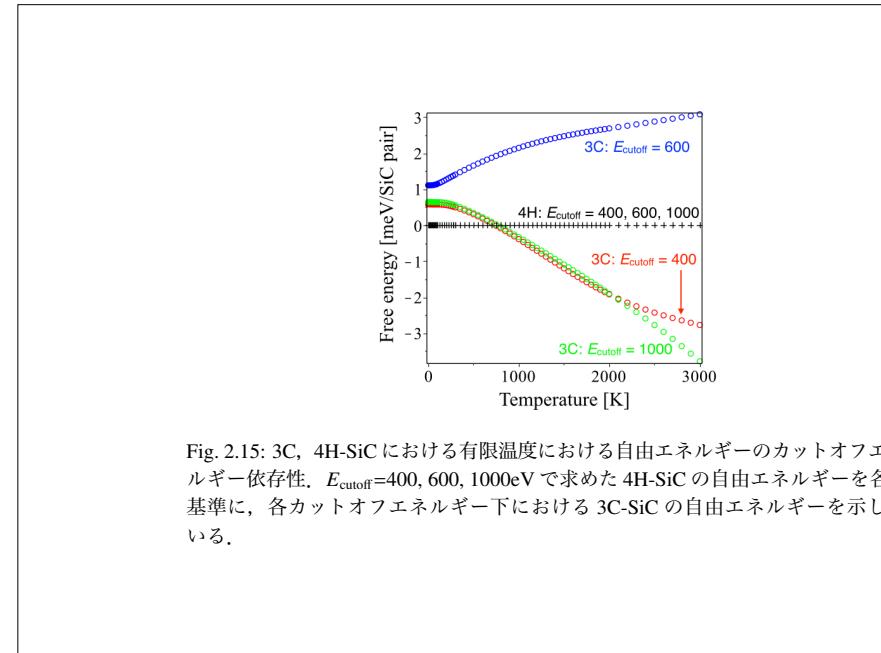
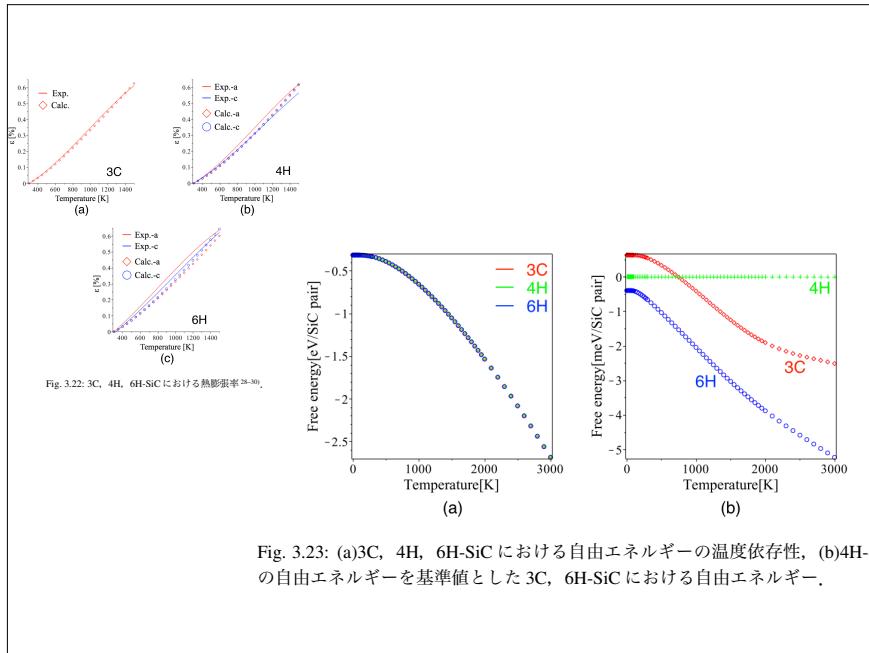
博士論文

固体材料の積層欠陥と溶質原子の第一原理計算

関西学院大学 理工学研究科
情報科学専攻 博士課程後期課程
山本 洋佑

2014年5月
指導教員 西谷 滌人 教授





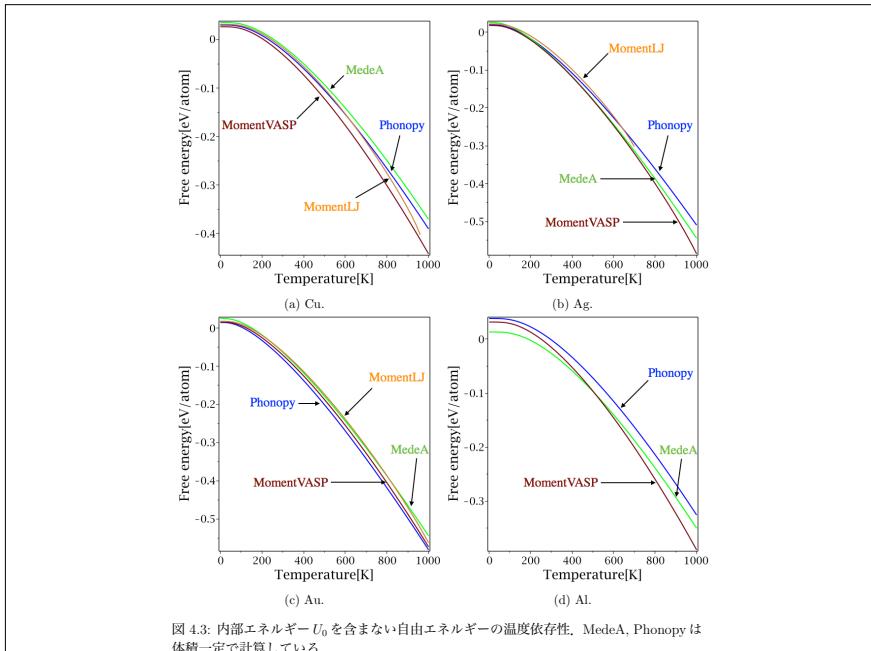


図 4.3: 内部エネルギー U_0 を含まない自由エネルギーの温度依存性。MedeA, Phonopy は体積一定で計算している。