Equilibrium crystal shape of GaAs and InAs by ab-initio thermodynamics

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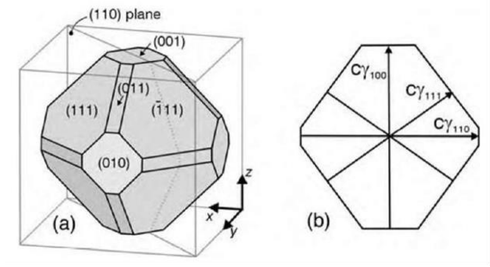
Computational Materials Design

Introduction

Equilibrium Crystal Shape(ECS) calculation



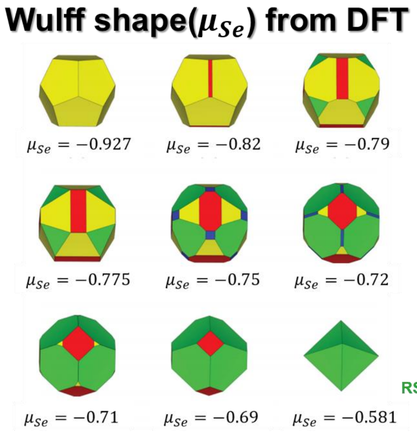
Wulff construction(ECS):
minimization of the total surface free energy for the given thermodynamic conditions

$$\frac{\gamma^{(n)}}{h^{(n)}} = constant,$$

$\gamma^{(n)}$=surface energy of specific orientation
$h^{(n)}$=surface normal

Limitations on the previous ECS calculation

Wulff shape(μ_{Se}) from DFT



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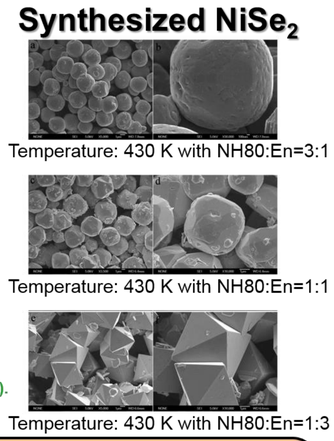
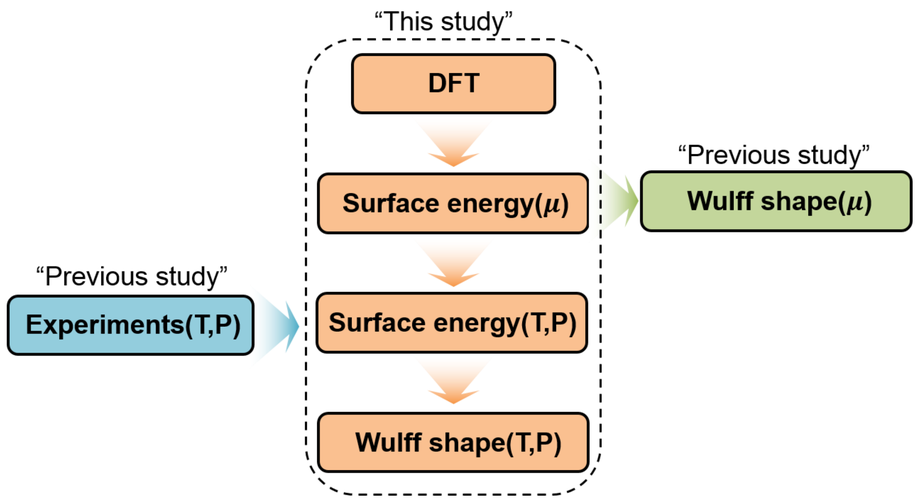
RSC Adv., 4, 13395 (2014).

Synthesized $NiSe_2$



Limitation:
Density Functional Theory(DFT) gives absolute surface energy but the energy(wulff shape) is given as a function of μ → "Gap between thermodynamic variables; μ vs. (T,P)"

Purpose of this study



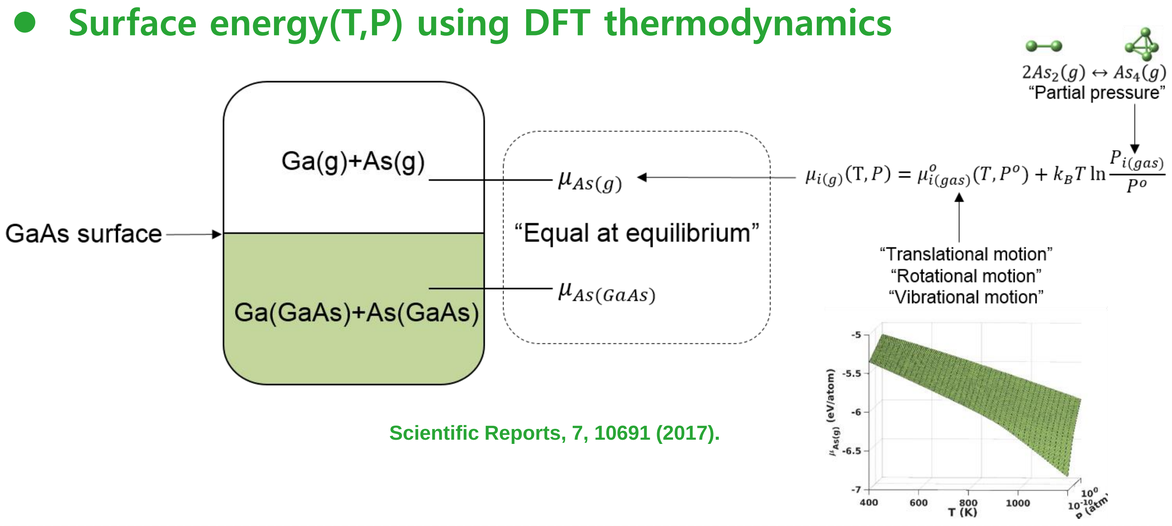
- **Calculation of ECS of GaAs and InAs as a function of (T,P)**
- **Comparison with the experimental growth shapes**

Calculation Methods

DFT conditions

- Vienna ab initio Simulation Package(VASP)
- xc-functional: LDA
- Valence electrons: Ga[$3d^{10}4s^24p^1$], In[$4d^{10}5s^25p^1$], As[$4s^24p^3$]
- Cutoff energy: 500eV
- K-points: 12*12*12 for conventional zinc-blende cell
- Energy(force) convergence: 10^{-6} eV(0.02 eV/Å)
- Surface slab structure with vacuum thickness >10 Å

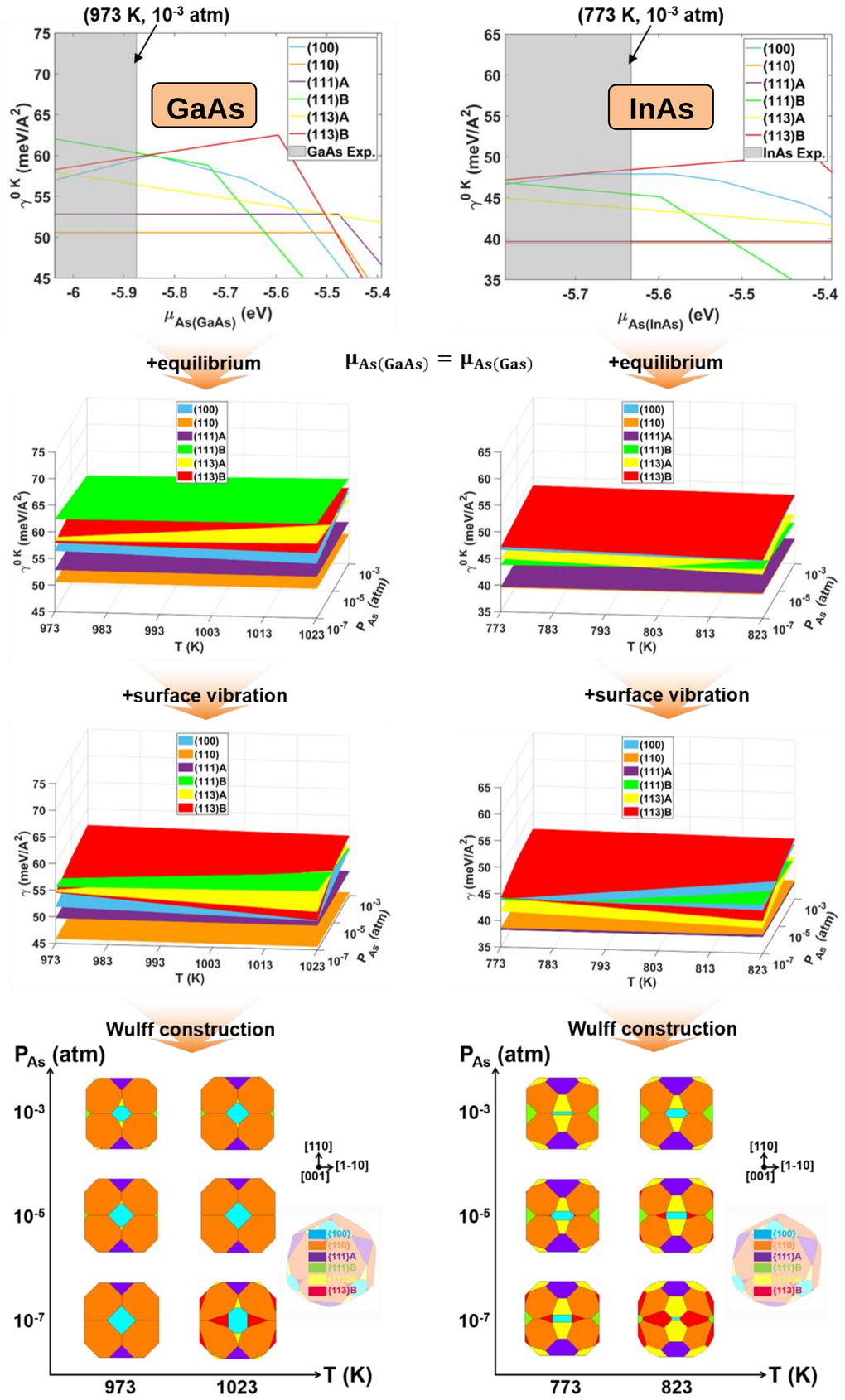
Surface energy(T,P) using DFT thermodynamics



Scientific Reports, 7, 10691 (2017).

Results

Calculation of ECS(T,P) of GaAs and InAs



Comparison with the experimental grown shapes

	Simulation	Experiments
GaAs	{100} {110} {111}A {111}B {113}A {113}B DFT calculation T: 973~1023 K P: ~10^{-5} atm	[1] SA-MOCVD T: 1023 K [TMGa]: 2.7×10^{-6} atm [AsH_3]: 5.0×10^{-4} atm [2] SA-MOCVD TMGa & TBAs or AsH_3 T: 973~1023 K [1] J. Cryst. Growth, 298, 616 (2007). [2] J. Mater. Res. ,26, 2127 (2011).
InAs	{100} {110} {111}A {111}B {113}A {113}B DFT calculation T: 773~823 K P: ~10^{-9} atm	[3] InAs on GaAs(001) by MBE T: 773 K P: 7.9×10^{-9} atm [4] InAs on GaAs(001) T: 773 K P: 7.9×10^{-9} atm [3] Phys. Rev. B 73, 205347 (2006). [4] Appl. Phys. Lett., 82, 3194 (2003).

Summary

- **Calculation of ECS(T,P) of GaAs and InAs including the effects of anisotropic surface vibration.**
- **Comparison with the experimental growth shapes confirms that the experimental growth was in near equilibrium.**

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