Surface morphology of InAs considering entropy effects

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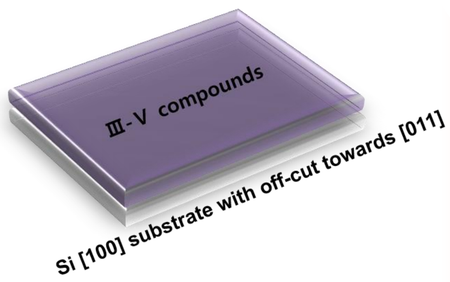
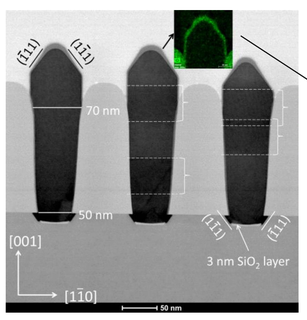
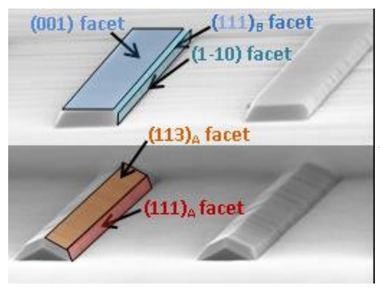
Computational Materials Design

INTRODUCTION

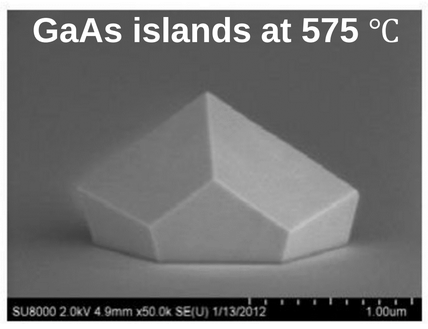
Ⅲ-Ⅴ compounds on Si [100] substrate

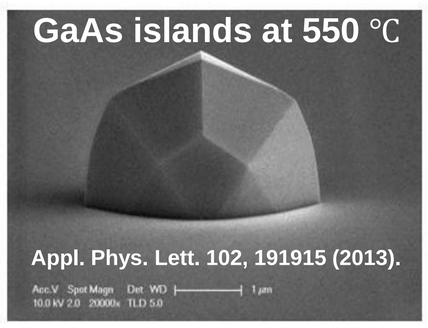






How can we predict the surface structures and morphology?





- Ⅲ-Ⅴ compounds are required to be grown on Si [100] substrate.
- The morphology is composed of some facets with different orientations.
- The surface morphology depends on the environment conditions (T, P).

COPMUTATIONAL DETAILS

Computational details

- VASP (Vienna *ab-initio* Simulation Package)
- xc-functional : LDA-CA
- Cutoff energy : 300 eV
- k-points : G 8×8×8 for the conventional cell of InAs.
- Valence treatment : As=$4s^2 4p^3$, In=$4d^{10} 5s^2 5p^1$
- Vacuum thickness : >10 Å
- The top 5 layers of the total 9 layers were allowed to move.
- The bottom layers were fixed and saturated with hydrogen.

METHODOLOGY

Chemical potential calculation of ideal gas

As_2

$$\mu_{As}(T,P) = \frac{1}{2}E_{As_2}^{total} + \frac{1}{2}E_{As_2}^{ZPE} + \Delta\mu_{As}(T,p^0) + \frac{1}{2}k_B T \ln\frac{p}{p^0}$$

Translation

$$\frac{1}{2}\Delta\mu_{As2}^{trans}(T,p^0) = -\frac{1}{2}k_B T \ln\left[\left(\frac{2\pi m}{h^2}\right)^{\frac{3}{2}}\frac{(k_B T)^{\frac{5}{2}}}{p^0}\right]$$

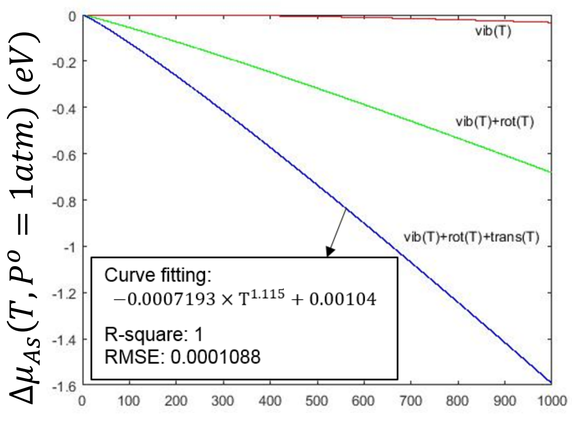
Rotation

$$\frac{1}{2}\Delta\mu_{As2}^{rot}(T,p^0) = -\frac{1}{2}k_B T \ln\left(\frac{2Ik_B T}{\sigma^{sym}\hbar^2}\right)$$

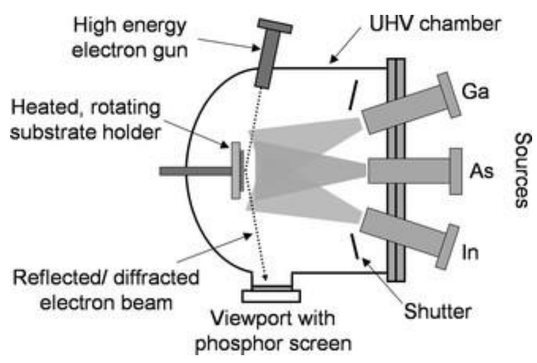
12.9758 THz

Vibration(3N-5=1 mode)

$$\frac{1}{2}\Delta\mu_{As2}^{vib}(T,p^0) = \frac{1}{2}k_B T \ln\left[1-\exp\left(-\frac{\hbar w_0}{k_B T}\right)\right]$$

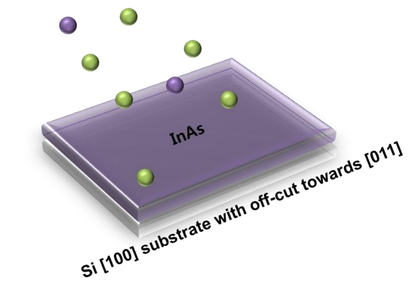


Arsenic as reservoir in Molecular Beam Epitaxy chamber

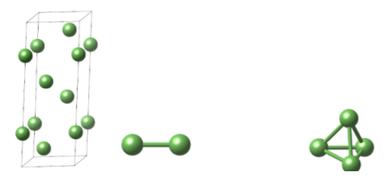


High Vacuum

In: from 1×10^{-10} to 2×10^{-10} atm
As: from 3×10^{-8} to 3×10^{-9} atm

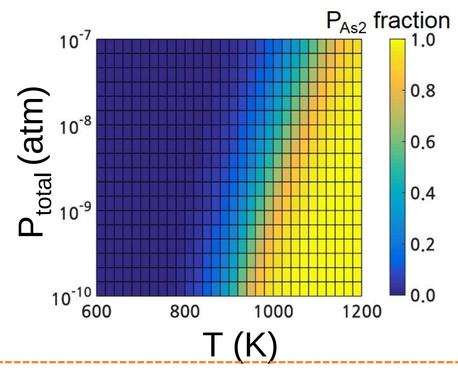


As(bulk) as reservoir in equilibrium with InAs surface, $\mu_{As(bulk)}=\mu_{As(InAs)}$



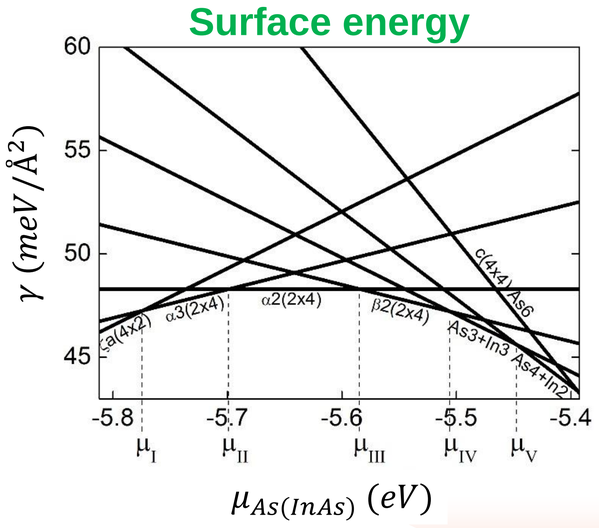
As(s) $2As_2(g) \leftrightarrow As_4(g)$

$P_{As2} + P_{As4} = P_{total}$

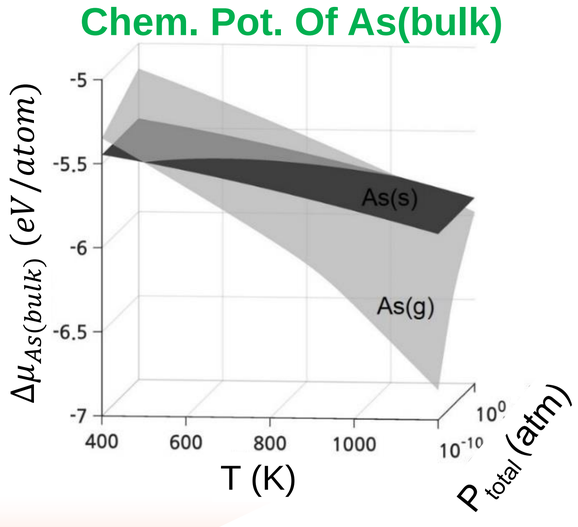


Results & discussions

Surface energy

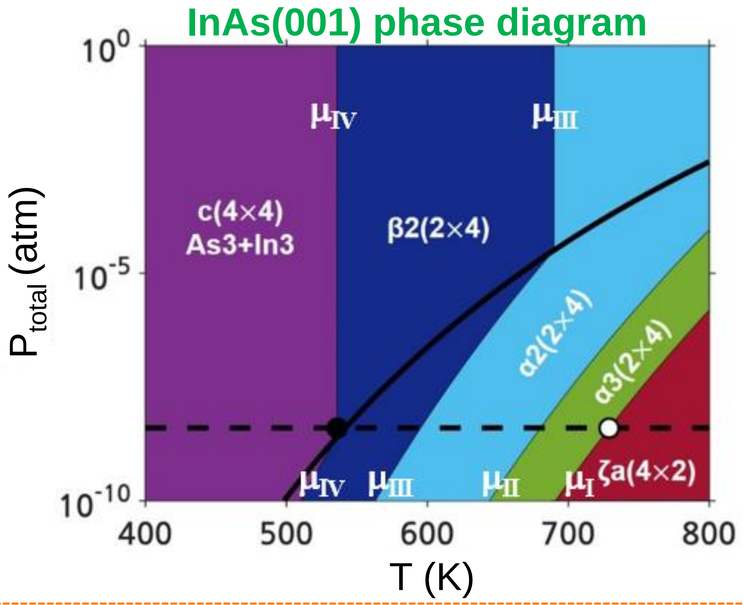


Chem. Pot. Of As(bulk)



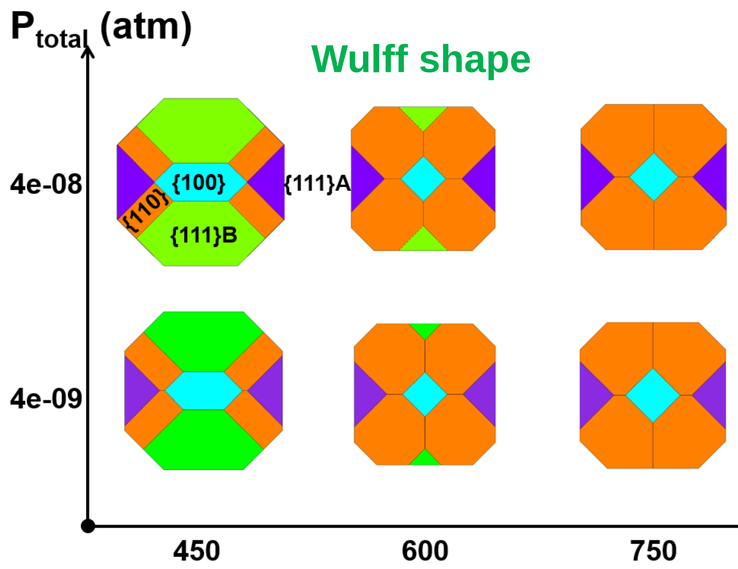
Equilibrium condition,
$\mu_{As(bulk)}=\mu_{As(InAs)}$

InAs(001) phase diagram



Consider Configuration entropy

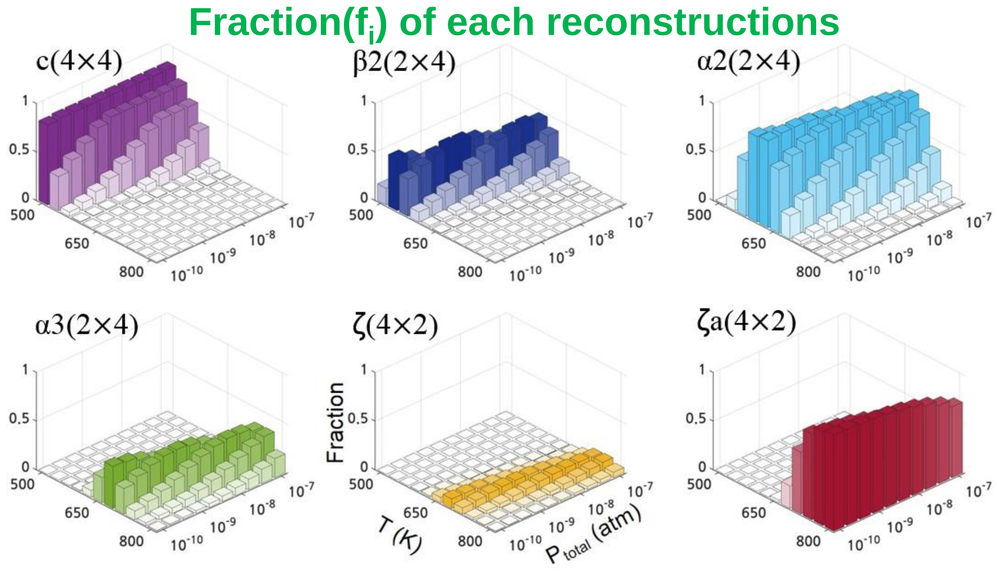
Wulff shape



$\gamma_{(100)} = \sum_i \gamma_i \times f_i$ where i∈(100) reconstructions

$\gamma_{(110)}, \gamma_{(111)A}, \gamma_{(111)B} = \cdots$

Fraction(f_i) of each reconstructions



Summary

Calculations of γ, μ, and S_{conf} enable to predict the surface structures & morphology as a function of (T,P).

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