Growth mechanism of III-V nanowires depending on the temperature and pressure: ab-initio thermodynamic study

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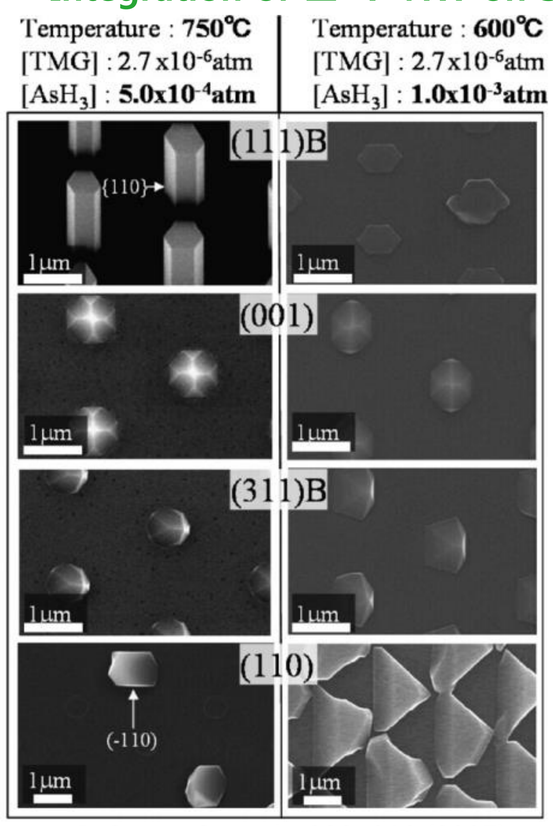
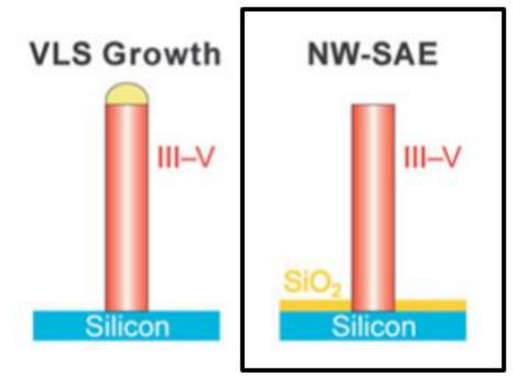
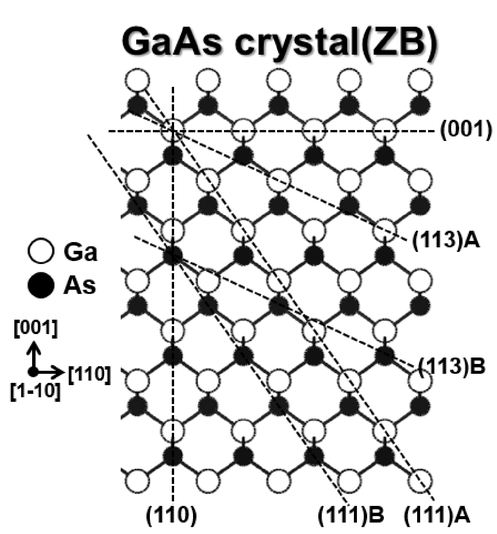
Introduction

Integration of Ⅲ-Ⅴ NW on Si



J. Cryst. Growth, 298, 616 (2007)





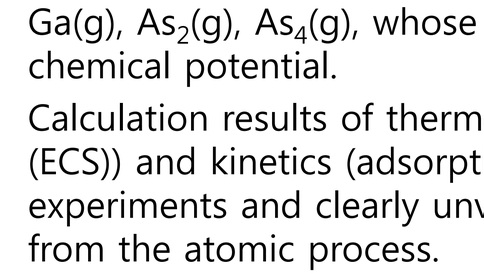
- Growth of GaAs depends on substrate orientation, growth temperature, and pressure.
- There are few theoretical studies about growth direction and condition dependence of the growth.
- Surface energies of various reconstructions were calculated as a function of (T, P) for several low-index orientations.
- The most stable reconstructions at common growth condition were considered as adsorbent to the incoming adsorbates: Ga(g), As_2(g), As_4(g), whose effects on surface are described by chemical potential.
- Calculation results of thermodynamics (Equilibrium Crystal Shape, (ECS)) and kinetics (adsorption and nucleation) agree well with experiments and clearly unveil the growth mechanism of GaAs from the atomic process.

Calculation Methods

Density functional Theory (DFT) calculations

- 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: 500 eV
- 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

Equilibrium Crystal Shape (ECS)

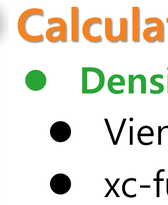


Wulff construction(ECS):
minimization of the total surface free energy for the given thermodynamic conditions

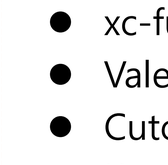
$$\frac{\gamma^{(n)}}{h^{(n)}} = constant,$$

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

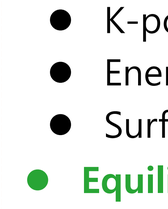
Chemical potential (T,P) of gas phase using DFT



$$F_{trans} = -k_B T \ln\left[\left(\frac{2\pi m}{h^2}\right)^{\frac{3}{2}} \frac{(k_B T)^{\frac{5}{2}}}{p}\right]$$

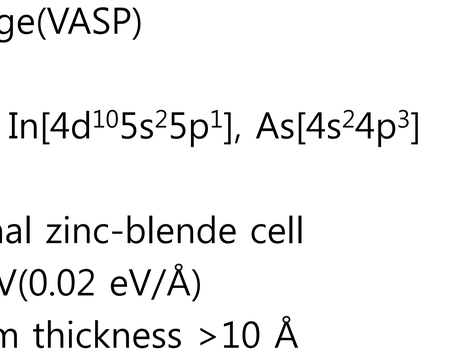


$$F_{rot} = -k_B T \ln\left(\frac{\pi^{1/2}}{\sigma}\sqrt{\frac{2I_A k_B T}{\hbar^2}}\sqrt{\frac{2I_B k_B T}{\hbar^2}}\sqrt{\frac{2I_C k_B T}{\hbar^2}}\right)$$



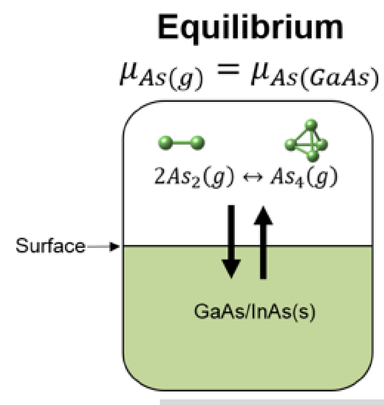
$$F_{vib} = \sum_{i=1}^{M}\frac{\hbar w_i}{2} + \sum_{i=1}^{M} k_B T \ln\left(1 - e^{-\frac{\hbar w_i}{k_B T}}\right)$$

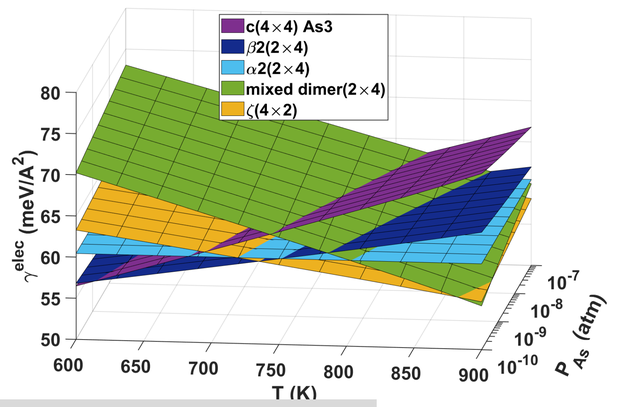
$$\mu_{i(g)}(T,P) = \mu^o_{i(gas)}(T,P^o) + k_B T \ln\frac{P_{i(gas)}}{P^o}$$



Results 1: surface energy of GaAs

Surface energy (T,P) of various (100) reconstructions

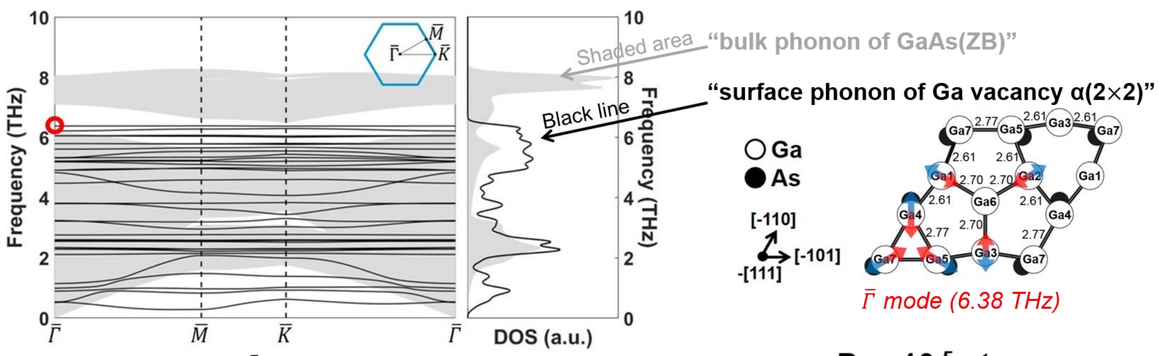


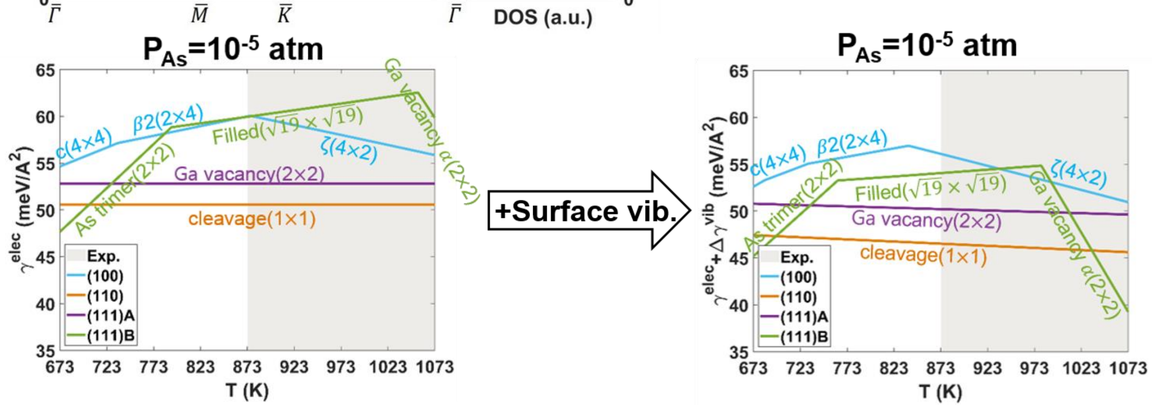


I. W. Yeu et al., Scientific Reports, 7, 10691 (2017)

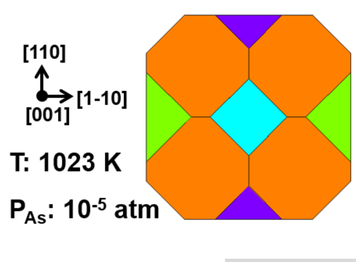
Results 2: equilibrium crystal shape of GaAs

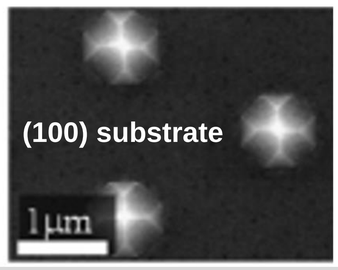
ECS with surface vibration and new (111)B reconstruction





ECS & SEM





SA-MOVPE

T: 1023 K

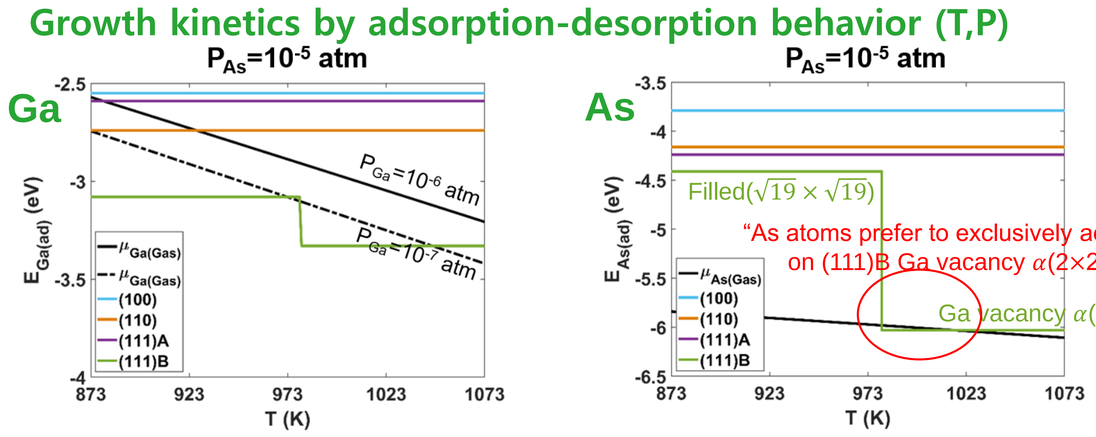
[TMGa]: 2.7×10^{-6} atm

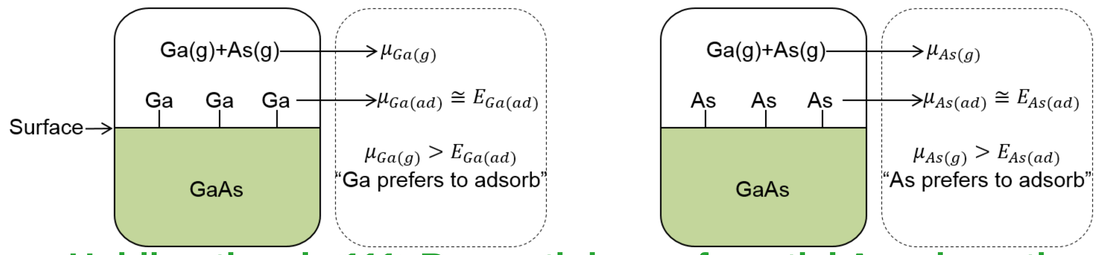
[AsH_3]: 5.0×10^{-4} atm

I. W. Yeu et al., Scientific Reports, 9, 1127 (2019)

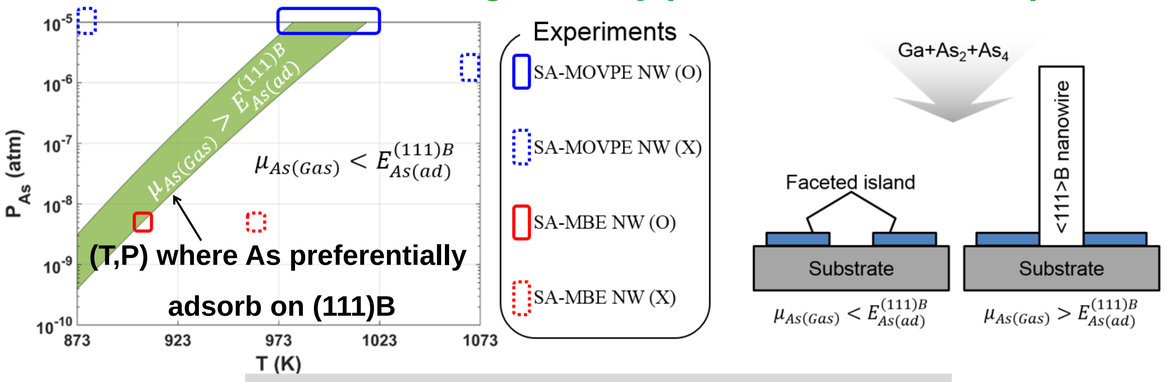
Results 3: growth of nanowire of GaAs

Growth kinetics by adsorption-desorption behavior (T,P)





Unidirectional <111>B growth by preferential As adsorption



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