Theoretical understanding on the growth and stacking-fault mechanism of GaAs nanowires grown by catalyst-free method

In Won Yeu[1,2], Gyuseung Han[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[1*]

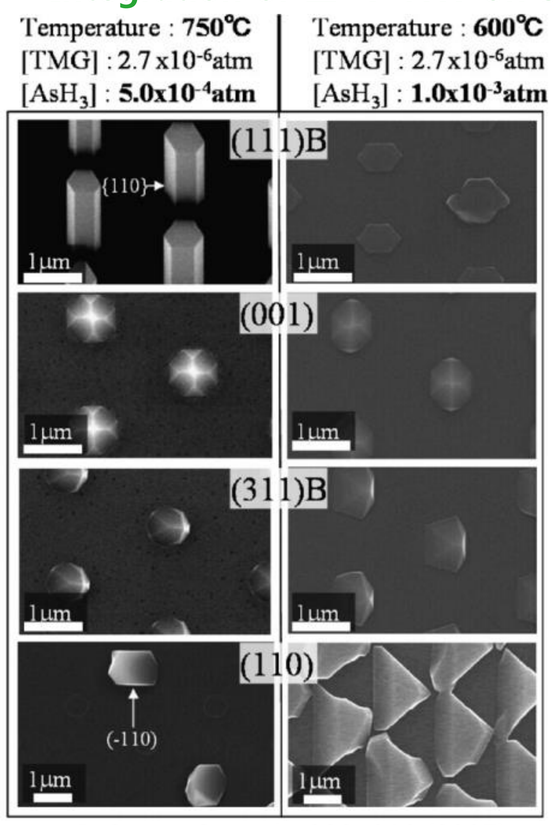
[1]Center for Electronic Materials, Korea Institute of Science and Technology, Seoul 02792, Korea

[2]Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea

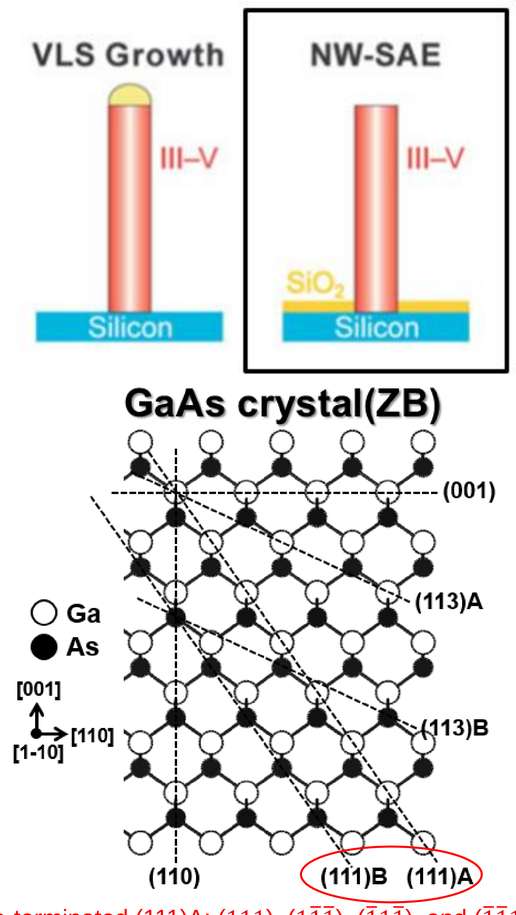
Computational Materials Design

Introduction

Integration of Ⅲ-Ⅴ NW on Si



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



Ga-terminated (111)A: (111), $(1\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, and $(\bar{1}\bar{1}1)$

As-terminated (111)B: $(\bar{1}\bar{1}\bar{1})$, $(\bar{1}11)$, $(1\bar{1}1)$, and $(11\bar{1})$

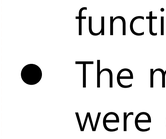
- Growth of GaAs depends on substrate orientation, growth temperature, and pressure.
- There are few theoretical studies about growth direction and condition dependence of the growth.
- Surface energies of various reconstructions were calculated as a function of (T, P) for several low-index orientations.
- The most stable reconstructions at a given 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

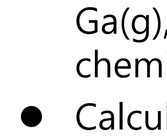
- Vienna ab initio Simulation Package(VASP)
- xc-functional: LDA
- Valence electrons: Ga[$3d^{10}4s^24p^1$], In[$4d^{10}5s^25p^1$], As[$4s^24p^3$]
- Cutoff energy: 500 eV
- K-points: 12*12*12 for conventional zinc-blende cell

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



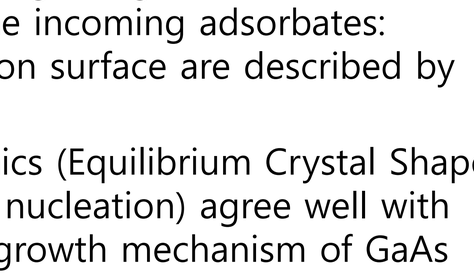
$$F_{trans} = -k_B T \ln\left[\left(\frac{2\pi m}{h^2}\right)^{\frac{3}{2}} \frac{(k_B T)^{\frac{5}{2}}}{p}\right]$$

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



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

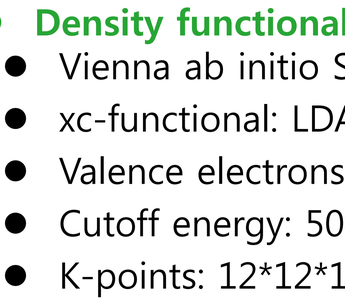
$$F_{vib} = \sum_{i=1}^{M} \frac{\hbar w_i}{2} + \sum_{i=1}^{M} k_B T \ln\left(1 - e^{-\frac{\hbar w_i}{k_B T}}\right)$$

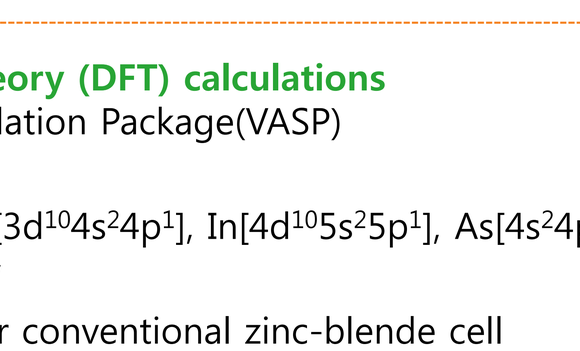


Surface energy (T,P) using ab-initio thermodynamics

Equilibrium

$$\mu_{As(g)} = \mu_{As(GaAs)}$$

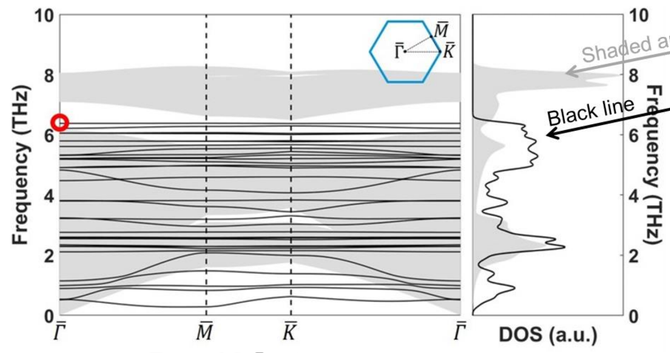


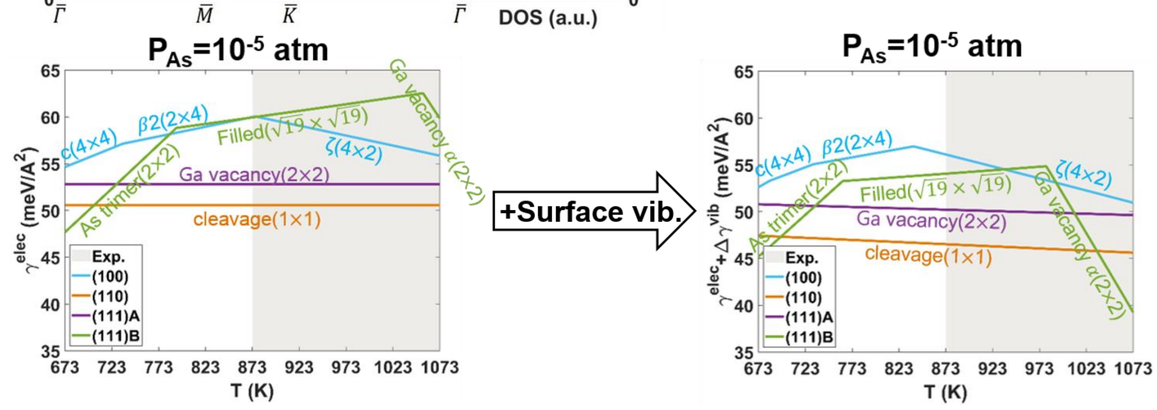


I. W. Yeu et al., Scientific Reports, 7, 10691 (2017)

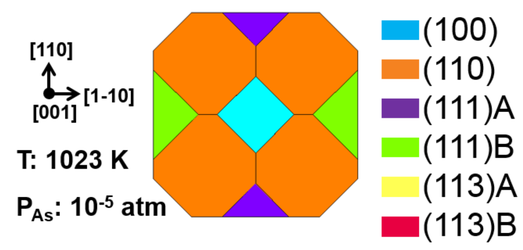
Results 1: equilibrium crystal shape of GaAs

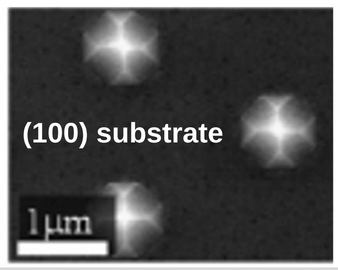
ECS with surface vibration and new (111)B reconstruction





ECS & SEM





SA-MOVPE

T: 1023 K

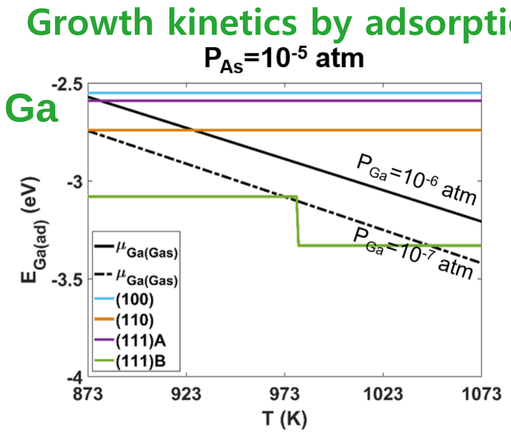
[TMGa]: 2.7×10^{-6} atm

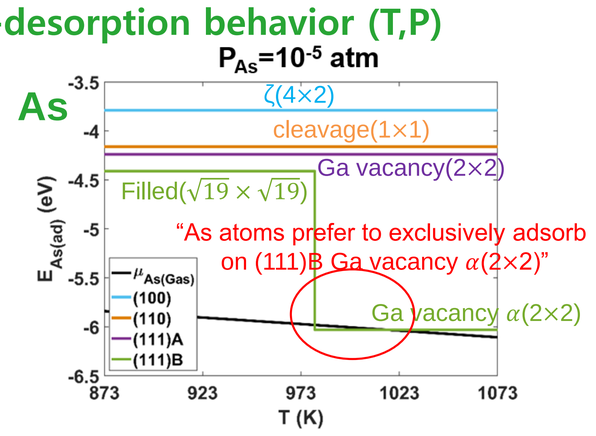
[AsH_3]: 5.0×10^{-4} atm

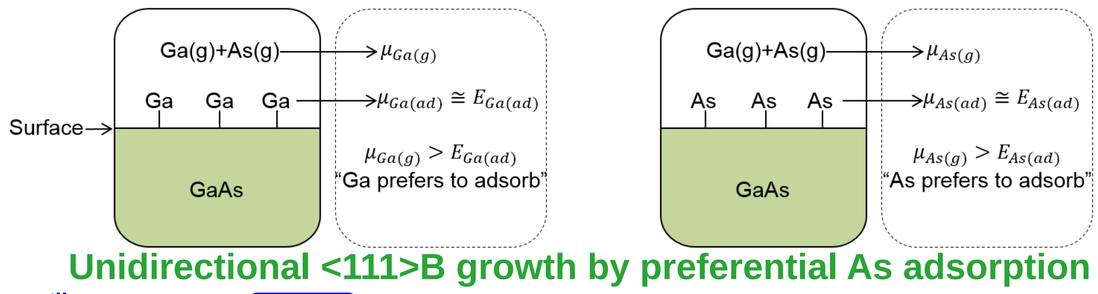
I. W. Yeu et al., Scientific Reports, 9, 1127 (2019)

Results 2: growth of nanowire of GaAs

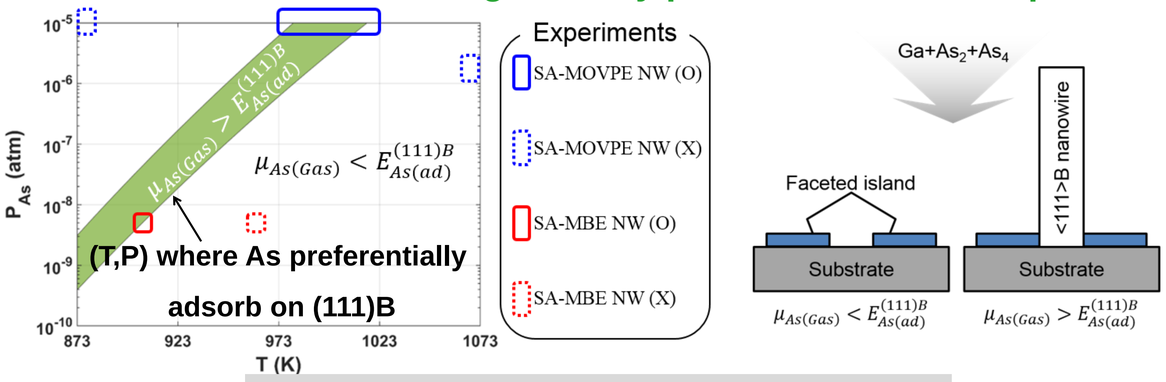
Growth kinetics by adsorption-desorption behavior (T,P)





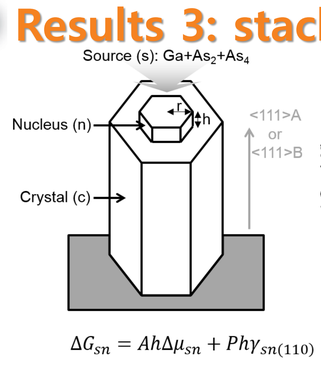


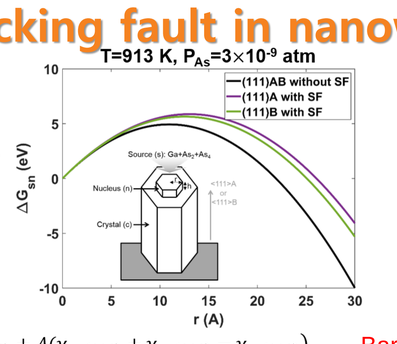
Unidirectional <111>B growth by preferential As adsorption

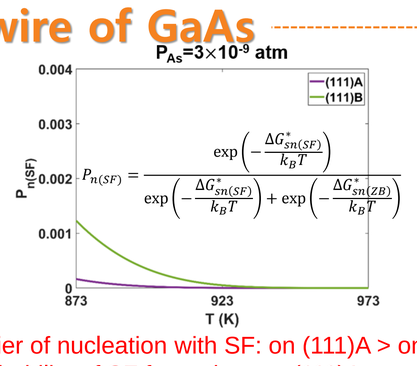


I. W. Yeu et al., Applied Surface Science, Submitted

Results 3: stacking fault in nanowire of GaAs



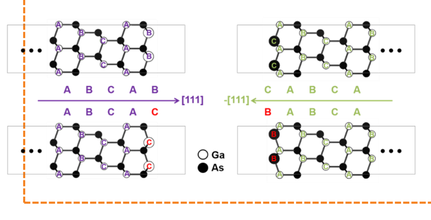


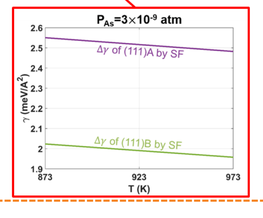


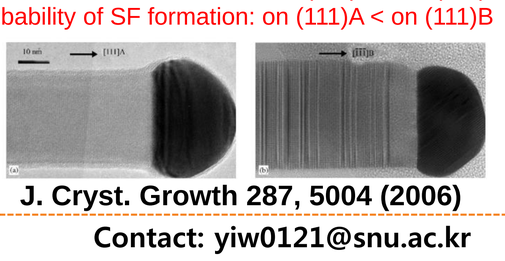
$$\Delta G_{sn} = Ah\Delta\mu_{sn} + Ph\gamma_{sn(110)} + A(\gamma_{cn(111)} + \gamma_{sn(111)} - \gamma_{sc(111)})$$

Barrier of nucleation with SF: on (111)A > on (111)B

Probability of SF formation: on (111)A < on (111)B







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Contact: yiw0121@snu.ac.kr