Atomistic understanding of the asymmetric growth and stacking behavior of GaAs nanowire grown by noncatalytic facet-driven method

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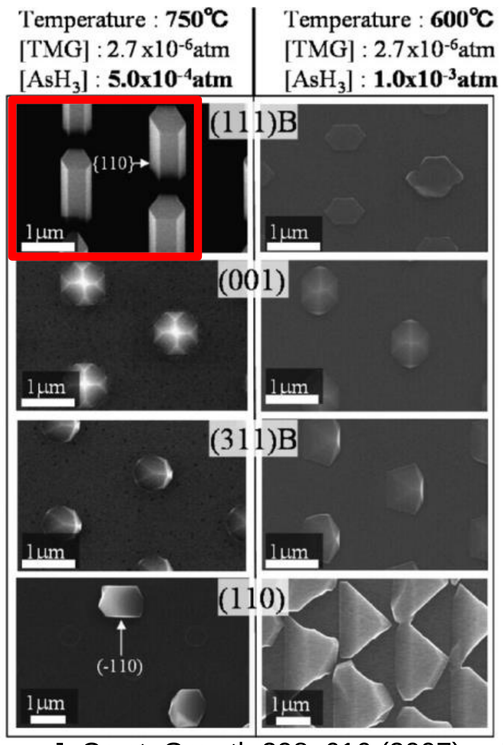
#TP1_069

Computational Materials Design

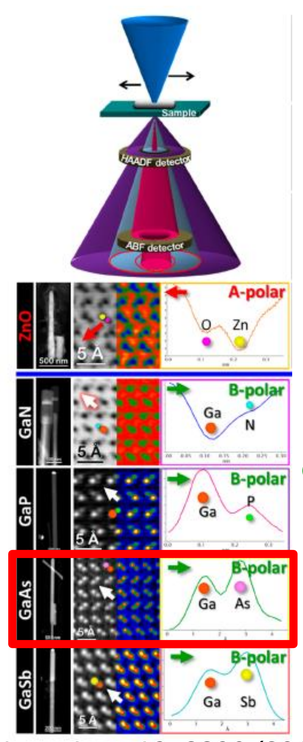
Introduction: GaAs nanowire (NW)

Asymmetric growth

✓ **"Among the various crystal directions, GaAs NW tends to grow along <111>B at narrow (T,P) range"**



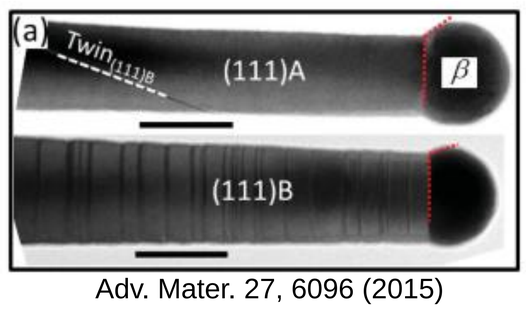
J. Cryst. Growth 298, 616 (2007)



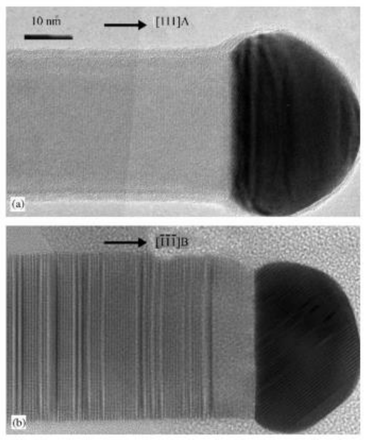
Nano. Lett. 19, 3396 (2019)

Asymmetric stacking

✓ **"Between the two opposite directions of <111>, density of planar defects is much higher in GaAs NW grown along <111>B (BNW) than <111>A (ANW)"**



Adv. Mater. 27, 6096 (2015)



J. Cryst. Growth. 287, 5004 (2006)

Purpose: Atomic simulation of NW growth

✓ Despite the tremendous developments in vapor-phase growth techniques, mechanism has not been understood and theoretical attempts remains at the heuristic level.

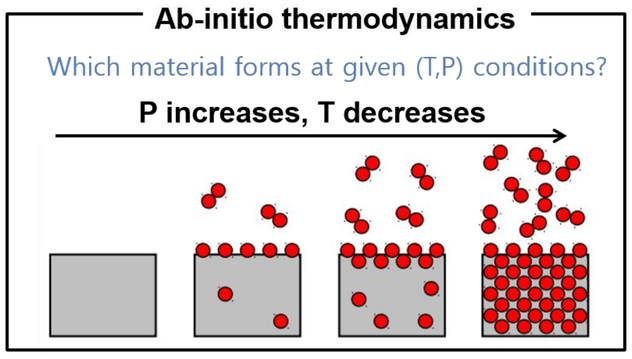
✓ In this presentation**, atomistic approach is suggested for thorough understanding of the T-P dependent asymmetric growth and stacking behavior considering enormous change in entropy between vapor-surface-solid**.

Calculation methods

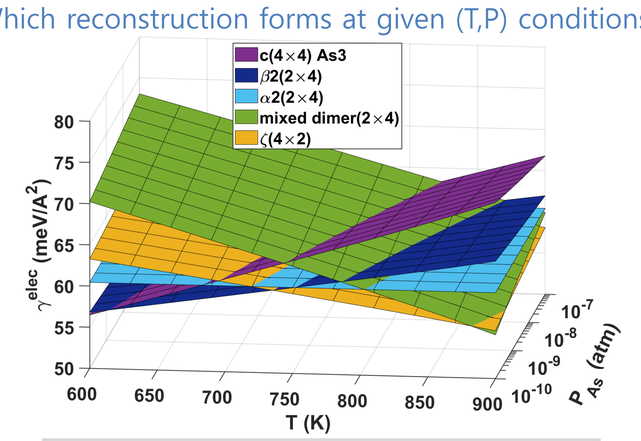
Surface energy (T,P)

Ab-initio thermodynamics

Which material forms at given (T,P) conditions?



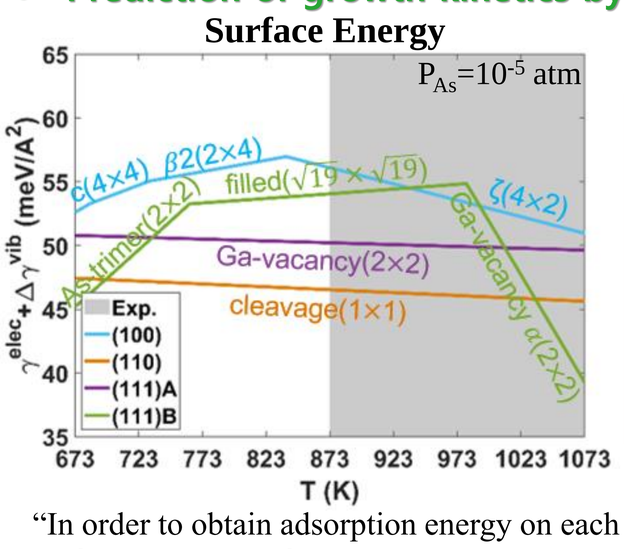
Which reconstruction forms at given (T,P) conditions?



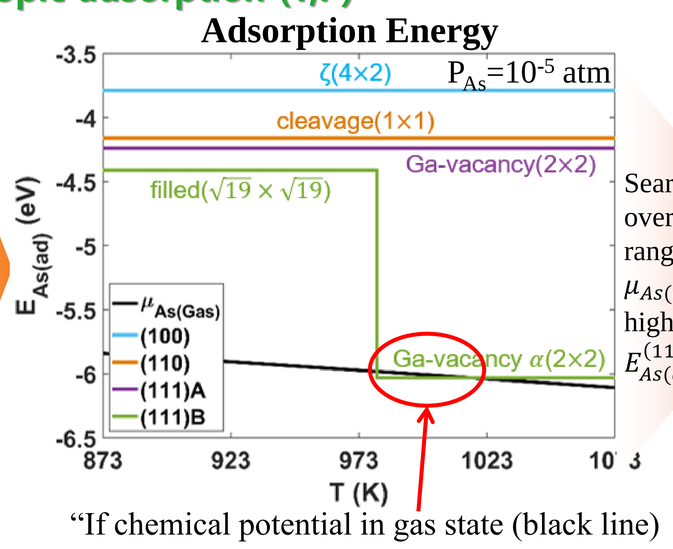
***I. W. Yeu et al.*, Sci. Rep. 7, 10691 (2017); Sci. Rep. 9, 1127 (2019)**

Results 1: Asymmetric growth of GaAs NW

Prediction of growth kinetics by anisotropic adsorption (T,P)



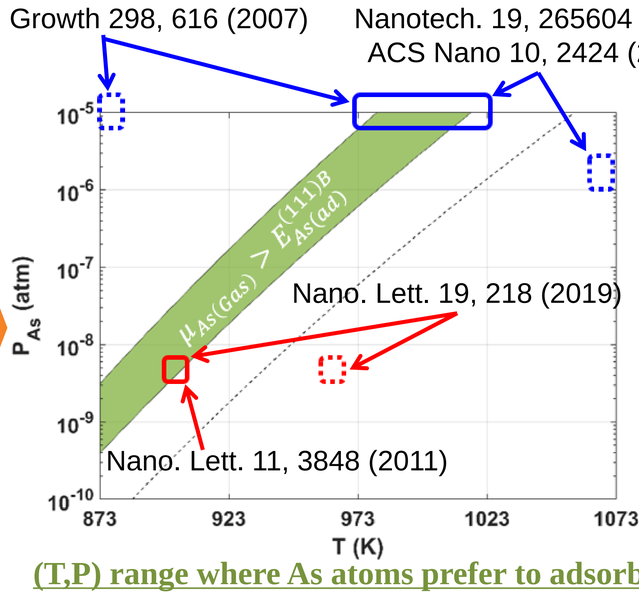
"In order to obtain adsorption energy on each surface, variation of reconstruction was identified by calculation of surface energy (T,P)"



"If chemical potential in gas state (black line) is higher than that in adsorbed state (colored lines), adsorption might be preferred"

Search the overall (T,P) range where $\mu_{As(Gas)}$ is higher than $E_{As(ad)}^{(111)B}$

J. Cryst. Growth 298, 616 (2007) Nanotech. 19, 265604 (2008) ACS Nano 10, 2424 (2016)



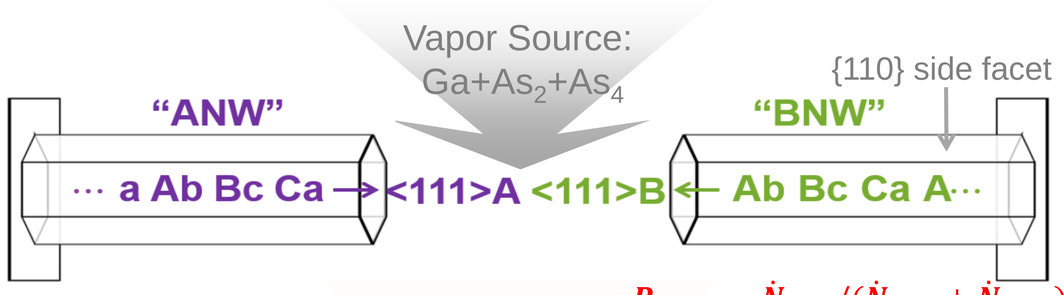
(T,P) range where As atoms prefer to adsorb exclusively on (111)B: "Preferential adsorption → nucleation → BNW growth"

***I. W. Yeu et al.*, Appl. Surf. Sci. 497, 143740 (2019)**

Results 2: Asymmetric stacking of GaAs NW

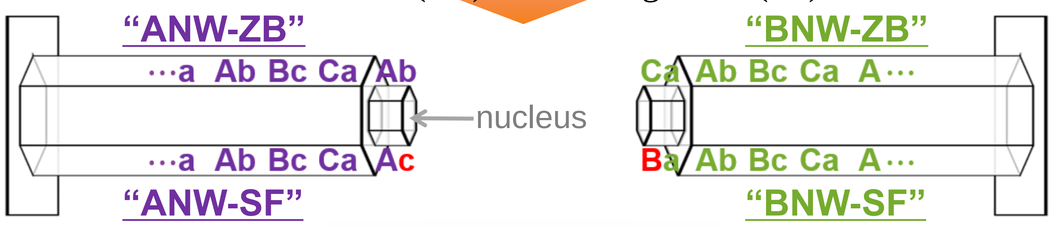
Prediction of stacking kinetics by asymmetric nucleation (T,P)

NW growth proceeds through layer-by-layer initiated by a nucleus:
"Stacking sequence on each layer is determined during nucleation"



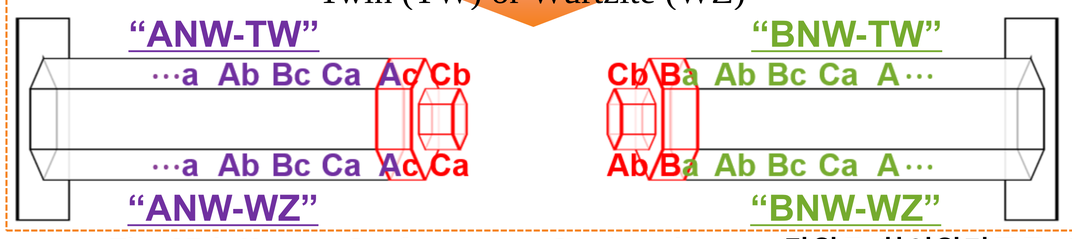
Nucleation I: $P_{n(SF)} = \dot{N}_{(SF)}/(\dot{N}_{(SF)} + \dot{N}_{(ZB)})$, $\dot{N}_{(i)}$: *nucleation rate with i − stacking*

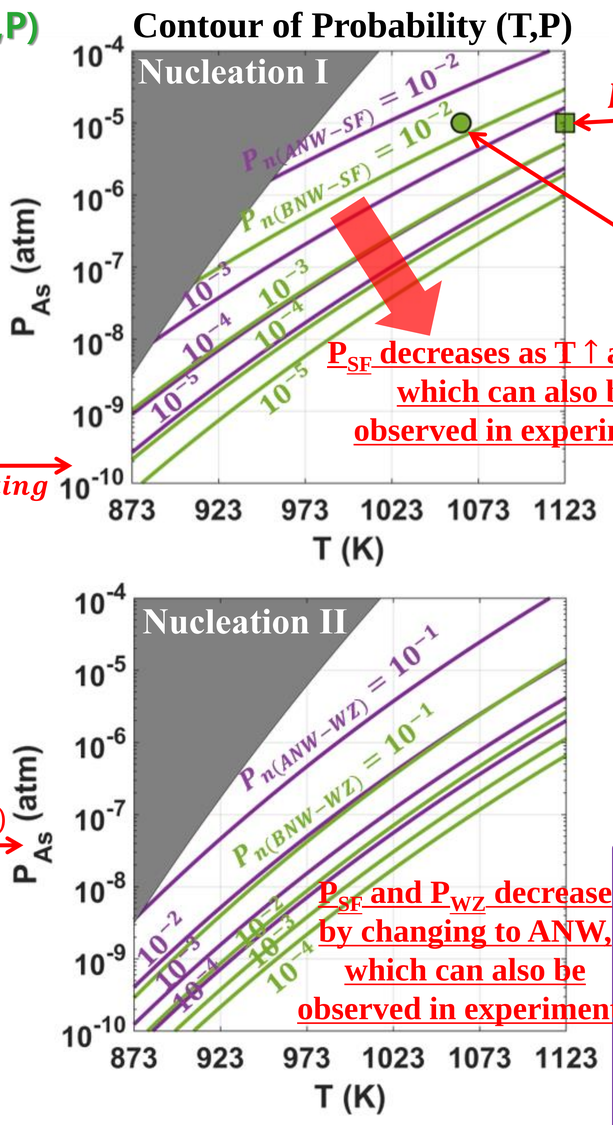
nucleus on ZB crystal surface:
Zinc-Blende (ZB) or Stacking-Fault (SF)

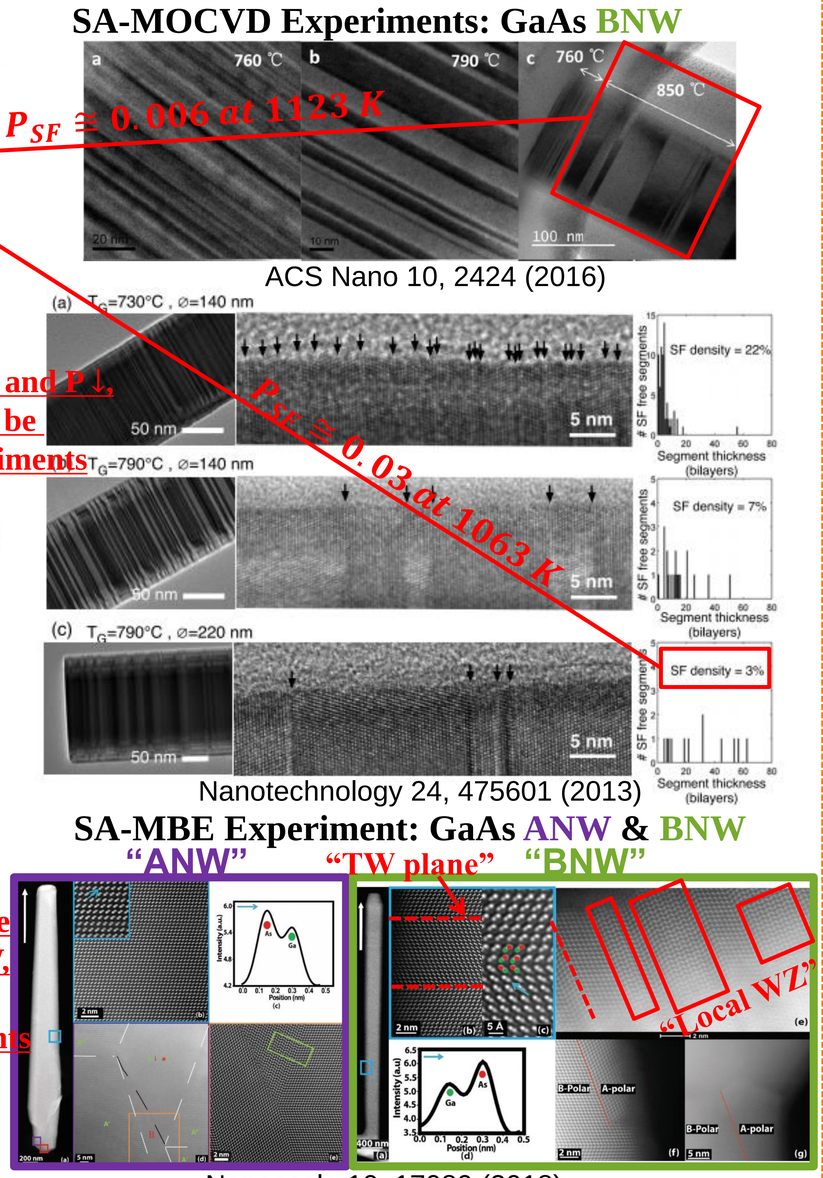


Nucleation II: $P_{n(WZ)} = \dot{N}_{(WZ)}/(\dot{N}_{(WZ)} + \dot{N}_{(TW)})$

nucleus on SF crystal surface:
Twin (TW) or Wurtzite (WZ)







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