

제 26회 한국반도체학술대회
세션: [TG2-C] Material Growth & Characterization



**Effect of the two-dimensional strain
on the equilibrium crystal shape of GaAs
by ab-initio thermodynamics**

2019. 02. 14.

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Contents

- **Introduction**

- Integration of GaAs on Si CMOS platform
- Purpose

- **Homo-epitaxy of GaAs on GaAs(001)**

- Unstrained crystal shape simulation of GaAs
- DFT + Statistical thermodynamics

- **Hetero-epitaxy of GaAs on Si(001)**

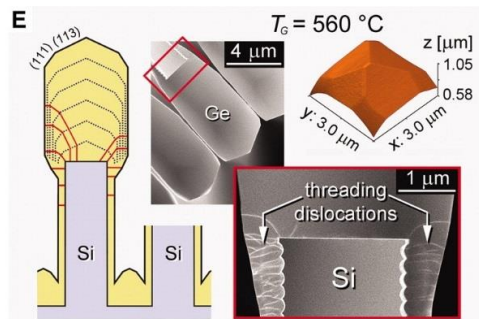
- Strained crystal shape simulation of GaAs
- DFT + FEM + Statistical thermodynamics

Integration of III-V on Si CMOS platform

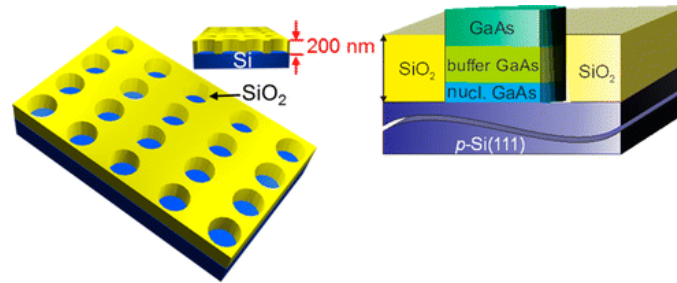
	e ⁻ mobility (cm ² /Vsec)	h ⁺ mobility (cm ² /Vsec)	Lattice constant (Å)
Si	1,400	500	5.43
Ge	3,900	1,900	5.65
GaAs	8,000	400	5.65
InAs	33,000	460	6.06

Difficulties

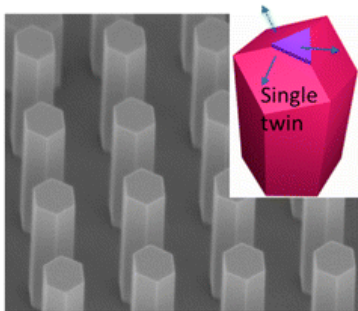
- Large lattice mismatch → **dislocation**
- Different thermal expansion coefficients → **crack**
- Polar material on a nonpolar substrate → **antiphase domain**



Science 335, 1330 (2012)



Cryst. Growth Des., 14, 593 (2014)



ACS Nano 10, 2424 (2016)



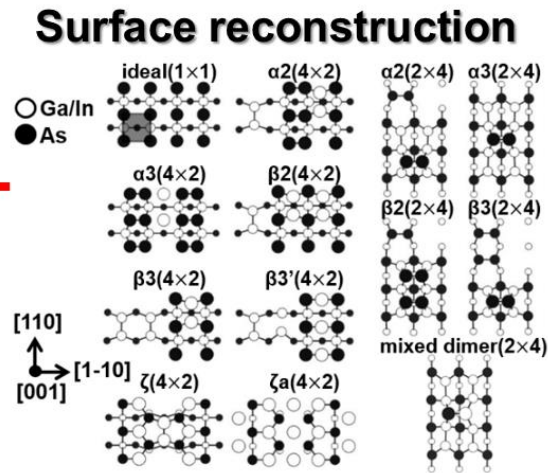
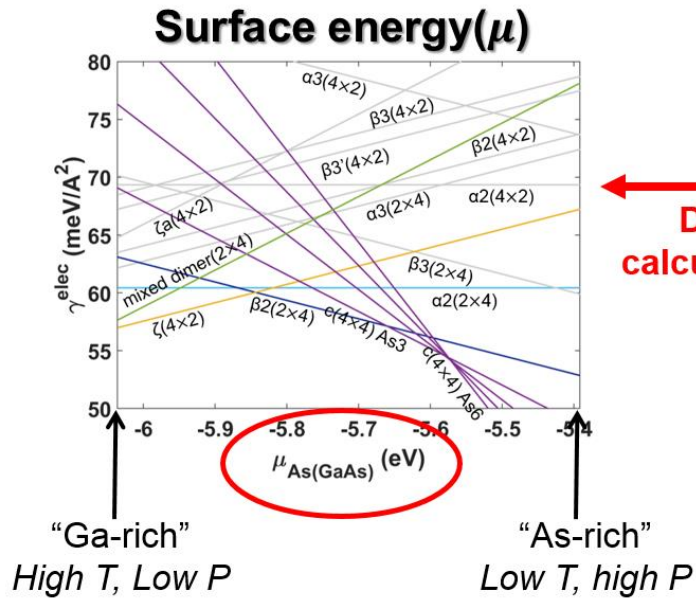
ACS Nano 11, 6853 (2017)

Selective Area Growth

- **Dislocation** → Confined to the bottom
- **Crack** → inhibition of propagation
- **Antiphase domain** → Reduction due to small number of nuclei

Understanding the surface energy & crystal shape

ab-initio thermodynamics

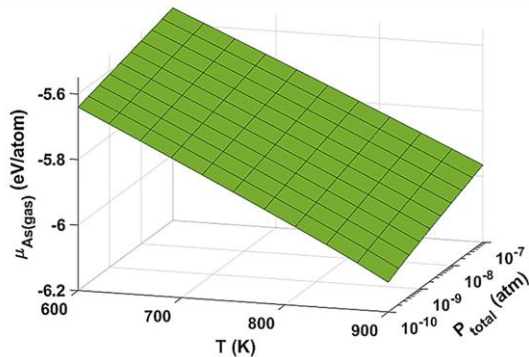


DFT calculation

x-axis: $\mu_{As(GaAs)} = \mu_{As(g)}(T, P) !!$

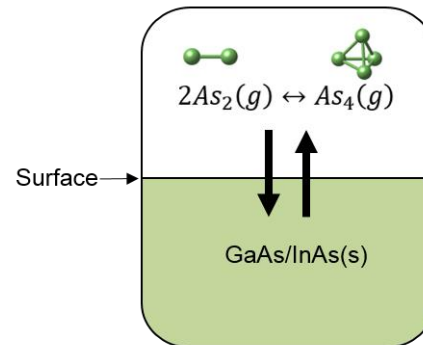
DFT calculation

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



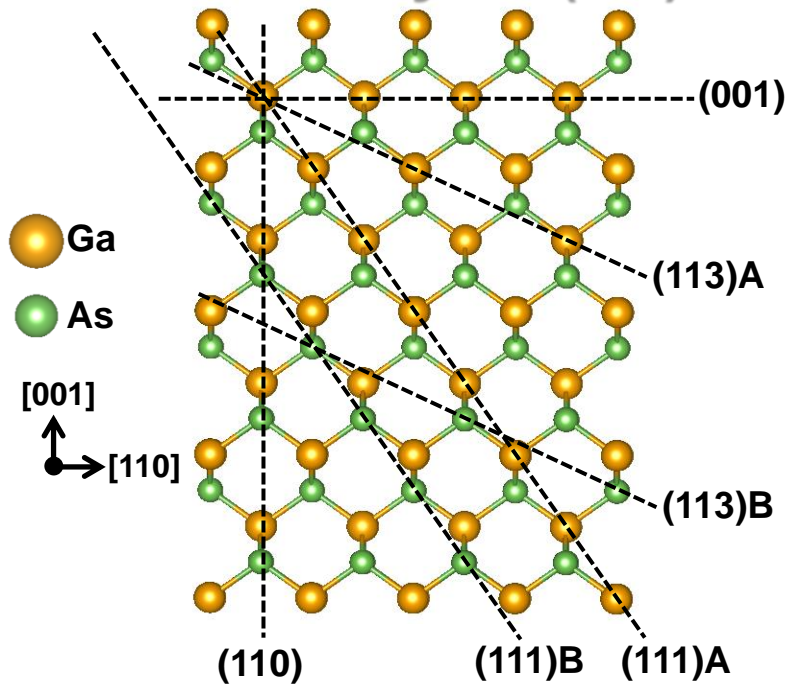
Equilibrium

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



Unstrained shape: Wulff shape

GaAs crystal(ZB)

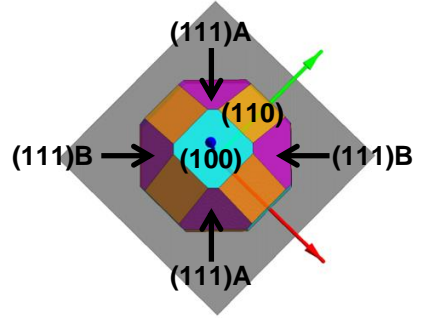
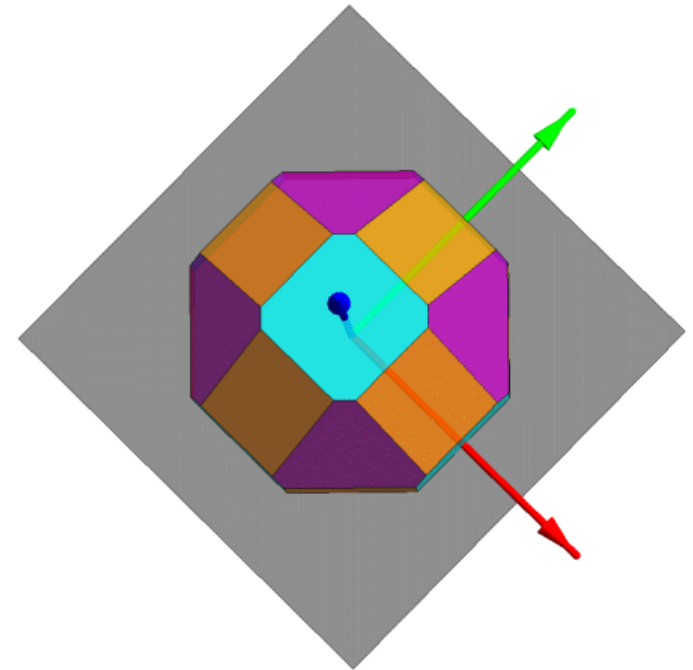


Wulff construction



$$\begin{aligned}
 &\text{when } \gamma^{(113)A} \\
 &= \gamma^{(113)B} \\
 &\gg \gamma^{(100)} \\
 &= \gamma^{(110)} \\
 &= \gamma^{(111)A} \\
 &= \gamma^{(111)B}
 \end{aligned}$$

Wulff shape



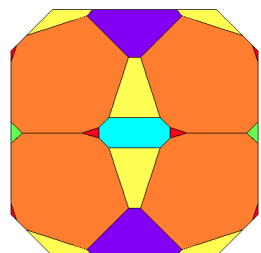
Wulff construction: $d^{(hkl)} \propto \gamma^{(hkl)}$

Wulff shape vs. homo-epitaxial shape

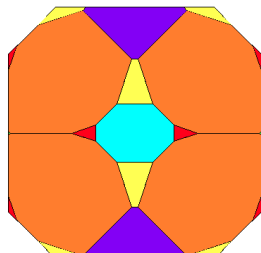
Simulation

Experiments

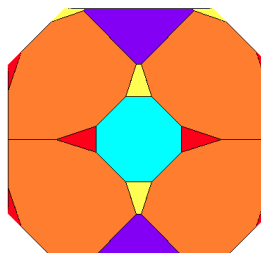
[110]
↑
[001]
→ [1-10]



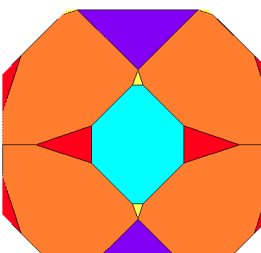
T: 973 K,
 $P_{As}: 10^{-3}$ atm



T: 973 K,
 $P_{As}: 10^{-5}$ atm

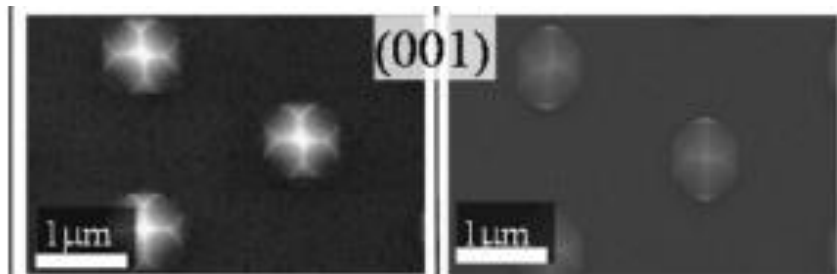


T: 973 K,
 $P_{As}: 10^{-7}$ atm



T: 973 K,
 $P_{As}: 10^{-9}$ atm

- (100)
- (110)
- (111)A
- (111)B
- (113)A
- (113)B



T: 1023 K

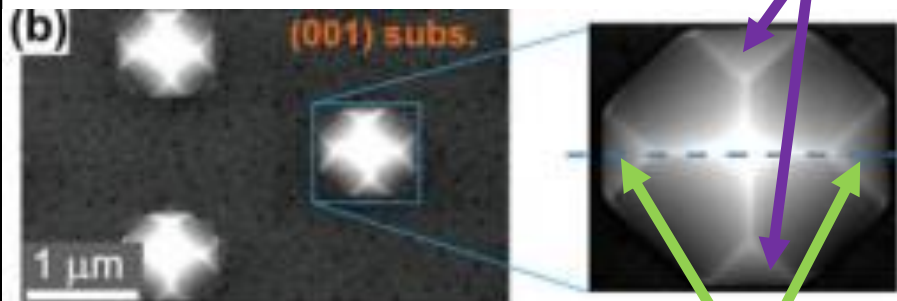
[TMGa]: 2.7×10^{-6} atm

[AsH₃]: 5.0×10^{-4} atm

T: 873 K

[TMGa]: 2.7×10^{-6} atm

[AsH₃]: 1.0×10^{-3} atm



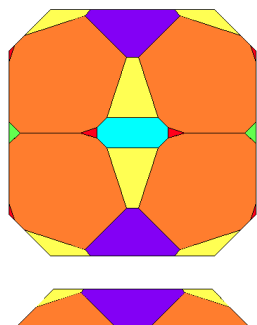
TMGa & TBAs or AsH₃

T: 973 K

J. Cryst. Growth, 298, 616 (2007)
J. Mater. Res., 26, 2127 (2011)

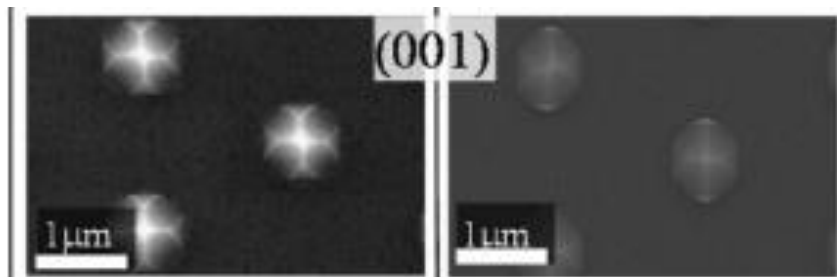
Wulff shape vs. homo-epitaxial shape

Simulation



T: 973 K,
 $P_{As}: 10^{-3}$ atm

Experiments



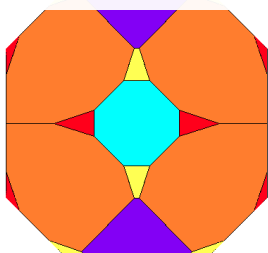
T: 1023 K

T: 873 K

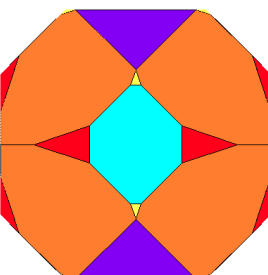
Experimentally found (111)B facet X

1. Experimental crystal shape is determined by kinetics
2. There is some unknown (111)B reconstructions

- (100)
- (110)
- (111)A
- (111)B
- (113)A
- (113)B



T: 973 K,
 $P_{As}: 10^{-7}$ atm



T: 973 K,
 $P_{As}: 10^{-9}$ atm



TMGa & TBAs or AsH₃

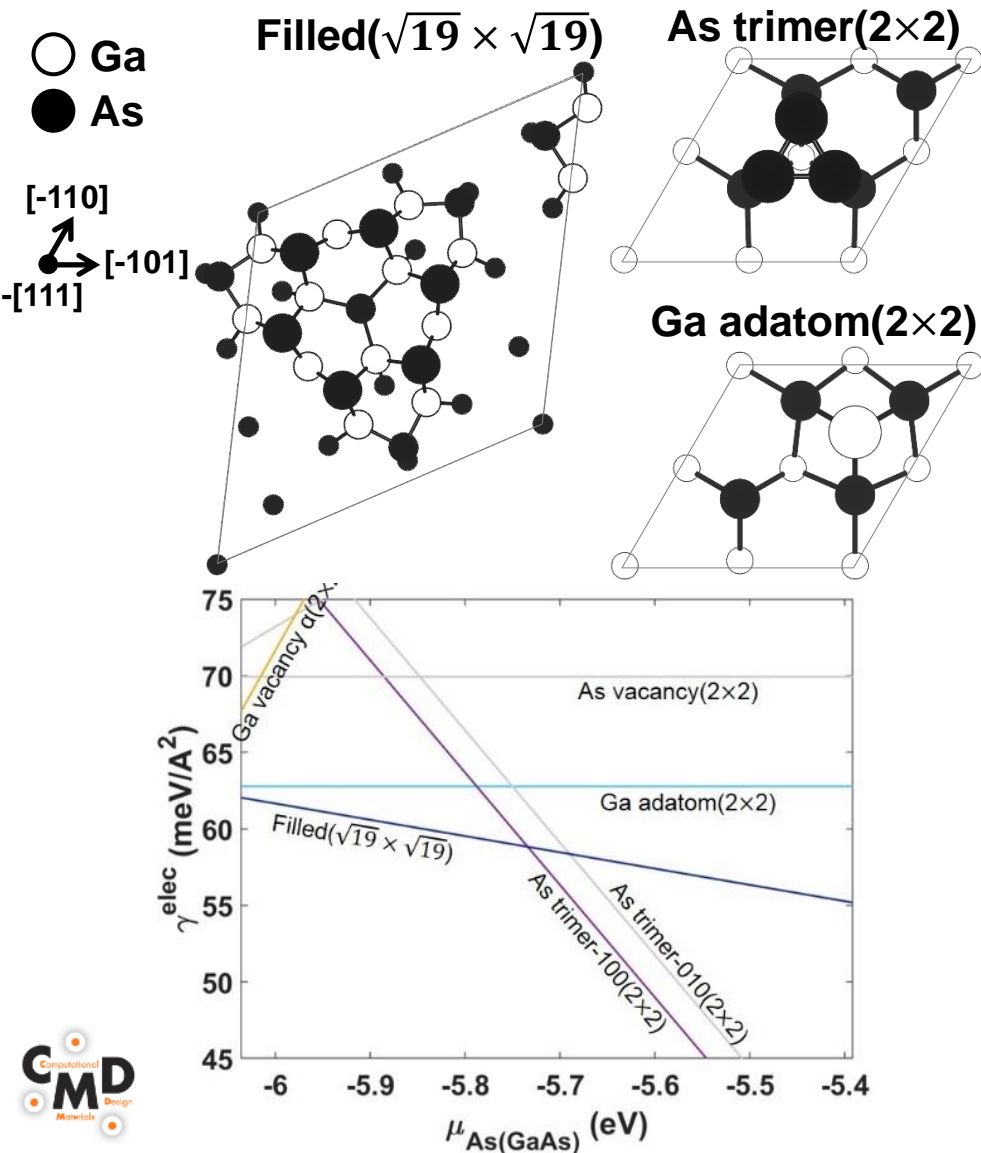
T: 973 K

{111}B

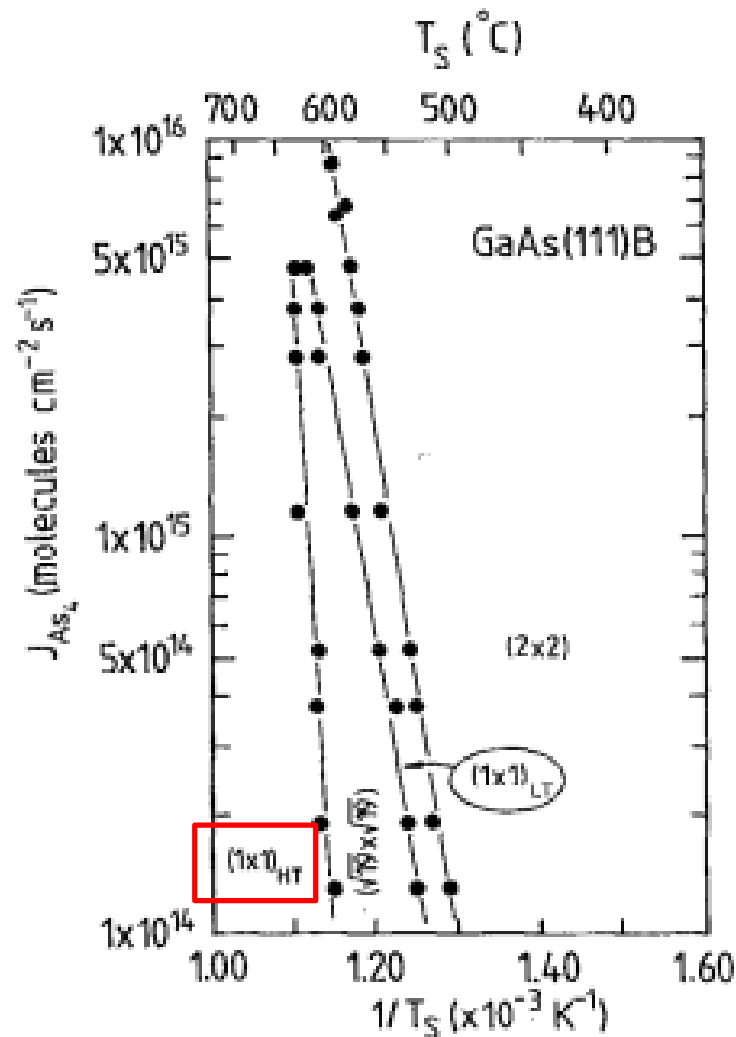
J. Cryst. Growth, 298, 616 (2007)
 J. Mater. Res., 26, 2127 (2011)

(111)B: other reconstructions?

Simulation

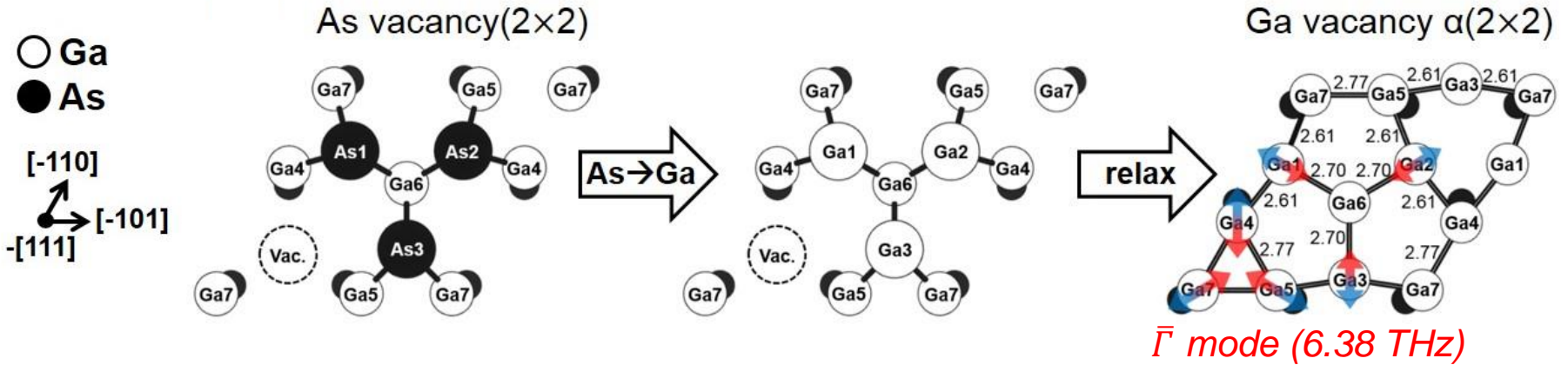


Experiments

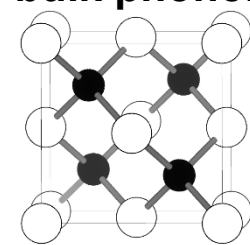
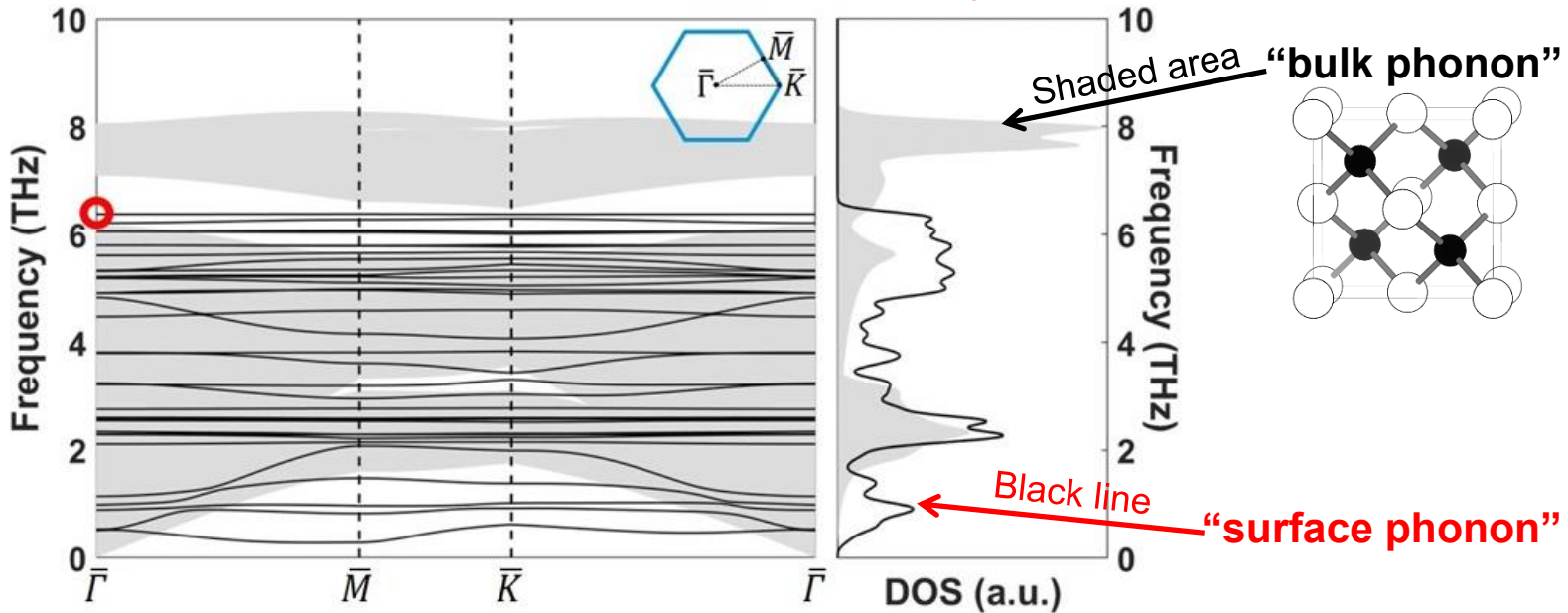


Appl. Phys. Lett., 62, 1370 (1993)

New GaAs(111)B reconstruction

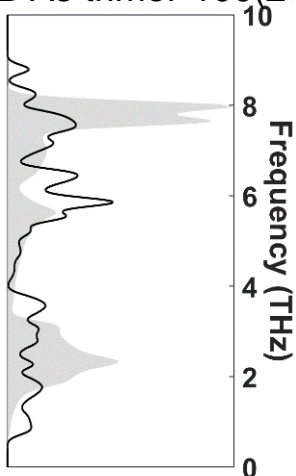


Surface phonon dispersion of Ga vacancy α (2×2)



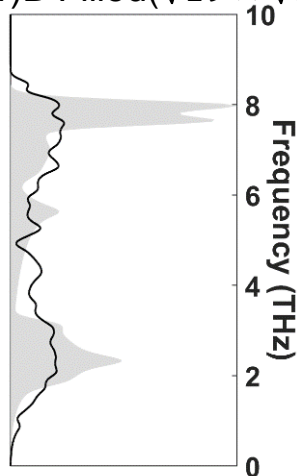
Surface vibration of GaAs(111)B

(111)B As trimer-100(2x2)



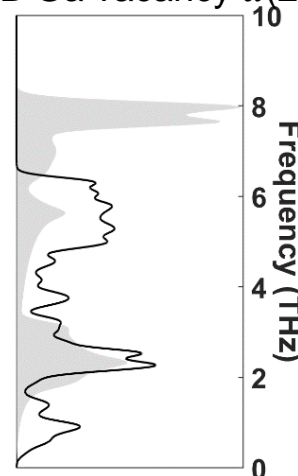
DOS (a.u.)

(111)B Filled($\sqrt{19} \times \sqrt{19}$)



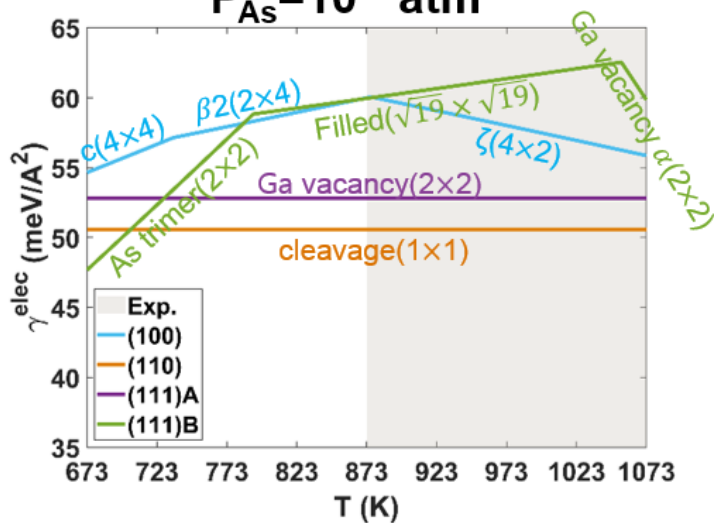
DOS (a.u.)

(111)B Ga vacancy $\alpha(2 \times 2)$



DOS (a.u.)

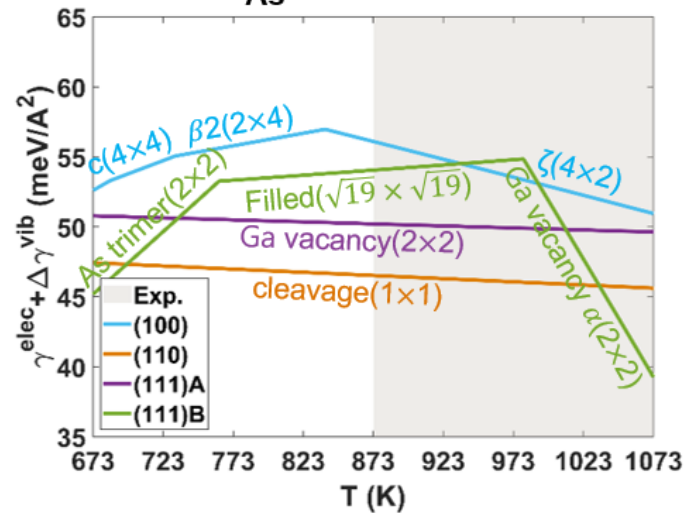
$P_{As} = 10^{-5}$ atm



Surface vib.

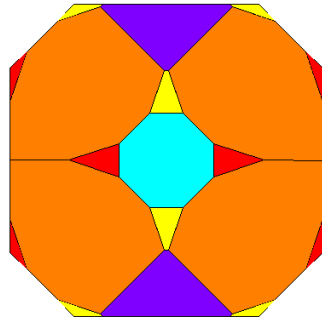
$$\gamma = \gamma^{\text{elec}} + \Delta\gamma^{\text{vib}}$$

$P_{As} = 10^{-5}$ atm



Wulff shape vs. homo-epitaxial shape

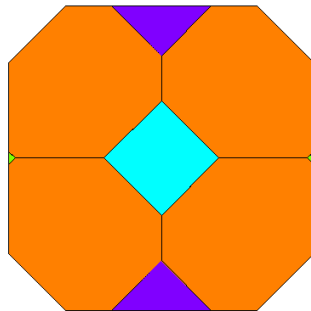
Simulation



$$\gamma^{elec}$$

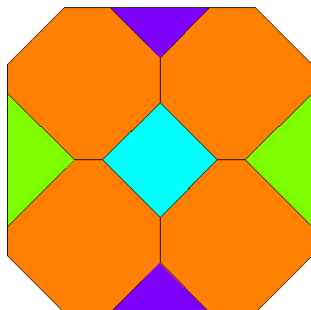
T: 1023 K

P_{As} : 10^{-5} atm



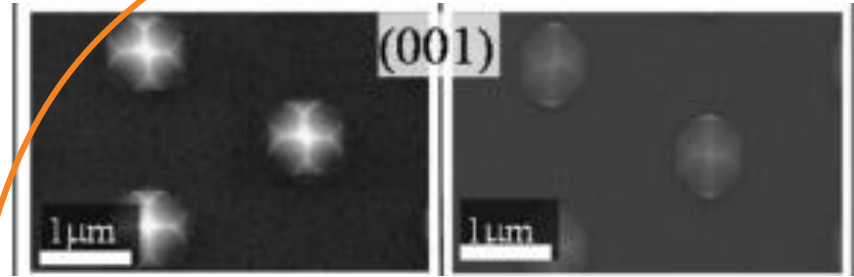
$$\gamma^{elec} + \Delta\gamma^{vib}$$

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



$\gamma^{elec} + \Delta\gamma^{vib}$
with
new (111)B
reconstruction

Experiments



T: 1023 K

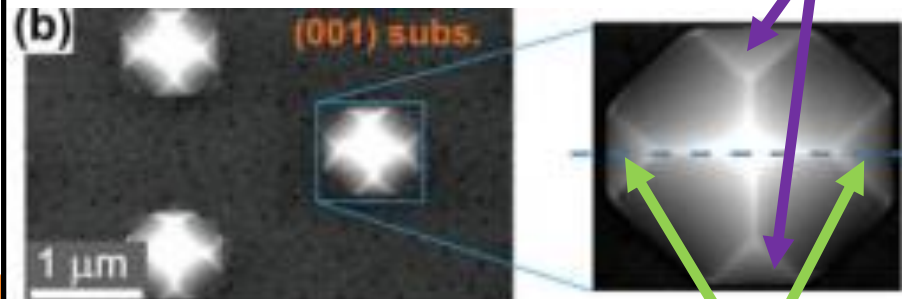
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TMGa & TBAs or AsH₃

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

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[110]
↑
[001]
→ [1-10]

- (100)
- (110)
- (111)A
- (111)B
- (113)A
- (113)B

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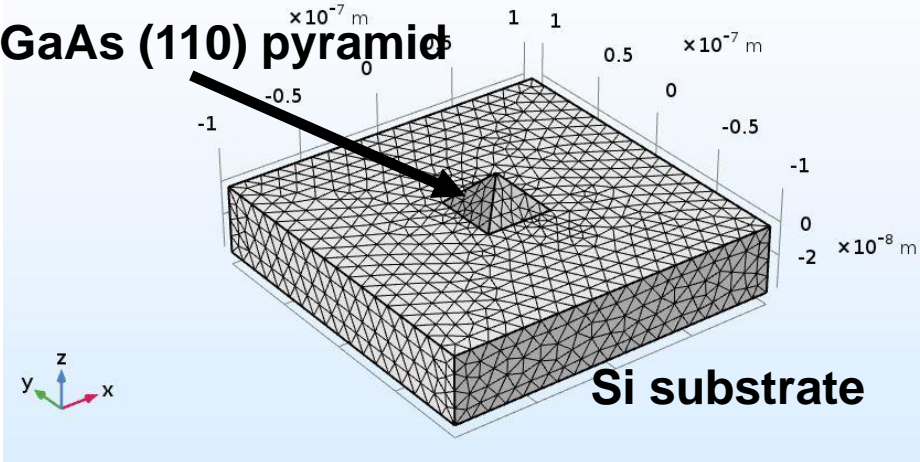
- Homo-epitaxy of GaAs on GaAs(001)

- Unstrained crystal shape simulation of GaAs
- DFT + Statistical thermodynamics

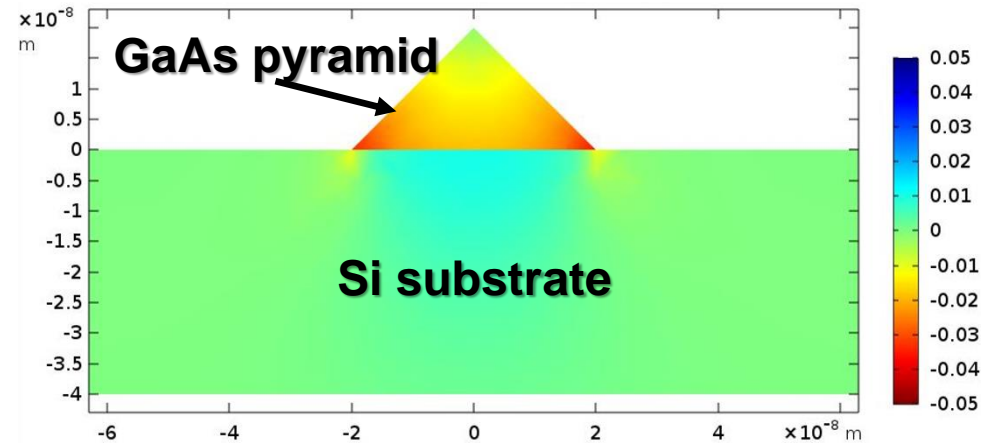
- **Hetero-epitaxy of GaAs on Si(001)**

- Strained crystal shape simulation of GaAs
- DFT + FEM + Statistical thermodynamics

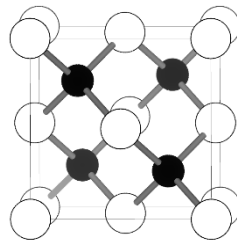
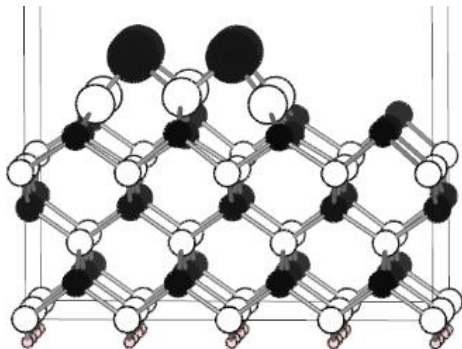
Strained shape: FEM + DFT



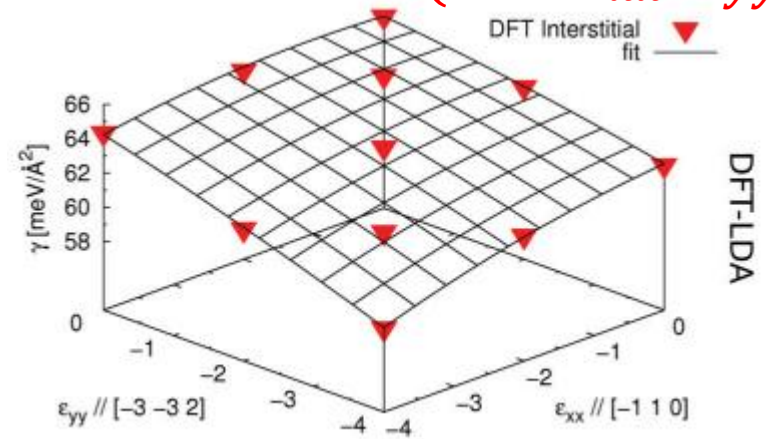
FEM: Strain distribution ($\epsilon_{xx}, \epsilon_{yy}$)



$$\gamma^{strained} = E_{surf}^{strained} - E_{bulk}^{strained}$$



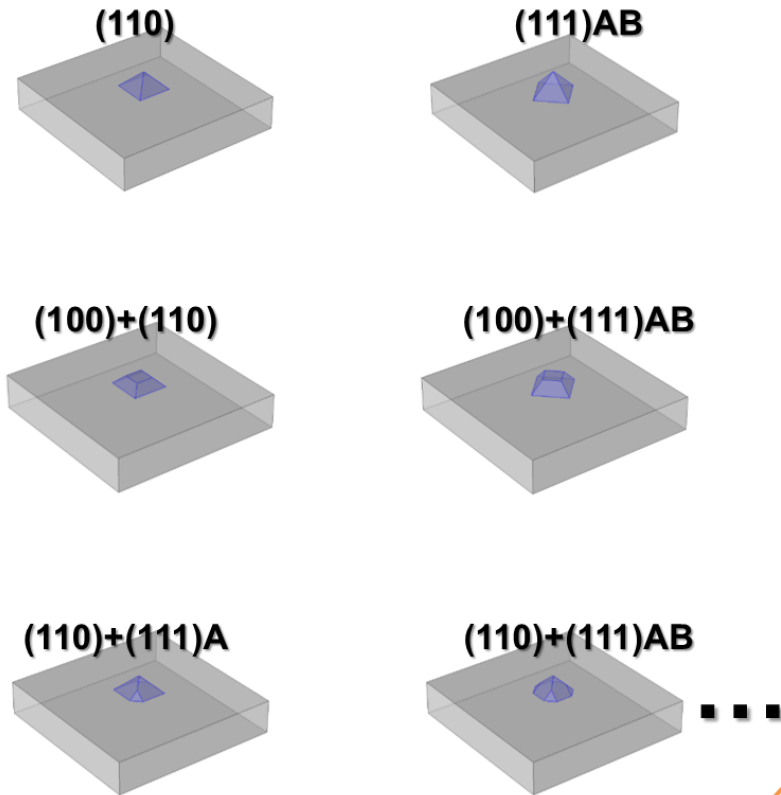
DFT: $\gamma^{strained}(T, P, \epsilon_{xx}, \epsilon_{yy})$



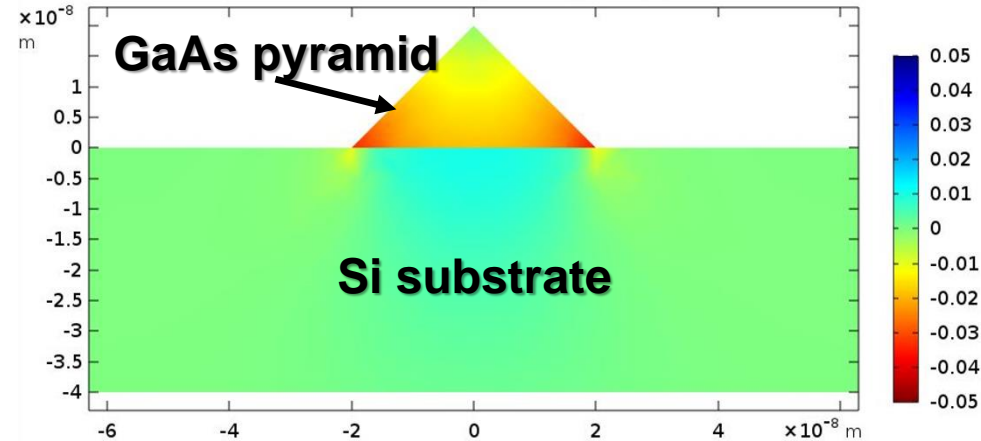
$$\gamma(\epsilon_{xx}, \epsilon_{yy}) = \gamma_0 + \sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + S_{xx}\epsilon_{xx}^2 + S_{yy}\epsilon_{yy}^2 + S_{xy}\epsilon_{xx}\epsilon_{yy}$$

Strained shape: FEM + DFT

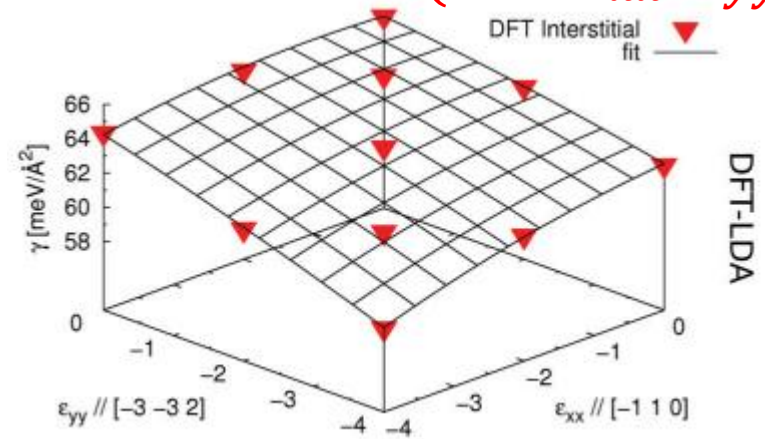
Various Faceted Forms



FEM: Strain distribution ($\epsilon_{xx}, \epsilon_{yy}$)



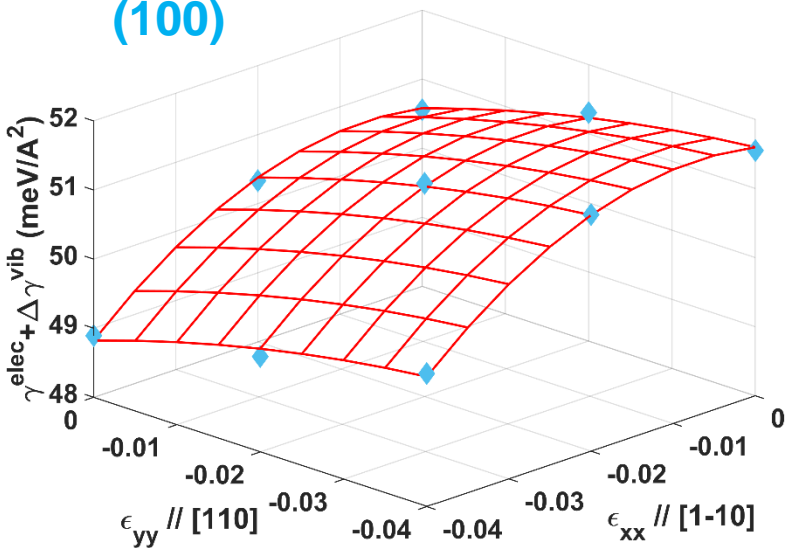
DFT: $\gamma^{strained}(T, P, \epsilon_{xx}, \epsilon_{yy})$



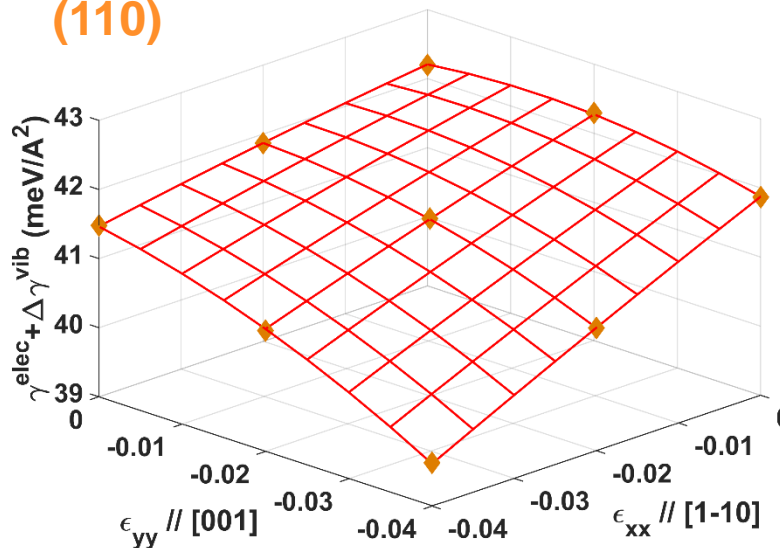
$$\gamma(\epsilon_{xx}, \epsilon_{yy}) = \gamma_0 + \sigma_{xx}\epsilon_{xx} + \sigma_{yy}\epsilon_{yy} + S_{xx}\epsilon_{xx}^2 + S_{yy}\epsilon_{yy}^2 + S_{xy}\epsilon_{xx}\epsilon_{yy}$$

Strained surface energy

(100)



(110)

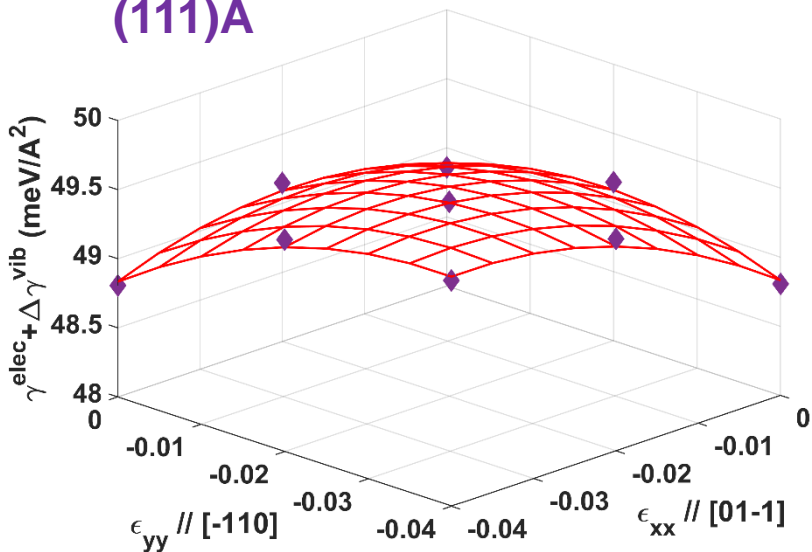


T: 1023 K

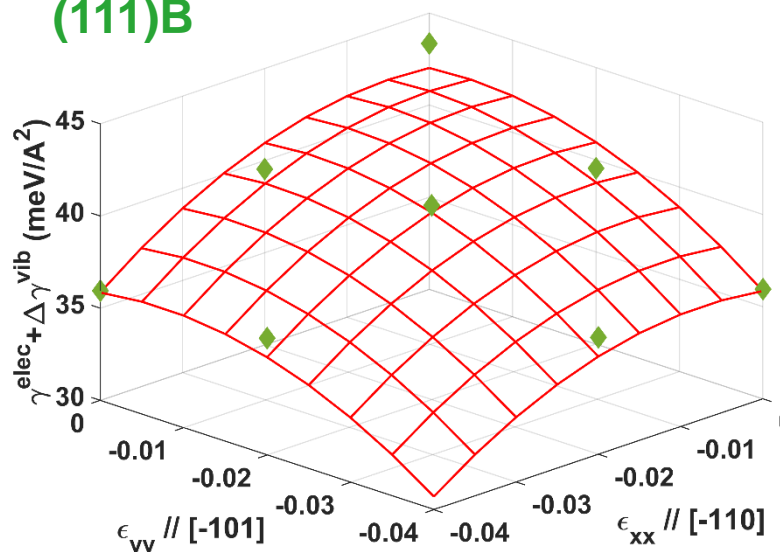
$P_{\text{As}}: 10^{-5} \text{ atm}$

- ◆ (100) DFT
- ◆ (110) DFT
- ◆ (111)A DFT
- ◆ (111)B DFT
- Fit

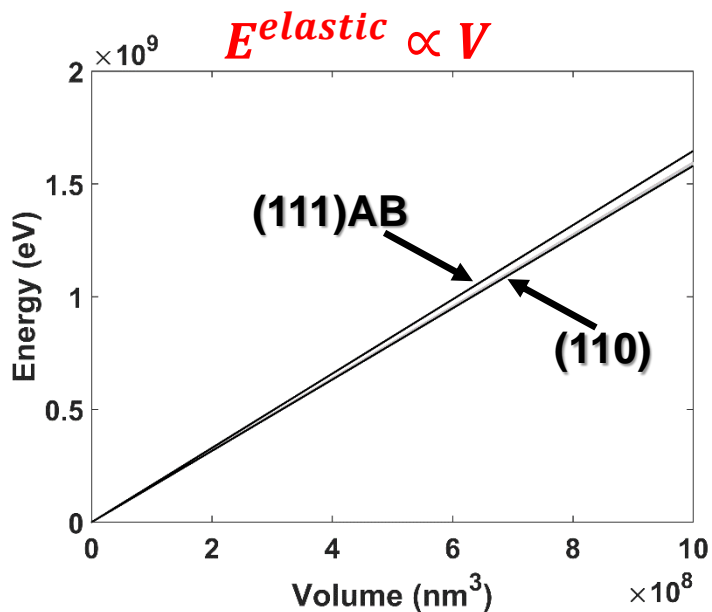
(111)A



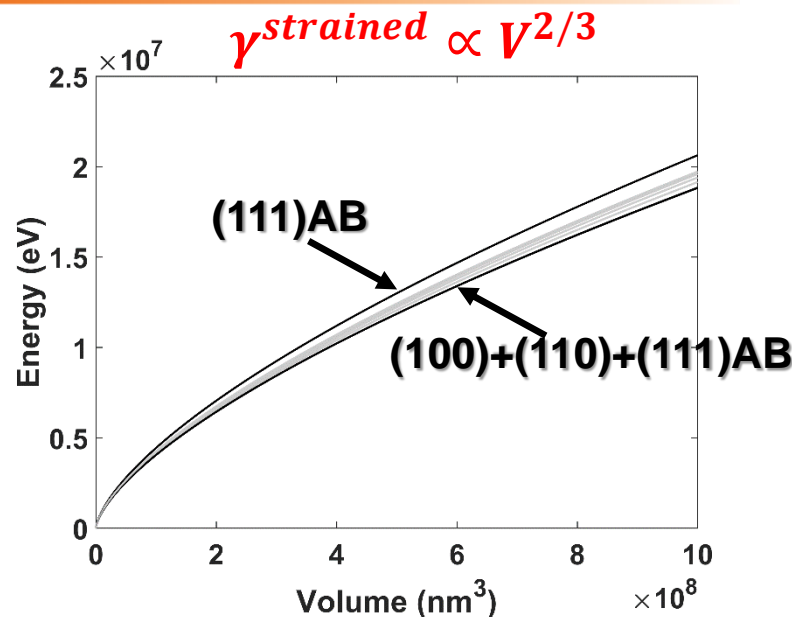
(111)B



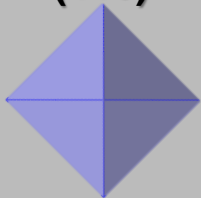
Energy(T, P, V) of strained crystal



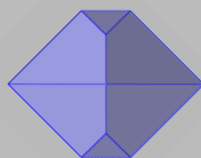
T: 1023 K
 $P_{As}: 10^{-5}$ atm



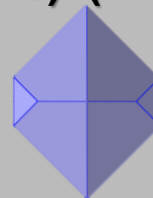
(110)



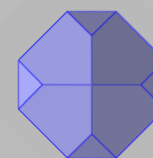
(110)+(111)A



(110)+(111)B

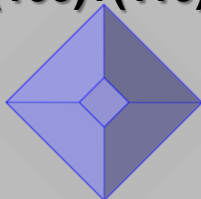


(110)+(111)AB

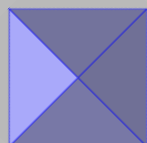


[110]
 [001]
 [1-10]

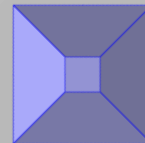
(100)+(110)



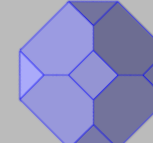
(111)AB



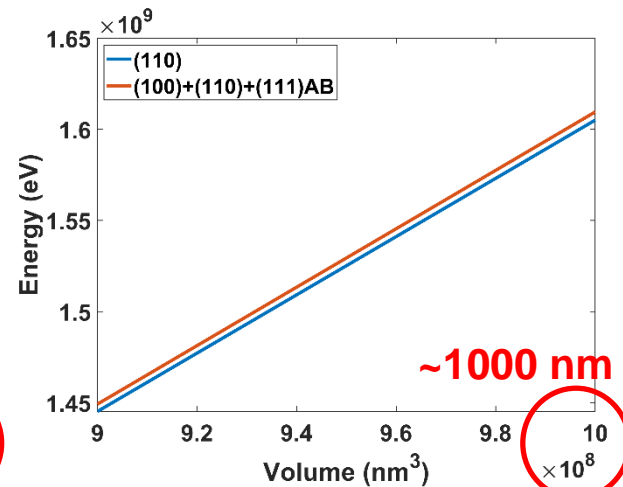
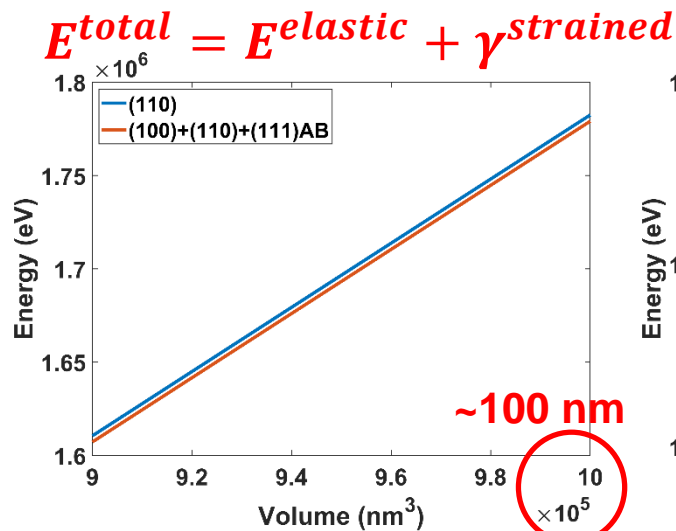
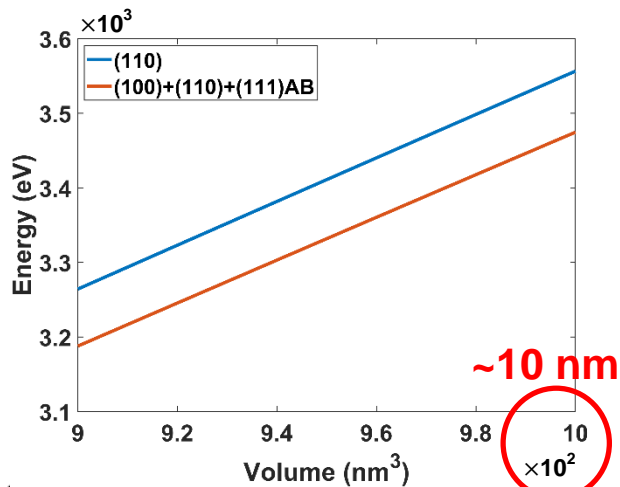
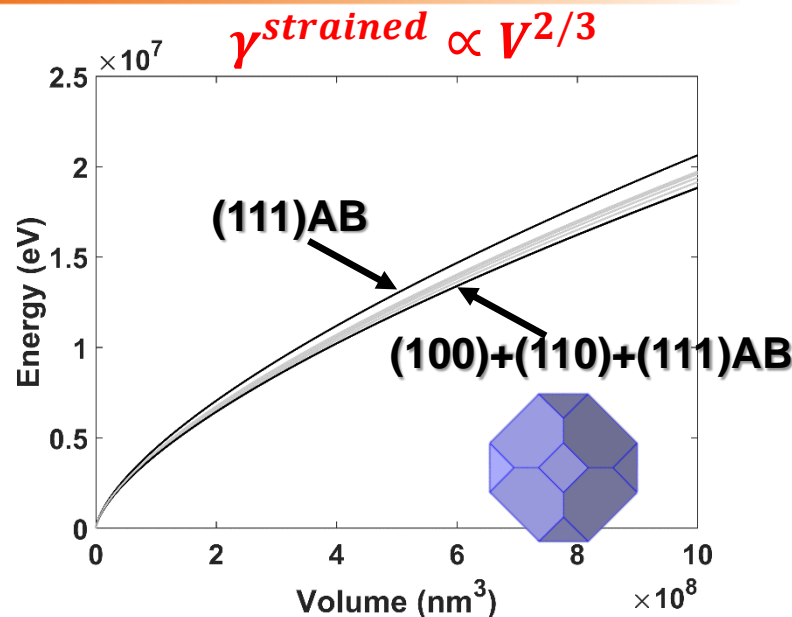
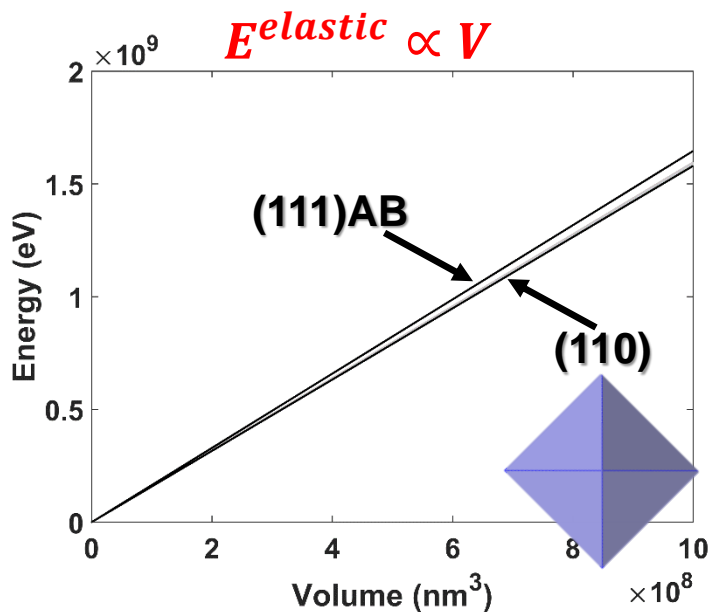
(100)+(111)AB



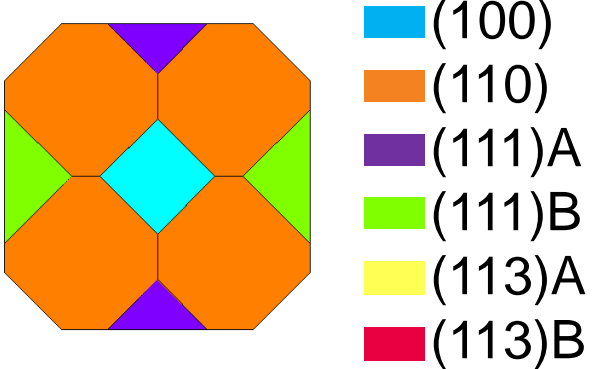
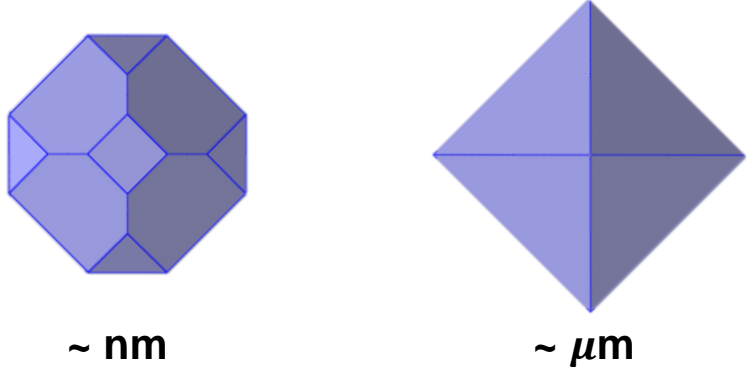
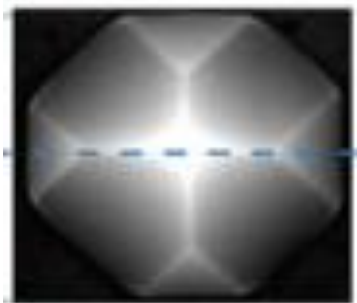
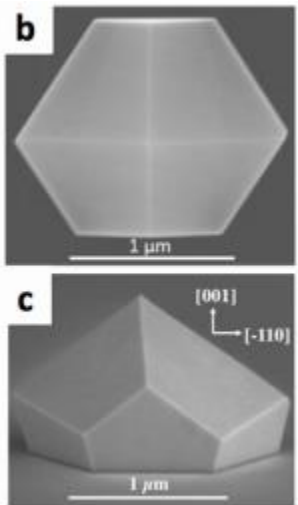
(100)+(110)+(111)AB



Energy(T, P, V) of strained crystal



Unstrained shape vs. Strained shape

	<h2>Unstrained GaAs on GaAs(100)</h2>	<h2>Strained GaAs on Si(100)</h2>
<p>Simulation</p> <p>T: 1023 K</p> <p>$P_{As}: 10^{-5}$ atm</p>		
<p>Experiment</p>	 <p>J. Mater. Res. ,26, 2127 (2011)</p>	 <p>Scientific Reports 6, 25328 (2016)</p>