Surface structure and surface energy of InAs

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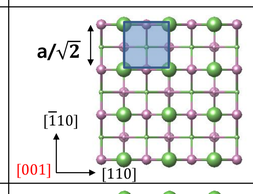
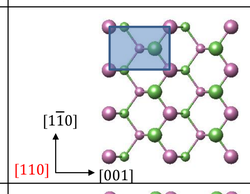
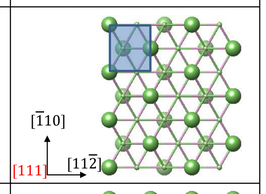
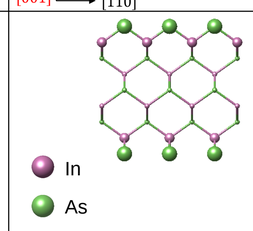
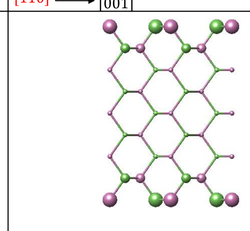
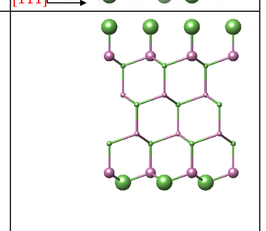
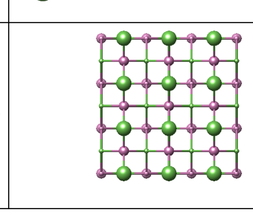
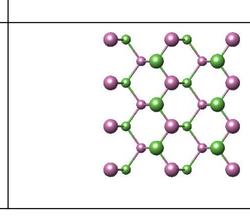
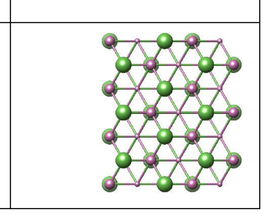
Computational Materials Design

INTRODUCTION

A. Zinc-blende unit surface

	(100) Surface	(110) Surface	(111) Surface
area	$a^2/2$ per one atom (100) = -(100)	$a^2/\sqrt{2}$ per two atom (110) = -(110)	$\sqrt{3}a^2/4$ per one atom (111) ≠ -(111)
Top			
Side			
bottom			

B. Motivation

- InGaAs : n-type channel material with high electron mobility (8000~30000 $cm^2V^{-1}s^{-1}$)
- GaAs & InAs surface : zinc-blende structure has some polar surfaces (ex. (111) and –(111))
- Polar surface energy : there were some results with energy density approximation approach
- New approach : by changing geometry, polar surface energy can be calculated directly

→ Purpose : calculation of InAs surfaces without approximation

COPMUTATIONAL DETAILS

A. Computational details

- VASP (Vienna *ab-initio* Simulation Package)
- xc-functional : GGA-PBE96, LDA-CA
- Cutoff energy : 300 eV
- k-points : According to convergence test for different slab structures
- Valence treatment : Ga=$3d^{10}4s^24p^1$, As=$4s^24p^3$, In=$4d^{10}5s^25p^1$
- Vacuum thickness : 10 Å
- The top 5 layers of the total 9 layers were allowed to move
- The bottom of the layers were saturated with hydrogen and fixed

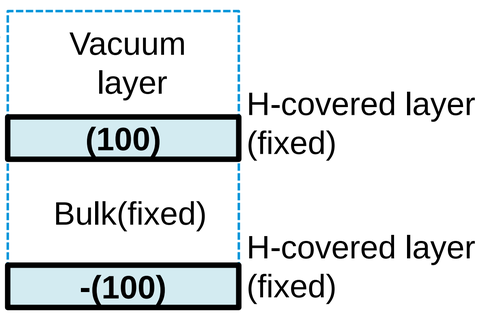
B. Equilibrium condition

- $\mu_{In} + \mu_{As} = \mu_{InAs} = \mu_{In(bulk)} + \mu_{As(bulk)} - \Delta H_f$
- $0 < -\mu_{In} + \mu_{In(bulk)} = \mu_{As} - \mu_{As(bulk)} + \Delta H_f$
- $-\Delta H_f < \mu_{As} - \mu_{As(bulk)} < 0$
- $\gamma_{surface}A = E_{tot} - \mu_{In}N_{Ga} - \mu_{In}N_{As} = E_{tot} - \mu_{InAs}N_{In} - \mu_{As}(N_{As} - N_{In})$

METHODOLOGY

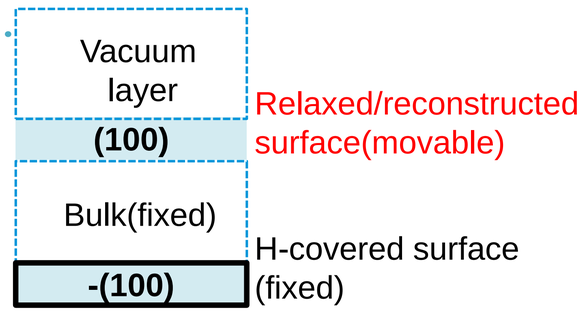
A. (100) surface

i.



$\gamma_{(100)\text{-}H} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/2A$

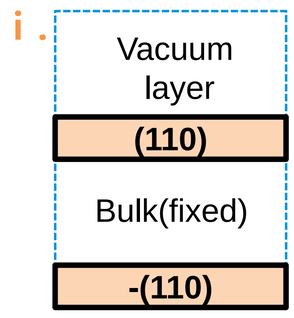
ii.



$\gamma_{(100)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(100)\text{-}H}$

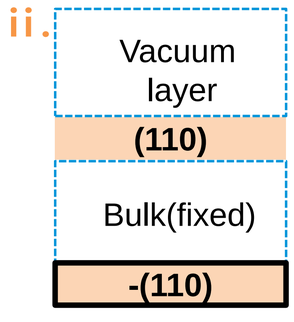
B. (110) surface

i.



$\gamma_{(110)\text{-}H} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/2A$

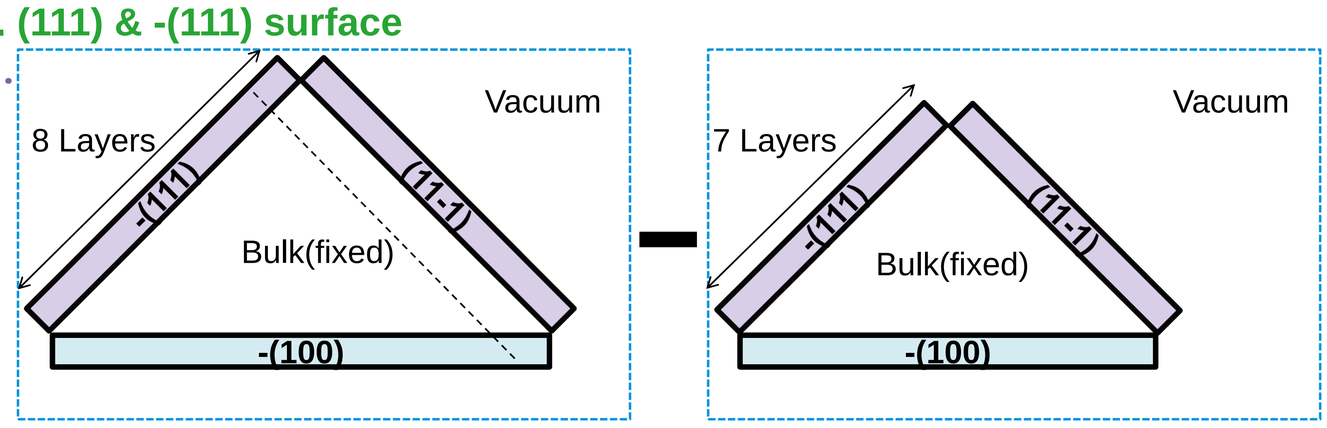
ii.



$\gamma_{(110)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(110)\text{-}H}$

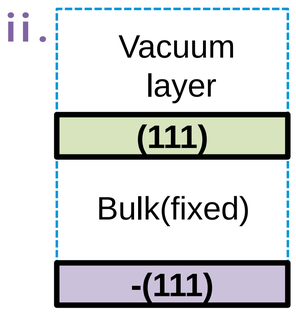
C. (111) & -(111) surface

i.



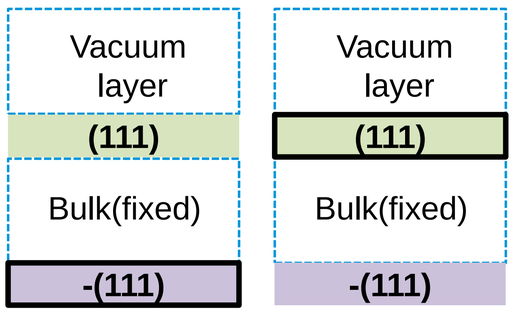
$\delta E = E_{tot}(n=8;\ 36AB) - E_{tot}(n=7;\ 28AB) - 8\mu_{AB} = 2\gamma_{(-1-1-1)\text{-}H} + \gamma_{(-1\ 0\ 0)\text{-}H}$

ii.



$\gamma_{(111)\text{-}H} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(-1-1-1)\text{-}H}$

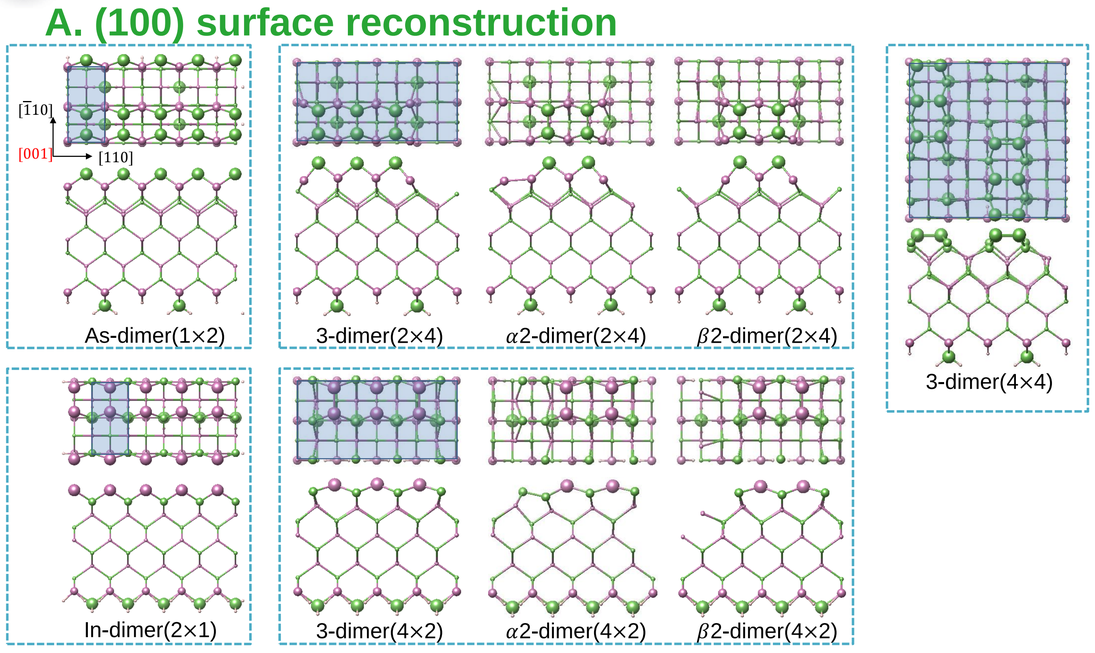
iii.



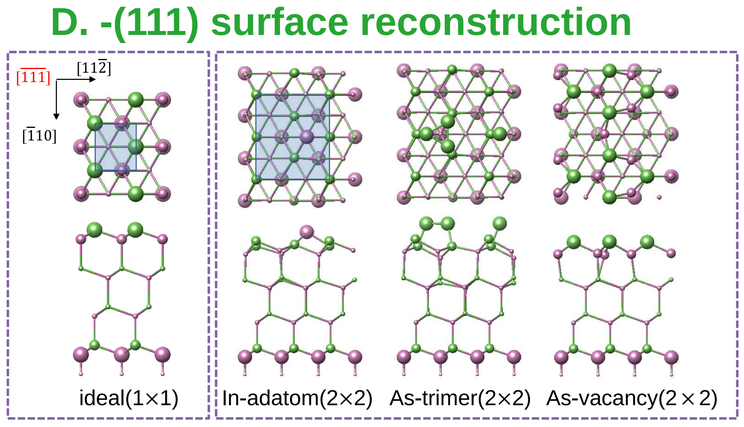
$\gamma_{(111)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(-1-1-1)\text{-}H}$
$\gamma_{(-1-1-1)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(111)\text{-}H}$

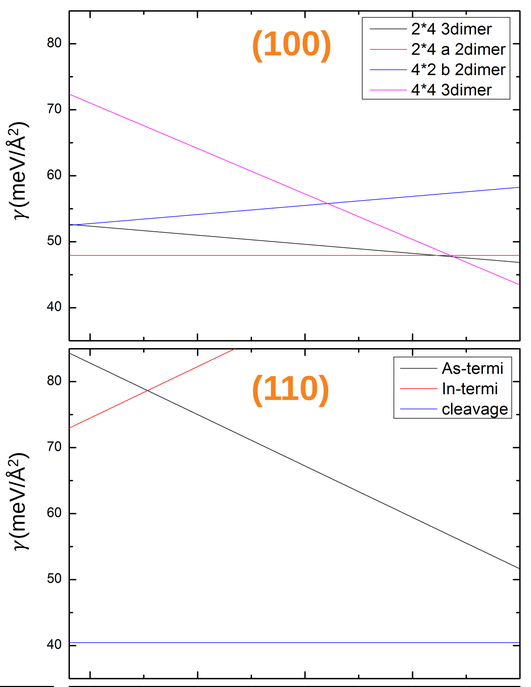
Results & discussions

A. (100) surface reconstruction

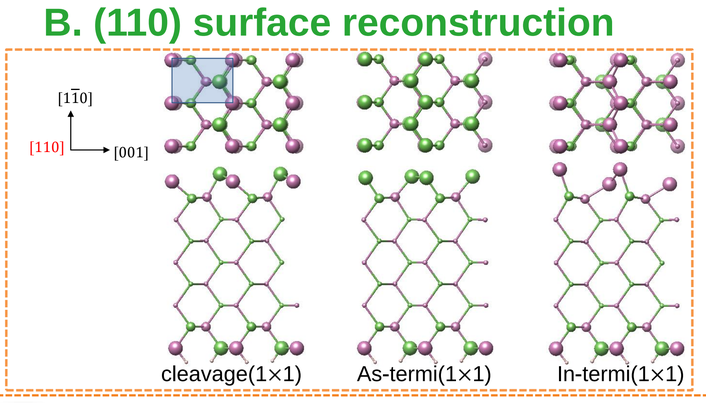


D. -(111) surface reconstruction

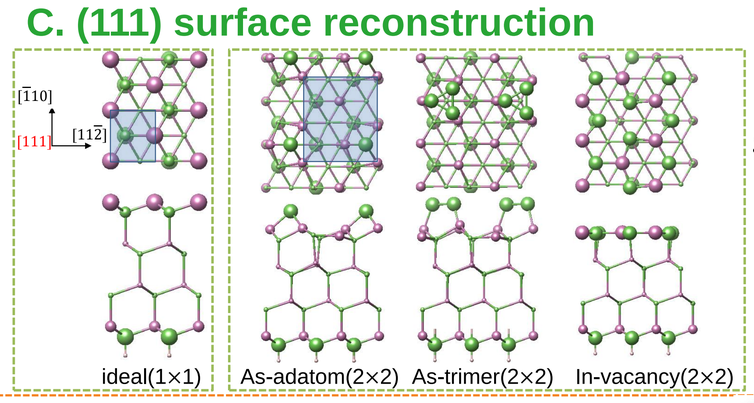




B. (110) surface reconstruction



C. (111) surface reconstruction



Summary

- Surface energies and surface structures were calculated by LDA functional
- In the In-rich region, E(110) < E(111) < E(100) < E(-1-1-1) : (110) cleavage is the most stable
- In the As-rich region, E(-1-1-1) < E(110) < E(111) < E(100) : -(111) As-trimer is the most stable

References

[1] Physical Review B. 1996;54(12):8844.
[2] Physical Review B. 1998;58(8):4566-71.
[3] Phys. Rev. Lett. Volume 92, Number 8 (2004)

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