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Atomistic Understanding on the Surface of GaAs By *Ab Initio* Thermodynamics; From Equilibrium Shape to Growth Shape

I. W. Yeu (Korea Institute of Science and Technology (KIST)), C. S. Hwang (Dep. MSE, and Inter-University Semicon. Res. Center), and J. H. Choi (Korea Institute of Science and Technology (KIST))

Abstract Text:

The III-V semiconductor nanowires (NWs) have attracted substantial attention as an ideal system for the study on the growth mechanism and electronic device applications. For the precise manipulation of the nanowire growth, understanding on the temperature–pressure (T–P) dependent variation in surface energy and reconstruction which governs the anisotropic interaction between vapor sources and crystal solids is crucial. Unfortunately, the quantitative values of the variation in surface energy cannot be obtained only using the conventional electronic structure calculation. To overcome this difficulty, we have developed a reliable *ab initio* thermodynamic method by which the T–P dependent surface energy is predicted from the atomic-scale calculations on: surface reconstructions of InAs[1]; equilibrium crystal shapes of GaAs and InAs[2]; and anisotropic adsorption and growth conditions of GaAs NW[3].

In this talk, we present an *ab initio* thermodynamics approach by combining the atomic-scale calculation with the thermodynamic treatment to take a step forward in the theoretical modeling on the growth of polar GaAs <111> nanowire by calculating the change in Gibbs free energy during the nucleation and growth process. By comparing the nucleation rate between different stacking sequences, the formation probability of stacking fault or wurtzite segment was quantitatively predicted under arbitrary vapor-phase growth conditions. The predicted T–P dependent probability from atomic-scale calculation is directly comparable to the experiments and remarkably consistent with the available results to date, elucidating the fundamental asymmetric growth mechanism. Our *ab initio* approach is truly independent of any empirical data, bridging to the experimentally controllable variables. This simulation can be applied to various nanomaterials, including two-dimensional materials as well as other III-V and II-VI NWs, where the precise control of the stacking sequence is significant for their properties.

[1] Yeu *et al.*, *Sci. Rep.*, 2017, **7**, 10691

[2] Yeu *et al.*, *Sci. Rep.*, 2019, **9**, 1127

[3] Yeu *et al.*, *Appl. Surf.*, *Sci.*, 2019, **497**, 143740

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Submitter's E-mail Address:
choijh@kist.re.kr
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First Author
Mr. In Won Yeu
Affiliation(s): Korea Institute of Science and Technology (KIST)
Phone Number:
E-mail Address: yiw0121@snu.ac.kr

Second Author
Prof. Cheol Seong Hwang
Affiliation(s): Dep. MSE, and Inter-University Semicon. Res. Center
Phone Number: 82-2-880-7535
E-mail Address: cheolsh@snu.ac.kr

Third Corresponding Author
Dr. Jung-Hae Choi
Affiliation(s): Korea Institute of Science and Technology (KIST)
Address:
Hwarangno 14-gil, Seongbuk-gu,
Seoul, 02792
Korea, Republic of (South)
Phone Number: +8229585488
E-mail Address: choijh@kist.re.kr

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