O20MF_0151

Effects of growth condition on the anisotropic growth and stacking behavior of GaAs polar nanowires: *ab initio* thermodynamics

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Over the past decades, the vapor-phase growth techniques of III-V nanowire (NW) have improved tremendously by careful control of the growth variables: growth mode, growth conditions of temperature (T) and pressure (P), and substrate orientation. It has been found that under narrow T–P range, the unidirectional growth along a certain crystallographic direction is induced by the anisotropic surface nucleation, and the involvement of stacking fault and polytypism in the grown NW depends on the T–P conditions. Nevertheless, the mechanism on the effects of the growth variables has not yet been fully elucidated and the lack of atomic-scale understanding deters the precise control of the NW growth.

This study provides an *ab initio* thermodynamic approach to take a step forward in the theoretical modeling on the growth of GaAs NW. We investigated the vapor-phase growth kinetics under arbitrary T–P conditions by combining the atomic-scale calculation with the thermodynamic treatment of vapor-solid system. Considering the entropy contribution as well as the electronic energy, the change in Gibbs free energy, composed of the chemical potential and surface energies of various reconstructions, was calculated as a function of T and P at each stage of adsorption, nucleation, and growth. It enabled us to predict the T–P dependent variation in nucleation rate along different crystallographic directions with possible stacking sequences: zinc-blende, stacking fault, twin, and wurtzite. As a result, the reason why GaAs NW tends to grow along one specific polar direction, <111>B, was identified as the excessive source supply on (111)B surface induced by preferential adsorption under narrow T–P conditions [1]. In addition, the intriguing asymmetry in stochastic determination of stacking sequence during the growth along the polar direction, <111>, and its dependence on growth condition were fundamentally elucidated, showing a perfect agreement with experimental observations [2]. The proposed *ab initio* approach is truly independent of any empirical data, bridging to the experimentally controllable variables: growth conditions and directions. Therefore, it will contribute to the nanoscale growth of various materials, including other III-V and II-VI NWs and two-dimensional materials, where the precise control of the stacking sequence is significant for their properties.

References

1. I. W. Yeu, G. Han, J. Park, C. S. Hwang and J.-H. Choi, *Appl. Surf. Sci.* 497, 143740, **(2019).**
2. I. W. Yeu, G. Han, C. S. Hwang and J.-H. Choi, under review**.**