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Atomistic Modeling for the Vapor-Phase Growth of GaAs Nanowires: from DFT to Growth Kinetics — •In Won Yeu[1], Gyuseung Han[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[2] — [1]Electronic Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Korea — [2]Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea

Based on density functional theory (DFT), this study introduces an ab initio approach tackling the vapor-phase growth kinetics of III-V nanowire (NW) depending on temperature (T) and pressure (P) conditions. By evaluating the vibrational entropy contribution to the surface energy through surface phonon calculations, the T-P dependent variation in surface reconstructions was successfully predicted by the authors. Considering the surface transitions, the change in Gibbs free energy is calculated as a function of T and P at each growth process on surfaces: adsorption and nucleation. The comparison of the free energy among different surfaces enables us to predict the relative rate of growth depending on crystallographic directions and stacking sequences. As a result, we identify the mechanism of extreme anisotropic growth of GaAs (spontaneous NW formation) along a certain polar direction, <111>B; the preferential adsorption of vapor sources on (111)B surface, allowed at narrow T-P range, induces the unidirectional growth. In addition, the asymmetric formation of stacking sequence during the growth along the two opposite directions of a polar direction, <111>A and <111>B, is elucidated, showing a perfect agreement with experimental observations.

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