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

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The control of the crystal shape is crucial to design materials for various applications. To predict the crystal shape exactly, the atomic scale understanding is essential in terms of both the thermodynamics and kinetics. The variation of crystal shape is determined by the relative surface energy of each orientation depending on temperature (T), pressure (P), and strain (ε). Recently, we established a thorough methodology to calculate the surface energy [1] and the equilibrium crystal shape (ECS) [2] as a function of temperature (T) and pressure (P) for the III-V compound materials in the combined framework of density functional theory (DFT) calculations and thermodynamics. This methodology is competitive compared to the previous DFT studies providing the surface energy and ECS as a function of chemical potential (μ). In this study, the effect of substrates, which induces two-dimensional strain, on the surface energy is also estimated. Then, we construct the ECS of GaAs as a function of T and P on Si substrate. They are compared with the unstrained GaAs [2] and also compared with the experimentally grown shapes on Si substrate.

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References [1] In Won Yeu *et al.*, Sci. Rep. 7, 10691 (2017). [2] The 25th Korean Conference on Semiconductors (2018).