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# Equilibrium crystal shape of GaAs by ab-initio thermodynamics

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The growth of the III-V compound semiconductors on Si is crucial to adapt their superior electronic properties to the silicon-based CMOS technology. In order to achieve the high-quality hetero-epitaxy preventing defects such as dislocation, crack, and anti-phase boundary, the selective area growth (SAG) method has been developed. To optimize this process, the atomic scale understanding is essential in terms of both the thermodynamics and kinetics. In this study, we establish a thorough methodology to calculate the surface energy 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 [1], which is competitive compared the previous DFT studies providing the surface energy as a function of chemical potential. Then, we construct the equilibrium crystal shape of GaAs as a function of T and P, including the effects of surface vibration. The calculated equilibrium shapes in various T and P conditions are compared with the experimentally grown shapes and explained in the viewpoint of the surface vibration, twin formation and kinetic factors.
[1] In Won Yeu *et al.,* Sci. Rep. 7, 10691 (2017).