First-principles thermodynamic theory of epitaxial alloys: Prediction of spontaneous rotation of epitaxial habits in InGaN and GaAsSb alloys

ZHE LIU, Mechanical Engineering Department, Monash University, Australia, GIANCARLO TRIMARCHI, Department of Physics, Northwestern University, ALEX ZUNGER, National Renewable Energy Lab — A general-purpose method for calculating the stablest ground state structures and finite-temperature thermodynamics of AC-BC alloys grown epitaxially on a coherent substrate is presented. In addition to the fact that such coherent epitaxy stabilizes certain ordered phases, we discovered that depending on the substrate and the film concentration there is a spontaneous rotation of the stablest film microstructure. This general behavior is revealed for both mixed-cation (In, Ga)N and mix-anion Ga(As, Sb) alloys on a variety of substrates. Such spontaneous rotation of the epitaxial habits can be understood by the tetragonal ratio \( \eta \neq 1 \) of the corresponding bulk structure.

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