

Abstract Submitted
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First-principles thermodynamic theory of epitaxial alloys: Prediction of spontaneous rotation of epitaxial habits in InGaN and GaAsSb alloys¹ 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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