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How nucleation can cause stacking faults on the GaAs (111) B surface: A DFT study JOSHUA SHAPIRO, ANDREW LIN, DIANA HUFFAKER, CHRISTIAN RATSCH, UCLA — GaAs grows along the [111] direction much faster than other crystal axes at high growth temperature. In this work, we leverage this anisotropy, using catalyst-free selective-area epitaxy, to grow high-aspect ratio nanopillars. However, we find that the resulting crystal structure exhibits a high density of stacking faults that can have detrimental effects on the electronic and optical properties of the material. Each stacking fault is equivalent to a monolayer of wurtzite embedded in an otherwise zinc-blende lattice. The origins of stacking faults are currently under debate, with both thermodynamic equilibrium arguments and nucleation arguments proposed to explain the segments of wurtzite that appear in the primarily zinc-blende crystal. Here we present a density-functional-theory study of nucleation and island growth on the (111)B surface of GaAs that demonstrates how the smallest stable nucleus can transition and stabilize in either a wurtzite or a zinc-blende orientation.

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