Absolute surface energies of polar and non-polar planes in GaN

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Growth of high quality single crystals and epitaxial layers of GaN is critical for producing optoelectronic and power electronic devices that reach the full potential of this material system. One of the fundamental material properties that govern growth of single crystals is the absolute surface energy of the crystallographic planes. Knowledge of these energies is required to understand and optimize growth rates of different facets in GaN, which determine bulk and selective area growth morphologies. In addition, surface energies provide brittle fracture toughnesses of the crystal, which determine the propensity for cracks to form in different crystallographic directions. By means of hybrid functional calculations, we have determined absolute surface energies for the non-polar {11-20} *a* and {10-10} *m* and polar (0001) +*c* and (000-1) -*c* planes in wurtzite GaN. Since polar surface energies are ill defined due to the low symmetry in the *c* direction of the wurtzite structure, we approximate their values using the zinc-blende phase. For all surfaces, we consider low-energy bare and hydrogenated reconstructions under a variety of conditions relevant to experimental growth techniques. We find that the energies of the *m* and *a* planes are similar, and constant over the range of conditions studied. In contrast, the energies of the polar planes are strongly condition dependent. Even so, we find that the +*c* polar plane is systematically lower in energy than the -*c* plane.

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