Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Absolute surface energies, fracture toughness, and cracking in nitrides CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Matrials Department, University of California, Santa Barabara — Growth of high quality single crystals and epitaxial layers of GaN is critical for producing high-efficiency optoelectronic and power electronic devices. 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, and provide fracture toughnesses for brittle fracture. By means of hybrid functional calculations, we have determined absolute surface energies for the non-polar {11-20} a and {10-10} m planes, and approximated values for polar (0001) $+c$ and (000-1) $-c$ planes in wurtzite GaN. 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. We have used our surface energies to determine brittle fracture toughnesses in AlN and GaN, as well as the critical thickness for cracking of AlGaN on GaN.

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Date submitted: 12 Nov 2013 Electronic form version 1.4