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Surface Energies and Cracking in GaN[1] CYRUS E. DREYER, CHRISTIAN CARBOGNO, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Cracking is one of the biggest limitations to growing thick GaN single crystals and films, caused by the buildup and release of strain energy. Cracking occurs along preferential crystallographic planes in the GaN wurtzite structure, and depends on the tensile stress on the given plane and the energetic balance between the strain energy released from the crack formation versus the cleaved surface area created. It is also well known that the equilibrium shape of a crystal is largely determined by its surface free energy. Therefore, to correctly predict the stresses under which certain planes will crack and aid in understanding crystal growth, knowledge of the absolute surface energy is required. We use first-principles calculations based on density functional theory and a hybrid functional to determine the surface energy for the nonpolar {11-20} *a*- and {10-10} *m*-planes, as well to as explore approximations to the surface energies of the polar {0001}/{000-1} *c*-planes in GaN. The effects of structure relaxations and reconstructions are fully taken into account, and the results are discussed in the light of available experimental observations.

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