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Effects of strain on effective masses in GaN and AlN[1] CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Strain caused by lattice mismatch or alloying is present in almost all heterostructure-based semiconductor devices. One of the fundamental effects of strain on semiconducting materials is to alter their band gap and thus the effective mass of their carriers. Because of the lack of native substrates for GaN and the mismatch between different layers, these effects are particularly important in GaN/AlGaN based devices. Using first-principles calculations, we have investigated the effects of hydrostatic and c-plane biaxial strain on the band structure of GaN and AlN, specifically on the band gap and effective mass in the direction parallel and perpendicular to the c direction. In general, the effective mass decreases with increased hydrostatic or biaxial tensile strain, as expected from k.p theory. However, the opposite trend is observed for the effective mass of AlN in the c direction under biaxial strain. This is explained by analyzing the strained band structure of AlN using a two-band Kane model.

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