MAR11-2010-002370

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Causes of yellow luminescence in GaN

ANDERSON JANOTTI, University of California Santa Barbara

Although GaN is already used in light-emitting diodes and laser diodes, the origins of a number of frequently observed sub-band-gap luminescence bands are still under debate. For instance, the broad yellow luminescence that is invariably seen in n-type GaN has been long attributed to Ga vacancies. However, its presence in semi-insulating or p-type material, in which the Ga-vacancy concentration is low, has remained unexplained. The yellow luminescence has also been associated with the presence of carbon impurities, yet no credible, C-related configuration has been suggested. Using first-principles calculations we investigate the electronic and structural properties associated with defects and impurities in GaN. We employ a hybrid functional method to overcome the well-known band-gap problem of density functional calculations, and obtain accurate, quantitative results for defect transition levels. We find that C substituting for N (C_N) is a deep acceptor in GaN, with an ionization energy of 0.90 eV, in contrast to the commonly accepted view that C_N acts as a shallow acceptor. Incorporating C_N will therefore not result in *p*-type conductivity [1]. By inspecting the calculated configuration coordinate diagrams, we find that the absorption and emission lines of C_N are in remarkable agreement with the experimental results for yellow luminescence. This solves the longstanding puzzle regarding the nature of the defect responsible for yellow emission in C-containing GaN, and suggests that previous experimental data, analyzed under the assumption that C_N acts as a shallow acceptor, should be revisited. Work performed in collaboration with J. L. Lyons and C. G. Van de Walle, and supported by the NSF and by the UCSB Solid State Lighting and Energy Center.

[1] J. L. Lyons, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. 97, 152108 (2010).