Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Native defects in GaN: a hybrid functional study[1] IBRAHIMA CASTILLO DIALLO, DENIS DEMCHENKO, None — Intrinsic defects play an important role in the performance of GaN-based devices. We present hybrid density functional calculations of the electronic and possible optical properties of interstitial N (N_i-N_i), N antisite (N_{Ga}), interstitial Ga (Ga_i), Ga antisite (Ga_N), Ga vacancy (V_{Ga}), N vacancy (V_N) and Ga-N divacancies ($V_{Ga}V_N$) in GaN. Our results show that the vacancies display relatively low formation energies in certain samples, whereas antisites and interstitials are energetically less favorable. However, interstitials can be created by electron irradiation. For instance, in 2.5 MeV electron-irradiated GaN samples, a strong correlation between the frequently observed photoluminescence (PL) band centered around 0.85 eV accompanied with a rich phonon sideband of ˜0.88 eV and the theoretical optical behavior of interstitial Ga is discussed. N vacancies are found to likely contribute to the experimentally obtained green luminescence band (GL2) peaking at 2.24 eV in high-resistivity undoped and Mg-doped GaN.

[1]National Science Foundation (DMR-1410125) and the Thomas F. and Kate Miller Jeffress Memorial Trust.

Ibrahima Castillo Diallo
None

Date submitted: 21 Jan 2016 Electronic form version 1.4