Sources of Shockley-Read-Hall recombination in III-nitride light emitters

CYRUS E. DREYER, Department of Physics and Astronomy, Rutgers University, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology, Vilnius, Lithuania and Kaunas University of Technology, Kaunas, Lithuania, JOHN L. LYONS, Center for Functional Nanomaterials, Brookhaven National Laboratory, JAMES S. SPECK, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Group-III nitrides are the key materials for high efficiency light-emitting diodes in the blue part of the visible spectrum, and a large research effort is aimed at extending this success to the green and the yellow range, where nitride LEDs are significantly less efficient. Though it has been noted that the efficiency of III-nitride devices may be limited by Shockley-Read-Hall recombination at point defects, the microscopic mechanism and defects responsible are unknown. Based on first-principles calculations of defect formation energies, charge-state transition levels, and nonradiative capture coefficients, we describe a mechanism by which complexes between gallium vacancies and oxygen and/or hydrogen can act as efficient channels for nonradiative recombination in InGaN alloys. The dependence of these quantities on alloy composition is analyzed. We find that modest concentrations of the proposed defect complexes, around $10^{16}$ cm$^{-3}$, can give rise to Shockley-Read-Hall coefficients $A = (10^7 - 10^9)$ s$^{-1}$. The resulting non-radiative recombination can significantly reduce the internal quantum efficiency of optoelectronic devices.

1This work was supported by DOE and by EU Marie Sklodowska-Curie Action.