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Auger recombination rates in nitrides from first principles

PATRICK RINKE, KRIS T. DELANEY, CHRIS G. VAN DE WALLE, University of California at Santa Barbara, CA 93106 — Indium gallium nitride (InGaN) alloys are successfully being used for light emitting and laser diodes in the green to ultraviolet part of the spectrum, but increases in internal quantum efficiency (IQE) are still required to allow broader applications. The IQE of InGaN devices is limited by loss mechanisms that, at high drive currents (i.e., high carrier concentrations) lead to a decrease in IQE, a phenomenon commonly referred to as "efficiency droop". We demonstrate by means of rigorous first-principles calculations (density-functional and many-body-perturbation theory), in which individual loss processes can explicitly be isolated, that Auger recombination is a key loss mechanism in wurtzite InGaN. Auger recombination had previously been proposed by Shen *et al.* [1] as a loss mechanism in optically pumped InGaN LED devices, but it is difficult to discriminate between different radiationless processes experimentally. We examine two different mechanisms – inter- and intra-band recombination – that affect different parts of the spectrum. In the blue to green spectral region and at room temperature the Auger coefficient can be as large as 2×10^{-30}cm^{6}s^{-1} and in the infrared even larger. Since Auger recombination scales with the cubic power of the free-carrier concentration it becomes an important non-radiative loss mechanism at high current densities. [1] Shen *et al.*, Appl. Phys. Lett. **91**, 141101 (2007).

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