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Abstract

First-principles calculation of Auger recombination
and internal absorption loss in nitride light emitters.

Carrier recombination processes play an important role in the operation of semiconductor optoelectronic devices. In particular, the competition between radiative and Auger recombination determines the efficiency of light emitters and may limit their high power performance. Despite its significance for devices, calculations of the Auger recombination rate are very challenging computationally and the number of reported theoretical results is limited. In this work, we calculate the Auger recombination rate in the group-III-nitrides, an important class of materials used for visible light emission. We show that the dominant Auger processes in these wide-band-gap materials are indirect ones, mediated by electron-phonon coupling and alloy scattering. The calculated values of the Auger coefficient indicate that it constitutes the dominant loss mechanism at high drive currents that limits the performance of nitride devices. Moreover, an additional loss mechanism in laser devices is the internal reabsorption of the generated light. We show that indirect free-carrier absorption is particularly strong in the nitrides and responsible for the observed modal loss in nitride lasers. Our calculations identify the importance of intrinsic loss mechanisms in optoelectronic devices and demonstrate the capabilities of first-principles calculations in energy materials research.