Trap-assisted Nonradiative Recombinations from First Principles

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Trap-assisted nonradiative recombination is a key mechanism limiting the efficiency of optoelectronic devices such as light emitting diodes. Trap-assisted recombination via multiphonon emission (MPE) has been studied from first principles;[1] its rate was found to become negligibly low in materials with band gaps larger than about 2.5 eV,[2] and it cannot explain the experimentally measured trap-assisted recombination rates in such materials[3]. We have proposed and developed a practical first-principles methodology to calculate the trap-assisted Auger-Meitner (TAAM) rate in semiconductors,[4] and shown that TAAM recombination can account for the experimental observations. As a first case study, we applied our formalism to a calcium substitutional impurity in InGaN. We found that for band gaps larger than 2.5 eV, the combination of hole capture by MPE and electron capture by TAAM results in recombination rates orders of magnitude larger than the recombination rate governed by MPE alone.[4] Our computational formalism is general and can be applied to any defect or impurity in any semiconducting or insulating material.

Building on this formalism, we have further investigated the role of substitutional carbon C_N as a nonradiative recombination center in GaN optoelectronic devices. We systematically analyzed the contributions of MPE, TAAM, radiative recombination, and thermal emission, revealing that TAAM plays a dominant role at the high carrier densities relevant for device operation.[5] Additionally, we identified the carrier-density regimes where thermal emission and radiative recombination become significant. Our results highlight that carbon concentrations exceeding $\sim 10^{17}$ cm^{-3} can have a noticeable impact on device efficiency, not just in GaN active layers but also in InGaN and AlGaN. Our work extend our formalism and provide a general framework for assessing the multiple processes that participate in trap-assisted recombination in semiconductors.[5]

References

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