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Theory of multiphonon inelastic scattering and carrier capture by defects in semiconductors - Application to capture cross sections[1]
GEORGIOS D. BARMPARIS, YEVGENIY S. PUZYREV, Vanderbilt University, X.-G. ZHANG, University of Florida, SOKRATES T. PANTELIDES, Vanderbilt University — Inelastic scattering and carrier capture by defects in semiconductors are the primary causes of hot-electron-mediated degradation of power devices. At the same time, carrier capture is a major issue in the performance of solar cells and light-emitting diodes. First-principles, parameter-free calculations of inelastic-scattering and capture cross sections as functions of carrier energy can provide guidance for modeling device degradation based on atomic-scale physical mechanisms. Here we report the construction of a comprehensive theory of multiphonon inelastic scattering by defects, with carrier capture being a special case. We resolve the old debate about what constitutes a correct theory of capture cross sections and report first-principles density-functional-theory calculations of capture cross section for three prototype defects. A Monte Carlo algorithm has been developed to obtain converged sum over all possible phonon configurations. The results reveal that the capture cross section depends strongly on the energy of the incoming electron.

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