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Multiphysics simulation of high-frequency carrier dynamics in conductive materials

Source

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Abstract

We present a multiphysics numerical technique for the characterization of high-frequency carrier dynamics in high-conductivity materials. The technique combines the ensemble Monte Carlo (EMC) simulation of carrier transport with the finite-difference time-domain (FDTD) solver of Maxwell's curl equations and the molecular dynamics (MD) technique for short-range Coulomb interactions (electron-electron and electron-ion) as well as the exchange interaction among indistinguishable electrons. We describe the combined solver and highlight three key issues for a successful integration of the constituent techniques: (1) satisfying Gauss's law in FDTD through proper field initialization and enforcement of the continuity equation, (2) avoiding double-counting of Coulomb fields in FDTD and MD, and (3) attributing finite radii to electrons and ions in MD for accurate calculation of the short-range Coulomb forces. We demonstrate the strength of the EMC/FDTD/MD technique by comparing the calculated terahertz conductivity of doped silicon with available experimental data for two doping densities and showing their excellent agreement. (C) 2011 American Institute of Physics.