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Title:Multiphysics simulation of high-frequency carrier dynamics in conductive materials
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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 EMCFDTDMD technique by comparing the calculated terahertz conductivity of doped silicon with available experimental data for two doping densities and showing their excellent agreement.
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