# A Generalized Drude Model for Doped Silicon at THz Frequencies Derived from FDTD/EMC/MD Simulations

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The characteristic scattering rate of doped silicon falls within the terahertz (THz) frequency band. Experimental characterizations have shown that for low and moderate doping densities (i.e. $< 10^{18}$ cm$^{-3}$) these materials cannot be adequately represented by the Drude model, which assumes that the electromagnetic frequency, $\omega$, is much smaller than the scattering rate, $\tau^{-1}$ (T. I. Jeon and D. Grischkowsky, Phys. Rev. Lett. 78, 1106, 1997). Experimental THz conductivity data for silicon is available for only a few specific doping densities, and a full description of electronic properties in this frequency range does not exist. Therefore, accurate numerical simulations based on a microscopic picture of carrier-field interactions offer a valuable characterization of doped silicon at these frequencies.

We present a full characterization of doped silicon conductivity over a broad range of frequencies (0-2.5 THz) and doping densities ($10^{14}$-$10^{18}$ cm$^{-3}$) using a recently-developed computational technique that accurately describes carrier dynamics under high-frequency electromagnetic excitation. The tool combines the finite-difference time-domain (FDTD) technique for Maxwell's equations with the ensemble Monte Carlo (EMC) technique for the Boltzmann transport equation and the molecular dynamics (MD) technique for close-range Coulomb interactions. EMC is a stochastic modeling technique that accurately describes carrier transport in materials, through the use of known material band structure and energy-dependent scattering rates. MD describes the short-range Coulomb forces between particles at distances smaller than an FDTD grid cell, and the exchange interaction between electrons. At each time step, microscopic currents from EMC carrier motion influence FDTD electric field updates according to Amperes law, while electrodynamic fields from FDTD and close-range Coulomb forces from MD influence EMC carrier motion according to the Lorentz force. The conductivity computed by the combined EMC/FDTD/MD technique shows excellent agreement with experimental data (K. J. Willis, S. C. Hagness, and I. Knezevic, J. Appl. Phys., 110, 063714, 2011).

We conducted many thousands of simulations to generate a comprehensive data set for the complex conductivity of silicon at five doping densities and 26 discrete frequencies. We show that the complex conductivity of doped silicon may be accurately described by the generalized Drude (GD) analytical model with doping-dependent fitting parameters, and we present these parameters for silicon. The resulting analytical description can be used readily to predict the complex conductivity of arbitrarily doped samples within the investigated range.