Abstract

Dynamic Effective Medium Theory of Nanosphere Materials

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A dynamical effective medium theory is developed for modeling the optical properties of square and cubic arrays of non-magnetic nanospheres in a dielectric medium. The theory yields dielectric functions, $e_{eff}(k, ø)$, for nanoparticle materials in terms of the polarizabilities of the individual nanospheres, the nanosphere volume fraction, and the dielectric constant of the medium (Lazarides and Schatz, Theochem 529, 2000). The dielectric functions satisfy the dispersion relation that characterizes plane wave propagation through the nanosphere lattice of spheres. The effective dielectric functions are calculated by inverting the lattice dispersion relation for lattice dipole polarizabilities derived by Draine and Goodman (Astrophysical J. 405, 1993) for use in discrete-dipole representations of bulk media. The dynamical effective medium theory is tested by comparing extinction spectra for finite samples calculated using the effective medium model with spectra calculated using an explicit model of the interacting nanosphere components and found to be accurate for 13 nm gold particles at metal volume fractions up to 0.4. The theory is compared with several other effective medium theories including Maxwell-Garnett theory, Torquato-Lado theory, and theories that apply partial dynamical corrections to quasi-static theory. Of the dipole theories, Maxwell-Garnett theory (with a particle-size dependent inclusion dielectric function) is found to provide the closest agreement with the dynamical effective medium theory and explicit coupled particle calculations. An explanation is provided for the well-documented observation that quasi-static theories provide surprisingly accurate continuum descriptions of materials that are heterogeneous on length scales that are substantial fractions of the wavelength of light. Higher-order static theory, tested against explicit coupled multipole electrodynamic calculations, is found to overestimate the interparticle interaction.

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