Abstract

This work reports the calculated dependence of the localized surface plasmon resonance (LSPR) parameters and damping mechanism on nanoparticle size of unconventional transition metals, including zinc, silver, rhodium, rhenium, molybdenum, tantalum, titanium, and scandium, within the size range of 10 to 400 nm. The study applies Mie theory to determine the peak energies, amplitude, and full width at half maximum (FWHM) of LSPR as a function of size, shape, and material type. We have found that the parameters of LSPR depend on electron structure and damping mechanisms. LSPR amplitude decreased systematically for individual nanoparticles (NPs) for sizes 10…200 nm, after which, a similar trend was exhibited due to radiative damping. Au, Sc and Ag are the only metal NPs that exhibited a significant FWHM of LSPR at sizes approximately below 40 nm. For all investigated transition metal NPs, smaller NPs exhibited higher absorption and lower scattering, while larger NPs showed narrower FWHM and red-shifted LSPR peaks due to retardation effects and multipolar plasmon excitations. The analysis highlights that some transition metal NPs exhibit optical characteristics similar to those of gold, silver, and copper, making them a good alternative for the mentioned ones at specific NP sizes.