A Theoretical Study on Optical - Thermal Energy Conversion in Metallic Nanoparticles

Y. He and T. Zeng[C,S]
Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, NC, U.S.A.
tzeng2@unity.ncsu.edu

Light-nanoparticle interaction is an interesting topic in thermal physics. It is known that the optical properties of nanoparticles differ significantly from that of bulk materials, and are dependent upon the shape and size of the particles. There has been much literature discussing the extinction spectral characters of metallic nanoparticles. These literatures mainly focus on the noble metals (e.g., Cu, Ag, and Au) [1]. However, two factors must be pointed out. First, the extinction coefficient of a nanoparticle consists of two parts, the absorption coefficient and the scattering coefficient. Only the former component transforms the radiation energy into heat, while the latter component just scatters the incidence into the space. Thus the extinction spectra cannot be used to characterize the optical – thermal energy conversion. As a part of a project on heat transfer in nanoparticle systems, this study aims to find the conversion of optical energy to thermal energy or the absorption coefficient in nanoparticles. Secondly, other than noble nanoparticles, metal nanoparticles such as nickel, especially those with complex composition such as FePt, have hardly been investigated. These nanoparticles are an object of the study.

We simulate the extinction and absorption spectra of nanoparticles of a set of common metals and some bimetal metals in order to investigate the optical - thermal energy conversion efficiencies for wavelengths in the range from 300 to 1200 nm. The discrete dipole approximation (DDA) method is utilized in the calculation [2]. The DDA method is a numerical finite element method. It meshes the target into a number of dipoles and performs calculations iteratively. Obtained optical properties of nanoparticles with a single composition (e.g. Fe particle and Pt particle) and a dual composition (e.g. FePt) are compared. The composition (structural) effect and the size effect are discussed.

[1] S. Link, M.A. Ei-Sayed, *Annual Rev. Phys. Chem.* **54**, 331 (2003).
[2] W.H. Yang, G.C. Schatz, and R.P.Van Duyne, *J. Chem. Phys.* **103,** 869 (1995).