Accuracy of the discrete dipole approximation for gold nanoparticles

Maxim A. Yurkin,[1,2] David de Kanter,[3] and Alfons G. Hoekstra[3]

[1]*Institute of Chemical Kinetics and Combustion, SB RAS, 3 Institutskaya St., 630090, Novosibirsk, Russia*
[2]*Novosibirsk State University, 2 Pirogova St., 630090, Novosibirsk, Russia*
[3]*Computational Science Research Group, Faculty of Science, University of Amsterdam, Science Park 107, 1098 XG, Amsterdam, The Netherlands*
e-mail: yurkin@gmail.com

Plasmon resonance in metal nanoparticles has gained increasing interest in recent years due to its ability to concentrate electromagnetic energy into subwavelength regions. One of the commonly used methods to simulate interaction of light with nanoparticles is the discrete dipole approximation (DDA, [1]). The agreement between the DDA simulations and experiments for extinction spectra of gold nanoparticles has never been perfect. However, the disagreement is attributed mostly to uncertainties in the particle shape and in the gold refractive index. The accuracy of the DDA itself for scattering of light by gold nanoparticles is usually quoted as "good enough if a large enough number of dipoles is used", i.e., the discussion is qualitative, with no error estimates available.

We studied the DDA accuracy for simulations of light scattering by gold nanoparticles in a vacuum. We chose three particle shapes (a sphere, a cube, and a rod) and two sizes (10–100 nm) and computed absorption and scattering spectra, using a range of discretizations (numbers of dipoles) and two DDA formulations: the standard lattice dispersion relation (LDR) and the relatively-new filtered coupled dipoles (FCD, [2]). The publicly available code ADDA [3] was used for simulations. At the conference we will show graphs of relative errors of calculated quantities versus wavelength, as well as errors in the position and amplitude of the main spectral peak.

The main conclusion is that caution should be exercised when using the DDA in this regime. With moderate dipole resolutions it is sufficiently accurate for scattering efficiencies or positions of spectral peaks, but very inaccurate for, e.g., values of absorption efficiencies in the near-IR. To keep relative errors of the latter within 10%, about 10^7 dipoles per sphere are required. The accuracy of the extinction efficiency shows a strong size dependence; in particular, it is unusually poor for nanoparticles smaller than 50–200 nm depending on the wavelength. Surprisingly, the errors for cubes are about 10 times smaller than those for spheres or rods, which we explain in terms of shape errors. The FCD is generally more accurate and leads to up to 2 times faster computations than the LDR. Therefore, we recommend FCD as the DDA formulation of choice for gold and other metallic nanoparticles.

Acknowledgement. M.Y. has been supported by the program of the Russian Government "Research and educational personnel of innovative Russia" (contract P2497).

References

[1] M. A. Yurkin and A. G. Hoekstra, "The discrete dipole approximation: an overview and recent developments," J. Quant. Spectrosc. Radiat. Transfer **106**, 558–589 (2007).

[2] N. B. Piller and O. J. F. Martin, "Increasing the performance of the coupled-dipole approximation: a spectral approach," IEEE Trans. Antennas Propag. **46**, 1126–1137 (1998).

[3] M. A. Yurkin, V. P. Maltsev, and A. G. Hoekstra, "The discrete dipole approximation for simulation of light scattering by particles much larger than the wavelength," J. Quant. Spectrosc. Radiat. Transfer **106**, 546–557 (2007).