Info taken from the Nano-Optics Module, 2015 BioNanotechology Summer Institute
Credit: Prashant K. Jain, Jeremy G. Smith

Background

The strongly enhanced surface plasmon resonance of noble metal nanoparticles at optical frequencies makes them excellent scatterers and absorbers of physical light. Superior optical properties, coupled with recent advances in nanoparticle synthesis, conjugation, and assembly, have stimulated interest in the use of plasmon- resonant nanoparticles and nanostructures for optical and photonic applications and, more recently, for biomedical applications. Nanoparticles composed of gold offer, in addition to their enhanced absorption and scattering, good biocompatibility, facile synthesis, and conjugation to a variety of biomolecular ligands, antibodies, and other targeting moieties, making them suitable for use in biochemical sensing and detection, medical diagnostics, and therapeutic applications. There have been several demonstrations of bioaffinity sensors based on the plasmon absorption and scattering of nanoparticles and their assemblies.

Another notable use of gold nanoparticles has been as contrast agents in cellular and biological imaging. Contrast agents in medical and biological imaging improve the sensitivity and diagnostic ability of the imaging modality by site-specifically labeling tissues or cells of interest. The effectiveness of nanoparticles as biomedical imaging contrast and therapeutic agents depends on their optical properties. For instance, a high-scattering cross- section is essential for cell imaging applications based on light-scattering microscopy. On the other hand, effective photothermal therapy with minimal laser dosage requires a high nanoparticle absorption cross-section with low scattering losses. Biosensing applications based on surface plasmon resonance shifts necessitate strong resonance in the wavelength sensitivity range of the instrument as well as narrow optical resonance line widths. For actual in vivo imaging and therapeutic applications, the optical resonance of the nanoparticles is strongly desired to be in the near-infrared (NIR) region of the biological water window, where the tissue transmissivity is the highest. In addition, the nanoparticle size is also an important consideration for nanoparticle uptake and retention by cells and tissue.

It is well-known that the plasmon resonance of metal nanoparticles is strongly sensitive to the nanoparticle size, shape, and the dielectric properties of the surrounding medium. Optical properties of gold nanoparticles can thus be readily tuned by varying their size and shape. In order to harness the full power of these phenomena, scientists need to understand the interactions of light with nanoparticles at very small length scales. There have been several experimental reports on the optical properties of metal nanoparticles, including gold nanospheres, nanorods, and nanoprisms, silver nanospheres, nanowires, and nanoprisms, copper nanospheres, aluminum

nanospheres, bimetallic nanoparticles, composite nanoparticles with a core-shell structure, and nanoparticle chains and assemblies. At the same time, well-established theoretical tools based on the Mie theory and the discrete dipole approximation (DDA) method have been readily exploited for a quantitative study of the nanoparticle optical properties of different size, shape, composition, and aggregation state, etc.

A very powerful method for determining the interaction of electromagnetic radiation with particles is known as the Discrete Dipole Approximation (DDA). Using DDA, the particle is discretized into an array of dipoles, or polarizable points. This method then solves Maxwell's equations for an incident field interacting with each of the dipoles individually. The resulting data can be used to compute scattering and absorption properties of the array of dipoles and, hence, the particle. This method relies on the assumption that the dielectric properties of the particle, and it's interaction with the incident field, are directly related to the polarizability of the constituent dipoles.

A popular code for the implementation of DDA calculations is called DDSCAT. DDSCAT allows for the computation of absorption and scattering properties of particles with arbitrary shapes and geometries, and provide outputs of light extinction, absorption, and scattering properties at various wavelengths of incident light.

The nanobioNODE at University of Illinois has developed a tool on nanoHUB.org that creates a simple and intuitive interface for using the DDSCAT code developed by Draine and Flatau. This allows experimental chemists and biologist not familiar with computational methods a visual interface in which they can simulate the interaction of light with nanoparticles of any geometry and compute light scattering, absorption, and plasmonic near field enhancement.

References

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