Nanocomposites and nanomaterials

The influence of the shape on the optical properties of nanoparticles

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Metal nanoparticles have attracted a great attention due to their strong interaction with light. The collective movements of electrons are resonant at optical frequencies and the surface charge and local electric field distribution depends on the shape of the nanoparticle [1].

In the real materials we deal with nanocomposites that have the nanoparticles of the irregular shape, different from sphere. A few analytical solutions are known for very simple geometrical shapes as spheres, cylinders or ellipsoids. Once the target is converted to a collection of simple particles, the scattering problem can be solved exactly for each particle shape.

The Blender is a 3D editor that can used to create and voxelize nanoparticles with different shapes and sizes and prepare the input data to the methods that will calculate optical response of the complex objects [2]. The discrete dipole approximation (DDA) is a method to compute scattering of radiation by particles of arbitrary shape [3] through approximating the target by an array of polarizable points (dipoles), assigning polarizabilities at these locations based on the physical properties of the target, and solving self-consistently for the polarization at each location in the presence of an incident radiation field.

The Blender tools and the discrete dipole approximation method were used to calculate optical spectra of silver nanoparticles of different shapes. The optical response was investigated for such shapes as a pyramid and a cube and compared with the optical response of the spherical nanoparticle.

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2. *Demchuk A.O., Bolesta I.M.* Voxel-based mesh generation for computational electromagnetics simulations // Abstracts of the International Conference "Nanotechnology and Nanomaterials – 2016". – 2016. -P. 54.

3. *Draine B. T.* The discrete-dipole approximation and its application to interstellar graphite grains // Astrophys. J.- 1988.- **333**.-P. 848-872.