Simulating nanoparticles interaction with an electron beam using the discrete dipole approximation

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Introduction

Studying the optical properties of plasmonic nanoparticles, scientists conduct experiments in which the nanoparticle is scanned by an electron beam [1]. The main advantage of an electron beam over optical methods (limited by the diffraction limit) is that it allows one to localize plasmon resonances on the surface of a nanoparticle with the accuracy of at least 1 nm. When scanning a nanoparticle, fast electrons lose energy (electron energy loss spectroscopy – EELS), and the particle emits light (cathodoluminescence – CL). As a result of the experiment, EELS and CL spectra are obtained for each position of the beam on the particle cross-section.

To correctly interpret the data obtained in the experiment, it is necessary to numerically simulate the experiment. The existing theory covers only the case of interaction of a particle and an electron in a vacuum - when there nothing else present. But in reality, the particle is placed on a substrate (or inside a substrate) to resist gravity and collisions with fast electrons.

Results

In this work, the volume-integral formulation of Maxwell's equations in terms of the Green's tensor was used [2]. As a result, we obtained a generalized solution for interaction of a particle and electron in an arbitrary (including absorbing) infinite host medium, including the case of Cherenkov radiation. This solution was not known previously, but its limiting case of vacuum matches the previously known theory.

The expressions obtained with this solution for simulating the EELS and CL were implemented in the open-source software ADDA (currently available in a separate fork – https://github.com/alkichigin/adda), based on the discrete dipole approximation [3]. The simulation results for spheres in a vacuum showed agreement with the exact reference solution (Lorentz-Mie theory). Moreover, the simulated spectrum for a silver sphere in a non-absorbing medium (SiNx plate, speed of light 0.55*c*, where *c* is the speed of light in vacuum) matched the experimental one, where electrons had the 120 keV energy (the corresponding speed is 0.59*c* – Cherenkov radiation case). This and other results will be demonstrated at the conference.

[1] F. J. García de Abajo, 'Optical excitations in electron microscopy', *Rev. Mod. Phys.*, vol. 82, no. 1, pp. 209–275, Feb. 2010, doi: 10.1103/RevModPhys.82.209.

[2] M. A. Yurkin and M. I. Mishchenko, 'Volume integral equation for electromagnetic scattering: Rigorous derivation and analysis for a set of multilayered particles with piecewise-smooth boundaries in a passive host medium', *Phys. Rev. A*, vol. 97, no. 4, p. 043824, Apr. 2018, doi: 10.1103/PhysRevA.97.043824.

[3] M. A. Yurkin and A. G. Hoekstra, 'The discrete dipole approximation: an overview and recent developments', *J. Quant. Spectrosc. Radiat. Transf.*, vol. 106, no. 1–3, pp. 558–589, 2007, doi: 10.1016/j.jqsrt.2007.01.034.