Electron Energy Loss Spectroscopy Simulation for Plasmonic Nanoparticles using a Time Domain Surface Integral Equation Solver

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Electron energy loss spectroscopy (EELS) is a well-known technique developed for analyzing atomic and electronic structure of various materials. In recent years, it has been adapted to investigate plasmonic properties of nanoparticles. In parallel to this shift in the experimental approach, various numerical techniques are modified to simulate the EELS experiments on a computer. These techniques include frequency-domain surface integral equation (FDSIE) solver (F. J. Garcia de Abajo and A. Howie, *Phys. Rev. B*, 65, 1-17, 115418), discontinuous Galerkin time domain (DGTD) scheme (C. Matyssek *et al.*, *Phot. Nano. Fund. Appl.*, 9, 367-373, 2011), and finite difference time domain (FDTD) method (Y. Cao *et al.*, *ACS Photonics*, 2, 369-375, 2015). The FDTD and DGTD schemes require volumetric discretization leading to large number of unknowns and they truncate computation domains using (approximate) artificial absorbing boundary conditions to mimic the radiation condition. On the other hand, FDSIE solver discretizes only the surfaces of nanoparticles and implicitly (and exactly) enforces the radiation condition without the need for absorbing boundary conditions. However, being a frequency-domain technique, it cannot easily account for nonlinear effects and may not be efficient when wideband simulations are required.

In this work, to overcome the shortcomings briefly described above, EELS for plasmonic nanoparticles is simulated using the marching-on-in-time (MOT) scheme developed for solving the time domain Poggio-Miller-Chan-Harrington-Wu-Tsai surface integral equation (TD-PMCHWT-SIE) (I. E. Uysal *et al.*, *J. Opt. Soc. Am. A*, 33, 1747-1759). In the simulations, electromagnetic fields generated by a fast moving electron are used to excite the plasmonic nanostructure and the scattered fields are computed along the electron's path to yield the energy loss probability of the electron. It should be noted here that this approach produces wideband data with a single simulation while maintaining the advantages of the FDSIE solver listed above.

Validity of the proposed approach will be demonstrated through its application to the computation of electron energy loss probability for different plasmonic nanoparticles including spheres and cuboids made of aluminum, gold or silver. The results will be compared to those obtained by analytical or other numerical methods whenever possible.