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Finite and Boundary Element Methods for Simulating Optical Properties of Plasmonic Nanostructures

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Abstract
In this study, a numerical investigation was done on the optical properties of silver nanostructures using the boundary element method (BEM) and finite element method (FEM). The BEM simulation was done using a freely available code called MNBEM in MATLAB with minor modifications. The FEM simulation was done by Comsol Multiphysics, a commercial software package. Silver nanostructures in the sphere, rod, and triangle geometries and the presence of different polarization angles were compared between these two methods. According to the obtained results, the absorption cross-sections for both BEM and FEM were consistent with their actual optical properties. For instance, both longitudinal and transverse resonance modes were observed in the case of nanorods, and all three in–plane dipole, in–plane quadrupole, and out–plane quadrupole plasmon resonances were observed successfully obtained for triangular nanostructures. Although both BEM and FEM results were similar to each other (from the number and position of the peaks in the final spectra), this similarity was decreased as the anisotropy was increased in the structure. For example, nearly 40 nm difference was observed between the BEM and FEM results in the triangular nanostructures, even though the trends and shape of the peaks were similar. It was revealed that specific points should be considered in the discretization process (especially the corner fillets) to close the gap in the obtained results from BEM and FEM. According to the obtained results, BEM significantly reduces the computational cost and time by discretizing only the boundary of the domain. A self-written software was developed to predict the optical cross-section of a plasmonic-ensemble consisting of spherical, rod-shaped, and triangular nanostructures, which can be used in different disciplines such as plasmon-enhanced solar cells, plasmon-enhanced photocatalysis, and plasmon-enhanced fluorescence.

Keywords Finite element method · Boundary element method · Surface plasmon resonance · Optical properties · Silver nanostructures · Plasmonics · Optical software · Optical simulation · Silver nanotriangle · Silver nanorod

Introduction

Localized surface plasmon resonance (LSPR) is an attractive optical phenomenon resulting from the confinement of electromagnetic waves within the immediate environment of metallic nanoparticles. During the last decade, the investment from multidisciplinary fields has been vastly increased in LSPR, and its application has been broadened from sensitive single-molecules detection to solar cells and biomedical practices [1–8]. The practical applications of plasmonic nanostructures are closely related to the physical characteristics of the generated SPR, which indeed is a function of size, geometry, composition, and the environment of the nanostructure [9–16]. In this regard, there is a great interest in predicting the performance of a desired plasmonic system. We have published a recent comprehensive review paper on the application of computational electromagnetics in plasmonic nanostructures, which one can refer to as a complete guide [17]. Theoretically, surface plasmon resonance and the related electric field enhancement can be described using classical electromagnetics, solving Maxwell's equations for the desired plasmonic material with the defined dielectric function in the presence of an external field [18]. Several methods are available for the numerical simulation of

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