Using the Lorentz Reciprocity Theorem with the Transfer Matrix Method in Python

Ekaterina Zossimova[1,2] **and Yuriy Akimov**[1]
1- Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, Singapore
2- Department of Physics and Astronomy, University of Exeter, Exeter EX4 4QD, UK
Author e-mail address: akimov@ihpc.a-star.edu.sg

Abstract: We present a simple way to calculate and visualize far-field radiation patterns due to polarizable particles at the surface of complex multilayer materials by means of the Lorentz reciprocity theorem and the python Jupyter notebook. © 2021 The Author(s)

1. Introduction

Many applications in optics and photonics require computation of light propagation through multilayer structures. In the natural sciences, such structures are intensively used to create state-of-the-art biosensors based on their resonant response to optical excitations. These types of calculations are already accessible to students through the open-source "tmm" Python software package [1], which implements the Transfer Matrix Method for propagation of light through multilayer planar stacks. In this work, we present a complementary feature to the tmm code, which enables computation of the far-field radiation pattern of a spherical particle at the top interface of the multilayer stack by means of the Lorentz reciprocity theorem. This theorem provides a computational ‘short-cut’ to explore the effect of a polarizable particle with tmm code, which would otherwise require computationally expensive grid-based methods to solve numerically.

2. Optical Simulations

1.1. Transfer Matrix Method

The Transfer Matrix Method is an analytical method to solve Maxwell’s equations in planar layered structures. The boundary conditions for Maxwell’s equations are solved at each interface, which makes this method much faster in comparison to methods that rely on solving Maxwell’s equations on discretized spatial grids.

The multilayer structure used in this study is based on the Kretschmann configuration and consists of an LaSFN9 substrate, Cr layer of 2 nm for better bonding, Au film of 48 nm, SiO2 spacer of 22 nm for optimized performance and water as a sensing medium [2]. This structure is known to have enhanced fields at the top interface when the incident light is in resonance with eigenmodes of the multilayer [3, 4]. The enhanced fields appear in the Kretschmann configuration under total internal reflection, enabling efficient dark-field spectroscopy of single particles/molecules.

The schematic representation of the Kretschmann configuration with a small polarizable particle on the top interface is shown in Fig. 1A. The field enhancement at the spacer/water interface is optimized for p-polarized light incident from the substrate at the wavelength of 780 nm. Fig. 1B shows the comparison between the field enhancement of the Kretschmann configuration and the bare substrate case as a reference. The Kretschmann configuration provides a three-fold enhancement at an incident angle of 49.8° in comparison to the bare substrate case.

1.2. Lorentz Reciprocity Theorem

The polarizable sphere is assumed to be subwavelength, so it can be effectively treated as a point dipole. We used the optimized field enhancement, $\mathbf{E}_{\mathrm{max}}$, at the dipole position ($\mathbf{r} = \mathbf{r}_{\mathrm{d}}$) to define dipole moment, $\mathbf{p} = \alpha\mathbf{E}_{\mathrm{max}}$, where α is a real scalar polarizability. By the Lorentz reciprocity theorem for two point dipoles [5], we reverse the order of the layers in the Kretschmann configuration and calculate the inverse incidence of plane waves from the water side. We calculate the electric near-field, $\mathbf{E}_{\mathrm{near}}^{\mathrm{S,P}}$, due to s- and p- polarized light at the position of the dipole. The relationship between the near-fields, at position $\mathbf{r}_{\mathrm{d}}$, and the radiated far-field, $\mathbf{E}_{\mathrm{rad}}$, is given by,

$$|\mathbf{E}_{\mathrm{rad}}|^2 = \left|\mathbf{E}_{\mathrm{rad}}^{\mathrm{S}}\right|^2 + \left|\mathbf{E}_{\mathrm{rad}}^{\mathrm{P}}\right|^2 = |\mathbf{E}_{\mathrm{near}}^{\mathrm{S}}(\mathbf{r}_{\mathrm{d}}) \cdot \mathbf{p}|^2 + |\mathbf{E}_{\mathrm{near}}^{\mathrm{P}}(\mathbf{r}_{\mathrm{d}}) \cdot \mathbf{p}|^2. \qquad (1)$$

Then, the Poynting vector can be calculated as $|\mathbf{E}_{\mathrm{rad}}|^2 n/2\eta_0$, where n is the refractive index of the water medium and η_0 is the vacuum impedance. Fig. 1C shows the radiation pattern for a particle with polarizability $\alpha = 1$ as a function of the angle of incidence from the water side. For a real scalar polarizability, the far-field intensity is proportional to α^2 as expected.

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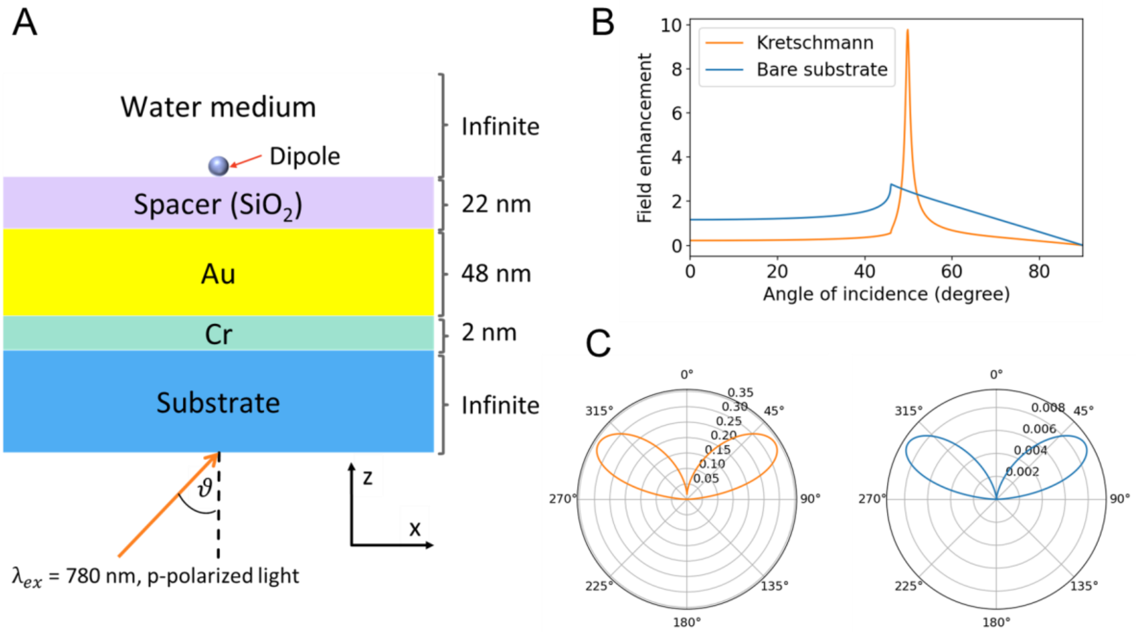

Fig. 1. A) Schematic representation of the Kretschmann configuration for detecting the dipole moment of a spherical particle at the sensor/water interface. B) Optimization of the field enhancement at the position of the dipole in Kretschmann and bare substrate configurations for a 780 nm p-polarized beam incident from the side of the substrate. The field enhancement is a maximum at an angle of 49.8° in the Kretschmann configuration and 46.0° in the bare substrate configuration. C) A polar plot of the far-field intensity due to the dipole at the surface of the multilayer stack, obtained by Lorentz reciprocity theorem.

We compare the radiation patterns for the Kretschmann and bare substrate configurations by integrating their respective radiation patterns. The integration gives a value of 1.15 $\alpha^2|\mathbf{E}_0|^2$ for the Kretschmann configuration and 0.0270 $\alpha^2|\mathbf{E}_0|^2$ in the bare substrate case, where $\mathbf{E}_0$ is the electric field amplitude of the incident light in the substrate. Thus, the Kretschmann configuration provides a 42-fold enhancement of the signal from the subwavelength dipole in comparison with the bare substrate case. This approach opens possibilities to study the radiation patterns of different types of polarizable particles in a classroom setting.

3. Expected usage and code availability

This work can be easily run and visualized in a Python Jupyter Notebook [6] without the need for large computational resources, which is often required to do this type of study with other methods. Students can study the effect of polarizable particles on an infinite variety of multilayer stacks and find inspiration from the literature about which materials might give the best results. This work touches on advanced topics such as plasmonics, whilst still being accessible to students. Easy to follow examples for teachers and students are available at: https://github.com/katya-zossi/tmm-sensors.

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