Nonlocal Fourier Modal Method

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We have developed a methodology to incorporate nonlocal optical responses, described with a simple hydrodynamic model, into the numerical Fourier modal method (FMM) technique, to enable broadening of simulation portfolio of such physical phenomena in plasmonic nanostructures.
Keywords: *Nonlocal optical response, Fourier modal method, plasmonics*

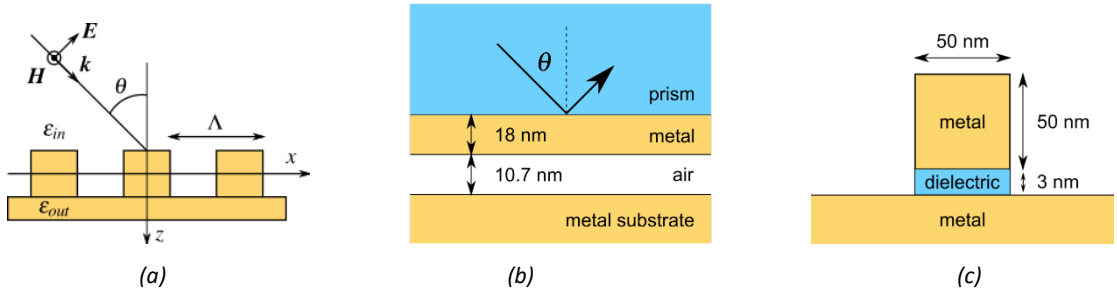
INTRODUCTION

Approximation of the local response of the material is a common approach in the analysis of the resonant behavior of the interaction of light with plasmonic nanostructures. However, as the characteristic dimensions of such structures decrease (in the order of nm), as has recently been shown, models based on nonlocal response (or even quantum interaction) are needed to describe such plasmonic systems [1]. These new models then provide an explanation of effects such as new types of resonances and their blue spectral shifts. In reality, in microscopic descriptions of light-matter interactions, such nonlocal optical response reveals due to the quantum mechanical uncertainties in material excitations. Up-to-date, there are several nonlocal models existing, based on different starting conditions, and predicting not always consistent and equivalent phenomena. Selected nonlocal models have already been successfully implemented in a number of numerical methods such as finite element method [2], finite-difference time-domain method, integral methods, Mie theory, and others. However, successful and effective implementation [3,4] using modal methods is missing.

NONLOCAL FOURIER MODAL METHOD

We have relied on our previous profound experience with both periodic (for one-dimensional - 1D and two-dimensional - 2D cases) and aperiodic version (i.e. isolated structures - for 2D and three-dimensional - 3D cases) of the FMM technique (or traditionally called rigorous coupled wave analysis, RCWA [5]), applied extensively in various rather complex problems, including, e.g. plasmonic gratings, periodic arrays exhibiting the extraordinary optical transmission (EOT) effects, plasmonic metasurfaces, etc., with traditional local-response approximation (LRA), and several important technical extensions implemented, such as proper Fourier factorization, adaptive spatial resolution, and symmetrization techniques [6-8]. Here, based on this experience, we have incorporated newly the nonlocal-response approximation (NRA) into the periodic FMM technique, described with a proper hydrodynamic model. In modifying the FMM method for these effects, our approach is based on [3]. We consider Maxwell's equations in the frequency domain with linearized hydrodynamic correction [2]. This model of nonlocal phenomena is one of the simpler (compared to more complex or quantum models) but it can well describe many experimental results.

Consider a one-dimensional diffraction grating with a grating period Λ (see Fig. 1a). A plane wave with a wavelength of λ is incident upon the diffraction grating at an angle θ (we consider only planar diffraction), due to the nonlocal effect in metals, we can focus only on TM polarization here. The FMM method is based on the evolution of the electromagnetic field and material parameters (within one layer) into a Fourier series. Because we have limited ourselves to TM polarization here, Maxwell's equations (frequency domain) contain only 3 electromagnetic field components: E_x, E_z, and H_y. The algorithm consists of two basic steps. First, the eigenvalue equation is solved, due to the non-locality, however, the electric intensity E_x is connected with the divergence of current density J. In the second step, the S matrix propagation algorithm is solved. Compared to the non-local variant, one equation for boundary conditions of J_z has to be added.

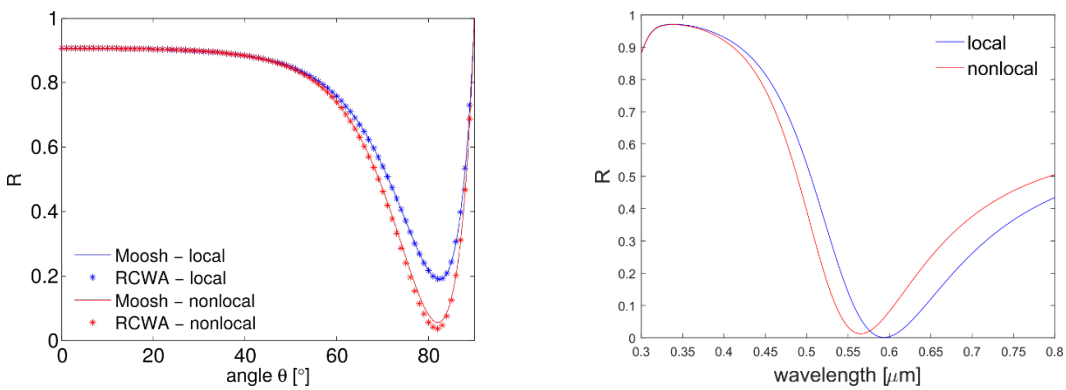


(a) (b) (c)

Fig. 1.: (a) Basic geometry and notation of a periodic diffraction grating, Λ represents the grating period, θ is the incident angle of the TM polarized plane wave, ε_{in} is the permittivity of a input medium, and ε_{out} is the permittivity of the output medium (substrate); (b) Schematic of the multilayer structure, parameters: λ=543 nm (TM polarization), prism is given with TiO_2 (n=2.5489-0.0003i), metal layer and metal substrate are made of silver (n=0.1442-3.1365i); (c) one period of the resonant diffraction grating, similar to (a), used for non-local simulations. The grating period is 200 nm.

RESULTS

A first example is a simple multilayer structure (see Fig. 1b), for simplicity, we applied the structure from the article [9] and here we checked the results of our novel non-local code with the Moosh program [9] (see also: https://github.com/AnMoreau/Moosh), applicable for nonlocal layers. The input TM polarized plane wave @ λ=543 nm propagates through a TiO_2 prism (n=2.5489-0.0003i), a plasmon mode is then generated on a silver layer with a thickness of 18 nm. The propagation properties of the plasmon mode are further influenced by a thin layer of air with a width of 10.7 nm. Below the air layer is a silver substrate. Since the metal layer is 18 nm thick (+ possible resonant effects), non-local effects are already expected here which was confirmed. Figure 2a shows the dependence of the reflectivity R on the incident angle θ, again, there is a comparison of our code with the program Moosh shown. Due to the fact that the condition for the generation of the plasmon mode is fulfilled for a certain angle, there is a decrease in reflection around θ=80°. If we take into account the nonlocal properties of silver, represented with the β parameter, $\beta=1.35\times10^6$ m/s , there is a further decrease in reflection and there is a small shift of the peak towards a smaller angle of incidence. In both cases, we can see very good agreement between our nonlocal tool and the software Moosh. Similarly, figure 2b shows the spectral dependence of the reflectivity R. The blue line shows the local behavior and the red line the nonlocal behavior. The angle of incidence is set to θ =82.61°.

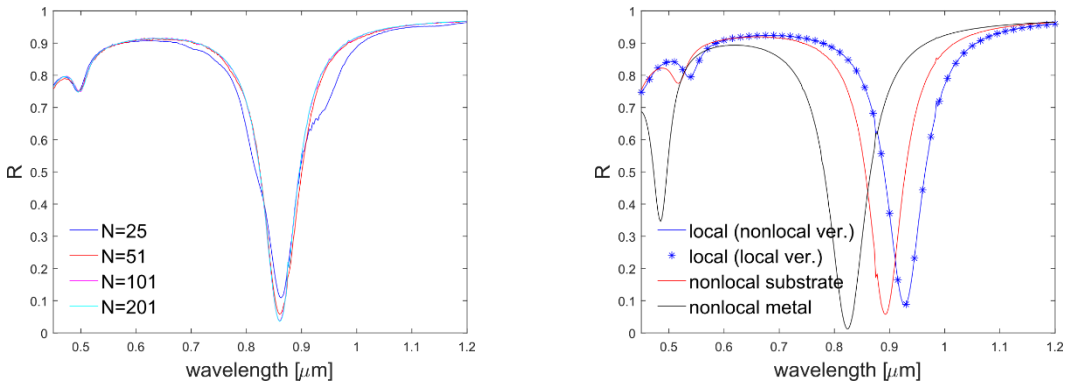


(a) (b)

Fig. 2.: (a) Dependence of the reflectivity R on the incident angle θ: comparison of our new implementation with the program Moosh. Local solutions are shown in blue, nonlocal solutions (for $\beta=1.35\times10^6$ m/s) are shown in red; (b) Dependence of the reflectivity R on the wavelength λ (θ =82.61°). Again, local solution is shown in blue, nonlocal solution (for $\beta=1.35\times10^6$ m/s) is shown in red.

A second example given here is a resonant diffraction grating (see Fig. 1c), this example is taken from [10]. An incoming plane wave (TM polarization) propagates perpendicularly to the 1D diffraction grating with a period of 200 nm. A silver rod with dimensions 50 nm x 50 nm is separated from the metal substrate (silver) by a thin dielectric layer (n=1.33) with a thickness of 3 nm. Figure 3a shows a comparison of the zero-order reflectivity spectra for different number of orders N showing a very good convergence behavior. Next, figure 3b shows the spectral dependence of the reflectivity. Clearly, there is a resonant peak present around the wavelength of 900 nm. To check

the performance of the nonlocal version of the FMM method, there is first a local calculation using the standard version of the FMM (blue line) shown, together with a local calculation using the non-local version of the FMM (blue dots, here, the nonlocality is just switched off). As can be seen, the results obtained are identical. Further, the red line shows a rather artificial (but numerically appreciative) case of switching on only the nonlocality of the substrate, while the black line represents the more realistic case where each metal component is considered nonlocally. Clearly, the expected blue shift of the resonance towards shorter wavelengths has gradually manifested itself, for the red and black lines, respectively. Finally, the applicability and flexibility of our nonlocal FMM have been shown, making it a useful tool for further investigations in the field of nanoplasmonics.



(b) *(b)*

Fig. 3.: (a) Comparison of the zero-order reflectivity spectra for different number of orders N; (b) Spectral dependencies of zero-order reflectivity efficiency. The blue curve represents the local calculation using the algorithm given here, which is checked (blue dots) by the standard RCWA algorithm, the red line shows the calculation of only nonlocal substrate, while the black curve shows the calculation where all metal components are considered nonlocaly.

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