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Rigorous coupled wave analysis for plasmonic nanoparticles

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Abstract

Electromagnetic simulation packages for nanoparticles have become of interest for science and engineering community because of interesting properties of nanomaterials, such as, plasmonics and localized field enhancement. There are several approaches to calculate electromagnetic wave responses including time domain and frequency domain; each approach does have its own pros and cons. In this paper, we discuss basic principle of Rigorous coupled wave analysis (RCWA) and some key issues of 2D Rigorous Coupled Wave Analysis (RCWA) for nanoparticle simulation, such as, the computing demands (long computation time and memory consumption) and staircase approximation. We also suggest some feasible approaches to get around the issues and speed up the calculation, such as, employing Li Feng Li's RCWA algorithm for circular and elliptical rods, making use of the symmetry of spherical shape particles to reduce redundancies in computation and building up an Eigenvector/Eigenvalue database of difference radii of disks, so that these disks can be stacked together to form various sizes of nanospheres.

Introduction

Rigorous coupled wave analysis (RCWA) is an electromagnetic modelling tool for periodic boundary condition, such as, 1D and 2D gratings. The method was invented by Moharam and Gaylord [1]. The RCWA for 1D grating has proved to be very successful; there are a number of commercial software packages in the market and a number of research publications [2-3] employed the RCWA in their study. Before we address the issues in nanoparticle simulation, let us consider the basic principle of 1D RCWA.

For RCWA 1D, the method solves an exact solution to Maxwell equations in Fourier-Space domain where electric and magnetic fields are represented as a sum of frequency harmonics (diffracted orders: N). The method is based on the mathematical expansion that the solutions to periodic differential equations can be expressed by Floquet function expansion [1]. Hence, the accuracy of the solution depends on the number of harmonics (diffracted orders) taken into account; the more diffracted orders the more accurate results, of course, this comes with an expense of a demand in computing power and computational time required. The method requires the grating to be modelled by rectangular grid blocks, where the permittivities of the grating profile can be expressed as a Fourier series as a function of position on the grating. Therefore, for a nonrectangular shape structure, such as, a triangular grating, a sine wave grating and a rod shape grating, it is necessary to approximate the shape of the grating using staircase approximation as shown in Fig.1. Electromagnetic wave modes for each of the slice layer are then calculated by matching the tangential electric and magnetic at the grating boundary (periodic boundary condition) and taking into account the phase due to the thickness of the layer Δz. Overall solution for all the layers can be calculated using scattering matrix approach or transfer matrix approach.

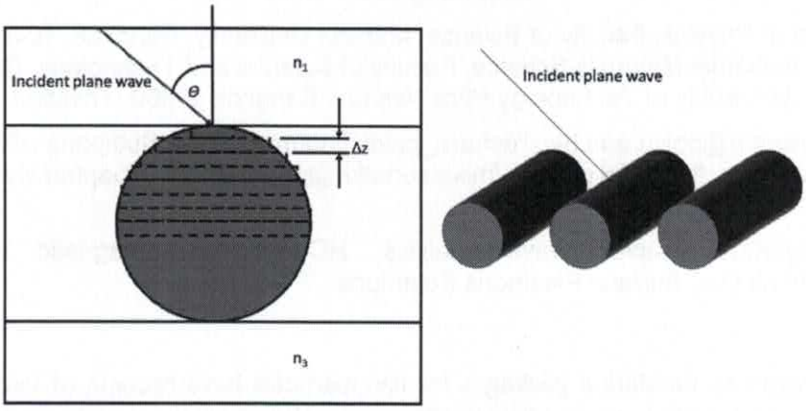

Fig. 1. shows staircase approximation on a rod shape grating for RCWA calculation

The principle for 2D case is essentially similar to the 1D case except for the 2D cases :

(1) The boundary matching has to be done in N times more than the 1D case. Hence the size of the matrices that need to be inverted for the 1D case is 2Nx2N, whereas for the 2D case $2N_x^2 x 2N_y^2$ where N_x and N_y are number of diffracted orders along x and y axes respectively. This leads to a big demand in computing power and memory for the 2D calculation.

(2) For the 2D case, not only the z direction suffers from the staircase approximation, but also along the xy-plane as shown in Fig. 2. Li Feng Li [4] has proposed a spherical coordinate transform approach enabling the circular shape and elliptical profile on the xy plane to be calculated with no staircase approximation.

(3) Fourier transform of the permittivity profile is a 2D FFT rather than 1D. This puts another load on the computational demand.

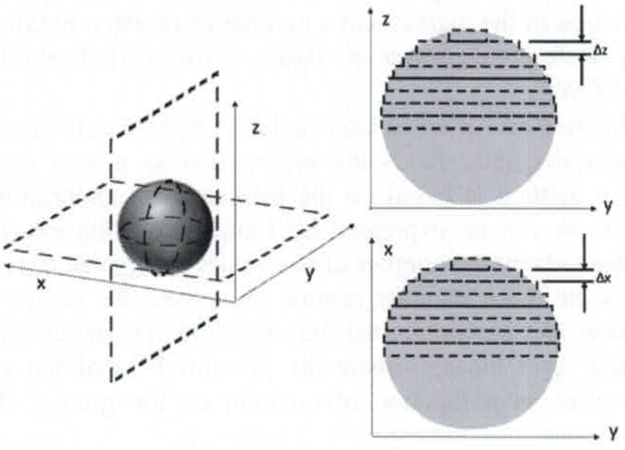

Fig 2. Shows staircase approximation along xy plane and yz plane for nanoparticles array

Software implementation and Results

In this paper, we have employed the following computational techniques to speed up the RCWA 2D calculation for nanoparticles array. The software is implemented in MATLAB and validated with results in literature.

(1) Li Feng Li's algorithm has been implemented [4] and we compared the simulation shown in Fig.3a for the nanopillars deposited on quartz substrate as shown in Fig.3b with the experimental and simulation results published by Si *et al.* [5]. In ref 5, the authors simulated the responses using Finite Difference Time Domain (FDTD) method. Their simulated results showed the same amount of spectral shift, although the central wavelength for the peaks are not the same. This may be due to differing refractive indices for the materials used in the two types of calculations.

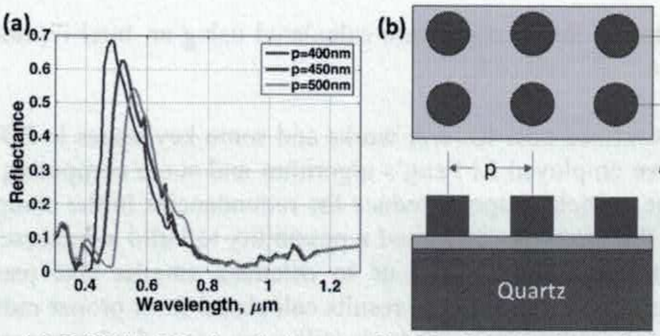

Fig 3. shows (a) RCWA 2D simulation results N_x=21, N_y=21 polarization direction parallel to the x axis for grating period of 400nm (blue curve), 450nm (red curve) and 500 nm (orange curve) and (b) Silver nanopillars deposited on quartz substrate with 6 nm Ti adhesion layer. Note that the refractive index values of Ag and Ti were from Johnson and Christy's paper [6] and refractive index of quartz used in this calculation was the values reported by Malitson [7].

(2) For nanoparticles, the shape of the profile is symmetric along z direction, for example, the bottom two rectangular pieces shown in Fig.2; they are, in fact, the same. This means there is a redundancy in the calculation, i.e. half of the nanosphere along z direction. We can avoid this redundancy by calculating only either the top half or bottom half the grating and reuse the Eigenvector and Eigenvalue calculated from the half sphere twice in by putting them in the reversed order in scattering matrix calculation.

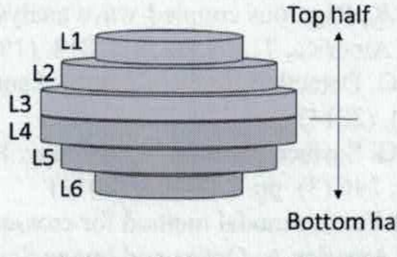

Fig. 4. shows a stack of disks consisting of 6 layers with grating period of 300nm. All the disks are 0.0167 μm high with radii of 0.0276 μm (L1), 0.0433 μm (L2), 0.0493 μm (L3), 0.0493 μm (L4), 0.0433 μm (L5) and 0.0276 μm (L6). Silver nano pillar using Johnson and Christy refractive index [6] on glass substrate (1.52). Incident wavelength of 633 nm with normal incident to the nano spheres grating. Nx=Ny=21

In this paper, we demonstrated this point by calculating a stack of disks consisting of 6 layers as shown in Fig 4. As mentioned earlier the L1 is identical to L6, L2 is identical to L5 and L3 is identical to L4. The results calculated from all the layers and from top half of the grating gave the same answer of R0=0.0145 and T0=0.9664. The computing required to for the conventional method and the half grating method were 53 seconds and 40 seconds respectively. The reason that the speed was not improved by factor of 2 was that the code required some time to store the Eigenvectors and Eigenvalues in the hard drive rather than just storing all the Eigenvectors and Eigenvalues in RAM.

(3) In the code, we employ parallel computing technique to speed up the calculation by calculating each of the layers in each separate CPU core.

(4) Since we store the Eigenvalues and Eigenvectors for each of the disk radii, we can then be able to calculate responses due to a smaller size of particles within the same grating period, such as, using L1 L2 L2 L1 profile by excluding the layer L3 in the scattering matrix calculation.

Note that the results presented in this section were calculated using an Intel i7(model Intel i7-4790@3.60GHz) computer with 32 GB of RAM.

Discussion and Conclusion

In this paper, we have described how RCWA works and some key issues in 2D RCWA for nanoparticle simulation. We have employed Li Feng's algorithm and some computing techniques, such as, use the symmetry of the particle shape to reduce the redundancies in the computation and employ the parallel computing. We have also discussed a possibility to build a database for a series of disks with different radii, this database allows us to calculate smaller size particles using scattering matrix approach directly by joining up the results calculated from proper radii sizes with no need to perform the RCWA calculation again. There is still some room for improvement for this MATLAB code, such as, employing the GPU (Graphic Processing Unit computation). Of course, another issue that cannot be overlooked is the matrix inversion; with a large number of diffracted orders this usually leads to an ill-conditioning. We might be able get around this by investigating a more sophisticated matrix inversion algorithm.

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