A Novel and Efficient Numerical Scheme Employing Characteristic Basis Functions for the Modelling of Optical Properties of Plasmonic Nanorods Array

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Abstract

In this paper we introduce a set of Characteristic Basis Functions (CBFs) for efficient representation of the currents induced on the elements in a 2D array of plasmonic nanorods. The use of these functions leads to a relatively small and well-conditioned matrix, only a 2×2 size for the normally incident plane wave. We show that the shape of the current can be found by solving a relatively small truncated array, 11×11 array for instance, and the level of the current can be computed by taking advantage of the fast convergence of the Galerkin testing integral in spectral domain circumventing the oscillatory behaviour of the solution in spatial domain.

1. Introduction

Arrays of plasmonic nanorods have potential applications in nanoantennas, sensors, focusing, and guiding and solar cells systems [i.e. 1, 2]. Solving an array of plasmonic nanorods comprising of dispersive and negative-permittivity materials by using conventional EM simulation packages are often inaccurate or highly time- and memory-consuming. This is because of the fine meshing required for solving the large aspect ratio rods and the fact that a large array must be solved. The periodic Green's function approach, typically used in the context of integral equation formulation, is known to suffer from a slow convergence rate [3, 4], which is undesirable. In this paper, we utilize the Characteristic Basis Function Method (CBFM) [5] to efficiently model the nanorods, followed by a spectral domain to enhance the convergence. The CBF method is a time- and memory-efficient technique for characterizing both the isolated and array-type problems. In this paper, we show that only two CBFs are sufficient for characterizing the current induced on each nanorod element. To determine the weight coefficients of the CBFs, we introduce a novel technique, which is based on finding the shape of the macro-CBF by first solving a 2×2 matrix equation, derived by using Galerkin's testing on the central element for a 11×11 truncated array. Next to find the level of that macro-CBF, we apply Galerkin in the spectral domain by using the Parseval theorem, which, in turn, serves to speed up the convergence of the partial sums considerably. The numerical scheme, described above, is very general and robust for simulating the scattering characteristics of periodic complex metamaterials.

2. Formulation and simulations

Fig. 1 depicts an array of plasmonic nanorods in *x*-*y* plane, illuminated at broadside by a vertically polarized incident plane wave. The unit cell is a plasmonic nanorod of length L=300 *nm*, radius a=10 nm, and its material is silver, which is characterized in the optical regime by using the Drude model: $\varepsilon_r = \varepsilon_{r\infty} - f_p^2 / [f(f - jf_d)]$, where f_p and f_d are plasma and damping frequencies. The method begins by solving for the polarization currents on the isolated nanorod for a number of different incident plane waves by representing the induced currents in terms of a few Macro Basis Functions (MBFs), according to Fig. 2. For the range of frequencies of interest here, 100-500 THz, we have found that it is sufficient to use just 5 MBFs to reach to a convergent solution [6].

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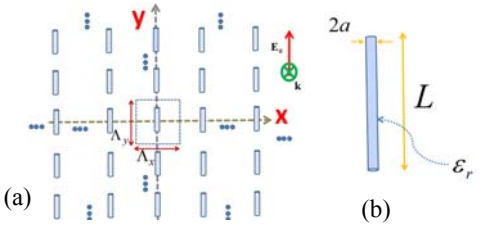

Fig. 1: (a) 2D array of plasmonic nano-rods (b) unit-cell

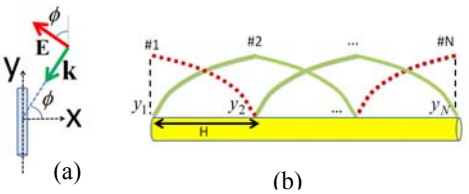

Fig. 2: (a) Solving the isolated element for different incident plane waves. (b) Representation of polarization current by *N* triangular sinusoidal MBFs.

Next, a Singular Value Decomposition (SVD) is applied to the obtained solutions in order to remove the redundancy and to generate a set of high level MBFs known as the Characteristic Basis Functions (CBFs) that are longitudinal in nature, i.e., they only vary along the *y*-direction. We see from Fig. 3 that at *f*=400 THz only the first three CBFs possess the singular values greater than than -20 dB. Moreover, CBF#2 is an odd function (see Fig. 3(b)), which does not contribute to the induced current for the normal incidence case being considered here. Hence, the CBFs#1 and #3 are sufficient to characterize the current induced on the single element. We call the CBF#1 and CBF#3 as s_1 and s_2.

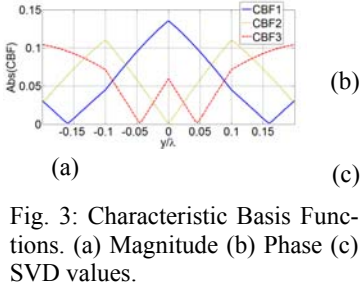

Fig. 3: Characteristic Basis Functions. (a) Magnitude (b) Phase (c) SVD values.

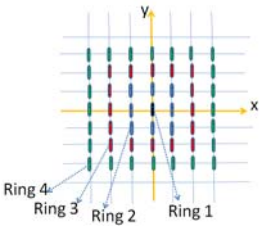

Fig. 4: Ring concept to apply Galerkin testing on the central element.

Next, we compute the truncated summation of the scattered field on the central unit-cell due to the elements of the 2-D array surrounding it, and then we test the electric field with CBFs (Galerkin's testing) that we have derived earlier to derive a small-size matrix equation. For the array problem, because of the normal incidence, we assume that all the elements have the same currents $I = c_1 s_1 + c_2 s_2$, where c_1 and c_2 are unknown coefficients, to be determined. The equation for polarization current of the central element is as follows:

$$j\omega\varepsilon_0(\varepsilon_r - 1)(E^i + E^s) = I/(\pi a^2) \tag{1}$$

In (1), E^i is the incident and E^s is the *y*-component scattered field due to the all of the elements in the array. To find the unknown coefficients c_1 and c_2, we need to test (1) by s_1 and s_2 and solve the resultant 2×2 matrix. Because we have infinitely many elements, we truncate the array by using the rings shown in Fig. 4, i.e., at stage #m we need to consider the truncated (2m-1)×(2m-1) array including the rings #1, #2,..., #m to find the corresponded coefficients $c_1(m)$ and $c_2(m)$. Such a computation has been performed and illustrated in Fig. 5. It is worth mentioning that for the relatively large number of rings the computation of E^s is time consuming. moreover, as depicted in Fig. 5, the convergence is slow and oscillatory due to owing to the1/*R* dependence of the fields computed byrelatively far rings. We observe from Fig. 5 that, after a few stages, the maxima and minima of these coefficients are essentially synchronized as we vary the number of rings, implying that the shape of macro CBF, comprising of a linear combination of the two CBFs, remains unchanged, and that only its level fluctuates as the size of the truncated array is increased. We can take advantage of this fact and avoid the computation of the mutual coupling contributions of the elements for relatively large number of rings. Specifically we have found that we can find the shape of the macro CBF by solving the 2×2 matrix equation corresponded to only 6 rings, i.e., for an 11×11 truncated array. Furthermore, to determine the level of the macro CBFs, we can take advantage of the fast convergence of the Galerkin integral in spectral domain by using the Parseval theorem. Indeed, the Galerkin integral in the spectral domain is turned out to be a series comprising of pq-Floquet modes corresponding to $2\pi p/\Lambda_x$ and $2\pi q/\Lambda_y$ Floquet wave numbers, where p and q are integers, and Λ_x and Λ_y are the periodicities along the x- and y-axis, re-

spectively, as shown in Fig. 1(a). The magnitude and phase of the macro-CBF ζ, which is the weighted sum of the CBFs# 1 and #3, are plotted in Fig. 6, as functions of the number of the truncated Floquet modes. We note that the convergence in the spectral domain does not depict the oscillatory behaviour similar to one encountered in the spatial domain summation (see Fig. 5). Moreover the speed of convergence in spectral domain is about 10 times faster than that in the spatial domain. Our next step is to take advantage of the closed form Floquet modes, to find the reflection coefficient of the array in a manner illustrated in Fig. 7. For Λ_x=200 nm and Λ_y=450 nm, only the Floquet mode corresponded to pq=00 contributes in the visible region is needed to compute the reflection coefficient, which can be expressed as:

$$\Gamma = 60\pi \tilde{I}(0)/\left(\Lambda_x \Lambda_y\right) \tag{2}$$

where $\tilde{I}(0)$ is the Fourier transform of the current at k_y=0. The computation of the reflection coeffient takes only 7 minutes for 401 frequency samples depicted in Fig. 7, on a 2.2 GHz Intel Core(TM)2 Duo CPU machine. Additionally, the SVD computation consumes about 23 minutes for $-90^\circ < \phi < 90^\circ$ (see Fig. 2(a)) with 1 degree increment and all the 401 mentioned frequency samples.

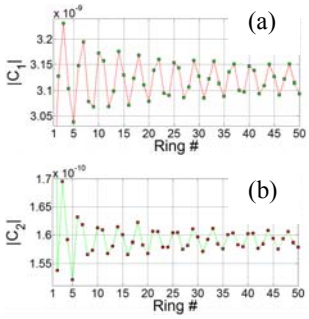

Fig. 5: Coefficients corresponded to each CBF versus the ring #. (a) first CBF (b) second CBF.

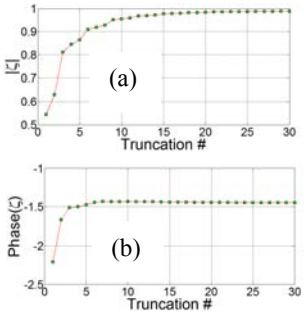

Fig. 6: Level of macro CBF interms of truncation number in the series comprising of Floquet modes. (a) Magnitude (b) Phase.

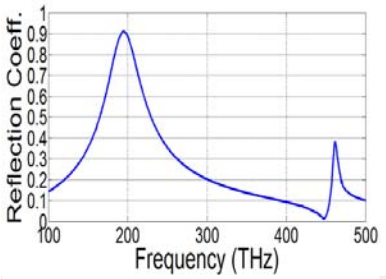

Fig. 7: Reflection coefficient of the infinite array of plasmonic nanorods over an optical range of frequency.

3. Conclusion

In this work, a fast and efficient computational scheme for modelling array of plasmonic nanorods has been proposed. Each rod has been successfully represented with only a few physics-based basis functions (CBFs). The periodicity has been accounted for by utilizing the ring concept, and Galerkin integrals have been computed in the spectral domain. The technique is capable for characterizing large clusters of metamaterials because the use of the proposed method is shown to reduce the burden on both the CPU memory and time

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