NUMERICAL OPTIMIZATION OF METALLIZED TITANIA NANOTUBE MORPHOLOGIES FOR NEGATIVE INDEX MATERIAL FLAT LENS APPLICATIONS

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Abstract

We perform numerical calculation in order to optimize the morphology of metallized titania nanotubes from the point of view of flat lens application based on NIM. An efficient multiple-scattering approach is used to calculate propagation of electromagnetic waves through the materials designed. The focusing properties of a flat lens constructed from a superlattice structure of nanotube clusters were found to be better as compared to a lens with a regular arrangement of nanotubes. A disorder of 20% introduced in the position of nanotubes of the optimized superlattice does not significantly influence the focusing properties of the lens.

1. Introduction

Negative-index materials (NIMs) are synthetic materials increasingly used for the development of optical elements. An interesting property of NIMs is the possibility to build a “perfect lens” that can focus electromagnetic waves to a spot size much smaller than a wavelength [1, 2]. Apart from composite wire, split ring resonator structures [2, 3], and backward-wave transmission lines [4], NIM lenses are designed also from dielectric rods [5, 6]. It was recently proposed to design NIM lenses from dielectric rods with a specific dielectric constant profile approximating a fish-eye geometry [7, 8]. This design was shown to provide improved focusing with a much thinner flat lens as compared to that assembled from homogeneous dielectric rods, it demonstrating also higher tolerances to the induced disorder in the rod assembly. The approach of designing NIMs on the basis of dielectric rods with a gradient of the dielectric constant was tested experimentally at microwave frequencies [9]. Most recently, it was proposed to assemble NIMs from titania nanotubes with inner and outer surfaces covered by thin metallic films [10]. The focusing properties of flat and concave lenses assembled from metallized titania nanotubes were compared with those of lenses made from nanorods with the refractive index $n = -1$ by performing numerical calculations using a multiple-scattering approach. Focusing was proved for both types of lenses.

The goal of this paper is to perform numerical calculation in order to optimize the morphology of metallized titania from the point of view of flat lens application based on NIM.

2. Methods employed

The mechanisms of obtaining materials with negative refractive index are associated with the reorganization of the electromagnetic oscillations spectra in periodical structures [11], and they were described previously in detail [12]. The necessary properties of optical metamaterials are usually obtained in the frequency range, where the reconstruction of the spectrum occurs [13-16]. The designing of metamaterials with necessary properties is complicated by the effects of spatial dispersion of a composite medium, and by the fact the wavelength is comparable with the mean distance between the elements of the composite medium (pores, rods, nanotubes, etc). Another problem is the production of perfect periodical structures with available technological methods. We suggest that the necessary optical properties can be obtained with an especial organization of the short-range order, and it is not necessarily to have a far-range order. Similarly to amorphous solid state materials, i.e., glasses with a non-ordered structure at atomic level [17, 18], the term of "amorphisity" can be applied to photonic structures. Disordered materials can be also described in terms of clusters with a non-regular structure called "*amorphon*", which are assembled in a super-structure [18].

The obtained titania nanotubular structures (Fig. 1b) represent a kind of "amorphous" structure when it is compared with different atomic arrangements shown in Fig. 1a. The diffraction pattern of a crystalline material represents well defined point spots as shown by the region 1 in Fig. 1a, while the diffraction pattern of an amorphous material consists of rings as illustrated by the region 2 in Fig. 1a. In order to analyze the degree of order in the produced structures, we have generated numerically the diffraction pattern (DP) by taking direct Fourier transform (DFT) from the SEM image. Thus, a DP can be obtained by calculating the direct 2D Fourier transform from the pixel-arrays of SEM pictures [19]. The two-dimensional Fourier transform of the image in Fig. 1b is composed of a diffuse ring which is characteristic of polycrystalline domains of pores, i.e., for structures with short range order.

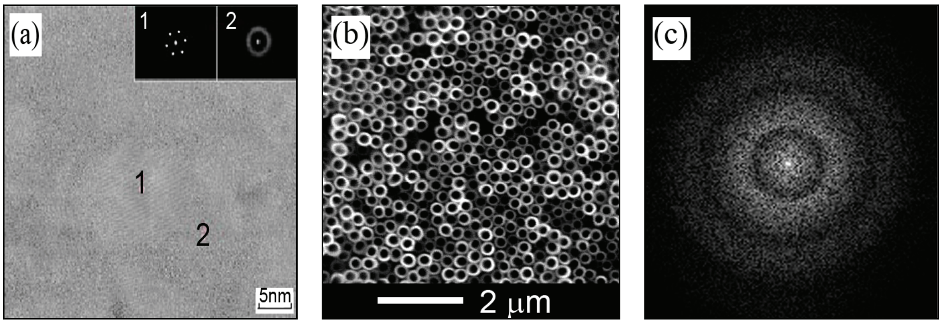

Fig. 1. (a) TEM image of a glass sample containing crystallized (1) and amorphous (2) regions, and inserted diffraction patterns of these regions; (b) SEM image of a sample with titania nanotubes; and (c) DFT of the titania nanotubes image.

We will model our "amorphous" structure of titania nanotubes using an elementary cluster with a non-regular arrangement of nanotubes, and will construct a superlattice from these clusters. Therefore, the nanotube system will represent a periodic photonic crystal with an elementary cell of big radius $l_{\text{eff}} >> a$, where a is the mean distance between the titania nanotubes [20]. We will use a cluster in the form of a hexagon with a non-regular arrangement of nanotubes inside the cluster as shown in Fig. 2a.

A highly efficient and accurate multiple-scattering approach [21] was used to calculate propagation of electromagnetic waves through the materials designed. Initially, the light scattering properties of individual rods are analyzed. Previously, we used an approach based on the effective medium concept [7, 22] to investigate the light scattering properties of individual rods. This method relies on using a hypothetic background medium with variable index of refraction in which the investigated rods are immersed. The scattering cross section of the rods is then calculated for each value of the refractive index of the background medium, and the dependence of the scattering cross section upon the refractive index of the medium involved is plotted. It is obvious that this dependence should exhibit a sharp decrease when the refractive index of the background medium approaches that of the rod being investigated. By performing calculations for different wavelengths and plotting the dependence of the refractive index of the rod as a function of wavelength, we determined the spectral range where the investigated rod behaves as NIM from the point of view of light scattering properties.

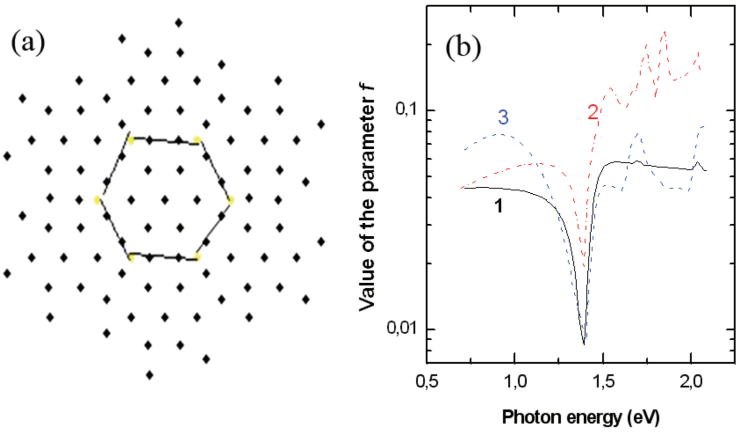

Fig. 2. (a) An elementary cluster of TiO_2 nanotubes; (b) Spectral dependence of the parameter *f* for a nanotube (1), a cluster with regular arrangement of nanotubes (2), and a cluster with non-regular arrangement (3).

In this work, we use a simplified method [10] which consists in the analysis of a parameter *f* describing the difference from the point of view of light scattering properties between the investigated unit (rod, or nanotube) and a similar unit with identical geometrical parameters but consisting of a material with the refractive index n = –1:

$$f = \max|D_m^{ni} - D_m|_{10>m>-10},$$

where D_m^{ni} and D_m are the parameters determining the light scattering properties [21] of the unit made from the material with n = –1 and the investigated unit, respectively; *m* is the index of the cylindrical function [21].

3. Results and discussions

The results of calculations for a TiO_2 nanotube covered by metal are shown in Fig. 2b by curve (*1*). The calculations were done for nanotubes with the inner diameter of 80 nm and the outer diameter of 160 nm, the outer and inner surfaces being covered with an Ag film with a thickness of 12 nm. Similar calculations were carried out for a cluster of nanotubes like that shown in Fig. 2a, but with a regular arrangement of nanotubes (curve *2*). In this case, the value of the parameter *f* was calculated not for a nanotube, but for a number of N nanotubes inside a cluster

$$f = \max\left| D^{ni\,(j)}{}_m - D^{(j)}{}_m \right|,$$

where j is the number of a nanotube in the cluster.

If we compare curves *1* and *2* in Fig. 2b, we can observe that the minimum value in curve *2* is higher as compared to curve *1*. That means that the light scattering properties of the cluster are poorer as compared to those of a nanotube. This is because $\lambda \sim l_{\mathrm{eff}}$ in spite of the fact that $\lambda >> a$. In these conditions, the system of nanotubes cannot be treated as a perfect effective homogeneous medium, and the spatial dispersion influences the optical properties of the medium [10]. However, the light scattering properties of the cluster can be improved by introducing some disorder in the arrangement of nanotubes in the cluster and optimising the positions of nanotubes. This is done by minimising the value of the *f* parameter as shown by curve 3 in Fig. 2b.

The focusing properties of flat lenses assembled from the investigated metallized TiO_2 nanotubes were studied by calculating the transmitted through the lens electromagnetic power $T = (E/E_0)^2$, where E is the electric field amplitude of the radiation passed through the lens, and E_0 is the electric field amplitude without the lens. The wavelengths of radiation are those determined from Fig. 3, i.e., the photon energy is 1.39 eV.

As one can see from Fig. 3, the focusing properties of a flat lens assembled from a superlattice of optimised clusters are much better that the focusing properties of a lens assembled from ordered nanotubes. A clear superlensing effect is observed with the superlattice of optimised clusters (Fig. 3b), i.e. $S/\lambda^2 < 1$, where S is the surface of the focal spot.

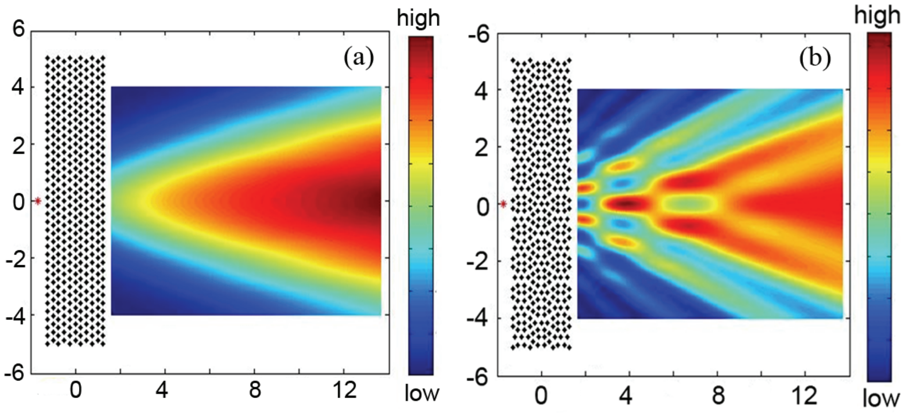

Fig. 3. Electric field intensity map of a cross-sectional view of the 2D source–image system when imaging by a photonic crystal flat lens consisting of ordered metallized TiO_2 nanotubes (a) and of a superlattice of optimized clusters (b).

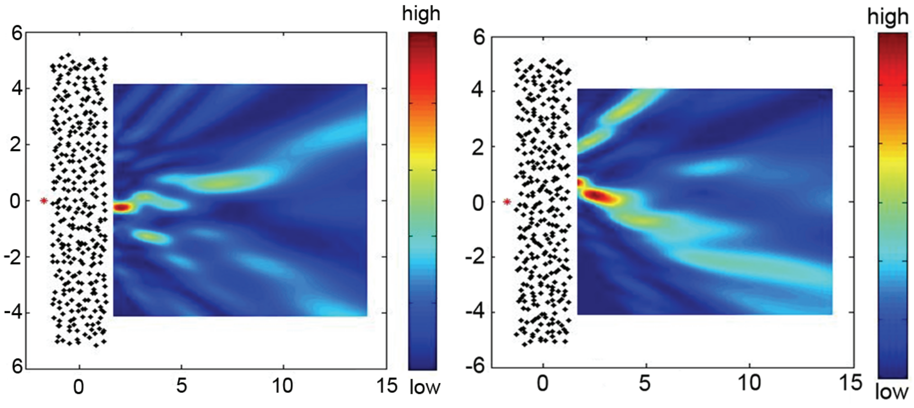

Fig. 4. Electric field intensity map of a cross-sectional view of the 2D source–image system when imaging by a photonic crystal flat lens assembled from nanotube clusters after two realizations of a random generator induced disorder of 20%.

One should mention that the lens assembled from the superlattice of optimized clusters is not very sensitive to the introduction of the disorder in the arrangement of nanotubes. Figure 4 represents the focusing properties of the flat lens after moving the nanotubes from the position represented in Fig. 3b by a random generator. We can conclude that the lens is not sensitive to the disorder.

As one can see from Fig. 5, which represents the direct Fourier transform (DFT) from three arrangements of nanotubes, the introduction of the disorder in the superlattice of clusters leads to an amorphous structure indicated by a nearly uniform spot in the DFT. Therefore, the design of an appropriate amorphisity makes it possible to construct lenses with excellent focusing properties.

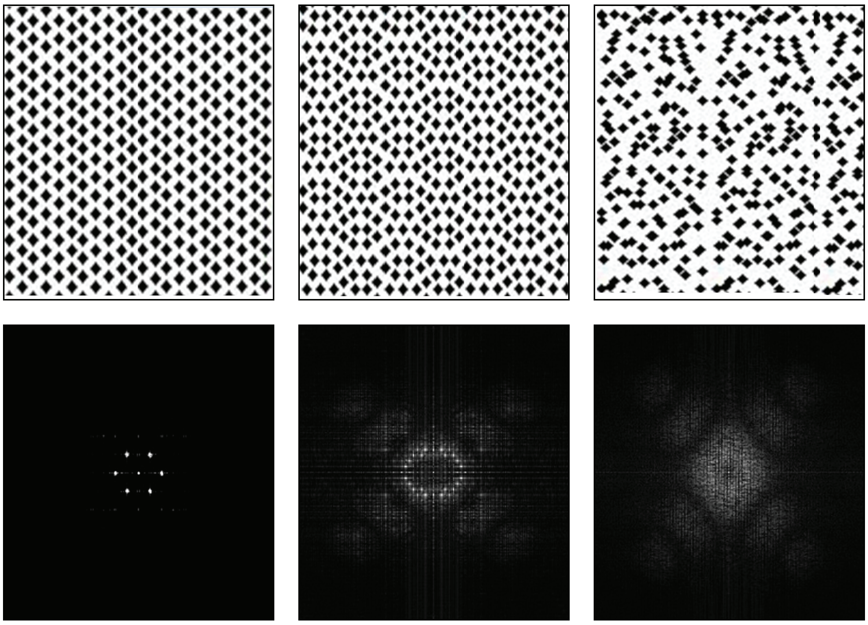

Fig. 5. DFT from three arrangements of nanotubes: an ordered arrangement, a superlattice of clusters, and a disordered arrangement.

4. Conclusions

The results of this work demonstrate that the focusing properties of a flat lens constructed from a superlattice structure of metallized TiO_2 nanotube clusters are better as compared to a lens with a regular arrangement of nanotubes. The lens assembled from the superlattice of optimized clusters is not sensitive to the introduction of the 20% disorder in the arrangement of nanotubes. The superlattice arrangement and the arrangement with a 20% disorder can be considered as two-dimensional amorphous photonic crystals with different degree of disorder. Therefore, it is shown that through the optimization of the degree of disorder in amorphous photonic crystals, it is possible to produce NIM lenses working at wavelengths which are much longer than the diameter and the distance between the metallized nanotubes.

Acknowledgments

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