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Authors

Sylvain, Lannebère
Campione, Salvatore
Aradian, Ashod
et al.

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Artificial Magnetism at Terahertz Frequencies in 3D Arrays of TiO_2 Microspheres Including Spatial Dispersion and Magnetoelectric Coupling

Sylvain Lannebère *, Salvatore Campione †, Ashod Aradian ‡, Matteo Albani*, and Filippo Capolino†

*Department of Information Engineering, University of Siena,53100, Siena, Italy
Email: lannebere@dii.unisi.it
†Department of Electrical Engineering and Computer Science, University of California, Irvine, California, 92697, USA
‡CNRS, Université Bordeaux 1, CRPP, UPR 8641, F-33600 Pessac, France

***Abstract*—In this work, we study the electromagnetic properties of a metamaterial made by a cubic array of TiO_2 microspheres embedded in a host medium at terahertz frequencies. By employing the method reported in [1] by Silveirinha, we are able to consider in the computation the effect of magnetoelectric coupling between TiO_2 microspheres, as well as spatial dispersion. After calculation of the dominant mode inside the structure, we show that the effect of spatial dispersion on the effective parameters for this kind of systems is relatively weak. Accuracy of the results and effectiveness of homogenized parameters have been demonstrated by comparison against full-wave simulations for a 5-layer slab of such a metamaterial.**

I. Introduction

In this work, we pursue the study of the magnetic properties of metamaterials made of nonmagnetic dielectric microspheres with large permittivity embedded in a host medium. These kind of structures, already studied in the gigahertz [2] and infrared frequency ranges [3], [4] can exhibit very strong magnetic response coming from the magnetic dipolar Mie resonance of the dielectric spheres. At terahertz frequencies, we have shown with the help of extended Maxwell Garnett theory, single dipole approximation and full-wave simulations that cubic arrays of TiO_2 microspheres give rise to strong magnetic response [5].

As a further step in the understanding of these systems, we are here interested in the dependence of the effective parameters on the wavevector, generally referred to as non-locality or spatial dispersion. To do so, we use the model reported in [1] by Silveirinha that consists in the generalization of the Lorentz-Lorenz formula to take into account the non-zero value of the wavevector. Thanks to this method, we are able to compute the eigenmodes propagating inside the structure and, when it is possible (only when one mode is dominant), to deduce the effective refractive index of the medium as well as the non-local effective parameters. By comparing these results to the ones obtained with full-wave simulations (finite element) and extended Maxwell Garnett theory, we show that spatial dispersion is relatively weak in these TiO_2 systems and it confirms their suitability to give rise to a large magnetic response.

II. Description of the Method

We use the model reported in [1] to compute the electromagnetic properties of an infinite cubic array of TiO_2 microspheres with permittivity $\varepsilon = 94 - j2.35$ embedded into a host medium. In this method, a modified Green's function of the periodic system (computed with the Ewald method for fast convergence and analytic continuation to the complex wavenumber domain [6]) is used to take all the interactions between point-like particles as well as the dependence on the wavevector $\mathbf{k}$ into account. All the information about the size of the microspheres is included inside their dynamic Mie polarizabilities.

Unlike the original publication [1], where the magnetoelectric coupling (electric dipole creating magnetic response and vice-versa) was neglected in the numerical examples, we choose to include this term to obtain more accurate results. The direct consequence of introducing such magnetoelectric coupling is that the composite medium becomes bi-anisotropic, and is then described by the four dyadics $\overline{\overline{\varepsilon}}(\mathbf{k}), \overline{\overline{\mu}}(\mathbf{k}), \overline{\overline{\xi}}(\mathbf{k}), \overline{\overline{\zeta}}(\mathbf{k})$ [7].

In [8] it is demonstrated that by using the homogenized parameters into the homogeneous medium wave equation one can calculate the frequency-wavevector dispersion relation of the metamaterial. In particular, the wavevector $\mathbf{k}$ in the effective bi-anisotropic medium is obtained by finding the solutions of the following wave equation:

$$\left[\left(\mathbf{k} \times \overline{\overline{I}} + \omega \overline{\overline{\xi}}(\mathbf{k})\right) \cdot \overline{\overline{\mu}}^{-1}(\mathbf{k}) \cdot \left(\mathbf{k} \times \overline{\overline{I}} - \omega \overline{\overline{\zeta}}(\mathbf{k})\right) + \omega^2 \cdot \overline{\overline{\varepsilon}}(\mathbf{k})\right] \cdot \mathbf{E} = 0 \quad (1)$$

III. Numerical Results

We observe that for well-designed filling fractions only one mode with transverse polarization (moving along one principal axis of the lattice) is dominant near the lowest order (magnetic) Mie resonance, and able to propagate with wavenumber $k(\omega)$. This wavenumber can be used to compute the effective refractive index of the composite medium $n(\omega) = \dfrac{k(\omega)}{k_0}$. This effective refractive index is compared in Fig. 1 to the one

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obtained from HFSS™ using the Nicolson-Ross-Weir (NRW) retrieval method [9] and the Maxwell Garnett (MG) one where neither spatial dispersion effects nor magnetoelectric coupling are considered. We observe an excellent agreement between the results of NRW based on full-wave simulations and the method in [1] taking into account both spatial dispersion and magnetoelectric coupling. The same conclusions are valid for the transverse component of the effective relative permeability $\overline{\overline{\mu}}_{\text{eff}}(\mathbf{k}(\omega))$ which is reported in Fig. 2. This is retrieved with the method in [1] using $\mathbf{k}(\omega) = k(\omega)\mathbf{u}$, with $\mathbf{u}$ the direction of propagation of the dominant mode. A fairly good agreement is observed also with the results retrieved with MG, and this makes us infer that spatial dispersion is weak in cubic arrays of TiO_2 microspheres.

Finally, to test the effectiveness of the retrieved parameters,

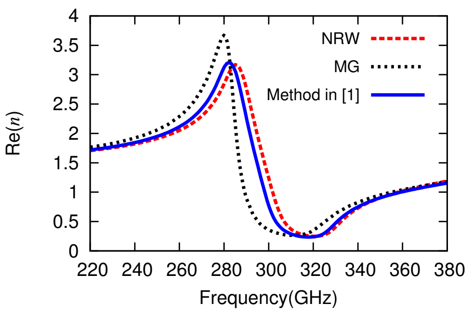

Fig. 1. Comparison between the effective refractive index obtained with HFSS (NRW), Maxwell Garnett (MG) and computed with the method in [1] for a cubic array of TiO_2 microspheres of 52 μm with a filling fraction of 29.44% in free space.

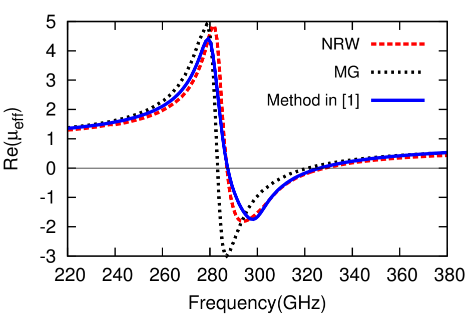

Fig. 2. Comparison between the effective relative permeability obtained with HFSS (NRW), Maxwell Garnett (MG) and computed with the method in [1] for a cubic array of TiO_2 microspheres of 52 μ_{eff}m with a filling fraction of 29.44% in free space.

we compare our results against full-wave simulations (Fig. 3). Namely, we calculate reflection and transmission coefficients for a 5-layer slab of TiO_2 metamaterial as the one of a homogeneous slab with thickness equal to 5 periods by using standard Fresnel formulas assuming the slab to have the refractive index with real part in Fig. 1. Again, we observe an excellent agreement between the different results which confirms the accuracy of the method in [1] (including both spatial dispersion and magnetoelectric coupling) to describe cubic arrays of TiO_2 microspheres.

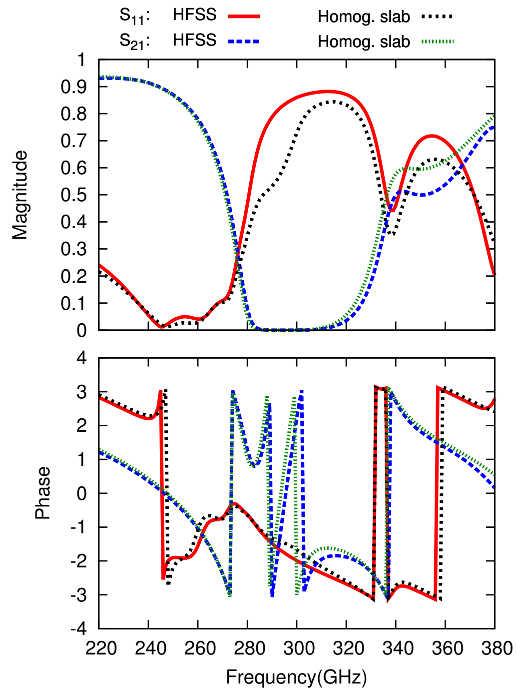

Fig. 3. Comparison between the magnitude and the phase of the S-parameters obtained with HFSS and computed with the method in [1] for a cubic array of TiO_2 microspheres of 52 μm with a filling fraction of 29.44% in free space.

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