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Electromagnetic characterization of submillimiter wave focusing devices based on TiO_2 microsphere metamaterials

Scientific Report on the Research Activity within the framework of the
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Waves Integrated Dielectric Focusing Systems“

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1 Introduction

The lack of strong magnetism in natural materials has motivated in recent years the use of metamaterials to generate artificial magnetism from non-magnetic constitutive materials, especially at high frequencies where natural magnetism disappears. Among the multitude of metamaterial configurations existing to overcome this natural limitation throughout the frequency spectrum [1, 2, 3, 4, 5, 6, 7, 8, 9, 10], one can choose to use magneto-dielectric particles (with high values of permittivity and/or permeability) embedded in a dielectric matrix [11, 12], or two sets of particles with different sizes and/or materials (one designed to resonate at the electric resonant mode, the other one designed to resonate at the magnetic resonant mode), to produce negative permeability [11, 13, 14] and/or an isotropic double negative material [15, 16]. The main advantage of this method is that one can use bottom-up techniques (chemical synthesis of microparticles together with self-assembly method) to create fully 3-dimensional metamaterials.

Following this approach, I have, during my PhD, examined how artificial magnetic properties can be obtained from arrays of dielectric spheres in the sub-millimetric range (from 300 GHz to 1 THz), by using the Mie dipolar magnetic resonance of the spheres. At this resonance strong polarisation current appears inside the spheres giving rise to strong magnetic response ; however, very high permittivity materials (epsilon around 100) are required to obtain an effective medium. In this range of frequency, we have shown after an investigation of a possible list of candidates [17], that titanium dioxide (TiO_2) is a good candidate to elaborate such self-assembled magnetic metamaterials since it presents a permittivity around 100 [18, 19]. Effective magnetic properties from arrays of such spheres, were studied analytically with the help of extensions of the well-known Maxwell Garnett theory, and numerically with finite element simulations. Both analysis showed that it exists range of reasonable filling fraction for which the material exhibits strong magnetic resonance with high positive, near-zero and negative permeability. These extraordinary values of the permeability are extremely interesting and would allow to create metamaterials able to focus far and near part of the magnetic field. Moreover this system could be integrated into more complex structures to create super or hyper lenses which enable to focus both propagating and evanescent part of the electromagnetic field.

The purpose of my visit in Siena in the LEA group under the supervision of Pr. Albani, was to study the applicability of the systems based on array of TiO_2 microspheres to create subwavelength focusing or imaging devices. This choice was motivated by previous collaboration with Pr. Albani's group during my PhD and to take advantage of the strong expertise of Pr. Albani in the modelization of complex electromagnetic systems.

2 Model under consideration

We aim to describe the focusing properties, at terahertz frequency range, of periodic systems composed of TiO_2 microspheres embedded in a host medium. To correctly understand and predict these focusing properties, it is important to evaluate with precision the global electromagnetic response of the structure arising from the collective response of the microscopic elements. Because it neglects the interaction between elements and the effect of wave-propagation, the homogenization model of Maxwell Garnett [20, 21], I used during my PhD, may be not precise enough to describe these systems.

Instead, we decided to use a more complete homogenization model, reported by Silveirinha in [22], that consists in the generalization of the Lorentz-Lorenz formula, and which takes into account interactions between particles as well the non-zero value of the wavevector.

In this method, it is assumed that the infinite array is exciting by an external plane wave with wavevector $\mathbf{k}$. Each microsphere of the infinite array is modelled as both electric and magnetic dipoles, and all interactions between these dipoles are taken into account through the Dyadic Green's function of the periodic array whose evaluation lies in the key point of the method. From the knowledge of the Green's function, it is reported in [22] how to retrieve the effective permittivity and permeability depending both on frequency ω and wavevector $\mathbf{k}$.

The first part of my work in Siena consisted in the implementation, in collaboration with the rest of the team, of the Matlab® code to compute the three dimensional dyadic Green's function for the periodic array. The reliability of the method depending on the fast (and correct) evaluation of the 3D Green's function, a particular care must be done to regularize the Green's function in space and spectral domain and to implement the Ewald's method [23, 24, 25] for fast convergence.

Then, we reformulate the original tensorial expression of the effective parameters to take into account the magnetoelectric coupling (the tensor $\overline{\overline{C}}_{\text{em}}(\omega, \mathbf{k})$ which was neglected in the original publication [22]). Such reformulation has for direct consequence that the medium becomes bianisotropic, i.e. is now described by the following bianisotropic constitutive relation :

$$\begin{aligned}\mathbf{D}_{\text{av}} &= \overline{\overline{\varepsilon}}_{\text{eff}}(\omega, \mathbf{k}) \cdot \mathbf{E}_{\text{av}} + \overline{\overline{\xi}}_{\text{eff}}(\omega, \mathbf{k}) \cdot \mathbf{H}_{\text{av}} \\ \mathbf{B}_{\text{av}} &= \overline{\overline{\mu}}_{\text{eff}}(\omega, \mathbf{k}) \cdot \mathbf{H}_{\text{av}} + \overline{\overline{\zeta}}_{\text{eff}}(\omega, \mathbf{k}) \cdot \mathbf{E}_{\text{av}}.\end{aligned} \tag{1}$$

where the expression of the four tensors $\overline{\overline{\varepsilon}}_{\text{eff}}, \overline{\overline{\mu}}_{\text{eff}}, \overline{\overline{\xi}}_{\text{eff}}, \overline{\overline{\zeta}}_{\text{eff}}$ is given by our code for an arbitrary couple $(\omega, \mathbf{k})$.

In the absence of any source, only a restricted number of modes $\mathbf{k}(\omega)$, so called eigenmodes, are supported by the array. From the Maxwell equations in absence of source, we derived the following equation whose complex solutions give the different complex eigenmodes of the system.

$$\underbrace{\left[\left(\mathbf{k} \times \overline{\overline{I}} + \omega \overline{\overline{\xi}}_{\text{eff}}(\omega, \mathbf{k})\right) \cdot \overline{\overline{\mu}}_{\text{eff}}^{-1}(\omega, \mathbf{k}) \cdot \left(\mathbf{k} \times \overline{\overline{I}} - \omega \overline{\overline{\zeta}}_{\text{eff}}(\omega, \mathbf{k})\right) + \omega^2 \cdot \overline{\overline{\varepsilon}}_{\text{eff}}(\omega, \mathbf{k})\right]}_{M} \cdot \mathbf{E}_{\text{av}} = 0 \tag{2}$$

The solutions of this equation are given by solving numerically $\det(M) = 0$ for a fixed direction of the propagation vector $\mathbf{k}$.

An important part of my work in Siena consisted in writing the Matlab code to numerically solve equation (2) and find the complex eigenmodes of the periodic system. The principle of this two-dimensional fit is to find a polynomial approximation of $\det(M)$ and then use Matlab's functions to find with good precision the roots of the polynomial which correspond to the eigenmodes. This numerical solve can give an infinite set of solutions, and an important part of the code is devoted to the selection and classification of the relevant eigenmodes.

Finally, the last part of my work consisted in the extension of the homogenization model to describe medium with several particles inside the unit cell. To do so, the interactions between particles inside the unit cell have to be taken into account correctly by the dyadic Green's function. This extension allows to obtain the four effective tensors $\overline{\overline{\varepsilon}}_{\text{eff}}(\omega, \mathbf{k})$, $\overline{\overline{\mu}}_{\text{eff}}(\omega, \mathbf{k})$, $\overline{\overline{\xi}}_{\text{eff}}(\omega, \mathbf{k})$, $\overline{\overline{\zeta}}_{\text{eff}}(\omega, \mathbf{k})$ and the possibility to study bidisperse systems like in [16], meant to provide negative index of refraction.

3 Numerical results

3.1 Monodisperse systems

The code Matlab developed in Siena was used to study an infinite three dimensional cubic array of lattice parameter a, composed of TiO_2 microspheres of radius 52 μm embedded in a host medium taken to be vacuum. The permittivity of TiO_2 was taken as $\varepsilon_{\text{TiO}_2} = 94 + 2.35i$ corresponding to the measured value at a frequency of 500 GHz (which is a good approximation for the frequency range between 200 and 500 GHz) [18].
After calculating the complex eigenmodes with longitudinal and transverse polarization propagating inside the structure when considering or not the magnetoelectric coupling, we were able to show that for a filling fraction in microspheres greater than 20%, the magnetoelectric coupling has a noticeable effect on the search of the eigenmodes near the fist magnetic Mie dipolar resonance. These results are consistent with the conclusions of [26].
Secondly, we noted that for filling fractions up to 44% only one complex transverse eigenmode $\mathbf{k}^{\text{tr}}_{\text{eff}}(\omega)$ dominates the electromagnetic behaviour of the structure and can consequently be used to deduce the effective properties of the material. From the value of this mode, we can assign a refractive index to the material with the relation : $n_{\text{eff}}(\omega) = \dfrac{k^{\text{tr}}_{\text{eff}}(\omega)}{k_0}$.
By comparing this index (with or without considering the $\overline{\overline{C}}_{\text{em}}$ tensor) to the one obtained from the full-wave simulation of a 5-layer slab with HFSS$^{\text{TM}}$ using the Nicolson-Ross-Weir (NRW) retrieval method [27] we could show that for frequencies around the lowest order Mie dipolar magnetic resonance of the microspheres, including the magnetoelectric coupling term $\overline{\overline{C}}_{\text{em}}$ results in an improved accuracy with respect to the full-wave simulations. This result is illustrated in Fig. 1 for a filling fraction in microspheres of 29.44%.

Secondly, by comparing the effective parameters corresponding to the eigenmodal propagation (in the absence of internal excitation) to the one obtained when considering $\mathbf{k} = \mathbf{0}$, we were able to highlight the effect of spatial dispersion on the effective parameters. As illustrated in Fig. 2 for the transverse component of the effective permeability tensor, the spatial dispersion (effect of the non zero value of $\mathbf{k}$) has an important effect on the amplitude of the first Magnetic dipolar resonance of the TiO_2 microspheres, but not any noticeable effect on the frequency of such resonance . We can say that to predict with accuracy the focusing properties of such an array of TiO_2 spheres, spatial dispersion effect as well as magnetoelectric coupling have to be taken into account.

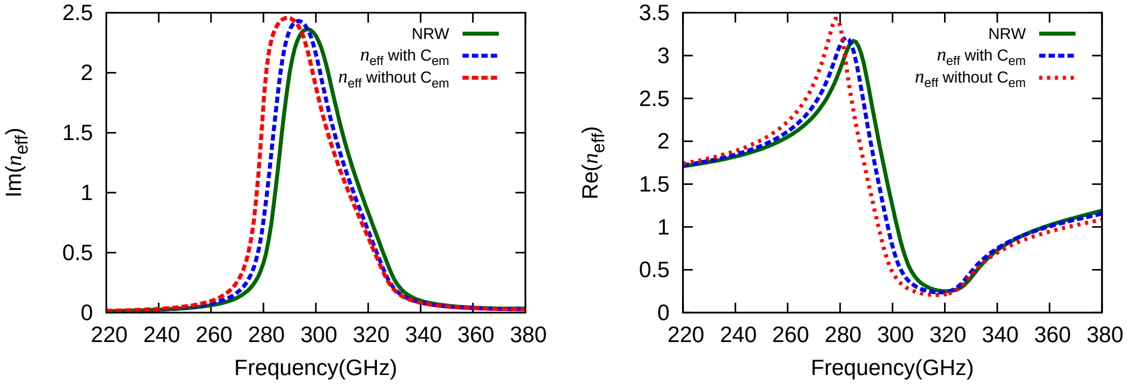

FIGURE 1 – Comparison between the effective refractive index obtained with HFSS (NRW), with the one computed with the present method taking into account or not the $\overline{\overline{C}}_{\mathrm{em}}$ dyadic, for a cubic array of $\mathrm{TiO_2}$ microspheres of 52 μm with a filling fraction of 29.44%.

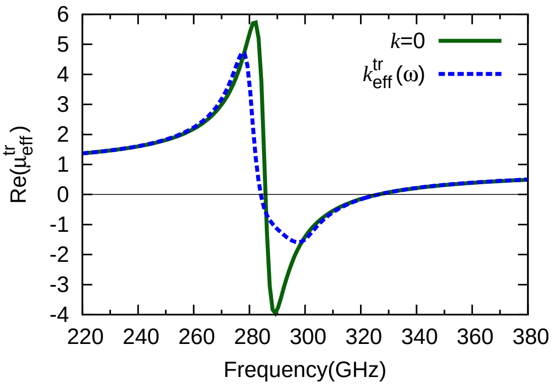

FIGURE 2 – Comparison between the transverse component of the permeability computed with the present method for $\mathbf{k} = \mathbf{0}$ or $\mathbf{k} = \mathbf{k}^{\mathrm{tr}}_{\mathrm{eff}}(\omega)$ for a cubic array of $\mathrm{TiO_2}$ microspheres of 52 μm with a filling fraction of 29.44%.

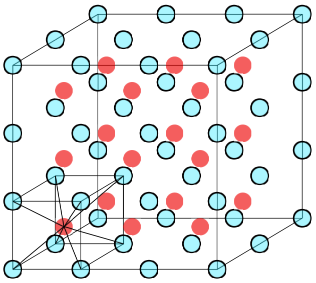

FIGURE 3 – Schematic representation of a BCC array.

3.2 Bidisperse systems

Thanks to the extension of the code to several particles inside the unit cell, we also studied infinite three dimensional bidisperse array of $\mathrm{TiO_2}$ microspheres embedded in a host medium taken to be vacuum. The bidisperse array under consideration is a Body-Centered Cubic (BCC) system as shown in Fig. 3 and consists in small spheres of TiO_2 located at the center of a cubic array made of big spheres of TiO_2. The small spheres mainly contribute to create negative permeability in a frequency band, whereas the big spheres contribute to create negative permittivity in the same band, giving rise, in theory, to a negative index band.

Like for the monodisperse case, we computed, using equation (2) and our Matlab code, the complex eigenmodes with transverse and longitudinal polarization inside the structure. This eigenmode calculation highlight the fact that a backward mode exists for some range of filling fraction (greater than 25 %), but it is a strongly attenuated mode coexisting with a forward mode as illustrated in Fig. 4 for a filling fraction of 29.44%. For this reason, we could conclude that these bidisperse systems of TiO_2 are unable to provide pure backward propagation (2 modes coexisting).

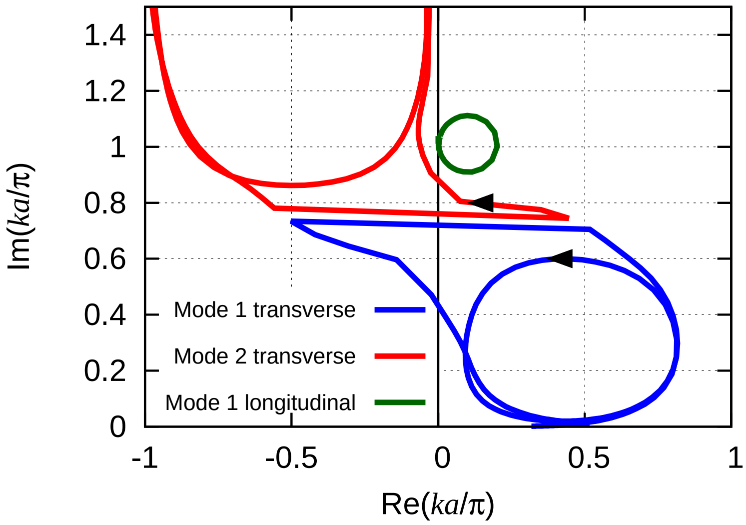

FIGURE 4 – Trajectories in the complex plane of both longitudinal and transverse normalized eigenmodes computed with equation (2) for a bidisperse cubic array of TiO_2 microspheres of 52 and 37 μm of radius with a filling fraction of 29.44%.

4 Publication

As a result of my work in Siena, an article about the the effect of spatial dispersion and magnetoelectric coupling on the magnetic properties of monodisperse array of TiO_2 spheres in terahertz frequency range was written. We are at the present time finishing the last corrections before submitting the article to a scientific journal.
Also, two abstracts were sent and accepted for presentations in a conference. The first one was sent to “EuCAP 2013, the 7th European Conference on Antennas and Propagation” which will be held in April 2013 at the Swedish Exhibition & Congress Centre in Gothenburg, Sweden. The second contribution was to the “2013 IEEE International Symposium on Antennas and Propagation” which will be held July 7-13, 2013, at the Hilton Orlando

Lake Buena Vista in Lake Buena Vista, Florida, USA.

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