Closed-form Expressions of Local Effective Bianisotropic Constitutive Parameters for Reciprocal Metamaterials

Valentina Sozio[1], Andrea Vallecchi[2], Matteo Albani[1], Filippo Capolino[3]
[1] Dept. of Information Engineering and Mathematics, University of Siena, Siena, Italy, valentina.sozio@unisi.it, matteo.albani@dii.unisi.it
[2] Dept. of Electronics and Electrical Engineering, University of Sheffield, Sheffield, United Kingdom, a.vallecchi@sheffield.ac.uk
[3] Dept. of Electrical Engineering and Computer Science, University of California Irvine, USA, f.capolino@uci.edu

***Abstract*—A straightforward approach is proposed to retrieve the local effective electromagnetic constitutive parameters of reciprocal bianisotropic metamaterials. The derivation is based on the Floquet representation of the field in periodic arrays and assumes that the metamaterial can be described by a nonlocal spatially dispersive generalized dielectric function incorporating all the polarization effects, including artificial magnetism, bianisotropy, and higher-order spatial dispersion effects. Closed-form expressions that directly relate the local bianisotropic model parameters to the nonlocal generalized effective permittivity are developed. The proposed formulas provide a homogenized description of the metamaterials that takes into account implicit weak spatial dispersion effects in terms of local nondispersive permittivity, permeability and magnetoelectric coupling parameters. Numerical examples are presented to demonstrate the applicability of these formulas for the retrieval of effective parameters of metamaterials with different types of lattices and inclusions.**

***Index Terms*—Metamaterials, bianisotropic media, constitutive relations, homogenization.**

I. Introduction

The potentiality of metamaterials highlighted in recent years has fueled research into understanding the interaction between these composite structures and electromagnetic radiation. The use of homogenization methods can provide a convenient characterization of such an interaction by describing metamaterials as bulk homogeneous materials with certain effective parameters that take into account their inherent qualities and complex nature, depending on both their elementary constituents and their spatial arrangement.

However, the application of the concept of homogenization encounters some difficulties when it comes to artificial materials because the size of the lattice constant is typically only moderately smaller than the wavelength of the electromagnetic radiation, in contrast to natural materials where the wavelength-to-lattice ratio is several orders of magnitude larger, even at optical frequencies. As a consequence, spatial dispersion effects are usually non-negligible in metamaterials and must be duly considered in the derivation of their homogenized description [1].

In [2], [3] a general homogenization approach for nonmagnetic periodic metamaterial has been recently introduced. It is based on the Floquet representation of the field in three dimensional periodic arrays and it is capable of providing a comprehensive description of both spatial and frequency dispersion phenomena. This homogenization method, so far limited to dielectric-only metamaterials, is characterized by the introduction of a single generalized permittivity tensor that takes into account all the polarization effects, including artificial magnetism, bianisotropy, and higher-order spatial dispersion effects. When spatial dispersion is weak, this nonlocal generalized permittivity can be connected with the local effective parameters of the classical bianisotropic constitutive model [2]. Whenever possible, it is more convenient to adopt a local homogenization scheme of material and describe the weak spatial dispersion effects in terms of local permeability and chirality parameters. In fact, the local bianisotropic constitutive model is valid in the spatial domain and can be used, for example, to establish boundary condition at an interface in a scattering problem, whereas the nonlocal generalized permittivity model only applies in the Fourier transformed (wavenumber) domain and implicitly assumes an infinite unbounded homogeneous structure [2].

The method subsequently proposed in [4], which is a generalization of the Floquet based homogenization approach developed in [2], provides an averaging procedure to define constitutive parameters that have local properties in the long-wavelength limit. A Taylor expansion of the polarization and magnetization currents is used to arrive at a description that explicitly takes into account weak spatial dispersion effects in the form of magnetoelectric coupling at the lattice level. However, the Taylor expansion relies upon the assumption of slow variation of the induced microscopic polarization and magnetization vectors within a unit cell.

To extract the local effective parameters of a generic composite material, it is suggested in [5] to expand the generalized permittivity tensor in a Taylor series. Nevertheless, there are inherent difficulties in calculating the local permeability through this procedure, because of the quadrupole moment contribution to the second order spatial derivatives of the nonlocal permittivity which of course cannot be taken into account by the local bianisotropic parameters.

The objective of this work is to develop an automatic and straightforward approach to retrieve the local effective bianisotropic parameters from the nonlocal generalized permittivity tensor. This local homogenization scheme can accurately describe the composite material when spatial dispersion is weak and an averaging of the fields can be performed.

II. FORMULATION

The *nonlocal* generalized dielectric function $\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})$ introduced in [2] to describe a homogenized metamaterial medium can be related to the parameters of the classical local bianisotropic constitutive model through the expression

$$\frac{\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})}{\varepsilon_h}=\left(\underline{\boldsymbol{\varepsilon}}_r-\underline{\boldsymbol{\xi}}\cdot\underline{\boldsymbol{\mu}}_r^{-1}\cdot\underline{\boldsymbol{\zeta}}\right)+\left(\underline{\boldsymbol{\xi}}\cdot\underline{\boldsymbol{\mu}}_r^{-1}\times\frac{c\mathbf{k}}{\omega}-\frac{c\mathbf{k}}{\omega}\times\underline{\boldsymbol{\mu}}_r^{-1}\cdot\underline{\boldsymbol{\zeta}}\right)+ \\ +\frac{c\mathbf{k}}{\omega}\times\left(\underline{\boldsymbol{\mu}}_r^{-1}-\underline{\mathbf{I}}\right)\times\frac{c\mathbf{k}}{\omega} \tag{1}$$

where $\underline{\boldsymbol{\varepsilon}}_r$ and $\underline{\boldsymbol{\mu}}_r$ are the local relative permittivity and permeability tensors, $\underline{\boldsymbol{\xi}}$ and $\underline{\boldsymbol{\zeta}}$ are dimensionless tensors that characterize the magnetoeletric coupling, and $\mathbf{k}$ denotes the wave vector.

To invert the above relation and extract from the nonlocal spatially dispersive generalized permittivity tensor the $\mathbf{k}$-independent local bianisotropic parameters, we assume that the metamaterial is reciprocal, implying that $\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})=\underline{\boldsymbol{\varepsilon}}_g^t(\omega,-\mathbf{k})$, where the superscript t denotes a transpose matrix, that in turn implies $\underline{\boldsymbol{\varepsilon}}_r=\underline{\boldsymbol{\varepsilon}}_r^t$, $\underline{\boldsymbol{\mu}}_r=\underline{\boldsymbol{\mu}}_r^t$, and $\underline{\boldsymbol{\xi}}=-\underline{\boldsymbol{\zeta}}^t$. It is convenient to introduce two novel operators acting on a dyad $\underline{\mathbf{A}}(\mathbf{k})$ function of the vector wavenumber $\mathbf{k}$: a "right-hand" curl

$$\underline{\mathbf{A}}\times\nabla_{\mathbf{k}}=-\left(\nabla_{\mathbf{k}}\times\underline{\mathbf{A}}^t\right)^t \tag{2}$$

(i.e., a curl applied to rows of $\underline{\mathbf{A}}$, in contrast to standard curl which operates on columns) and, related to this, the second order differential operator

$$\nabla_{\mathbf{k}}\times\underline{\mathbf{A}}\times\nabla_{\mathbf{k}}=-\nabla_{\mathbf{k}}\times\left(\nabla_{\mathbf{k}}\times\underline{\mathbf{A}}^t\right)^t, \tag{3}$$

where $\nabla_{\mathbf{k}}=\sum_{p=1}^{3}\frac{\partial}{\partial k_p}\hat{\mathbf{u}}_p$ is the nabla differential operator with respect to $\mathbf{k}$.

By applying the above defined operators to (1), the following closed form expressions can be derived for the retrieval of the local parameters

$$\begin{cases}\underline{\boldsymbol{\mu}}_r=\left\{\underline{\mathbf{I}}+\frac{k_h^2}{6}\left[\nabla_{\mathbf{k}}\times\frac{\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})}{\varepsilon_h}\times\nabla_{\mathbf{k}}\right]_{\mathbf{k}=\mathbf{0}}\right\}^{-1}\\ \underline{\boldsymbol{\zeta}}=k_h\underline{\boldsymbol{\mu}}_r\cdot\left[\nabla_{\mathbf{k}}\times\frac{\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})}{\varepsilon_h}\right]_{\mathbf{k}=\mathbf{0}}\\ \underline{\boldsymbol{\xi}}=k_h\left[\frac{\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})}{\varepsilon_h}\times\nabla_{\mathbf{k}}\right]_{\mathbf{k}=\mathbf{0}}\cdot\underline{\boldsymbol{\mu}}_r\\ \underline{\boldsymbol{\varepsilon}}_r=\frac{\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{0})}{\varepsilon_h}+\underline{\boldsymbol{\xi}}\cdot\underline{\boldsymbol{\mu}}_r^{-1}\cdot\underline{\boldsymbol{\zeta}}\end{cases} \tag{4}$$

To calculate the generalized dielectric function we apply the Lorentz-Lorenz homogenization method proposed in [3] and recently extended to the case when the unit cell of a 3D periodic array contains more than one inclusion in [6]. Within this homogenization scheme, we consider non bianisotropic particles and introduce a dual dipole approximation for the induced currents assuming that the microscopic electric and magnetic current distributions in the unit cell can be described by a superposition of electric and magnetic dipole moments. Specifically, here we consider a unit cell with N inclusions located at $\mathbf{r}_n$, each characterized by both electric $\underline{\boldsymbol{\alpha}}_{ee,n}$ and a magnetic $\underline{\boldsymbol{\alpha}}_{mm,n}$ dyadic polarizabilities. Based on these assumptions, the *nonlocal* generalized permittivity tensor, valid for multiple inclusions in the unit cell, can be expressed as follows

$$\frac{\tilde{\underline{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})}{\varepsilon_h}=\underline{\mathbf{I}}+\frac{1}{V_{cell}}\sum_{n,j=1}^{N}\left[\underline{\mathbf{A}}_{ee,nj}\cdot\underline{\boldsymbol{\alpha}}_{ee,j}-\frac{\mathbf{k}}{k_h}\times\underline{\mathbf{A}}_{me,nj}\cdot\underline{\boldsymbol{\alpha}}_{ee,j}\right. \\ \left.+\underline{\mathbf{A}}_{em,nj}\cdot\underline{\boldsymbol{\alpha}}_{mm,j}\times\frac{\mathbf{k}}{k_h}-\frac{\mathbf{k}}{k_h}\times\underline{\mathbf{A}}_{mm,nj}\cdot\underline{\boldsymbol{\alpha}}_{mm,j}\times\frac{\mathbf{k}}{k_h}\right] \tag{5}$$

where, by resorting to block matrix notation,

$$\begin{bmatrix}\underline{\mathbf{A}}_{ee,nj} & \underline{\mathbf{A}}_{em,nj}\\ \underline{\mathbf{A}}_{me,nj} & \underline{\mathbf{A}}_{mm,nj}\end{bmatrix}_{6N\times6N}=\begin{bmatrix}\underline{\mathbf{B}}_{ee,nj} & \underline{\mathbf{B}}_{em,nj}\\ \underline{\mathbf{B}}_{me,nj} & \underline{\mathbf{B}}_{mm,nj}\end{bmatrix}_{6N\times6N}^{-1} \tag{6}$$

with

$$\begin{aligned}\underline{\mathbf{B}}_{ee,nj}&=\underline{\mathbf{I}}\delta_{nj}-\underline{\boldsymbol{\alpha}}_{ee,n}\cdot\underline{\mathbf{C}}_{\text{int}}(\mathbf{r}_n-\mathbf{r}_j;\omega,\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_n)}\\ \underline{\mathbf{B}}_{em,nj}&=-\underline{\boldsymbol{\alpha}}_{ee,n}\cdot\underline{\mathbf{C}}_{e,m}(\mathbf{r}_n-\mathbf{r}_j;\omega,\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_n)}\\ \underline{\mathbf{B}}_{me,nj}&=\underline{\boldsymbol{\alpha}}_{mm,n}\cdot\underline{\mathbf{C}}_{e,m}(\mathbf{r}_n-\mathbf{r}_j;\omega,\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_n)}\\ \underline{\mathbf{B}}_{mm,nj}&=\underline{\mathbf{I}}\delta_{nj}-\underline{\boldsymbol{\alpha}}_{mm,n}\cdot\underline{\mathbf{C}}_{\text{int}}(\mathbf{r}_n-\mathbf{r}_j;\omega,\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_n)}+\frac{\underline{\boldsymbol{\alpha}}_{mm,n}}{V_{cell}}\end{aligned} \tag{7}$$

The indices (n, j) correspond to the 3×3 dyadic coefficients describing the contribution of the j -th electric and magnetic dipoles to the microscopic field at $\mathbf{r}_n$ arranged along the rows and columns of the linear system block matrix. The host medium intrinsic wavenumber is indicated by k_h, and V_{cell} is the volume of each unit cell containing the N inclusions The dyadic regularized Green's functions $\underline{\mathbf{C}}_{\text{int}}(\mathbf{r}_n - \mathbf{r}_j; \omega, \mathbf{k})$ and $\underline{\mathbf{C}}_{e,m}(\mathbf{r}_n - \mathbf{r}_j; \omega, \mathbf{k})$ introduced in [3], rigorously take into account the electromagnetic interaction among the constituent particles within each unit cell, in a 3D periodic environment.

The *nonlocal* generalized permittivity tensor (5) is then used in (4) to calculate the *local* bianisotropic parameters. The derivatives with respect to $\mathbf{k}$ appearing in (4) are implemented numerically as centered finite differences. The resulting parameters allow the *local* representation of the weakly dispersive part of the generalized permittivity. A residual term

$$\mathbf{\Delta}(\omega, \mathbf{k}) = \frac{1}{\varepsilon_h}\left[\tilde{\underline{\boldsymbol{\varepsilon}}}_g(\omega, \mathbf{k}) - \underline{\boldsymbol{\varepsilon}}_g(\omega, \mathbf{k})\right], \qquad (8)$$

which vanishes in the long wave length limit $\mathbf{k} \to 0$, might be in general present when a non-negligible spatial dispersion is included in $\tilde{\underline{\boldsymbol{\varepsilon}}}_g(\omega, \mathbf{k})$ because of quadruple or other higher order effects.

III. Numerical Results

To validate and illustrate the application of the formulas presented in the previous section, we homogenize a few sample configurations of metametarials, whose unit cells are formed by spherical inclusions arranged in different types of lattices.

In the first example, we consider the homogenization of a periodic cubic lattice with a *single* spherical dielectric inclusion in the unit cell. In particular, we refer to the array of dielectric particles previously analysed in [7]. The radius of the spherical inclusion is $a = 1.069$ mm, its permittivity is equal to $\varepsilon_{inc} = 400$, and the lattice period is $s_i = 4$ mm. Fig. 1 shows the yy-component of the relative generalized effective permittivity (with spatial dispersion) of the composite material for three different values of the wave vector $\mathbf{k}$ which is directed along the x-axis, i.e. $\mathbf{k} = k_x\hat{x}$.

The bianisotropic *local* parameters computed according to (4), that equivalently describe the material electromagnetic response, are depicted in Fig. 2. By comparing the dispersive generalized permittivity in Fig. 1 and the local parameters in Fig. 2, it appears that the resonance of the generalized permittivity occurring at about 10 GHz is an intrinsic electric resonance of the medium, subject to negligible spatial dispersion, which is accurately reproduced by the extracted local permittivity in Fig. 2. It is noted that in a small bandwidth near the resonance of the permittivity, the magnetic permeability exhibits an anomalous behaviour and tends to

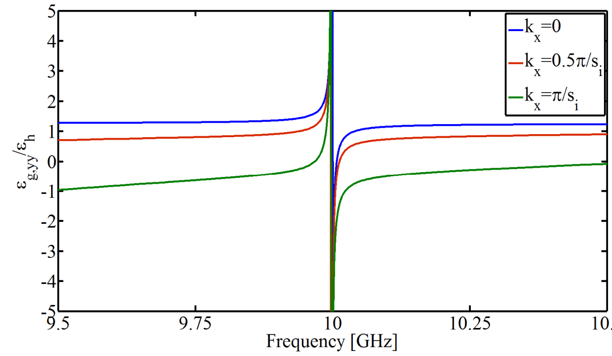

Fig. 1. Generalized permittivity for a periodic cubic lattice of dielectric spherical inclusions with permittivity $\varepsilon_{inc} = 400$ and radius $a = 1.069$ mm for different values of k_x.

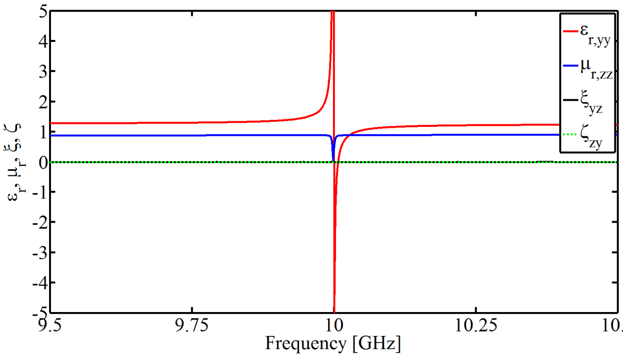

Fig. 2. Local bianisotropic parameters for a periodic cubic lattice of dielectric spherical inclusion with permittivity $\varepsilon_{inc} = 400$ and radius $a = 1.069$ mm.

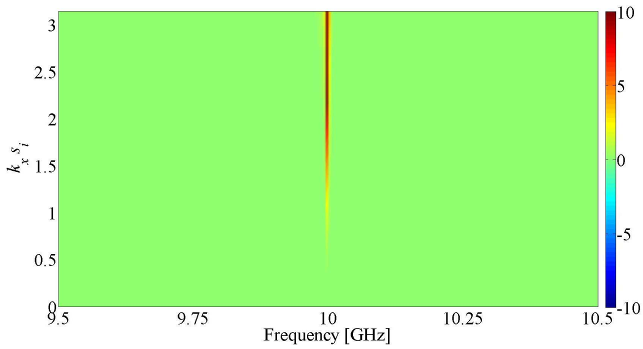

Fig. 3. Plot of $\mathbf{\Delta}(\omega, \mathbf{k})$ at variable frequency and wavenumber for a metamaterial made of a periodic cubic lattice of dielectric spherical inclusion with permittivity $\varepsilon_{inc} = 400$ and radius $a = 1.069$ mm.

vanish at the electric resonance. In fact, as explained in [2], across rapid variation of the permittivity it cannot be expected that a Taylor expansion of the dielectric function be accurate, and spatial dispersion can become dominant.

To assess the validity of the *local* bianisotropic representation of the metamaterial electromagnetic response, we check the amplitude of the yy-component of the residual term (8) which is plotted in Fig. 3 for varying frequency and wavenumber. Generally, $\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})$ calculated as in (1) from the local parameters well approximates the original nonlocal permittivity $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$ except that in the narrow frequency region close to the resonance of the nonlocal permittivity.

In a second example, we consider again a metamaterial lattice with a single dielectric inclusion per unit cell with the same permittivity as in the previous example but with a smaller radius ($a = 0.748$ mm). The results for the nonlocal generalized permittivity and the local parameters are presented in Figs. 4 and 5, respectively. In this case, it can be observed that the resonance of the nonlocal generalized permittivity strongly depends on the value of $\mathbf{k}$ (note also that the resonance occurs just for the values of $\mathbf{k}$ different from zero). This resonance has a magnetic nature, as can be clearly detected by examining the extracted local permeability that provides a neat local characterization of this phenomenon.

Similarly to the previous example, in Fig. 6 we plot the yy-component of $\boldsymbol{\Delta}(\omega,\mathbf{k})$. As apparent, the discrepancy between $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$ and $\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})$ is significant over a larger portion of the considered frequency and wavenumber range. This is not unexpected because, as shown in Fig. 4, spatial dispersion effects are particularly evident in $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$, and cannot be adequately described by means of the Taylor expansion at $\mathbf{k} = 0$; i.e., it is not "weak".

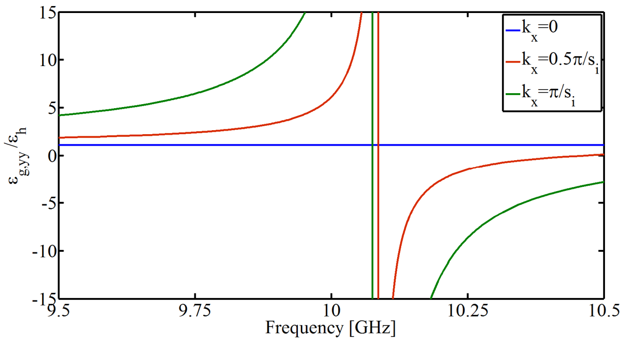

Fig. 4. Generalized permittivity of a periodic cubic lattice of spherical inclusions with permittivity $\varepsilon_{inc} = 400$ and radius $a = 0.748$ mm for different values of k_x.

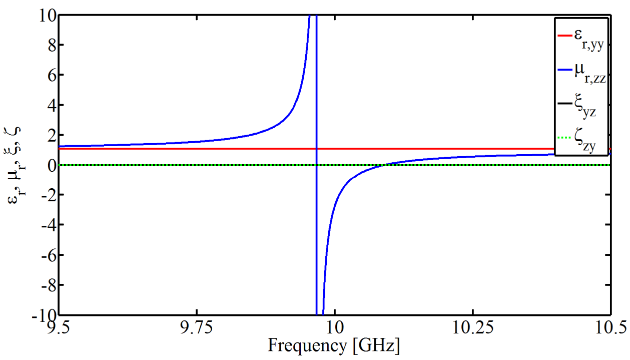

Fig. 5. Local bianisotropic parameters for a periodic cubic lattice of spherical inclusions with permittivity $\varepsilon_{inc} = 400$ and radius $a = 0.748$ mm.

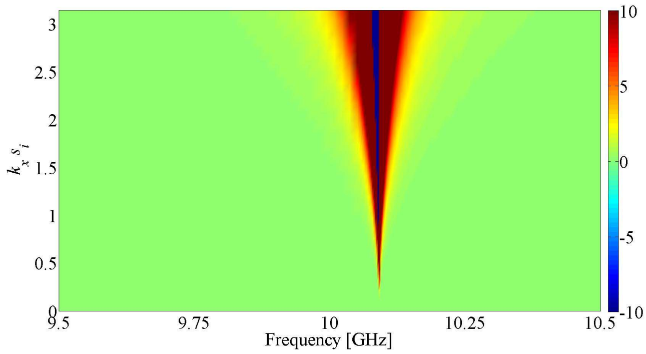

Fig. 6. Plot of $\boldsymbol{\Delta}(\omega,\mathbf{k})$ at variable frequency and wavenumber for a periodic cubic lattice of dielectric spherical inclusion with permittivity $\varepsilon_{inc} = 400$ and radius $a = 0.748$ mm.

In a last example, we electromagnetically homogenize a metamaterial whose unit cells are formed by arranging in the binary face-centered cubic lattice (fcc) shown in Fig. 7 the two types of inclusions that we have individually analysed in the previous examples. As suggested in [7], this structure can constitute a 3D isotropic medium with simultaneous negative effective permittivity and permeability.

The results of both the nonlocal and local homogenization approaches applied to this composite material are shown in Figs. 8 and 9, respectively. In this case the generalized permittivity apparently exhibits a double resonance at two close frequencies (one is narrower than the other), which eventually results in both resonant local permittivity and local permeability.

In the plot of the yy-component of $\boldsymbol{\Delta}(\omega,\mathbf{k})$ shown in Fig. 10 it is noted that the disagreement between $\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})$ and $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$ is concentrated at the resonance of $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$ with an electric nature, at ~10 GHz, and in the vicinity of the narrower resonance of $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$ with a magnetic nature, particularly in the region of vanishing $\underline{\boldsymbol{\mu}}_r$ at ~10.05 GHz. Due to the smaller density of each kind of inclusion in this binary array configuration, the bandwidth of both resonances is narrower and accordingly $\underline{\boldsymbol{\varepsilon}}_g(\omega,\mathbf{k})$ fails to accurately reconstruct $\underline{\tilde{\boldsymbol{\varepsilon}}}_g(\omega,\mathbf{k})$ over a limited but important frequency range.

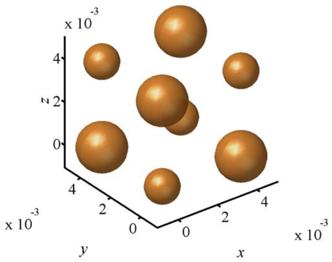

Fig. 7. Geometry of a binary fcc lattice of dielectric inclusions of the same dielectric material but of different radii ($a_1 = 0.748$, $a_2 = 1.069$ mm).

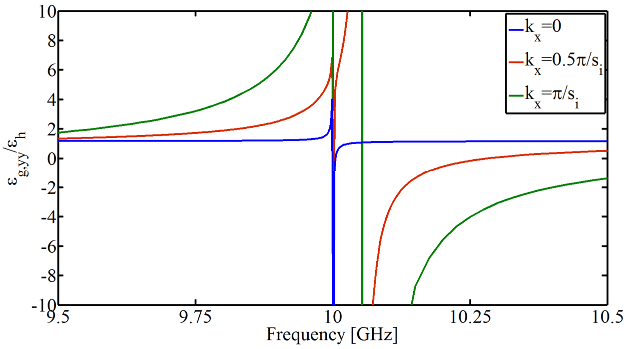

Fig. 8. Generalized permittivity for the periodic binary fcc lattice in Fig. 7.

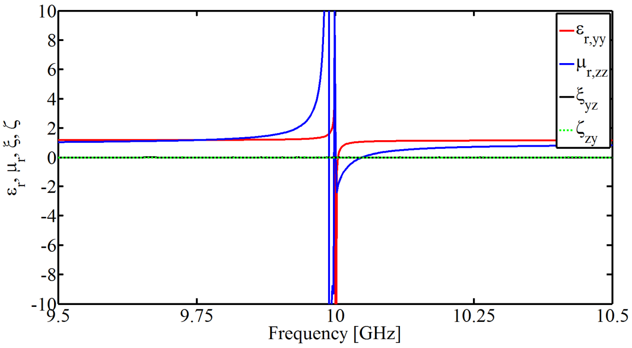

Fig. 9. Local bianisotropic parameters for the periodic binary fcc lattice in Fig. 7.

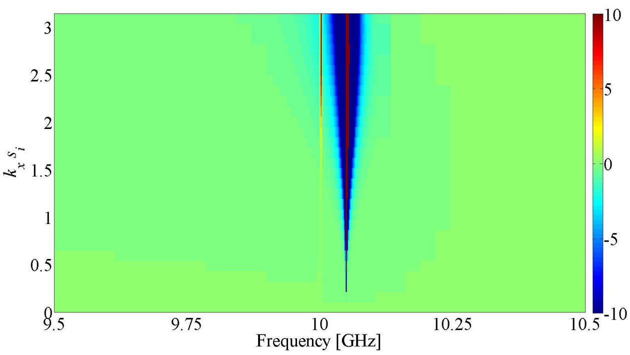

Fig. 10. Plot of $\Delta(\omega, \mathbf{k})$ at variable frequency and wavenumber for the periodic binary fcc lattice in Fig. 7.

Further examples of homogenization of metamaterials formed by periodic arrangements of spherical plasmonic nanoclusters, which have been proposed as building blocks for new magnetic and negative index materials at optical frequencies [8]-[10], will be presented at the conference.

IV. Conclusion

A retrieval procedure has been devised to extract the *local* bianisotropic model parameters of reciprocal metamaterials from the *nonlocal* spatially dispersive generalized dielectric function, incorporating all the polarization effects. Closed-form expressions have been derived for the *local* nondispersive permittivity, permeability and magnetoelectric coupling parameters. These formulas have been demonstrated to be applicable for the electromagnetic homogenization of metamaterial constitutive parameters with different types of lattices and inclusions, taking into account implicit weak spatial dispersion effects.

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