Homogenization of Negative-Index Composite Metamaterials: A Two-Step Approach

A. I. Căbuz, D. Felbacq, and D. Cassagne

Groupe d'Etude des Semiconducteurs UMR CNRS-UM2 5650, CC074, Université Montpellier II, Pl. E. Bataillon, F-34095 Montpellier Cedex 05, France

(Received 11 December 2005; published 17 January 2007)

We present a two-step homogenization method for composite metamaterials. First, each layer of wires or resonators is homogenized as a slab with negative permittivity or permeability, respectively. Second, the single negative stack which results is homogenized to form the effective medium. Comparing the predictions of the first and second step can serve as a gauge of the homogeneity of the composite. We thus take a gradual approach to homogenization, asking not *whether*, but *to what extent* a composite metamaterial approaches the sought after effective medium. Our two-step approach can also capture phenomena which otherwise may be wrongly attributed to effective medium behavior. We illustrate by qualitatively reproducing and reinterpreting a set of experimental data from the literature.

DOI: 10.1103/PhysRevLett.98.037403 PACS numbers: 78.20.Ci, 41.20.Jb, 42.70.Qs, 78.67.−n

Metamaterials with a possibly negative index of refraction have been under intense study since the results of Pendry [1,2] suggested that they might be fabricated by interspersing effective negative permittivity media (thin metal wires or electric resonators) with effective negative permeability media (magnetic resonators such as split rings or high dielectric fibers). Negative permittivity and negative permeability can be obtained separately, but the way in which they mix in order to obtain a *negative-index* medium is less well understood. Attempts to model the composites have been primarily based on black-box experimental or numerical reverse engineering methods [3] which provide only limited information about the physics of the structure.

Our aim in this Letter is to put forward and illustrate a bottom up, constructive approach to understanding negative-index composites. It basically consists of treating the material as a stack of single negative parameter monolayers (Fig. 1). There are some compelling arguments for conceiving of negative-index composites this way.

First, is the pragmatic argument. The majority of experimental and numerical work available in the literature has concentrated on periodic structures built by alternating monolayers of wires and monolayers of resonators in different configurations (e.g., Fig. 1 of Ref. [4]). Thus experimental data is already widely available.

Second, there is the theoretical work of Pokrovsky and Efros [5] and Marques and Smith [6] which has shown that the negative epsilon property of metallic gratings is fragile with respect to the brutal mixing of the wires with other objects. The negative permittivity of thin wire structures is essentially an interference phenomenon and anything that perturbs the interference of waves scattered by neighboring wires is liable to destroy it. Resonators should therefore not be placed between wires, as much as possible, which immediately leads to the idea of stacking them monolayer by monolayer. This conclusion is supported by more recent work [7,8] which has shown that near field coupling between wires and resonators is detrimental to negative-index phenomena. Placing resonators at nodes of the magnetic field of the wire structure, halfway between successive wire rows [8], is a way to minimize inductive coupling, which leads us again to the idea of the alternating monolayers. Also supporting our approach is the classical result that in a periodic 3D network of dipoles (atoms in the classical Clausius-Mosotti model) over 92% of the local field seen by any particular dipole is due to other atoms in the same plane [9].

The third and perhaps most compelling argument is that by comparing the predictions of the partial homogenization with the full homogenization we can distinguish in a simple way phenomena which are truly due to effective medium behavior from other features (transmission peaks) which are due to non effective medium behavior. It gives us important information regarding how large a wavelength to

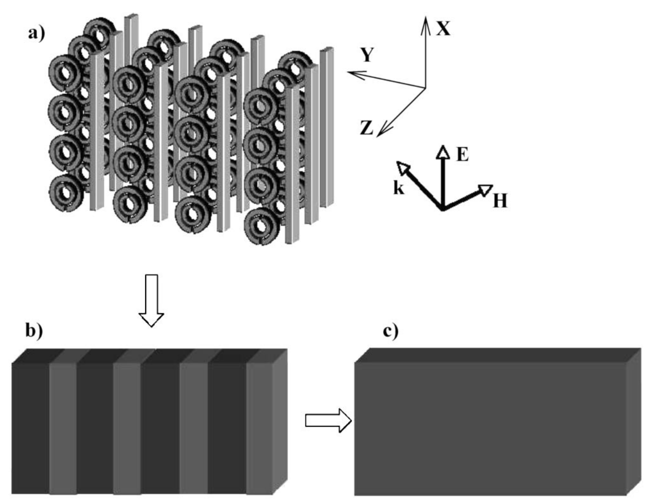

FIG. 1. First each monolayer making up the composite is homogenized giving a 1D stack composed of two anisotropic layers, each characterized by a permittivity and a permeability tensor. Second, the 1D stack is homogenized to give the effective medium. The three media are referred to below as (a) ''the composite'' (the 3D structure), (b) ''the 1D stack'', and (c) ''the effective medium''.

 © 2007 The American Physical Society

period ratio is required for effective medium operation. In effect, the intermediate 1D medium serves as an *upper bound*, in a sense, on the ''homogeneity'' of the composite and can therefore be used to gauge the validity of the effective medium model. We illustrate by qualitatively reproducing experimental results available in the literature and using it to reinterpret those results. We now discuss the meta-"atoms'' available and their layerwise homogenization.

There have been different proposals for resonating elements, from Pendry's initial suggestions: the split rings and the high dielectric fibers [1,10] to the more recent nanorods [11], gold dots [12], or short wires [13]. For instance, high dielectric rod media [14] have been shown rigorously to exhibit magnetic activity of the form

$$\mu_{\rm eff}(k_0) = I + C\frac{k_0^2}{(k_p^2 - k_0^2)}, \tag{1}$$

where C and k_p are constants related to the geometry of the resonator and k_0 the wave number in vacuum. The various kinds of split ring resonators are now well understood as well, see, for example, Sauviac *et al.* [15]. A 2D medium composed of wires directed along x can be described by a diagonal permittivity tensor with diagonal elements (ε_{xx}, 1, 1), where

$$\varepsilon_{xx} = 1 - \frac{2\pi\gamma}{k_0^2 - k_x^2}, \tag{2}$$

and $\gamma = 1/[d^2 \ln(\frac{d}{2\pi a})]$, where d is the period, a the wire radius and k_x the wave vector component along the x direction [16].

It is important to note that even though effective medium models such as those cited above concentrate on infinite two dimensional media filled with either wires or resonators, as the case may be, single rows of the respective elements continue to exhibit the same effective medium properties.

For the case of the wire medium, it has recently been shown that a single thin wire grating can be homogenized to a very good approximation as a negative permittivity slab [17,18]. For the case of the magnetic resonating medium, the analogous result can be verified numerically. This is done in [14] for a 3 row dielectric structure, but continues to hold for a single row. Because of the strong localization of the field in the high dielectric rods, the transfer matrix of a single grating is only weakly dependent on the presence of the neighboring rows. In the case of metallic resonators the layer parameters can be obtained by treating it as a monolayer of point dipoles [9,19,20] characterized by dispersive polarizabilities which can be obtained analytically [15]. Stronger field localization can be achieved by using designs with higher internal capacitance such as the broadside-coupled resonators of Ref. [21]. The benefits of weak evanescent coupling among neighboring elements justify this design decision [7,8].

We can therefore perform the first step of the homogenization procedure, by approximating the composite metamaterial with a single negative 1D stack. The remaining step is now that of homogenizing this structure to obtain the overall effective medium model.

The effective medium of a 1D stack of anisotropic slabs can be obtained using a variety of well known methods such as the powerful two-scale expansion method [22]. We consider that each homogeneous slab is described by two diagonal tensors $\varepsilon_h = \mathrm{diag}(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz})$ and $\mu_h = \mathrm{diag}(\mu_{xx}, \mu_{yy}, \mu_{zz})$ grouping a total of six y dependent functions since the medium is invariant in x and z. The effective medium parameters are given by

$$\varepsilon_h = \mathrm{diag}(\langle\varepsilon_{xx}\rangle, \langle\varepsilon_{yy}^{-1}\rangle^{-1}, \langle\varepsilon_{zz}\rangle), \tag{3}$$

$$\mu_h = \mathrm{diag}(\langle\mu_{xx}\rangle, \langle\mu_{yy}^{-1}\rangle^{-1}, \langle\mu_{zz}\rangle), \tag{4}$$

where the brackets denote averaging over the period. It is clear that the effective medium is very rich in possible configurations and properties [23]. The unboundedness of the harmonic mean (the y components) is a particularly promising avenue for realizing media with exotic behaviors, and is also behind the resonant behavior of the Wiener bounds [24].

We now concentrate on comparing the predictions of our approach and the experimental data made available and interpreted in Figs. 2 and 3 of Ref. [25]. In this work, the metamaterial corresponds to the one represented in Fig. 1(a). Following our analysis the metamaterial is replaced by the *partially* homogenized two-layers medium of Fig. 1(b) and finally by the *fully* homogenized medium of Fig. 1(c). The two layers of Fig. 1(b) are characterized by parameters ε_1, μ_1 and ε_2, μ_2, where $\varepsilon_1 = \mathrm{diag}(\varepsilon_r, \varepsilon_r, 1)$, $\mu_1 = \mathrm{diag}(1, 1, \mu_{\rm eff})$, and $\varepsilon_2 = \mathrm{diag}(\varepsilon_{xx}, 1, 1)$, $\mu_2 = \mathbf{1}$ and where $\mu_{\rm eff}$ and ε_{xx} are given by Eqs. (1) and (2), respectively. The effective medium of Fig. 1(c) is characterized by parameters $\varepsilon_h = \varepsilon_1\theta_1 + \varepsilon_2\theta_2$ and $\mu_h = \mu_1\theta_1 + \mu_2\theta_2$, where θ_1 and θ_2 are the filling fractions, 0.8 and 0.2, respectively, as estimated from Ref. [25]. We have assumed the resonators to be symmetrical in x and y and that the permittivity ε_r is constant over the wavelengths under study. It is known that this permittivity is only weakly dispersive [14,26]. In order to simulate the wires with the closed resonators we can then simply set $\mu_{\rm eff} = 1$ and to simulate the resonators alone, without the wires, we set $\varepsilon_{xx} = 1$.

The incident field is polarized with the electric field along the wires (x direction) and the magnetic field along the resonators (z direction). The period we used was 5 mm [25], and we plot transmission curves as a function of frequency in GHz.

The form of the permeability was chosen to resonate around 8.6 GHz as seen from the dash-dot curves, the transmission of resonators alone. In the case of Fig. 2 the plasma frequency of the wires plus closed resonators was chosen to the left of the magnetic resonance, while in Fig. 3

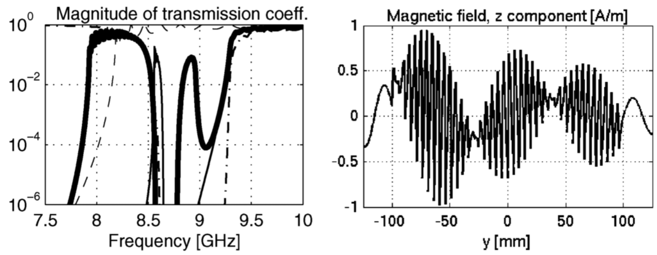

FIG. 2. Left—transmission curves for the case of plasma frequency (~8.3 GHz, wires and closed resonators—dashed line) below the magnetic resonating frequency (8.6 GHz, resonators alone—dot-dashed line). Right—the field profile for a stack of 40 periods, at $f = 8.93$ GHz ($\lambda = 33.6$ mm).

the plasma frequency is to the right. This can be seen from the dashed curves, the transmission of wires and *closed* resonators. The thick solid lines then give the transmission for the *partially* homogenized structure [Fig. 1(b)] while the thin solid lines give the transmission for the *fully* homogenized structure [Fig. 1(c)].

The main feature one must notice in these two figures is that in Fig. 2 the transmission peak around 8.9 s GHz is predicted only by the partial (thick solid curve) but *not* the fully homogenized (thin solid curve) model, while in Fig. 3, both the partial and the fully homogenized model show a transmission peak in that frequency range. This indicates not only that the peak of Fig. 2 is not a left-handed peak, it is a peak that is not an effective medium feature at all. In fact the structure of Fig. 2 is not homogenized over the whole interval between 8 and 9.1 GHz. Since the configuration of Fig. 2 reproduces the conditions of Ref. [25] we are inclined to interpret their ''right-handed peak'' rather as an inhomogeneous peak. A transmission peak can therefore be obtained even when the average permittivity and the average permeability of a structure have different signs, as for the peak at 8.9 GHz. The high transmission around 8 GHz is likewise inhomogeneous in character as the mean permittivity is negative but the mean permeability is positive. The situation is different in the case of Fig. 3, even though the frequency and the period are the same as in the first case. We can therefore confirm the negative-index nature of the ''left-handed peak'' of Ref. [25]. We should also note that the small nonhomogeneous peak at 8.5 GHz in Fig. 3, is also visible in the experimental data of Fig. 3 of Ref. [25], at the same frequency.

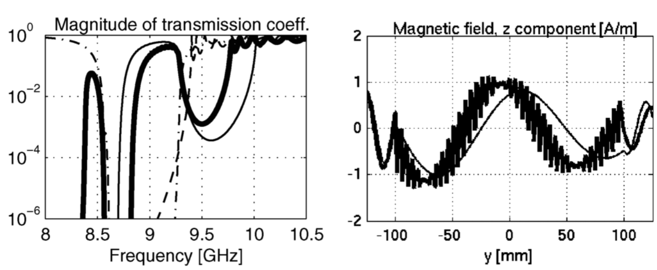

FIG. 3. Left—Transmission curves for the case of plasma frequency (~10 GHz) above the magnetic resonating frequency (8.6 GHz). Right—The field profile for a stack of 40 periods, at $f = 9.2$ GHz ($\lambda = 32.6$ mm). The period is $d = 5$ mm.

We have therefore shown that it is possible to reproduce the experimental data using our simple 1D model. Moreover homogeneous and nonhomogeneous features coexist on the same figure, and our model can be used to distinguish between them.

A better understanding of the physical character of the transmission peaks is obtained by a study of the field profile in the partially homogenized medium. The plots on the right sides of Figs. 2 and 3 show the magnetic field in a 40 period thick structure. In both cases the wavelengths are between 6 and 7 times larger than the period.

The field profile in the nonhomogeneous peak of Fig. 2 shows that the variation of the field across individual layers is very strong. Homogenization is therefore not justified. In fact, this type of transmission has been previously described in terms of a tight bindinglike model based on modes bound to the interfaces between successive layers [27]. It is clear that this type of propagation is incompatible with effective medium theory and an effective index of refraction cannot be defined.

Inspection of the field profile in the left-handed peak of Fig. 3 shows that this case is in the intermediate region where the medium exhibits homogeneouslike features to a certain extent, but cannot be said to truly behave as a homogeneous effective medium. The spatial field profile in the medium is vaguely sinusoidal, but the oscillations within one period are still relatively large, while the transmitted fields of the partially homogenized and the fully homogenized models are somewhat out of phase. It is clear that a smaller period is required for a *better* effective medium to be obtained. These results therefore suggest that for $\lambda \sim 6d$ the effective medium theory is only marginally valid. It is likely that most applications will have more stringent requirements on the material used, especially those involving negative refraction which are more sensitive to spatial dispersion. The most direct way to improve our effective medium is to increase the wavelength to period ratio by reducing the period (experimentally this would require designing smaller resonators with the same resonance frequency). This is illustrated in Fig. 4 for which we have $\lambda \sim 12d$. We have simply halved the layer thicknesses and doubled the number of periods. The nonhomogeneous features between 8 and 8.5 GHz which we observe in Figs. 2 and 3 disappear and the agreement between the transmission curves (left) as well as the field profiles (right) is far better. This confirms that what we see in Fig. 3 is indeed an intermediate case.

Using this approach, we emphasize the gray scale, gradual nature of the homogenization of composites. The question we should ask is generally not *whether* a composite is homogenized at a given wavelength, but *to what extent* it is, or even, to what extent it *needs* to be. The approach described here gives us a handle on how close we are to the medium needed for a given application.

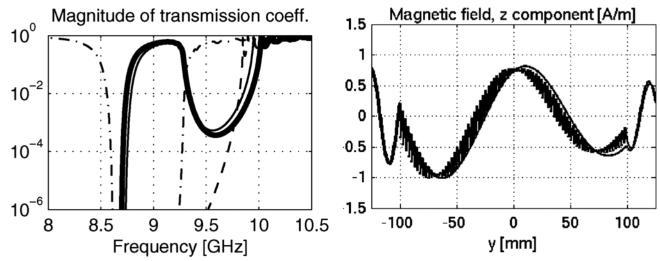

FIG. 4. Left—Transmission curves for the case of plasma frequency (~10 GHz) above the magnetic resonating frequency (8.6 GHz). Right—The field profile for a stack of 80 periods, at $f = 9.2$ GHz ($\lambda = 32.6$ mm). The period is $d = 2.5$ mm.

The way to the design of better effective media seems to be through the design of smaller resonators, with higher quality factors and more localized fields. In other words, resonators must be designed with resonances at wavelengths larger with respect to their size. Since the resonance wavelength is on the order of $\sqrt{LC}$, where L and C are the internal inductance and capacitance of the resonator, a simple way to increase it is to use a broadside-coupled design such as that proposed in Ref. [21].

Our approach can also be used to evaluate the homogeneity of composites not only as a function of frequency but of angle of incidence as well. The rich range of refraction behaviors accessible, for different polarizations and orientations, is listed in Fig. 2 of Ref. [23]. However it is not clear how far one can tilt away from normal incidence before nontrivial spatial dispersion features typical of nonhomogeneous structures become important. Our approach can be used in that case as well to delimit incidence angle domains where homogenization is justified from domains where it is not, without the use of cumbersome 3D simulations.

In conclusion we have outlined a simple approach to the analysis of composite metamaterials. Our approach consists of building the effective medium model layer by layer, as an anisotropic single negative stack. We qualitatively reproduce experimental data available in the literature, suggesting that the composites commonly being studied have a size that places them at the borderline of homogenization theory: they can exhibit features of heterogeneous materials (e.g., the peak at 8.5 GHz, Fig. 3) in addition to the effective medium left-handed properties (e.g., the peak at 9 GHz, Fig. 3). Our indirect homogenization approach provides a way to distinguish between the former and the latter as well as a means to evaluate how well the effective medium approximates the behavior of a given structure. The single negative stack can be seen as an *upper bound* on the effective medium quality of the composite. This allows a designer to quickly and effectively evaluate the usefulness of a given composite using widely shared and straightforward 1D methods. Our approach can also be easily adapted to the study of cylindrical geometries, e.g., the electromagnetic cloak [28].

[1] J. B. Pendry, A. J. Holden, D. J. Robbins, and W. J. Stewart, J. Phys. Condens. Matter **10**, 4785 (1998).
[2] J. B. Pendry, A. J. Holden, D. J. Robbins, and W. J. Stewart, IEEE Trans. Microwave Theory Tech. **47**, 2075 (1999).
[3] D. Smith, S. Schultz, P. Markos, and C. Soukoulis, Phys. Rev. B **65**, 195104 (2002).
[4] M. Bayindir, K. Aydin, E. Ozbay, P. Markos, and C. M. Soukoulis, Appl. Phys. Lett. **81**, 120 (2002).
[5] A. L. Pokrovsky and A. L. Efros, Phys. Rev. Lett. **89**, 093901 (2002).
[6] R. Marques and D. R. Smith, Phys. Rev. Lett. **92**, 059401 (2004).
[7] J. F. Woodley, M. S. Wheeler, and M. Mojahedi, Phys. Rev. E **71**, 066605 (2005).
[8] S. I. Maslovski, Tech. Phys. Lett. **29**, 32 (2003).
[9] C. R. Simovski, S. A. Tretyakov, A. H. Sihvola, and M. M. Popov, Eur. Phys. J. Appl. Phys. **9**, 195 (2000).
[10] S. O'Brien and J. B. Pendry, J. Phys. Condens. Matter **14**, 4035 (2002).
[11] V. M. Shalaev, W. S. Cai, U. K. Chettiar, H. K. Yuan, A. K. Sarychev, V. P. Drachev, and A. V. Kildishev, Opt. Lett. **30**, 3356 (2005).
[12] A. N. Grigorenko, A. K. Geim, H. F. Gleeson, Y. Zhang, A. A. Firsov, I. Y. Khrushchev, and J. Petrovic, Nature (London) **438**, 335 (2005).
[13] J. F. Zhou, L. Zhang, G. Tuttle, T. Koschny, and C. M. Soukoulis, Phys. Rev. B **73**, 041101 (2006).
[14] D. Felbacq and G. Bouchitte, Phys. Rev. Lett. **94**, 183902 (2005).
[15] B. Sauviac, C. R. Simovski, and S. A. Tretyakov, Electromagnetics **24**, 317 (2004).
[16] P. A. Belov, R. Marques, S. I. Maslovski, I. S. Nefedov, M. Silveirinha, C. R. Simovski, and S. A. Tretyakov, Phys. Rev. B **67**, 113103 (2003).
[17] D. Felbacq, F. Zolla, and G. Bouchitte, Phys. Rev. E (to be published).
[18] A. Căbuz and D. Felbacq, *Proceedings of the MRS* (MRS, Warrendale, PA, 2006), Vol. 919E, p. 0919-J03-02.
[19] R. E. Collin and W. H. Eggimann, IEEE Trans. Microwave Theory Tech. **9**, 110 (1961).
[20] M. J. Dignam and M. Moskovits, J. Chem. Soc., Faraday Trans. **69**, 56 (1973).
[21] R. Marques, F. Medina, and R. Rafii-El-Idrissi, Phys. Rev. B **65**, 144440 (2002).
[22] G. Allaire, SIAM J. Math. Anal. **23**, 1482 (1992).
[23] D. R. Smith and D. Schurig, Phys. Rev. Lett. **90**, 077405 (2003).
[24] T. G. Mackay and A. Lakhtakia, Opt. Commun. **234**, 35 (2004).
[25] N. Katsarakis, T. Koschny, M. Kafesaki, E. N. Economou, E. Ozbay, and C. M. Soukoulis, Phys. Rev. B **70**, 201101 (2004).
[26] T. Koschny, P. Markos, E. N. Economou, D. R. Smith, D. C. Vier, and C. M. Soukoulis, Phys. Rev. B **71**, 245105 (2005).
[27] H. Jiang, H. Chen, H. Li, Y. Zhang, J. Zi, and S. Zhu, Phys. Rev. E **69**, 066607 (2004).
[28] D. Schurig, J. J. Mock, B. J. Justice, S. A. Cummer, J. B. Pendry, A. F. Starr, and D. R. Smith, Science **113**, 3628 (2006).