On the signs of the imaginary parts of the effective permittivity and permeability in metamaterials

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The signs of the imaginary parts of the permittivity and permeability in metamaterials such as split ring resonators and strip wires are investigated. It is shown that the Lorentzian model often used to describe the effective parameters (i.e., the permittivity and permeability) of these metamaterials does not physically allow their imaginary parts to be negative. Moreover, a popular technique used to retrieve the effective parameters of a structure from its S-parameters is also investigated. By comparing the effective parameters for an array of dielectric spheres obtained both from S-parameter simulations and analytical calculations, it is shown that an often observed negative imaginary permittivity obtained from the S-parameters is a result of numerical error in the simulations. This is shown both for the finite element method and finite-difference time-domain simulations. © 2010 Optical Society of America

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1. INTRODUCTION

In 1967 Veselago posed that a medium in which the real parts of the electric permittivity and magnetic permeability were simultaneously negative would exhibit a negative index of refraction [1]. Such a medium, characterized by a left-handed relationship between the electric field vector $\vec{E}$, magnetic field vector $\vec{H}$, and wave vector $\vec{k}$, would exhibit new phenomena such as negative refraction and reversed Doppler shift. However, at the time, no materials with either a negative permittivity or negative permeability were available that could conveniently be combined to test Veselago's hypothesis, and it was not for 30 years that such convenient materials became available.

In 1996 Pendry *et al.* showed that an array of thin metallic rods could be made to display a plasma frequency at microwave frequencies [2]. Because of the low value of the plasma frequency, this structure could be used to produce a negative real part of the permittivity at low frequencies without the large losses resulting from the corresponding imaginary part. Later, in 1999 the same group showed that an array of split ring resonators (SRRs) produced a magnetic plasma frequency in the microwave regime [3]. This structure, even though it is composed of nonmagnetic materials, exhibits a negative real part of the permeability in the region between the resonance and plasma frequencies. Soon after, Smith *et al.* combined these two structures and showed that there was a transmission peak in the region where the real parts of both the permittivity and permeability were negative implying a negative index of refraction [4]. The existence of a negative index was then confirmed when a similar medium was shown to refract waves with a negative angle [5]. Since then, many new negative index media, also referred to as left-handed media (LHM), have been created [6–9] based on Veselago's original proposal.

Recently, there have been claims that these media can exhibit a negative imaginary part of either the electric permittivity, ϵ'', or the magnetic permeability, μ'', while remaining passive. More specifically, it was shown using numerical studies that a negative index medium composed of SRRs and strip wires (SWs) could exhibit a negative imaginary permittivity ($\epsilon''<0$) [10–12]. It was then later shown that an array of split strip wires by themselves exhibits a negative imaginary permeability ($\mu''<0$) and that an array of SRRs by themselves exhibits a negative imaginary permittivity ($\epsilon''<0$) [13]. In these cases the permittivity and permeability were obtained from the simulated scattering parameters of the structure using a process which will be referred to as the retrieval technique [14]. In this paper the validity of the retrieval technique will be examined, and it will be shown that in the case considered $\epsilon''<0$ is predicted as a result of numerical error in the simulations.

It should be noted that, in order for a medium to be considered passive, one of the conditions it must satisfy is that the heat dissipation in the medium given by

$$Q=\omega(\epsilon''|\vec{E}|^2+\mu''|\vec{H}|^2) \quad (1)$$

be positive, where $\vec{E}$ is the electric field and $\vec{H}$ is the magnetic field [15]. Unfortunately, the sign of Q in a medium with $\epsilon''<0$ or $\mu''<0$ is unclear, so that in a medium with only $\epsilon''<0$ or $\mu''<0$ passivity is not necessarily violated as pointed out in [10,13]. However, passivity is only one of the conditions that must be satisfied, causality and analyticity must also be considered. In this paper it will be shown that the Lorentzian model most commonly used to describe metamaterials such as SRRs and SWs cannot be used to model a medium with $\epsilon''<0$ or $\mu''<0$ without violating analyticity or assuming population inversion.

This paper is divided as follows. In Section 1 the Lorentzian model often used to describe the permittivity and permeability in these metamaterials will be examined, and the validity of using this model to describe media with a negative imaginary permittivity or permeability will be discussed. In Section 2 the effective parameters (i.e., the index, impedance, permittivity, and permeability) of an array of dielectric spheres will be determined both analytically and by using the retrieval technique. The results will then be contrasted and discussed in Section 3. Finally, we will give our final thoughts and conclusions in Section 4.

2. LORENTZIAN MODEL FOR PERMITTIVITY AND PERMEABILITY

The dispersive natures of the SWs and SRRs are often described by the Lorentzian model where the effective permittivity and permeability are given by [2,3,10,14]

$$\epsilon = 1 + \frac{\omega_{pe}^2}{\omega_{oe}^2 - \omega^2 - i\gamma_e\omega}, \tag{2}$$

$$\mu = 1 + \frac{\omega_{pm}^2}{\omega_{om}^2 - \omega^2 - i\gamma_m\omega}, \tag{3}$$

where ω_{pi} is the plasma frequency, ω_{oi} is the resonance frequency, γ_i is the damping constant, and $i=e,m$ represents the electric or magnetic response. From a purely mathematical standpoint, the imaginary part of the permittivity in Eq. (2) can be negative under two conditions: $\gamma_e<0$ or $\omega_{pe}^2<0$. In order to examine the first condition, $\gamma_e<0$, recall that the permittivity, ϵ, relates to the displacement vector, $\vec{D}$, and the electric field vector, $\vec{E}$. In the time domain this relationship is expressed by the well-known result,

$$D(\vec{r},t) = \epsilon_0\left\{E(\vec{r},t) + \int_{-\infty}^{\infty} G(\tau)E(\vec{r},t-\tau)d\tau\right\}, \tag{4}$$

where $G(\tau)$ is the susceptibility kernel given by

$$G(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\epsilon(\omega)}{\epsilon_o} - 1\right)e^{-i\omega\tau}d\omega. \tag{5}$$

Substituting Eq. (2) into Eq. (5), the susceptibility kernel becomes

$$G(\tau) = \omega_p^2 e^{-\gamma\tau/2}\frac{\sin(\nu_o\tau)}{\nu_o}\Theta(\tau), \tag{6}$$

where $\Theta(\tau)$ is the step function and $\nu_o^2=\omega_o^2-\gamma^2/4$. If $\gamma<0$ in Eq. (6), the susceptibility kernel is not bounded on the complex plane as $\tau\to\infty$ and hence, from Eq. (5) the permittivity is not analytic. Therefore the case with $\gamma<0$ is not causal and cannot be considered [16].

The second case, $\omega_{pe}^2<0$, implies that the plasma frequency must be imaginary. In the electron oscillator model, the plasma frequency is given by

$$\omega_{pe} = \sqrt{\frac{Ne^2f}{m_e}}, \tag{7}$$

where N is the atomic number density, e is the electron charge, m_e is electron mass, and f is the oscillator strength. Of all the parameters in Eq. (7), only the oscillator strength can be negative, which corresponds to the case of a medium undergoing population inversion [17,18]. Since population inversion is not a viable physical mechanism for the SRR and SW structures, the case of $\omega_{pe}^2<0$ is not physical and cannot be considered. Therefore, although the Lorentzian model is used to describe the SRRs and SWs for which $\epsilon''<0$ and $\mu''<0$ are predicted, this model does not in fact allow such behavior.

3. EFFECTIVE PARAMETERS OF AN ARRAY OF SPHERES

Many of the metamaterial structures under investigation are composed of arrays of metallic inclusions with complex shapes for which no exact analytical expressions exist that describe their effective material parameters. In order to estimate the values of these parameters, several procedures have been developed [14,19]. One of the most popular techniques is the retrieval technique, which involves obtaining the parameters (permittivity and permeability) from the numerically simulated scattering parameters (S-parameters) of the structure using

$$n = \frac{1}{kd}Cos^{-1}\left[\frac{1}{2S_{12}}(1-S_{11}^2+S_{12}^2)\right] + \frac{2l\pi}{kd}, \tag{8}$$

$$z = \sqrt{\frac{(1+S_{11})^2+S_{12}^2}{1-S_{11})^2+S_{12}^2}}, \tag{9}$$

$$\epsilon = \frac{n}{z}, \tag{10}$$

$$\mu = nz. \tag{11}$$

Here S_{11} and S_{12} are the S-parameters for reflection and transmission through the structure; respectively; k is the wavevector in free space and l is an integer, which accounts for the different possible branches of the inverse cosine function. This retrieval technique has been used to estimate the effective parameters of media such as arrays of SRRs and SWs [10,13,14]. As mentioned above, in some cases the retrieval technique has predicted $\epsilon''<0$ or $\mu''<0$, and since Eq. (1) does not require both ϵ'' and μ'' to be positive there is no indication that passivity has been violated. Unfortunately, there is no direct way to check the validity of these results, since accurate analytical expressions for the effective parameters of these structures, derived from first principles, are not available.

In order to check the validity of the retrieval procedure, we require a resonant structure for which the index, impedance, permittivity, and permeability can be calculated analytically from fundamental considerations and whose S-parameters can be simulated numerically. The retrieval technique could then be applied to the simulated S-parameters, and the results can be compared to the analytically calculated parameters. If the results obtained from the two different approaches (analytical and retrieval) do not agree, we must conclude that the retrieval technique based on simulated S-parameters is not a proper tool when characterizing such resonant structures. Moreover, the process can help shed light on the possible sources of errors within the retrieval technique.

The structure which will be considered is an array of dielectric spheres with $\epsilon = 200 + i10$ immersed in air with radius $r = 4$ μm and unit cell size $a = 10$ μm. Using Mie theory and the Clausius–Mossotti relation, we have previously shown that the permittivity and permeability for an infinite array of spheres is given by

$$\epsilon_{an} = \frac{k_0^3 + 4\pi i N_V a_1}{k_0^3 - 2\pi i N_V a_1}, \tag{12}$$

$$\mu_{an} = \frac{k_0^3 + 4\pi i N_V b_1}{k_0^3 - 2\pi i N_V b_1}, \tag{13}$$

where N_V is the volume density of the spheres and a_1 and b_1 represent electric and magnetic dipole terms [20]. The analytical index of refraction, impedance, permittivity, and permeability are shown in Figs. 1–4, respectively [the real parts are shown in part (a) and the imaginary parts are shown in part (b)]. From the plots it is clear that the structure exhibits a magnetic resonance at approximately 2.5 THz so that $\lambda/a = 12$. Also, the S-parameters for propagation through a 10 μm thick slab with material parameters obtained from Eqs. (12) and (13) were calculated and are shown in Fig. 5 for comparison with the simulated results.

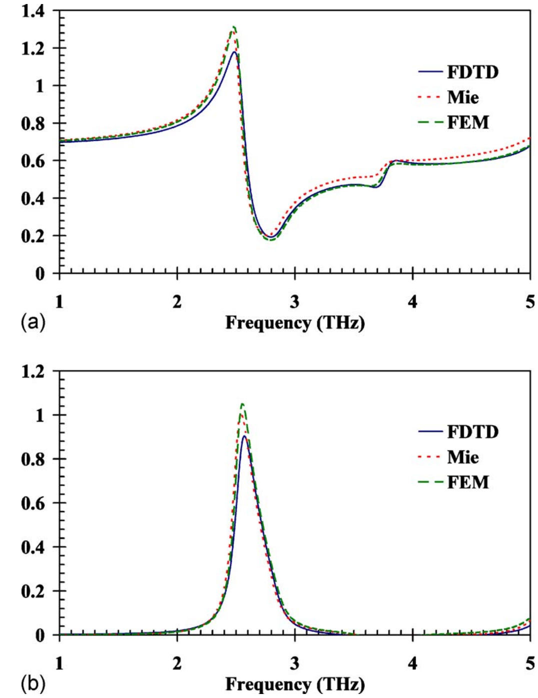

Fig. 2. (Color online) Real (a) and imaginary (b) parts of the effective impedance obtained analytically (dotted curve) and from using the retrieval technique on S-parameters obtained from FDTD (solid curve) and FEM (dashed curve) simulations.

The scattering parameters for propagation through an array of spheres infinite in the transverse plane and one

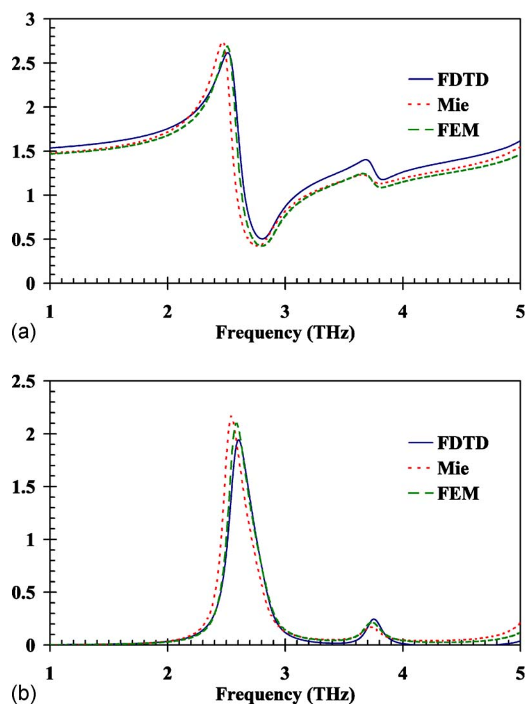

Fig. 1. (Color online) Real (a) and imaginary (b) parts of the effective index of refraction obtained analytically (dotted curve) and from using the retrieval technique on S-parameters obtained from FDTD (solid curve) and FEM (dashed curve) simulations.

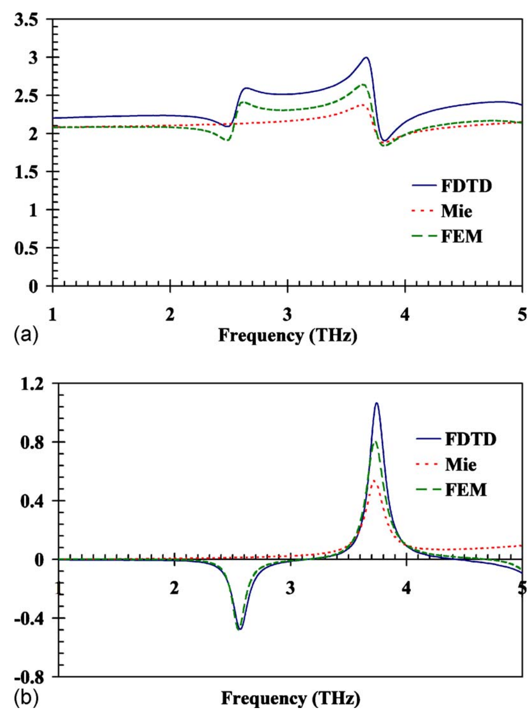

Fig. 3. (Color online) Real (a) and imaginary (b) parts of the effective permittivity obtained analytically (dotted curve) and from using the retrieval technique on S-parameters obtained from FDTD (solid curve) and FEM (dashed curve) simulations.

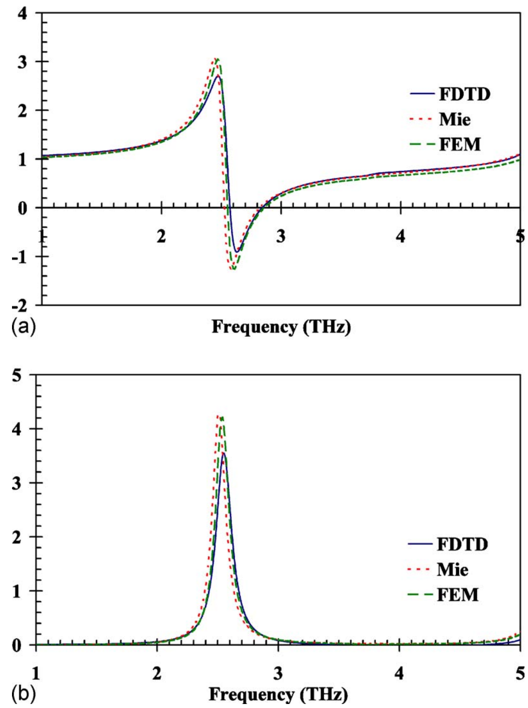

Fig. 4. (Color online) Real (a) and imaginary (b) parts of the effective permeability obtained analytically (dotted curve) and from using the retrieval technique on S-parameters obtained from FDTD (solid curve) and FEM (dashed curve) simulations.

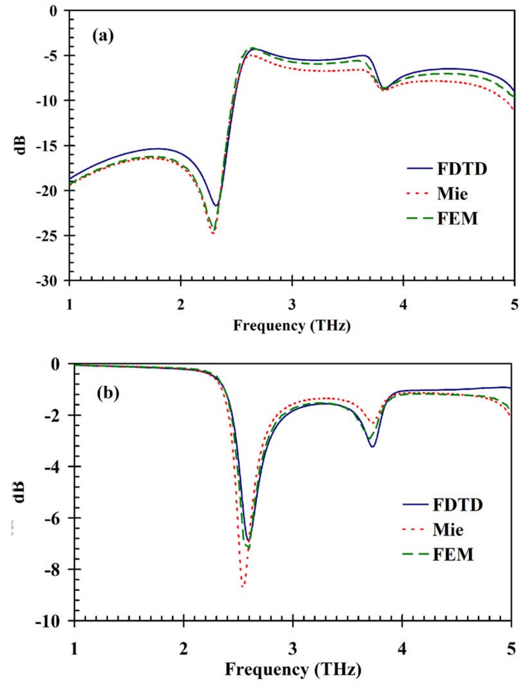

Fig. 5. (Color online) (a) S11 and (b) S12 calculated analytically for propagation through a 10 μm thick slab (dotted curve) and determined from FDTD (solid curves) and FEM (dashed curves) simulations for propagation through a sheet of dielectric spheres infinite in the transverse plane and one unit cell thick in the propagation direction.

unit cell thick in the propagation direction were simulated using both Ansoft HFSS, a commercial finite element method (FEM) field solver, and Lumerical, a commercial finite-difference time-domain (FDTD) solver. In both cases, perfect electric boundary conditions were defined on the faces perpendicular to the electric field and perfect magnetic boundary conditions were defined on the faces perpendicular to the magnetic field. The simulated S-parameters for propagation through this structure are shown in Fig. 5. Using Eqs. (8) and (9), the retrieved index and impedance of the array were obtained from both the FEM and FDTD results and are shown in Figs. 1 and 2, respectively [the real parts are shown in part (a) and the imaginary parts are shown in part (b)]. The permittivity and permeability were then obtained using Eqs. (10) and (11) and are shown in Figs. 3 and 4, respectively [the real parts are shown in part (a) and the imaginary parts are shown in part (b)].

4. DISCUSSION

Comparing Figs. 1–5 the shapes of the curves for the S-parameters, indices, impedances, and permeabilities match. On the other hand, the permittivities resulting from the numerical and analytical methods differ significantly. In particular, Fig. 3 shows that an antiresonance appears at 2.56 THz, which results in a negative imaginary permittivity. The question then arises as to why the permittivities differ while the other parameters match. In order to understand this difference it is helpful to expand Eq. (10):

$$\epsilon' + i\epsilon'' = \frac{n' + in''}{z' + iz''} = \frac{(n' + in'')(z' - iz'')}{z'^2 + z''^2} = \frac{n'z' + n''z'' + i(n''z' - n'z'')}{z'^2 + z''^2}. \tag{14}$$

From Eq. (14) any change in the sign of the imaginary part of the permittivity will be due to the numerator. For an array of SRRs *by themselves* the real and imaginary parts of the effective index and impedance are positive so that the sign of the imaginary part in Eq. (14) is determined by the relative magnitudes of the terms $|n'z''|$ and $|n''z'|$. Figure 6 shows the magnitudes of $|n'z''|$ and $|n''z'|$ for the analytical and retrieved cases. In the analytical

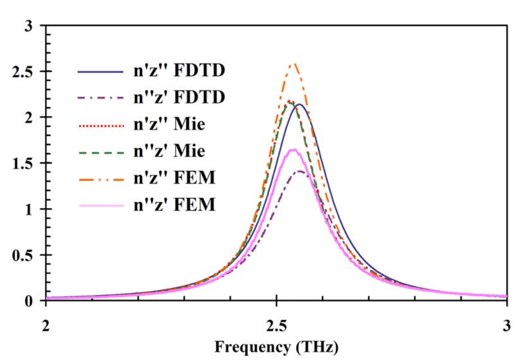

Fig. 6. (Color online) Magnitude of the terms $n'z''$ and $n''z'$ calculated from the analytical expressions and retrieved from the FDTD and FEM simulations.

case, these two terms have nearly identical magnitudes so that the numerator in Eq. (14) is small (but positive). On the other hand, in the case of the retrieved parameters these two terms diverge for both the FEM and FDTD results in the resonance region as a result of numerical error in the simulated S-parameters used to obtain n and z. Because $|n'z''| \approx |n''z'|$ in this region, this divergence results in significant deviation of the retrieved permittivity from its expected value (i.e., a negative imaginary part). Therefore, although the simulation errors do not cause problems in the retrieval procedure when obtaining the effective index, impedance, and permeability, these same small errors cause unacceptable errors when obtaining the permittivity due to the form of Eq. (14). The fact that the FEM and FDTD simulations both give good results for the S-parameters, index of refraction, impedance, and permeability but that both result in this behavior for the permittivity emphasizes the sensitivity of the retrieval procedure to any small deviation from the expected results. The discrepancy between the analytical and simulated results can be attributed to numerical error (due to approximation, truncation, round off) in the FEM and FDTD simulations.

In the case considered above, the real and imaginary parts of the index and impedance were positive (i.e., $n'>0$, $n''>0$, $z'>0$, and $z''>0$.) If a similar positive index medium was considered but with $z''<0$ (i.e., an array of SWs) then the effective permeability and not the permittivity would possibly exhibit a negative imaginary part. This can be seen by expanding Eq. (11):

$$\mu' + j\mu'' = (n' + jn'')(z' + jz'') = n'z' - n''z'' + j(n''z' + n'z''). \tag{15}$$

Imposing the conditions $n'>0$, $n''>0$, $z'>0$, and $z''<0$ the imaginary parts of the permittivity and permeability can be written as

$$\epsilon'' = \frac{(|n''z'| + |n'z''|)}{z'^2 + z''^2},$$

$$\mu'' = |n''z'| - |n'z''|. \tag{16}$$

In this case the permeability now has the term $|n''z'| - |n'z''|$ so that any errors in the numerically obtained S-parameters will cause problems when calculating Eq. (15). Therefore, considering Eqs. (14) and (15) it is clear that any time the retrieval technique is used one of the two parameters, the permittivity or the permeability, will have the form $|n''z'| - |n'z''|$ and may be problematic. As a general rule, the retrieval technique can be used to obtain the effective index and impedance. Then, the form of Eqs. (14) and (15) will determine which of the two parameters, the permittivity or permeability, can be determined reliably and which may be problematic.

5. CONCLUSION

In this paper it was shown that the Lorentz model, often used to describe SRRs and SWs, does not allow the imaginary parts of the permittivity or permeability to be negative in these structures. This implies that, to the extent that the Lorentz model is an appropriate model for describing the dispersive nature of the SRRs and SWs metamaterials, the presence of negative ϵ'' or μ'' is not allowed. Moreover, by using a test case such as an array of dielectrics for which the effective parameters can be obtained both analytically and via the retrieval technique (using both FDTD and FEM simulations), we have demonstrated that the observation of negative ϵ'' and μ'' are the consequence of simulation errors. Finally, it has been pointed out that, due to the particular from of ϵ'' and μ'', whenever a retrieval technique is used one has to be careful to assign the proper signs to the imaginary parts of the effective medium parameters.

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