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Sign of the refractive index in lossy metamaterials

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ABSTRACT

One of the criteria for determining the existence of negative index of refraction in artificial electromagnetic structures (metamaterials) is the occurrence of opposite directions of the group and phase velocities. In this work, we study specific examples of metamaterials where we show that the above criterion does not hold when losses are taken into account and dominate the interaction of light with the metamaterial. The structure are three-dimensional superlattices of consisting of plasmonic and polaritonic particles and are studied by a rigorous multiple-scattering theory and effective-medium approximation. © 2009 Elsevier B.V. All rights reserved.

1. Introduction

The field of metamaterials is one of the most fascinating disciplines in optics as properties and phenomena which cannot be met in naturally occurring materials are realized via man-made structures. Negative refractive index (NRI) [1,2] and invisibility cloaking [3] are the most prominent features of the above materials. The mainstream route for obtaining a negative refractive index is to achieve a simultaneous occurrence of negative electric permittivity and permeability which gives rise to NRI [4]. This is literally true for the case of negligible losses in the constituent materials. When absorption comes into play, the spectral region of NRI is also determined by the imaginary parts of the effective permittivity $\epsilon_{e\!f\!f}$ and permeability $\mu_{e\!f\!f}$. It is not, therefore, necessary to have a strict coincidence of the spectral regions with negative real parts in the permittivity and permeability in the case of lossy materials. The occurrence of NRI can also be inferred directly from the frequency band structure of a metamaterial. Namely, in the subwavelength limit and in the case where a single frequency band exists over a given spectral region, a NRI is attributed to the metamaterial when the group velocity $\mathbf{v}_g = \nabla_{\mathbf{k}} \omega(\mathbf{k})$ is opposite to the phase velocity $\mathbf{v}_{ph} = \hat{\mathbf{k}}\omega/k$ [5]. This is true in the limit of zero

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losses where the group velocity assumes real values. In the case where the inherent losses of the constituent metamaterials are taken into account, the group velocity is a complex function and the definition of a NRI becomes problematic [6].

In this work, specific examples are studied where the criterion described above does not hold. Namely, we calculate the complex frequency band structure of a superlattice of plasmonic nanospheres as well as superlattices of alternating plates of plasmonic and polaritonic spheres exhibiting NRI. We show, in particular, that, within the frequency region of the surface-plasmon (SP) band, although the real part of the (generally complex) group velocity is opposite to the real part of the phase velocity, a NRI cannot be assumed. The amount of losses is so high that light attenuation dominates propagation within the superlattice of NPs and blurs the occurrence of NRI. Our predictions are made on the basis of rigorous multiple-scattering electrodynamics calculations as well as on effective-medium theory and corroborate with previous requirements for the definition of negative refractive index.

2. Fcc crystal of plasmonic spheres

Our first case study is an fcc crystal consisting of Drude-type spheres, i.e., their dielectric function is provided by

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\tau^{-1})},\tag{1}$$



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where ω_p is the bulk plasma frequency of a given metal and τ is the relaxation time of conduction-band electrons. We have taken $(\omega_p \tau)^{-1} = 0.05$, a typical value of losses in metallic nanoparticles. The first-neighbor distance is taken to be $a_0 = c/\omega_p$ (the lattice constant is $a = \sqrt{2}a_0$) and the radius of the spheres $S = 0.2a_0$. The superlattice is intentionally taken to be dilute so that the dipole approximation is enough for the description of the interaction of light with the structure.

The above structure is studied by means of the layer-multiplescattering (LMS) method. It is an efficient computational method for the study of the EM response of three-dimensional photonic structures consisting of non-overlapping spheres [7,8] and axisymmetric nonspherical particles [9]. The LMS method is ideally suited for the calculation of the transmission, reflection and absorption coefficients of an electromagnetic (EM) wave incident on a composite slab consisting of a number of lavers which can be either planes of non-overlapping particles with the same 2D periodicity or homogeneous plates. For each plane of particles, the method calculates the full multipole expansion of the total multiply scattered wave field and deduces the corresponding transmission and reflection matrices in the plane-wave basis. The transmission and reflection matrices of the composite slab are evaluated from those of the constituent layers. By imposing periodic boundary conditions one can also obtain the (complex) frequency band structure of an infinite periodic crystal. The method applies equally well to nonabsorbing systems and to absorbing ones. Its chief advantage over the other existing numerical methods lies in its efficient and reliable treatment of systems containing strongly dispersive materials such as Drude-like and polaritonic materials.

We view the superlattice as a succession of (001) planes of Drude-type spheres, i.e., planes of spheres parallel to the (001) surface of fcc. The lattice corresponding to this surface is square. In Fig. 2a we show the complex frequency band structure for $\mathbf{k}_{\parallel} = \mathbf{0}$ [normal to the (001) surface] where \mathbf{k}_{\parallel} is the parallel component of the Bloch wavevector **k**. reduced within the surface Brillouin zone (SBZ) of the (001) surface. The component of the Bloch wavevector along the *z*-axis is given in dimensionless units, i.e., $k_{z}a/2\pi$, where *a* is the lattice constant defined above. A calculation of the complex frequency band structure offers, for a given frequency ω , both the real and imaginary parts of k_z , the component of the wavevector normal to the (001) surface. So, for a given dispersion relation $\omega = \omega(k_z)$, one can define the effective refractive index as $n_{eff} = ck_z/\omega$. It is evident that the curve of $\Re k_z$ exhibits a strongly resonant behavior due to the excitation of SP modes within the spheres. The interaction of SP modes of neighboring spheres gives rise to the resonant frequency band of Fig. 2a [10]. Within the shaded spectral region of Fig. 2, $\Re k_z$ decreases with increasing frequency, i.e., the real part of the group velocity $\Re v_g = \partial \omega / \partial \Re k_z$ is negative. This would signify the occurrence of NRI. In Fig. 2b we show the effective refractive index $n_{eff} = ck_z/\omega$ for the two possible scenarios: negative and positive refractive index (PRI). We observe that the choice of PRI looks as a more natural choice of n_{eff} as it is a smooth and continuous function of frequency. The corresponding NRI band exhibits discontinuities at both its edges. We note, however, that the discontinuities in n_{eff} is not an uncommon phenomenon since it has also been reported in cases where n_{eff} is retrieved by inverting the Fresnel's equations for a finite slab of a metamaterial [11]. Fig. 2c shows the corresponding real part of the group index $\Re n_g = c \partial \Re k_z / \partial \omega$ which is inversely proportional to the group velocity v_g . The negative values of $\Re n_g$ signify backward wave propagation which, is usually associated with NRI. We note that in Fig. 2, as well as in Fig. 3 below, there exist several, generally complex bands, within the studied spectral region. However, we only show the frequency band with the smallest $\Im k_z$ at every frequency since wave propagation/attenuation within a finite slab of the crystal is determined by this par-



Fig. 1. Unit cell of an fcc superlattice of Drude-type spheres. *a* denotes the lattice constant, a_0 the first-neighbor distance and *S* the radius of the spheres.

ticular band. It is worth noting that the structure of Fig. 1 is a truly subwavelength metamaterial since the wavelength-to-structure ratio is $\lambda/a_0 = 2\pi c/(\omega_{mid}a_0) \approx 11$ where ω_{mid} is the middle frequency of the shaded area of Fig. 2.

It should be pointed out that one can argue that in the NRI case the phase and group velocities point to the same direction and not to opposite directions since both n_{eff} and n_g are negative. At the same time, in the PRI case, n_{eff} is positive whilst n_g is negative and therefore the phase and group velocities point to opposite directions. In reality, the sign of the group velocity does not depend on the material (and hence on the frequency band structure) but from the direction of energy flow of a pulse incident on the given material. So, when a pulse is launched towards a slab of a material, the group velocity points at the direction of the pulse propagation which is taken as the positive direction by default. When a lossless material has a dispersion relation with negative derivative of frequency versus the wavevector, the corresponding n_{eff} has to be negative in order to preserve causality [12].

In Fig. 2b and c, we also show the corresponding imaginary parts of n_{eff} and n_g , respectively. In an absorbing medium, the real



Fig. 2. (a) Complex frequency band structure normal to the (001) surface of an fcc crystal (lattice constant $a = \sqrt{2}c/\omega_p$) of Drude-type metallic spheres ($S\omega_p/c = 0.2$) in air, as calculated by the rigorous LMS method. (b) The corresponding effective refractive index n_{eff} . (c) The group index n_g . The solid (broken) lines refer to the real (imaginary) parts of the quantities in the abscissas.

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