Retrieving effective parameters for quasiplanar chiral metamaterials

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We introduce and compare two approaches for retrieving quantitatively the effective chirality of metamaterials at normal incidence. The retrieval employs either the reflected and transmitted amplitude of a plane wave illuminating a finite three-dimensional (3D) metamaterial or the dispersion relation of the pertinent Bloch modes in an infinite metamaterial. Both approaches are applied to characterize a 3D metamaterial consisting of a stack of metallic gammadions separated by dielectric films. It will be shown that the results coincide if transitional effects between the metamaterial and the environment can be neglected.
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Recently, the transmission behavior of chiral metamaterials (CMs) fabricated by planar technologies, i.e., single, thin textured metal films on dielectric substrates, has attracted a considerable deal of interest.[1–5] Frequently, these structures are termed quasiplanar CMs, although they consist at least of two different layers required for fulfilling the chirality condition, i.e., a unit cell cannot be mapped onto its mirror image by proper rotations (lack of inversion symmetry). Such typical unit cell is shown in Fig. 1. A genuine bulk CM can be formed by periodically arranging these unit cells in both planar directions and perpendicular to this plane. For a periodic arrangement of identical unit cells, bianisotropic material equations have to be used to describe chiral media.[6] The tensorial treatment of the material equations is not necessary if light propagation is considered only normal to the C_4-symmetry plane of the material.[5] In the following we focus on geometries, which show this type of symmetry.

Up to now CMs were usually regarded to be composed of a single functional layer (metal on substrate). Interaction of light with this structure causes a polarization rotation in transmission. The required inversion symmetry breaking of the unit cells is provided by the substrate. The magnitude of the achievable polarization rotation typically exceeds the rotation capability of natural available media, such as quartz or sugar solutions, by a few orders of magnitude. Although more elaborated schemes with two coupled functional layers exist, such media remain to be effectively thin films only. Even in this case the modulus of the rotation remains typically smaller than a single degree.[7] Recently, Kwon *et al.*[8] published a similar method to assign effective chiral parameters, considering only one functional layer of helical chiral objects. Contrary to their work, we compare two different methods and show their convergence and thereby the applicability of an effective description.

For applications in optical devices this absolute rotational power is significantly too low. Thus it is required to extend this approach toward a genuine bulk CM, i.e., a stack of metal-dielectric functional layers, to achieve a significant polarization rotation. The aim of this letter is to describe the properties of these three-dimensional (3D) CMs in assigning effective chirality parameters. This will allow a simplified comparison among various structures.

To reveal the absolute value of the chirality parameter κ, two approaches will be used. In the first approach κ is determined employing the dispersion relation of an infinite bulk medium. In the second approach an inversion of the transmission and reflection coefficients for a slab made of a stack of quasiplanar CMs is used. We then show that the values of κ determined by R/T-retrieval converge toward the bulk values determined by the dispersion relation if a sufficiently large number of quasiplanar CMs are used. Furthermore, the relation between the polarization rotation and the effective parameters is elaborated.

To calculate the effective chirality parameter κ, it is necessary to investigate the propagation properties of light in such media at first. The bianisotropic media we are considering obey material equations of the form $\vec{D}=\varepsilon_0\hat{\varepsilon}\vec{E}-i(\hat{\kappa}/c)\vec{H}$ and $\vec{B}=\mu_0\hat{\mu}\vec{H}+i(\hat{\kappa}/c)\vec{E}$, where both the displacement vector $\vec{D}$ and the magnetic induction $\vec{B}$ depend linearly on the electric field $\vec{E}$ and the magnetic field $\vec{H}$. Here $\hat{\varepsilon}=\mathrm{diag}(\varepsilon_n,\varepsilon_t,\varepsilon_t)$ is the tensor of the permittivity, $\hat{\mu}=\mathrm{diag}(\mu_n,\mu_t,\mu_t)$ is the permeability, $\hat{\kappa}=\mathrm{diag}(\kappa_n,\kappa_t,\kappa_t)$ is the chirality parameter, and c is the vacuum speed of light. Two elements of each tensor are equal due to the C_4 symmetry. In the following we focus on light propagation in the x-direction, i.e., $\vec{k}=k_x\vec{e}_x=k\vec{e}_x$. For this particular case only the tangential field components are relevant and the material equations for those relevant components can be written as $\vec{D}=\varepsilon_0\varepsilon_t\vec{E}-i(\kappa_t/c)\vec{H}$ and $\vec{B}=\mu_0\mu_t\vec{H}+i(\kappa_t/c)\vec{E}$ being equal to the relations for a Pasteur medium.[6] For convenience the index t will be omitted in the following. The eigenmodes of such medium are right-circularly polarized (rcp) and left-circularly polarized (lcp) plane waves with wave vectors given by the dispersion relation,

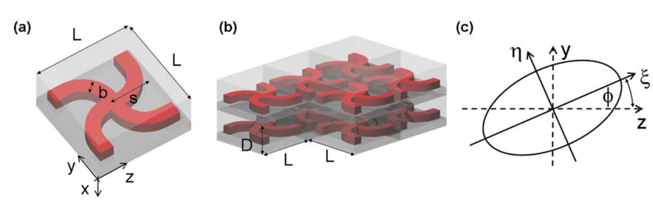

FIG. 1. (Color online) Schematics of the unit cells. (a) Metallic gammadion on substrate embedded in dielectric. (b) Sketch of the periodic arrangement. (c) The polarization ellipse along with the definition of relevant qualities.

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$$|k_x(\omega)| = \frac{\omega}{c}[\sqrt{\varepsilon(\omega)\mu(\omega)} \pm \kappa(\omega)]. \quad (1)$$

In the following the dependence of all quantities on frequency ω is kept in mind but suppressed in equations.

The eigenmodes do not couple in a homogenous medium and the following abbreviations can be introduced: $\vec{E}^{+} = (E_0/2)(0,1,+i)^T$:$k^{+}_{\pm} = k_0(\pm\sqrt{\varepsilon\mu} - \kappa)$ and $\vec{E}^{-} = (E_0/2)(0,1,-i)^T$:$k^{-}_{\pm} = k_0(\pm\sqrt{\varepsilon\mu} + \kappa)$, where the $\pm$-sign in the subscript indicates forward- and backward-propagating waves, respectively. These solutions are well known and examined, e.g., in Ref. 6.

The chiral parameter for an infinite medium can be obtained by taking the difference in the propagation constants $k^{\pm}$ of both eigenmodes, i.e., by

$$\kappa = (k^{-}_{\pm} - k^{+}_{\pm})/2k_0. \quad (2)$$

This approach can be also applied to metamaterials (MM) in considering them as media with effective parameters. Thus, the first step consists in deriving the dispersion relations $k^{-}_{\pm}(\vec{k}_{\perp},\omega)$ and $k^{+}_{\pm}(\vec{k}_{\perp},\omega)$ for the Bloch modes of the 3D periodic structure. Then Eq. (2) may be used to derive κ. At this stage it is important to keep in mind that this chirality parameter κ is derived from the dispersion relations $k^{\pm}_{\pm}(\vec{k}_{\perp},\omega)$ at $\vec{k}_{\perp}=0$. Thus, the effective chirality of a MM κ is likewise a wave parameter and characterizes the material only at a certain transverse wave vector, here a vanishing one. This effective parameter serves thus only to simplify the MM characterization. To date no genuine material parameters for any MM are available (for details of this issue, see Ref. 9). On the other hand, to retrieve κ from the complex reflection and transmission at a multilayer CM of thickness d, it is necessary to obtain an analytical expression for $R_{\pm}$ and $T_{\pm}$ at normal incidence at first. The rather cumbersome but straightforward calculation yields

$$R_{\pm} = R \quad \text{and} \quad T_{\pm} = Te^{\pm ik_0\kappa d}, \quad (3)$$

where R and T are the reflected and transmitted amplitudes for $\kappa=0$ at normal incidence, respectively.[10] The rotation of the polarization only affects the transmitted fields as required by reciprocity.

To analyze the polarization rotation we assume the incident electric field, arbitrarily to a certain extent, to be y-polarized. It can be decomposed into a rcp- and lcp waves by $\vec{E}_I = \vec{E}^{+} + \vec{E}^{-} = E_0\vec{e}_y$. The transmitted electric field is then given by $\vec{E}_T = T_+\vec{E}^{+} + T_-\vec{E}^{-} = E_0T[0,\cos(k_0\kappa d),\sin(k_0\kappa d)]^T = E_0(0,T_y,T_z)^T$. The chirality parameter κ can be calculated as

$$\kappa = \frac{1}{k_0 d}\arctan\left(\frac{T_z}{T_y}\right). \quad (4)$$

In absorptive media $\kappa=\kappa'+i\kappa''$ is usually complex. Therefore the output beam is in general elliptically polarized. In the system of the principal axis (see Fig. 1) the equation for the ellipse is $\xi^2/\alpha^2+\eta^2/\beta^2=1$. The real part κ' describes the rotation angle ϕ of the ellipse, which can be easily shown by algebraic manipulation. The imaginary part κ'' determines the ratio between the small and the large axes of the ellipse $\alpha/\beta=\tanh[k_0\kappa'' d]$, i.e., the imaginary part κ'' determines the ellipticity of the polarization state. It is therefore responsible for the effect of circular dichroism. Obviously κ' and κ'' are connected by a Kramers–Kronig relation since κ has to be a meromorphic function.[11] Therefore dispersive circular dichroism cannot occur without a polarization rotation resulting from a nonvanishing real part κ'. For large absolute values of κ'' the tanh function tends to ± 1, i.e., either lcp waves or rcp waves are transmitted. For vanishing κ'' the polarization remains linear. There are no constraints on the value of κ except that $\Im(k^{\pm})$ has to remain positive for the reason of causality.[6,11]

The transmission coefficient T is then given by

$$T = \frac{T_y}{\cos(k_0\kappa d)} = \frac{T_z}{\sin(k_0\kappa d)}. \quad (5)$$

The effective parameters n, Z, ε, and μ of the MM can be obtained by retrieving them, as given in Ref. 12, using R and T from Eqs. (3) and (5), although they will depend on the propagation direction.[13] It is evident that these retrieved parameters are also only wave parameters as discussed in Ref. 9.

For the sake of providing an application of the theory we focus here on the chirality of metallic gammadions. They can be understood as prototypical unit cells for chiral metaatoms. The sketch of the unit cell and the definition of all geometrical parameters is given in Figs. 1(a) and 1(b). The period in the y- and z-directions is $L=660$ nm. The gammadions are deposited on a thin dielectric film with a height of $h_{\text{sub}}=50$ nm and a refractive index of $n=1.73$. The height of the metallic gammadions on top of the dielectric film is $h_{\text{met}}=50$ nm [dispersive material parameters were taken from the literature (Ref. 14)]. For the purpose of stacking these layers the gammadions are embedded in a dielectric with $n=1.44$. The remaining quantities are defined as $b=75$ nm and $s=220$ nm. Note that the dielectric substrate is an essential part of the unit cell. Hence the unit cell cannot be described as planochiral.[15] A bulk medium is constructed by forming a stack of such functional layers. The fabrication of those media is generally feasible with current state-of-the-art technology.[16] The period in the x-direction (separation among subsequent functional layers) is chosen to be $D=200$ nm. Note that the unit cell consists of three layers: the metallic gammadion, a homogenous dielectric substrate below, and a homogeneous dielectric on top with a thickness of $d=D-h_{\text{met}}-h_{\text{sub}}=100$ nm, rendering the unit cell being chiral without any form of twist or anisotropy in propagation direction. The smallest wavelength (1.14 μm) of interest will be much larger than all relevant geometrical feature sizes, hence, rendering the homogenization procedure to be valid.

The dispersion relation and the scattering coefficients of the system under consideration are calculated numerically with the Fourier Modal Method (FMM).[17] As described before all quantities of interest can be inferred from these simulations. The transmission and reflection calculations were obtained for both propagation directions for the structures and its mirror image. The results for the gammadions for a particular propagation direction are shown in Fig. 2. Note that in no configuration any effect of polarization rotation on reflected waves is observed. To access the bulk properties and to answer the question whether and to which extent the properties of the multilayer MM coincide with those of the infinite medium, the chirality κ was retrieved for an increasing

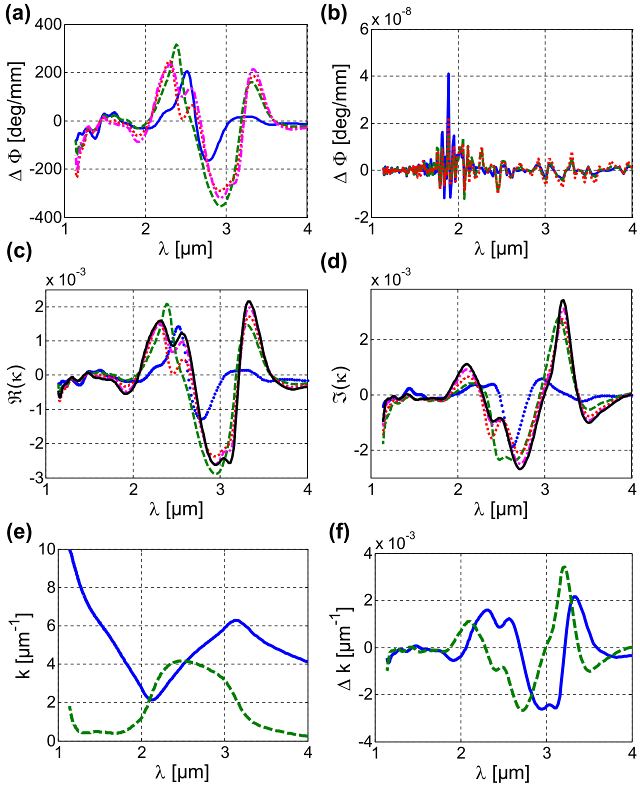

FIG. 2. (Color online) Polarization rotation with (a) and without (b) substrate and embedding dielectric. The real part (c) and the imaginary part (d) of the corresponding effective chirality parameter as a function of the wavelength λ and the number of layers that form the metamaterial stack. The lines are labeled as follows: blue dots—one layer, green dashed—two layers, red dotted—five layers, magenta dash-dotted—ten layers, and black solid—infinite bulk medium. The blue, green, red, and magenta data are determined by R/T coefficients, the black line by the dispersion relation. (e) Real (blue solid lines) and imaginary (green dashed lines) parts of the dominating Bloch modes and (f) the half of their difference being equivalent to κ.

number of functional layers (1, 2, 5, and 10). These results are compared with results of the infinite system for which chirality can be deduced from the dispersion relation. In the FMM, which discretizes the problem, $4\times N^2$ eigenvalues are computed at a fixed frequency, where N denotes the number of Fourier orders retained in the expansion. The factor of 4 results from the two polarization states and the forward and backward propagating solutions. For calculating effective parameters only the eigenmode with the smallest imaginary part of the propagation constant is considered since it will dominate light propagation in the medium.[18]

The angle of rotation $\Delta\phi$ [Fig. 2(a)] is clearly identical to $\Re(\kappa)$ [Fig. 2(c)]. In Fig. 2(b) the angle of rotation is shown for the periodic arrangement of gammadions without substrate and embedding dielectric. The unit cells are not chiral anymore; hence, the polarization rotation vanishes except for numerical noise. In Fig. 2(e) the real part of the propagation constants for the (lcp) and (rcp) eigenmodes with the smallest positive imaginary part is shown. Their difference required for calculating κ by using Eq. (2) cannot be inferred from the figure and is thus shown in Fig. 2(f).

The rotation maximum reaches more than 300 deg/mm at a wavelength of $\lambda=2.95\ \mu$m. For a single functional layer of a thickness of $D=200$ nm, this value corresponds to an absolute value of $\Delta\phi$ of less than a single degree. Nevertheless the rotation capability of such structures can exceed that of the natural available material. Both the real part and the imaginary part of $\kappa(\omega)$ are strongly dispersive [Figs. 2(c) and 2(d)]. Their resonances are coupled to the resonances of the structure. It holds generally that the stronger such resonances are excited, the larger the polarization rotation. The spectral positions of such resonances can be easily deduced from R/T spectra.[19,20] Traces can be seen in the induced strong dispersion in the effective propagation constant [Fig. 2(e)]. Clearly for an increasing number of layers the chirality parameters as retrieved from R and T converge toward the respective values obtained form the dispersion relation. Already five layers are sufficient to assign bulk properties to the stacked medium. Effects associated with the boundaries tend to be negligible then (see, e.g., Refs. 9 and 21).

In conclusion, our results confirm that the polarization rotation achieved by quasiplanar CMs due to optical activity can exceed that of natural available media. Since chirality is a genuine bulk property, we have introduced an approach to assign effective chirality parameters to these CMs. Both methods, the approach based either on reflection or transmission of a multilayer MM or by employing the dispersion relation provide identical results if boundary effects are negligible. This approach therefore paves the way toward the description of bulklike CMs on the basis of effective material parameters. However, these parameters are wave rather than material parameters and depend on the propagation direction in the MM.

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