Local constitutive parameters of metamaterials from an effective-medium perspective

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The reason of the nonlocality of constitutive (material) parameters extracted from the Fresnel-type reflection-transmission coefficients of composite slabs at moderately low frequencies is explained, and the physical meaning of these parameters is clarified. Local constitutive parameters of metamaterial lattices are discussed, and their existence at moderate frequencies is demonstrated. It is shown how to extract local material parameters from the dispersion characteristics of an infinite lattice and from reflection and transmission coefficients of metamaterial layers.

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I. INTRODUCTION

In the modern scientific literature, the so-called metamaterials (see, e.g., Refs. 1–3) correspond to a lot of exciting results. Metamaterials (MTMs) are sometimes defined as media which possess constitutive (material) parameters not observed in nature. Thanks to these material properties, many exotic phenomena were predicted and discovered in MTM structures. As a rule, MTM are realized as lattices of reciprocal optically small resonant particles, such as complex-shape metal inclusions (in different frequency ranges) and plasmonic and polaritonic nanospheres and nanowires (at infrared frequencies and in the visible). A particle characteristic size δ and the maximal period of lattices a at the frequency of particle resonance are assumed in many MTMs to be much smaller than the wavelength λ in the lattice matrix. This assumption is usually considered as allowing one to homogenize MTMs and to explain their exotic properties in terms of conventional material parameters (MPs) introduced in the quasistatic theory of lattices.[4,5] However, it is important that δ and a in MTM, though small, are not negligible with respect to λ. In most practical cases, they lie within the frequency band

$$0.01 < \frac{(a,\delta)}{\lambda} < 0.2. \tag{1}$$

Also, the effective wavelength in MTM (which, in cases of small attenuation, can be expressed though the propagation constant q as $\lambda_{\text{eff}}=2\pi/\text{Re}\{q\}$) being shortened at the particle resonance compared to λ can approach $2a$. At such frequencies, the lattice spatial resonance (*Bragg's resonance*) takes place in spite of the low-frequency condition (1) being satisfied. Then the Bragg (staggered) mode which has a complex wave number $q=\pi/a+j\,\text{Im}(q)$ even in lossless lattices can be excited. Within the band of the staggered mode, the homogenization of the metamaterial lattice is meaningless. If one formally introduces material parameters for such a regime, they will not be measurable response functions, and it will be not possible to use them for a sample of other dimensions or for a sample excited in another way. In particular, such formally introduced material parameters cannot satisfy the following conditions of *locality* (see, e.g., in Ref. 4):

(a) Passivity. For the temporal dependence $e^{-i\omega t}$, it implies $\text{Im}(\varepsilon)>0$ and $\text{Im}(\mu)>0$ simultaneously at all frequencies; for $e^{j\omega t}$, the sign of both $\text{Im}(\varepsilon)$ and $\text{Im}(\mu)$ should be negative.

(b) Causality (for media with negligible losses $\partial(\omega\varepsilon)/\partial\omega>1$ and $\partial(\omega\mu)/\partial\omega>1$). This also means that in the regions of negligible losses, material parameters obviously grow versus frequency: $\partial(\text{Re}(\varepsilon))/\partial\omega>0$ and $\partial(\text{Re}(\mu))/\partial\omega>0$).

(c) Absence of radiation losses. Though this principle is often attributed in the literature to a more recent work,[6] it was, in fact, postulated for periodic structures in Ref. 7, then proved for dipole lattices in Ref. 8.

(d) Independence of the material parameters on the wave propagation direction. For planar slabs, this means independence from the incident angle.

Constitutive parameters, of course, have no physical meaning at the frequencies of staggered modes: for a lossless medium the wave number of a staggered mode is complex; however, material parameters (whose product must determine this wave number) cannot be complex in lossless structures.[4,5] From this fact, some researchers deduce that it is impossible to introduce local MPs over the whole resonant band of a metamaterial (e.g., Ref. 9). This is not so. Local material parameters can be introduced within the part of the resonant band of particles which is free from the staggered mode.

The staggered mode of a lattice never covers the whole region in Eq. (1), and there are bands where $a<\lambda_{\text{eff}}/2$. At these frequencies, one intuitively expects that MPs satisfy the locality conditions listed above. However, inspecting well-known works[10–17] and many others devoted to the extraction of MP from measured or simulated reflection (R) and transmission (T) coefficients of a MTM slab, one notices that it is apparently not so. At least one of the two extracted MP in all these works violates all the locality conditions. This violation happens not only within the resonance band but over the whole frequency range in Eq. (1) even well below the lower edge of the resonant band. In the present work, we will show that the reason for this contradiction between our expectance and the results of these works is a *special* physical meaning of calculated MPs, different from the meaning of the local constitutive parameters.

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In Ref. 18, it is properly noticed that *special* MPs introduced for orthorhombic lattices in Refs. 19 and 20 are nonlocal. It is possible to prove that these special MPs are equal to MPs measured or simulated in Refs. 10–17 through R and T. The main goal of this paper is to introduce local MPs for the frequency range in Eq. (1) which can be also extracted from same reflection and transmission coefficients (R and T) of a layer. This extraction is possible over the band in Eq. (1), except the frequencies of staggered modes.

II. LOCAL AND NONLOCAL MATERIAL PARAMETERS

It was probably first noticed by Drude[21] that in the case when the lattice period is smaller but comparable with the wavelength (e.g., $a=0.01,\ldots,0.1\lambda$) the approximation of a sharp boundary for the homogenized lattice loses validity. In this case, a finite lattice cannot be replaced by a homogeneous medium with a permittivity being uniform over the whole volume of the sample. This is so because the phase shift of the field over the lattice period cannot be neglected. Moreover, in this case one cannot define the location of physical boundaries of natural lattices in an unambiguous way. At the interface, the normal components of averaged electric and magnetic fields should experience a jump, but we cannot define the position of this interface. Drude suggested to spread this field jump over a thin transition layer where the local effective permittivity varies from its bulk value (the local permittivity calculated for the unbounded lattice) to its value in free space outside the sample. The reason why this theory has not been popular is quite simple: In natural media, the influence of Drude transition layers is negligible since $a \ll 0.01\lambda$. However, to ignore Drude's surface effect for MTM is not possible: it is just the case when it becomes significant. The Drude theory was revisited and extended in our works.[22–25] We have considered microscopic fields and polarizations near the sample boundary. An extended model of Drude transition layers allowed one to increase the accuracy in the prediction of the reflection coefficient from a composite slab compared to the Drude approximate formulas. From these earlier results, it becomes clear that neglecting transition layers in the calculation of the reflection and transmission coefficients for a composite slab through its local MPs leads to significant errors in the frequency band in Eq. (6), especially at oblique incidence.

It is important to note, on the other hand, that the problem of reflection and transmission of plane waves in composite slabs can be formulated in different ways. First, we can consider this problem using conventional (local) MP that, however, implies the Drude effect of the spread lattice boundary. Second, it is possible to introduce formal MPs that determine the transfer matrix of the lattice unit cell for the fixed propagation direction (and have no other physical meaning). Then, the problem of transition layers does not arise and these MPs can be directly related to the reflection and transmission coefficients. However, these MPs turn out to be nonlocal.[10–17] Third, it is possible to extract local MPs through exact calculations of microscopic fields in the structure and their averaging.[26,27] However, in our interpretation, homogenization should offer a tool for fast (approximate) evaluation of electromagnetic properties of systems containing metamaterial layers. Here, we suggest a *simple analytical* homogenization model of metamaterials and prove that based on this model we can extract local MPs through reflection and transmission coefficients of slabs.

Though the presence of the transition layer makes the problem of the plane-wave reflection [in the frequency range in Eq. (1)] more difficult to solve as in the case of uniform effective-medium model (in the quasistatic limit), MPs used in this model are local, and the locality is an important advantage. Once extracted, tensors of local MPs are independent of the wave incidence angle and polarization, whereas nonlocal MPs at the same frequency are different for different directions of the wave vector. Local MPs can describe the interaction between the medium with wave packages and with evanescent waves. Nonlocal MPs are applicable only for propagating waves; moreover, a given pair of nonlocal MPs is applicable for an individual plane wave only, and only in this simple situation they do not violate the passivity condition in the effective medium. Really, in a plane wave, its electric and magnetic fields are related through the wave impedance. In this situation, the negative electric or magnetic losses (the wrong sign of $\varepsilon_{\rm eff}$ for magnetic MTM was obtained in Refs. 10–17 or, vice versa, the wrong sign of $\mu_{\rm eff}$ for dielectric MTM) are compensated by positive magnetic or electric losses, and the individual electromagnetic wave properly attenuates. A similar speculation can be done about causality. For wave packages and for evanescent waves, the behavior of the medium described through nonlocal MP is not passive and not causal. In this case, the electric field and magnetic field are locally decoupled. For example, in the near zone of a wire antenna the electric field dominates. Then, the wrong sign of electric losses in the substrate material implies electric power generation in the substrate (assuming that nonlocal material parameters of the substrate describe its response to the antenna field). This is impossible for passive materials. It is also easy to see violation of causality in the near-field zone of antennas. Thus, nonlocal MPs are not applicable to problems related to evanescent waves (for example, they are not applicable to describe antenna substrates). The same concerns the packages of propagating waves, e.g., a standing wave, where the maxima of the electric field correspond to minima of the magnetic field. As a result, the use of nonlocal MP violates the passivity and causality in the same way. Only local MPs can be used to describe materials in such problems.

The approximation of a uniform slab[10] allows to extract nonlocal MPs $\varepsilon_{\rm eff}$ and $\mu_{\rm eff}$ for lattices of thickness d through the direct inversion of reflection and transmission coefficients R and T which, for the normal incidence and temporal dependence $\exp(j\omega t)$, take the form

$$R=\frac{r(1-e^{-2jq_{\rm eff}d})}{1-r^2e^{-2jq_{\rm eff}d}}, \quad T=\frac{e^{-jq_{\rm eff}d}(1-r^2)}{1-r^2e^{-2jq_{\rm eff}d}}. \tag{2}$$

Here, $q_{\rm eff}=\omega\sqrt{\varepsilon_0\mu_0\varepsilon_{\rm eff}\mu_{\rm eff}}\equiv k_0\sqrt{\varepsilon_{\rm eff}\mu_{\rm eff}}$ is the wave number of the effective-medium filling the layer, and r is the reflection coefficient from semi-infinite medium expressed through Z (the medium wave impedance normalized to that of free space) as

$$r = \frac{Z-1}{Z+1}, \quad Z = \sqrt{\frac{\mu_{\mathrm{eff}}}{\varepsilon_{\mathrm{eff}}}}. \tag{3}$$

As it was already noticed, formulas (2) lead to nonlocal constitutive parameters of artificial crystals in the frequency region of our interest. Let us understand why MPs obtained in Refs. 10–17 are nonlocal. Below, we will show that these parameters enter the so-called Bloch impedance which is not equal to the wave impedance of the refracted wave. The Bloch impedance is the ratio of the amplitudes of the fundamental Bloch harmonics of electric and magnetic fields, whereas the wave impedance is that of the averaged electric and magnetic fields. And we will see that the substitution of the fundamental Bloch harmonics instead of the averaged fields into Maxwell's equations implies introduction of *fictitious* material responses. As the medium response described by the MP extracted from relations (2) is fictitious, one cannot expect causality and passivity of these MP.[28,30]

Consider a problem of plane-wave reflection from a semi-infinite lattice of electric dipole scatterers (named below as p *lattice*). The exact analytical solution of this problem was found in Ref. 31. For simplicity, let us restrict the analysis by the special case of the normal incidence on an orthorhombic lattice of dipoles located in free space. Also, we assume that the frequency range satisfies the condition $k_0 a = \omega a\sqrt{\varepsilon_0\mu_0} < \pi$, where a is the lattice period along the direction of propagation (in this frequency region only one eigenwave can propagate). Then, the reflection coefficient from a semi-infinite lattice takes the form[31]

$$r = \frac{\sin\dfrac{(k_0-q)a}{2}}{\sin\dfrac{(k_0+q)a}{2}}\Pi. \tag{4}$$

Here, q is the eigenwave wave number and factor Π for which a closed-form expression was obtained in Ref. 31 takes into account all polaritons excited at the interface. It was proven in Ref. 31 that at the frequencies of our interest, this factor has the unit of absolute value. So, it can be represented as an imaginary exponential $\Pi = e^{j\Phi}$ with a real parameter Φ. The influence of polaritons can be taken into account by a displacement of the effective interface to which the new reflection coefficient r' is referred [the reflection coefficient r in formula (4) refers to the first crystal plane hit by the incident wave]. After this shift, we can rewrite Eq. (4) in the form

$$r' = r\exp(-j\Phi) = \frac{Z_B-1}{Z_B+1}, \quad Z_B = \frac{\tan(k_0 a/2)}{\tan(qa/2)}. \tag{5}$$

The phase shift Φ is rather small for $qa<1$.[31] Notice that knowing Φ one can avoid introduction of an effective interface and obtain the exact reflection coefficient as $r' = (Z_B' - 1)/(Z_B'+1)$ with redefined Z_B' related to Z_B from Eq. (5) through the standard formula for the input impedance of a loaded transmission line.

If $\max(qa/2, k_0 a/2) \ll 1$, the sine and tangent functions in Eqs. (4) and (5) can be replaced by their arguments. Then, we obtain from Eq. (5) $Z_B = k_0/q$ that gives the continuous medium approximation. Indeed, if we compare $Z_B = k_0/q = 1/\sqrt{\varepsilon_{\mathrm{eff}}\mu_{\mathrm{eff}}}$ with Z from Eqs. (3), we obtain $\mu_{\mathrm{eff}}=1$ and $q = k\sqrt{\varepsilon_{\mathrm{eff}}}$, and Eq. (5) transforms to the correct Fresnel reflection formula for a continuous dielectric half-space. Nonlocality of the effective permittivity extracted through R in this case is negligible. The practical condition of applicability of this approximation follows from numerical properties of the tangent function and reads as

$$\max\left(\frac{a}{\lambda}, \frac{a}{\lambda_{\mathrm{eff}}}\right) < 0.01. \tag{6}$$

This condition gives the upper frequency limit up to which formulas (2) and (3) are compatible with the continuous medium approximation. The frequency region [Eq. (6)] is the same for which the transition layers in the theory[24] have no visible influence. However, for practical implementations of MTM, the frequencies satisfying Eq. (6) are not interesting.

Consider the normalized impedance $Z = Z_B$ from Eq. (3) at frequencies in Eq. (1). Formulas (5) obtained as the *strict* solution of the boundary lattice problem are known also in the theory of periodically loaded transmission lines (TLs). The second formula in Eq. (5) represents the so-called *Bloch impedance* of a TL loaded by shunt lumped impedances with period a [see, e.g., formula (5.117) from Ref. 32]. The Bloch impedance describes properties of the fundamental Bloch mode in an infinite lattice (or periodically loaded transmission line), and it is equal to the ratio of the amplitudes of the electric and magnetic fields $\mathbf{E}_0$ and $\mathbf{H}_0$ of this mode. If an eigenmode with the wave vector $\mathbf{q}$ propagates along the axis z in a lattice of electric and/or magnetic inclusions with the periods along Cartesian axes denoted as (b_x, b_y, a), the Bloch expansion for the microscopic fields reads

$$\begin{Bmatrix} \mathbf{E}(\mathbf{r}) \\ \mathbf{H}(\mathbf{r}) \end{Bmatrix} = \begin{Bmatrix} \mathbf{E}_0 \\ \mathbf{H}_0 \end{Bmatrix} e^{-jqz} + \sum_{\mathbf{n}\neq\mathbf{0}} \begin{Bmatrix} \mathbf{E}_\mathbf{n} \\ \mathbf{H}_\mathbf{n} \end{Bmatrix} e^{-j(qz+\mathbf{G}_\mathbf{n}\cdot\mathbf{r})}, \tag{7}$$

where $\mathbf{G}_\mathbf{n} \equiv (G_x, G_y, G_z) = (2\pi n_x/b_x, 2\pi n_y/b_y, 2\pi n_z/a)$ are multiples of the generic lattice vector and $\mathbf{n} = (n_x, n_y, n_z)$, $n_{x,y,z} = 1, 2, \ldots, \infty$. To find the amplitudes of the fundamental Bloch mode $\mathbf{E}_0$ and $\mathbf{H}_0$ from the microscopic fields represented by Eq. (7), we should average the fields in the transverse plane, calculating

$$\begin{Bmatrix} \mathbf{E}_{TA} \\ \mathbf{H}_{TA} \end{Bmatrix} \equiv \frac{1}{b_x b_y}\int_{-b_x,-b_y/2}^{b_x,b_y/2} \begin{Bmatrix} \mathbf{E}(\mathbf{r}) \\ \mathbf{H}(\mathbf{r}) \end{Bmatrix} dxdy, \tag{8}$$

and then calculate integrals

$$\begin{Bmatrix} \mathbf{E}_0 \\ \mathbf{H}_0 \end{Bmatrix} = \frac{1}{a}\int_{-a/2}^{a/2} \begin{Bmatrix} \mathbf{E}_{TA}(z) \\ \mathbf{H}_{TA}(z) \end{Bmatrix} e^{+jqz} dz. \tag{9}$$

Indeed, from definition (8), we see that

$$\begin{Bmatrix} \mathbf{E}_{TA} \\ \mathbf{H}_{TA} \end{Bmatrix} = \begin{Bmatrix} \mathbf{E}_0 \\ \mathbf{H}_0 \end{Bmatrix} e^{-jqz} + \begin{Bmatrix} \mathbf{E}_{n_z} \\ \mathbf{H}_{n_z} \end{Bmatrix} e^{-j[q+(2\pi n_z/a)]z}. \qquad (10)$$

The transverse averaging [Eq. (8)] eliminates the higher-order modes in the transverse plane, so that terms with G_x and G_y disappear, but the terms with G_z and the corresponding higher-order amplitudes $\mathbf{E}_{n_z}$ and $\mathbf{H}_{n_z}$ are retained.

Formulas (9) and (10) clearly indicate that the Bloch impedance is a nonlocal parameter because for calculating $\mathbf{E}_0$ and $\mathbf{H}_0$ beyond the quasistatic limit it is not enough to know the microscopic fields in the vicinity of the observation point. They depend explicitly on the propagation constant of the fundamental Bloch mode. So, the effective material parameters extracted from Z_B should be nonlocal at the frequencies of our interest.

Formulas (9) indicate that the Bloch impedance defined in Ref. 2 as the ratio of the effective voltage and current at the input or output of a lattice unit cell $Z_B = E_{TA}(\pm a/2)/\eta H_{TA}(\pm a/2)$ (normalized to the wave impedance η of the matrix) is also equal to the ratio of fundamental Bloch harmonics of electric and magnetic fields in the lattice.

Unlike the zeroth Bloch harmonic of electric and magnetic fields, the volume-averaged microscopic fields $\langle \mathbf{E} \rangle$ and $\langle \mathbf{H} \rangle$ are simply the integrals of microscopic fields around the observation point divided by the cell volume $V = ab_x b_y$,

$$\begin{Bmatrix} \langle \mathbf{E} \rangle(\mathbf{r}) \\ \langle \mathbf{H} \rangle(\mathbf{r}) \end{Bmatrix} \equiv \frac{1}{V}\int_V \begin{Bmatrix} \mathbf{E}(\mathbf{r}+\mathbf{r}') \\ \mathbf{H}(\mathbf{r}+\mathbf{r}') \end{Bmatrix} d^3\mathbf{r}'. \qquad (11)$$

Here, the local position vector $\mathbf{r}'$ refers to the unit-cell center. Comparing Eqs. (9) and (11), one can see that the averaged fields *are not equal* to the fundamental Bloch modes of the true fields. The difference is determined by the factor $\exp(+jqz)$ which is absent in the integrand of Eq. (11). High-order terms of expansion (7) give nonzero contributions into $\langle \mathbf{E} \rangle$ and $\langle \mathbf{H} \rangle$,

$$\begin{Bmatrix} \langle \mathbf{E} \rangle(z) \\ \langle \mathbf{H} \rangle(z) \end{Bmatrix} = e^{-jqz}\left[\begin{Bmatrix} \mathbf{E}_0 \dfrac{\sin qa/2}{qa/2} \\ \mathbf{H}_0 \dfrac{\sin qa/2}{qa/2} \end{Bmatrix} + \sum_{n_z=1}^{\infty} \begin{Bmatrix} \mathbf{E}_{n_z} \dfrac{\sin[(qa+2\pi n_z)/2]}{(qa+2\pi n_z)/2} \\ \mathbf{H}_{n_z} \dfrac{\sin[(qa+2\pi n_z)/2]}{(qa+2\pi n_z)/2} \end{Bmatrix} \right]. \qquad (12)$$

We have just seen that the effective material parameters introduced for the fundamental Bloch harmonic amplitudes $\mathbf{E}_0$ and $\mathbf{H}_0$ via the Bloch impedance are nonlocal parameters. Let us next consider if one can write Maxwell's equations for fields averaged in this this way. Integrating Maxwell's equations for the microscopic fields

$$\nabla \times \mathbf{E} = -j\omega(\mu_m \mathbf{H} + \mathbf{M}), \quad \nabla \times \mathbf{H} = j\omega(\varepsilon_m \mathbf{E} + \mathbf{P}), \qquad (13)$$

one does not change these equations, and they still hold for $\langle \mathbf{E} \rangle$ and $\langle \mathbf{H} \rangle$ and the averaged polarizations $\langle \mathbf{P} \rangle$ and $\langle \mathbf{M} \rangle$. Here, ε_m and μ_m are, respectively, absolute permittivity and permeability of the matrix which, in the general case, are not equal to ε_0 and μ_0. In the case of propagation along one of the lattice axes (we consider propagation along z), we can assume without any loss of generality that the averaged electric field has only one Cartesian component $\langle E \rangle$ (as well as the averaged magnetic field and the averaged electric and magnetic polarizations). For example, $\langle \mathbf{E} \rangle = \langle E \rangle \mathbf{x}_0$, $\langle \mathbf{P} \rangle = \langle P \rangle \mathbf{x}_0$ and $\langle \mathbf{H} \rangle = \langle H \rangle \mathbf{y}_0$, $\langle \mathbf{M} \rangle = \langle M \rangle \mathbf{y}_0$. Then, Maxwell's equations for the averaged fields read

$$q\langle H \rangle = \omega\varepsilon_m \langle E \rangle + \omega \langle P \rangle, \qquad (14)$$

$$q\langle E \rangle = \omega\mu_m \langle H \rangle + \omega \langle M \rangle. \qquad (15)$$

Substituting expressions (12) and similar expressions for $\langle P \rangle$ and $\langle M \rangle$ into Eqs. (14) and (15), we obtain

$$qE_0 = \omega(\mu_0 H_0 + M_0 + M_{\rm fict}), \qquad (16)$$

$$qH_0 = \omega(\varepsilon_0 E_0 + P_0 + P_{\rm fict}), \qquad (17)$$

where we had to introduce fictitious polarization and magnetization defined as

$$M_{\rm fict} = \left(\frac{qE_0}{\omega} - \mu_0 H_0\right)\left(1 - \frac{\sin qa/2}{qa/2}\right) + \sum_{n_z=1}^{\infty} (M_{n_z} + \mu_0 H_{n_z}) \frac{\sin[(qa+2\pi n_z)/2]}{(qa+2\pi n_z)/2}, \qquad (18)$$

$$P_{\rm fict} = \left(\frac{qH_0}{\omega} - \varepsilon_0 E_0\right)\left(1 - \frac{\sin qa/2}{qa/2}\right) + \sum_{n_z=1}^{\infty} (P_{n_z} + \varepsilon_0 E_{n_z}) \frac{\sin[(qa+2\pi n_z)/2]}{(qa+2\pi n_z)/2}. \qquad (19)$$

Treating the fundamental Bloch harmonic of electric and magnetic fields in Maxwell's equations written in forms (16) and (17) as the averaged fields, one comes to additional terms in these equations which can be interpreted as fictitious magnetization of p lattices and fictitious electric polarization of m lattices. Substituting the standard relations $E_0 = Z_B \eta H_0 = \sqrt{\mu_0\mu_{\rm eff}/\varepsilon_0\varepsilon_{\rm eff}}$ and $q = \omega\sqrt{\mu_0\varepsilon_0\mu_{\rm eff}\varepsilon_{\rm eff}}$ in Eqs. (16) and (17), we obtain the following artifacts: $\mu_{\rm eff} \neq 1$ for a lattice of purely electric inclusions and also $\varepsilon_{\rm eff} \neq 1$ for a lattice of magnetic inclusions. This is so because $P_{\rm fict}$ and $M_{\rm fict}$ are not equal to zero in these cases and are negligible only when $qa \ll 1$. Fictitious polarizations and material parameters relating them with the zeroth Bloch harmonic of the fields have little physical meaning for three-dimensional lattices. These artifacts follow from the known fact that the zeroth Bloch harmonics of microscopic fields *do not satisfy* Maxwell's equations (whereas the averaged fields do).

III. EXTRACTION OF LOCAL MATERIAL PARAMETERS

In this section, we will show that despite the difficulties discussed above, local material parameters can be introduced

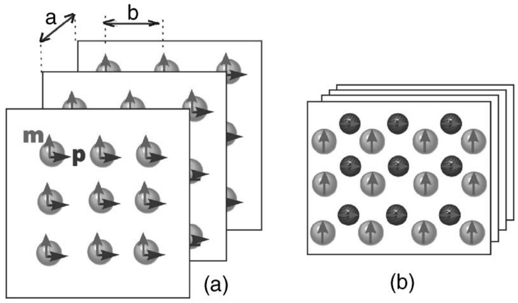

FIG. 1. Presentation of a p-m lattice as a set of dipole crystal planes. (a) Every particle has both electric and magnetic moments. (b) Electric and magnetic particles are different.

for metamaterial lattices in a reasonably wide frequency range, and there exists a simple way to extract these local parameters from reflection and transmission coefficients for normal incidence of a plane wave. We will do this using an example of a periodical lattice of electric and magnetic dipole particles. To proceed, we will need to write the dispersion equation for waves in such lattices.

A. Dispersion equation for p-m lattices

The dispersion equation of a wave propagating along a coordinate axis of an orthorhombic p lattice in the frequency region $ka<\pi$ was derived in Ref. 32 [Eq. (5.226)]. It turned out to be the same as the dispersion equation of a periodically loaded transmission line with shunt loads (e.g., Ref. 33):

$$\cos(qa) = \cos(ka) + \frac{j}{2Z_{\text{load}}}\sin(ka), \tag{20}$$

where $k=\omega\sqrt{\mu_0\varepsilon_0}$ is the wave number of the unloaded line (host medium) and Z_{load} is the impedance of loads normalized to the wave impedance η of the unloaded line. In this section, we generalize this equation to the case of p-m lattices.

Let us consider propagation of a plane wave with the wave vector $\mathbf{q}=q\mathbf{z}_0$ in an infinite lattice shown in Fig. 1. The lattice unit cell is $b\times b\times a$, i.e., $b_x=b_y$ [possible anisotropy in the x-y plane brings no new effects]. In Fig. 1(a), the particles are assumed to possess both electric and magnetic moments. In Fig. 1(b), the electric and magnetic scatterers are different particles. The formulas written below are the same for both these geometries. This is so since the quasistatic interaction between electric ($\mathbf{p}$) and magnetic ($\mathbf{m}$) dipoles is absent in both these structures. Any $\mathbf{p}$ dipole is not affected by $\mathbf{m}$ dipoles lying in the same crystal plane and vice versa, $\mathbf{m}$ dipoles do not interact with $\mathbf{p}$ dipoles of the same crystal plane. The p-m and m-p interactions between adjacent crystal planes are wave processes (except an impractical special case $a\ll b$) and therefore are not sensitive to the transverse displacement of $\mathbf{m}$ dipoles with respect to $\mathbf{p}$ dipoles in the lattice shown in Fig. 1(b).

Let a reference (0 numbered) p-m particle located at the coordinate origin have electric and magnetic polarizabilities a_{ee} and a_{mm}. These polarizabilities can be resonant in the same frequency range. Let E^{loc} and H^{loc} denote the x component of the local electric field and the y component of the local magnetic field, respectively. Then the $\mathbf{p}$ dipole and $\mathbf{m}$ dipole of the particle can be expressed as

$$p_0 = a_{ee}E^{\text{loc}}, \quad m_0 = a_{mm}H^{\text{loc}}. \tag{21}$$

The local fields are produced by other particles located at points $(x=n_xb, y=n_yb, z=n_za)$ and can be expressed through p_0 and m_0 since $p(\mathbf{n})=p_0\exp(-jn_zqa)$ and $m(\mathbf{n})=m_0\exp(-jn_zqa)$,

$$E^{\text{loc}} = C_{ee}p_0 + C_{em}m_0, \quad H^{\text{loc}} = C_{mm}m_0 + C_{me}p_0. \tag{22}$$

Substituting Eq. (22) into Eq. (21), we come to a linear system of equations

$$\frac{1}{a_{ee}}p_0 = C_{ee}p_0 + C_{em}m_0, \tag{23}$$

$$\frac{1}{a_{mm}}m_0 = C_{mm}m_0 + C_{me}p_0. \tag{24}$$

A closed-form expression for the cross-coupling interaction factor $C_{em}=C_{me}$ was derived in Ref. 34. For p-p and m-m interaction factors, the duality principle gives $C_{ee}=C_{mm}/\eta^2$. One can find in Ref. 32 the following expression for these coefficients:

$$C_{ee} = \frac{C_{mm}}{\eta^2} = \frac{\eta\omega}{2b^2}\left(C_0 + C_{NF} + \frac{\sin ka}{\cos ka - \cos qa}\right) + j\frac{k^3}{6\pi\epsilon_m}, \tag{25}$$

where $k=\omega\sqrt{\mu_m\varepsilon_m}$ is the host matrix wave number and $\eta=\sqrt{\mu_m/\varepsilon_m}$ is its wave impedance. In Eq. (25), the trigonometric term describes the wave interaction of the reference $\mathbf{p}$ dipole with $\mathbf{p}$ dipoles of other crystal planes. The real parameter C_{NF} describes the near-field interaction with $\mathbf{p}$ dipoles of other crystal planes. Finally, the real parameter C_0 is responsible for the near-field interaction of the reference $\mathbf{p}$ dipole with the other $\mathbf{p}$ dipoles of the reference crystal plane. For C_0, a simple expression was derived in Ref. 32:

$$C_0 = \frac{1}{2}\left(\frac{\cos kbs}{kbs} - \sin kbs\right), \tag{26}$$

where $s\approx 0.6954$. At low frequencies, $kb<0.5$, the approximation $C_0\approx 0.36$ is quite accurate.[32] The term C_{NF} can be neglected if $a\geqslant b$,[32] and below we restrict our study by this case.

Equating the determinant of Eqs. (23) and (24) to zero, we obtain the dispersion equation for waves in the lattice (an alternative equivalent form was derived in Ref. 34):

$$\cos qa = \cos ka - \sin ka\left(\frac{G}{4} + \frac{X}{4}\right) - \sqrt{\sin^2 ka\left(\frac{G}{4} - \frac{X}{4}\right)^2 + \frac{GX}{4}\sin^2 qa}. \tag{27}$$

Here, the following notations have been introduced:

$$\left\{\begin{matrix} G \\ X \end{matrix}\right\} = \frac{k_0 a}{V\left(\left\{\begin{matrix} \dfrac{\varepsilon_m}{a_{ee}} \\ \dfrac{\mu_m}{a_{mm}} \end{matrix}\right\} - j\dfrac{k^3}{6\pi}\right) - C_0}. \tag{28}$$

In Eq. (28), $V = ab^2$ is the unit-cell volume. In lossless structures, the following fundamental relations hold for electric and magnetic polarizabilities (derived initially in Refs. 7 and 8 and reproduced later inRef. 6):

$$\mathrm{Im}\,\frac{1}{a_{ee}} = \frac{k^3}{6\pi\varepsilon_m}, \quad \mathrm{Im}\,\frac{1}{a_{mm}} = \frac{k^3}{6\pi\mu_m}. \tag{29}$$

This means that parameters G and X in Eq. (27) are real valued in lossless lattices. Equation (20) is a special case of Eq. (27) which holds when there is no magnetic polarization ($a_{mm}=0$ and consequently $X=0$).

B. Local material parameters

At the reference particle position $x=y=z=0$, we have $\langle P\rangle = p_0/V$ and $\langle M\rangle = m_0/V$. Let us now define the absolute local material parameters ε_L and μ_L by formulas

$$\left\{\begin{matrix} \langle P\rangle \\ \langle M\rangle \end{matrix}\right. = \left\{\begin{matrix} (\varepsilon_L - \varepsilon_m)\langle E\rangle \\ (\mu_L - \mu_m)\langle H\rangle \end{matrix}\right. . \tag{30}$$

Substitution of these definitions into Eqs. (14) and (15) at $z=0$ leads to relations

$$q^2 = \omega^2 \varepsilon_L \mu_L, \quad Z_L \equiv \frac{\langle E\rangle}{\langle H\rangle} = \sqrt{\frac{\mu_L}{\varepsilon_L}}. \tag{31}$$

These MPs are expected to be *local* even at moderately low frequencies [Eq. (1)] since they relate volume-averaged fields and polarizations. It is difficult to prove strictly this fact (see also the discussions in Refs. 24 and 35), but the explicit examples confirm it.

Let us assume that we know parameters G and X which describe the crystal plane response defining the dispersion relation (27). The local MP can be estimated expressing polarizabilities a_{ee} and a_{mm} through G and X using formula (28) and then applying the well-known Clausius-Mossotti formula to find ε_L via a_{ee} and μ_L via a_{mm}. However, this quasistatic formula is hardly accurate at moderate frequencies. Formulas (31) offer another (dynamic) way for obtaining local MPs through G and X. Really, from Eqs. (23) and (24) with substitutions of Eqs. (25) and (28), it follows that

$$\eta p_0\left(\frac{2}{G} - \frac{\sin ka}{\cos qa - \cos ka}\right) = m_0 \frac{\sin qa}{\cos qa - \cos ka}, \tag{32}$$

$$m_0\left(\frac{2}{X} - \frac{\sin ka}{\cos qa - \cos ka}\right) = \eta p_0 \frac{\sin qa}{\cos qa - \cos ka}. \tag{33}$$

These relations give an auxiliary coefficient one needs in order to find the "local wave impedance" Z_L:

$$\gamma = \frac{\eta p_0}{m_0} = \frac{\eta\langle P\rangle}{\langle M\rangle} = \sqrt{\frac{G}{X}}\sqrt{\frac{\cos qa - \cos ka - \dfrac{X\sin ka}{2}}{\cos qa - \cos ka - \dfrac{G\sin ka}{2}}}. \tag{34}$$

From Eq. (30), we obtain (see also in Refs. 34 and 35):

$$\gamma = \eta Z_L \frac{(\varepsilon_L - \varepsilon_m)}{(\mu_L - \mu_m)}.$$

On the other side, from Eq. (31) we have

$$\varepsilon_L = \frac{q}{\omega Z_L}, \quad \mu_L = \frac{q}{\omega} Z_L. \tag{35}$$

Therefore, Z_L can be expressed as

$$\frac{Z_L}{\eta} = \frac{\gamma k + q}{\gamma q + k}. \tag{36}$$

Knowing G and X, one can find q. Then, through G, X, and q, one finds γ. Then, through q and γ, one finds Z_L. Finally, one determines local MPs through q and Z_L.

Practically, what is suggested is the generalization of the quasistatic approach based on the Clausius-Mossotti formula to the range of moderate frequencies. In the quasistatic limit, our result for ε_L and μ_L must be the same as that classical result. Let us check it, for simplicity, for a cubic p lattice. In this case $X=0$ and Eq. (27) simplifies to Eq. (20), which we can rewrite as

$$\cos(qa) = \cos(ka) - \frac{G}{2}\sin(ka). \tag{37}$$

Substitution of $\gamma \to \infty$ into Eqs. (35) and (36) gives $Z_L = \eta k/q$ and $q = k_0\sqrt{\varepsilon_L}$. For very low frequencies $\max(ka, qa) \ll 1$, we take into account two terms of the Taylor expansion of trigonometric functions in Eq. (37), and substituting expression (28) for G, we obtain

$$1 - \frac{(k_0 a)^2 \varepsilon_L}{2\varepsilon_0} = 1 - \frac{(k_0 a)^2 \varepsilon_m}{2\varepsilon_0} - \frac{(k_0 a)^2 \varepsilon_m \left[1 - \dfrac{(k_0 a)^2 \varepsilon_m}{6\varepsilon_0}\right]}{2\left[V\varepsilon_m \mathrm{Re}\left(\dfrac{1}{a_{ee}}\right) - C_0\right]}. \tag{38}$$

Neglecting the small term $(ka)^2/6 \ll 1$, we obtain the Clausius-Mossotti equation for the local permittivity,

$$\varepsilon_L = \varepsilon_m + \frac{1}{V\,\mathrm{Re}\left(\dfrac{1}{a_{ee}}\right) - \dfrac{C_0}{\varepsilon_m}}. \tag{39}$$

Our factor $C_0 \approx 0.36$ differs slightly from the classical term 0.33 in the denominator of expression (39). This difference is related to the ignorance of near-field interaction between adjacent crystal planes [we have neglected $C_{NF} \ll C_0$ in formula (25)]. The needed correction can be introduced in the theory.

Taking into account three terms of the Taylor expansion of cosine and sine functions in Eq. (38), one can obtain a frequency-dependent correction of the order $(k_0a)^2$ to the Clausius-Mossotti relation. Also, in the lossy case, the inverse polarizability after subtraction of the term $k^3/6\pi\varepsilon_m$ [see formula (28)] will be not purely real. One has to substitute $\mathrm{Re}(1/a_{ee})$ by $(1/a_{ee}-jk^3/6\pi\varepsilon_m)$. The Clausius-Mossotti equation following from Eq. (38) and generalized to the lossy case can be rewritten in the Lorentz form

$$3\varepsilon_m V\frac{\varepsilon_L-\varepsilon_m}{\varepsilon_L+2\varepsilon_m}=\frac{1}{\left(\frac{1}{a_{ee}}-j\frac{k^3}{6\pi\varepsilon_m}\right)\left[1-\frac{(ka)^2}{24}\right]+\frac{(k_0a)^2}{24\varepsilon_m V}}.$$

This result was obtained earlier in Ref. 24 in a totally different way. A similar check can be done for p-m lattices where one comes in the limit case $(k_0a,qa)\ll\pi$ to the Clausius-Mossotti relations for both ε_L and μ_L.

C. Relations between local and nonlocal material parameters

Next, let us relate ε_L, and μ_L to reflection and transmission coefficients R and T for a slab of a finite thickness. Involving transition layers in this extraction would make the problem rather difficult. A simpler way is to find q and $Z=Z_B$ through R and T using Eqs. (3) and (2) and then express G and X through q and Z_B. Knowing G and X, it is easy to calculate the local MP. Let us then relate the Bloch impedance Z_B with G and X. To do this, one can apply the transfer-matrix method. For the case under consideration [the normal propagation with respect to $(x$-$y)$-crystal planes], the transfer matrix $\mathbf{F}$ of a crystal plane defined at $z=0$ [matrix components (A,B,C,D)] reads as

$$\begin{bmatrix} E_{TA}(z=-0)/\eta \\ H_{TA}(z=-0)\end{bmatrix}=\begin{bmatrix} A & B\\ C & D\end{bmatrix}\begin{bmatrix} E_{TA}(z=+0)/\eta \\ H_{TA}(z=+0)\end{bmatrix}. \quad (40)$$

Even if particles have sizes comparable to period a, one can attribute effective currents to the crystal plane $z=0$. This procedure is basically the same as replacing the finite particles by point p and m dipoles which is a good approximation for many practical cases. The transversally averaged electric field experiences a jump across the crystal plane. This jump is proportional to the effective magnetic current on this plane, i.e., to the magnetic dipole m_0. The transversally averaged magnetic field also experiences a jump across the crystal plane. It is proportional to the effective electric current, i.e., to p_0. It can be shown that

$$\frac{\eta[H_{TA}(z=+0)-H_{TA}(z=-0)]}{E_{TA}(z=+0)-E_{TA}(z=-0)}=\frac{\eta p_0}{m_0}\equiv\gamma, \quad (41)$$

where parameter γ is expressed in Eq. (34) through G and X. The transmission-line representation of the lattice unit cell (see Fig. 2) helps to understand that the Bloch impedance [which is equal to the ratio of voltages (transversally averaged electric fields) and currents (transversally averaged magnetic fields) at the input or output of every unit cell of a loaded transmission line[2,29]] is equal to

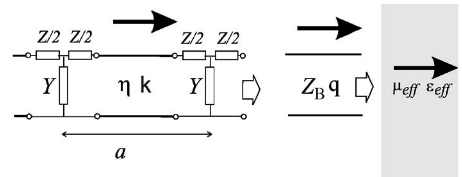

FIG. 2. Presentation of a lattice with electric and magnetic inclusions (p-m lattice) as (1) periodically loaded transmission line, (2) homogenized transmission line with Bloch impedance Z_B and wave number q (k and η are unloaded wave number and characteristic impedance, respectively), and (3) effective magnetodielectric medium with nonlocal MP $\varepsilon_{\mathrm{eff}}$ and μ_{eff}.

$$Z_B=\frac{E_{TA}\left(z=\pm\frac{a}{2}\right)}{\eta H_{TA}\left(z=\pm\frac{a}{2}\right)}. \quad (42)$$

Equations (41) and (42) allow us to find all the components of the transfer matrix of a crystal plane,

$$\mathbf{F}=\begin{bmatrix} A & B\\ C & D\end{bmatrix}=\begin{bmatrix}\frac{\gamma Z_{in}}{\gamma Z_{in}-1} & \frac{Z_{in}}{\gamma Z_{in}-1}\\ \frac{1}{\gamma Z_{in}-1} & \frac{1}{\gamma Z_{in}-1}\end{bmatrix}. \quad (43)$$

Here, Z_{in} is the input impedance of the crystal plane, obtained from the Bloch impedance by referring it to the point $z=0$,

$$Z_{in}=\frac{Z_B-j\tan\left(\frac{ka}{2}\right)}{1-jZ_B\tan\left(\frac{ka}{2}\right)}. \quad (44)$$

From the circuit representation of a p-m-crystal plane (see Fig. 1), it is evident that $A=D$ (the equivalent scheme is symmetric), and therefore

$$Z_{in}=\frac{1}{\gamma}=\sqrt{\frac{X}{G}}\sqrt{\frac{\cos qa-\cos ka-\frac{G\sin ka}{2}}{\cos qa-\cos ka-\frac{X\sin ka}{2}}}. \quad (45)$$

Equations (44) and (45) relate Bloch impedance with local parameters G and X which are determined only by the individual polarizabilities of particles and their concentration. If one knows q and Z_B, one can express the local material parameters using relation (36) together with Eqs. (35), (44), and (45), yielding

$$\varepsilon_L=\frac{q(q+kZ_{in})}{\omega(k+qZ_{in})},\quad \mu_L=\frac{q(k+qZ_{in})}{\omega(q+kZ_{in})}, \quad (46)$$

where Z_{in} is expressed through Z_B by relation (44). Being found from R and T of a layer containing N lattice unit cells across it, the nonlocal MP related to the Bloch impedance by Eq. (3) and local MP related to Bloch impedance by Eqs. (46) and (44) can be used for slabs with arbitrary thicknesses

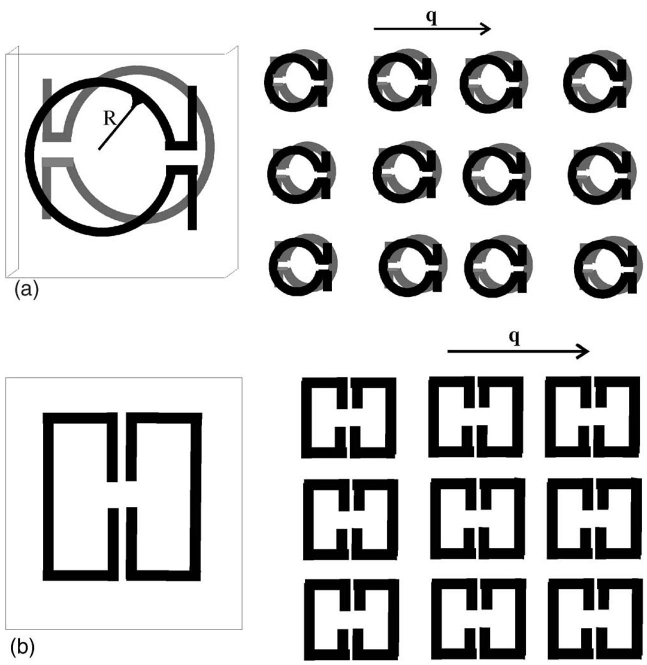

FIG. 3. (a) Lattice of pairs of Ω particles operating at microwaves. (b) Lattice of SRRs operating at infrared suggested by O'Brien and Pendry (Ref. 11).

(if divisible by a). Therefore, one can attribute both sets of material parameters found for finite slabs and even for a monolayer (one unit cell across the slab) to infinite lattices.

IV. EXAMPLES

To illustrate the locality of one set of MPs and the nonlocality of the other one, two numerical examples of a direct calculation of them through the known polarizabilities of particles will be presented. The algorithm of this calculation is as follows:

$$(a_{ee},a_{mm}) \to (G,X) \to \begin{cases} (q,Z_B) \to (\varepsilon_{\rm eff},\mu_{\rm eff}) \\ (q,Z_L) \to (\varepsilon_L,\mu_L). \end{cases} \tag{47}$$

The first arrow implies the use of formula (28); the second one implies the solution of Eq. (27) and the use of formula (36) in the upper case and (45) in the lower case. To find the local MP, formulas (34)–(36) have been used. The first numerical example corresponds to a cubic lattice formed by capacitively loaded wire dipoles. The second example corresponds to a lattice of pairs of Ω particles shown in Fig. 3(a). In the first example, the polarizability of particles is nearly static: $a_{ee} \approx l^2 C_0$, where l is the effective length of a wire dipole and C_0 is the loading capacitance. However, with a

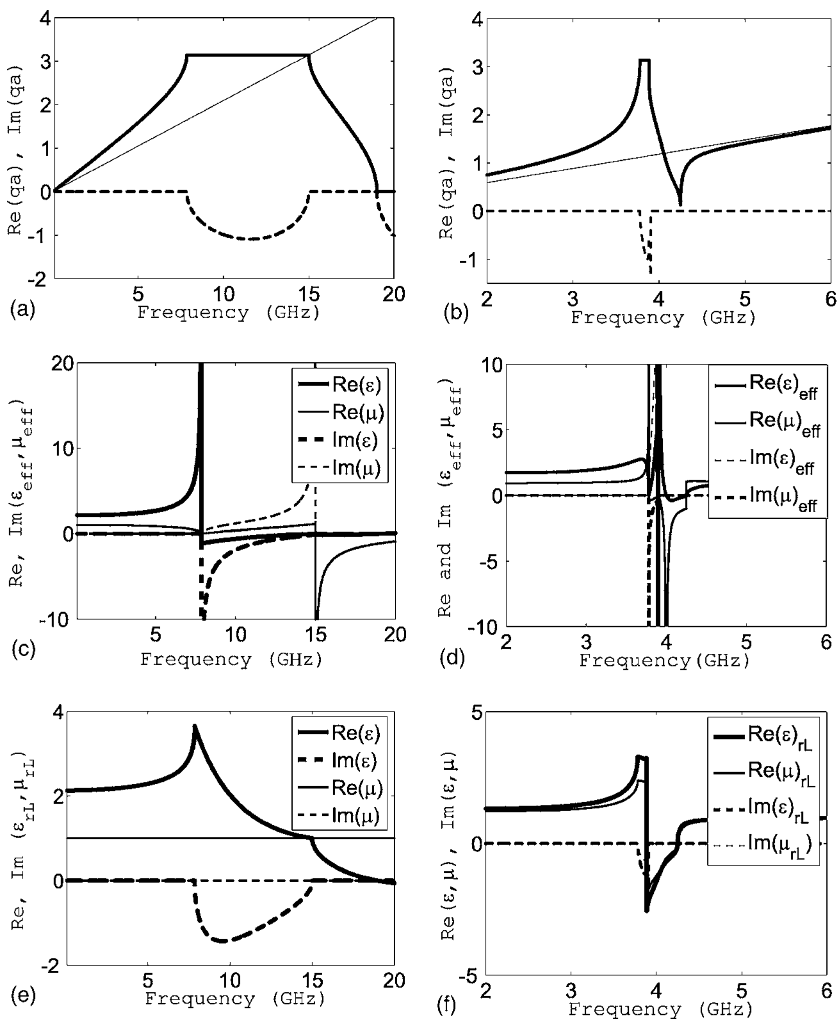

FIG. 4. (a) Dispersion in a lattice of nonresonant dipoles. (b) Dispersion in a lattice of resonant p-m particles (pairs of Ω particles). (c) Nonlocal MP for the lattice of nonresonant dipoles. (d) Nonlocal MP for p-m particles. (e) Local MP for nonresonant dipoles (locality is satisfied up to the spatial resonance of the lattice at 7.5 GHz). (f) Local MP for p-m particles (pairs of Ω particles).

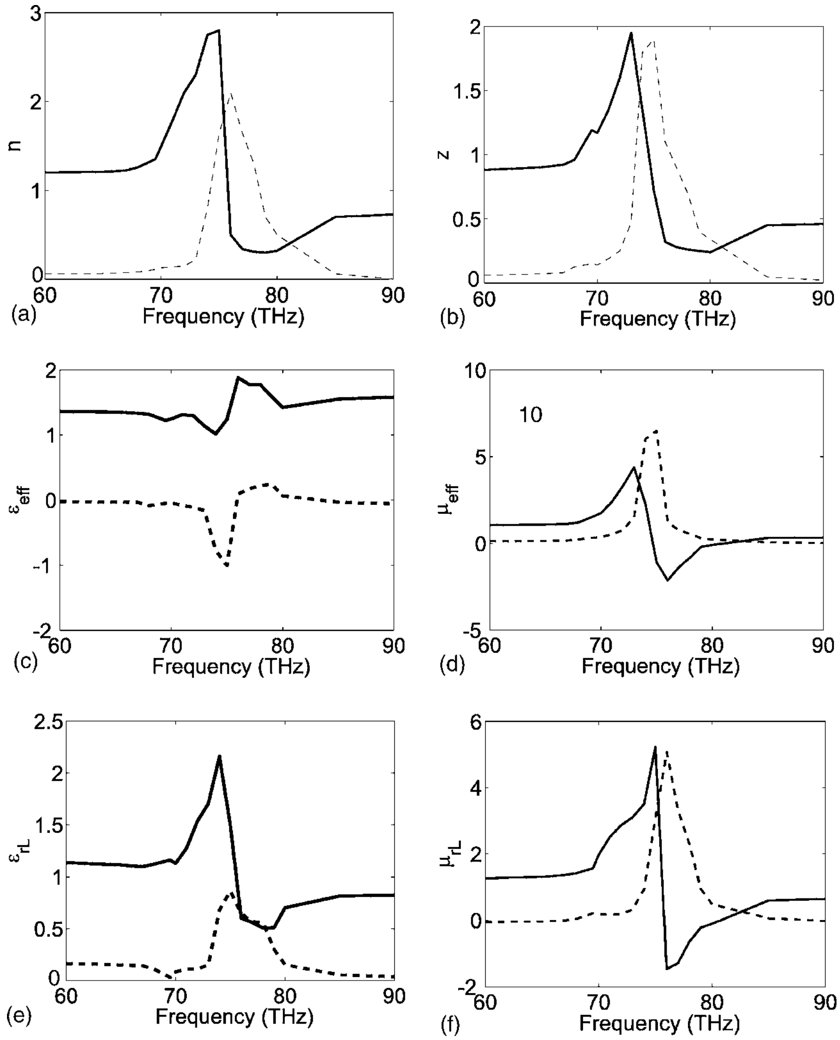

FIG. 5. (a) Refraction index extracted in Ref. 13 from R and T coefficients of a slab comprising the lattice of silver SRRs with period $a=600$ nm. (b) Normalized Bloch impedance extracted in Ref. 13 (c) Nonlocal permittivity extracted for this lattice. (d) Nonlocal permeability. (e) Relative local permittivity. (f) Relative local permeability.

rather large C_0, the effect of the presence of nonresonant dipoles can be significant. This is seen as a wide stop band with a staggered mode near the first lattice resonance [Fig. 4(a)]. Notice that, qualitatively, the same results as shown in Figs. 4(a), 4(c), and 4(e) should correspond also to lattices of metal spheres of radius 2–4 mm which also behave below 15 GHz (the lattice period was chosen to be $a=10$ mm in both examples and the host matrix was a free space) as nonresonant dipoles with rather high static polarizability. A lattice of electric dipoles cannot have local magnetic susceptibility. Correspondingly, the relative local permeability μ_{rL} is an identical unit in Fig. 4(e). The locality conditions are satisfied until the first lattice resonance which occurs at 7.5 GHz. Nonlocal MPs in Fig. 4(c) contain a nontrivial permeability, and imaginary parts of ε_{eff} and μ_{eff} have the opposite signs. Even below 7.5 GHz, we observe in Fig. 4(c) a violation of causality.

In the second example, both electric and magnetic polarizabilities of double Ω particles are resonant. We calculate them using formulas[34]

$$a_{ee}=\frac{A}{\omega_0^2-\omega^2+j\omega\Gamma}, \quad A=\frac{l^2}{L_0}, \tag{48}$$

$$a_{mm}=\frac{B\omega^2}{\omega_0^2-\omega^2+j\omega\Gamma}, \quad B=\frac{\pi^2\mu_0^2R^4}{L_0}, \tag{49}$$

where L_0 is the inductance of metal rings, l is the effective length of the electric dipole induced in the particle, and R is the ring radius shown in Fig. 3. In this example, a single p-m particle resonates at 4 GHz, and the backward-wave regime in the lattice exists within 3.9–4.2 GHz. The loss factor Γ was assumed to be negligibly small in order to avoid complications of complex solutions of Eq. (27). The second example is illustrated by plots in Figs. 4(b), 4(d), and 4(f). The staggered mode exists in the 3.75–3.92 GHz band, in which the local MPs have no physical meaning. However, in the present example, the calculated relative MPs $\varepsilon_{rL}=\varepsilon_L/\varepsilon_0$ and $\mu_{rL}=\mu_L/\mu_0$ in Fig. 4(f) apparently satisfy the locality conditions (up to 12 GHz), whereas the frequency behavior of transmission-line (Bloch) parameters in Fig. 4(d) is nonphysical.

In our third example, we study a structure for which the input data are R and T coefficients of a slab. The slab is filled by a lattice of silver split-ring resonators (SRRs) shown in Fig. 3(b). This structure operating in the infrared range was studied in Refs. 11 and 13. For this case, the algorithm of extracting the local material parameters is as follows:

$$(R,T) \rightarrow (q,Z_B) \rightarrow (\varepsilon_L,\mu_L). \qquad (50)$$

In algorithm (50), the first arrow corresponds to the inversion of formulas (2) and (3). In fact, q and Z_B were already found in Refs. 11 and 13 and one can use the data presented on p. 56 of Ref. 13 for $n=q/k_0$ and Z_B. At the second step of Eq. (50), one can use formulas (44) and (46).

The period a in this case is equal to $a=600$ nm and the time dependence is $\exp(-i\omega t)$, as it is adopted in optics. The input data taken from Ref. 13 are shown in Figs. 5(a) and 5(b), and the results are presented in Fig. 5(c)–5(f). The difference between the results obtained for local and nonlocal material parameters confirms the theory developed in this paper. Parameters extracted by direct inversion of Fresnel formulas (2) and (3) are nonlocal, and parameters obtained using the suggested theory satisfy the locality conditions.

V. CONCLUSION

In this paper, it is demonstrated that local material parameters (MPs) of lattices can be introduced not only at very low frequencies but also in the region of moderately low frequencies where various metamaterials (MTMs) usually operate. These local MPs complement the pair of nonlocal MPs of MTMs which were introduced in earlier papers. Though at moderate frequencies the local MPs allow to solve boundary problems for MTM slabs only at the expense of introducing two transition layers near the slab surfaces, these MPs are very important. Only local material parameters do not depend on the incidence angle, and only they can be used to study the interaction of metamaterial samples with wave packages and evanescent waves. It is then important to learn to extract these parameters from R and T coefficients of composite slabs. The simple algorithm of this extraction is explained in the present paper and is illustrated by numerical examples.

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