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Resonant Negative Refractive Index Metamaterials

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1. Introduction

Negative refractive index (NRI) media are extensively studied nowadays. The interest in these materials keeps on increasing since the year 2000 when a team at the university of California in San Diego (UCSD) published an experimental demonstration of the existence of a material presenting both a negative permittivity and negative permeability (Shelby et al. (2001); Smith, Padilla, Vier, Nemat-Nasser & Schultz (2000)). They also showed that it is necessary to attribute a negative refractive index to such media (Smith & Kroll (2000)). Novel physical phenomena such as the inversion of Doppler's effect, Cerenkov effect and focusing using flat slabs are then predicted based on the theoretical publication V. G. Veselago dating back to 1967 (Veselago (1968)).

Though different terminologies are used for these media (the actual terms are "left handed media", "double negative metamaterial", "negative refractive index metamaterial"), the concept of backward wave propagation (wave with a phase velocity propagating in the opposite direction with respect to the propagation of energy) dates back to at least 1904 (Moroz (n.d.); Tretyakov (2005)). Indeed, H. Lamb has studied this concept for mechanical systems and A. Schuster in the field of electromagnetism. Independently, H. C. Pocklington (Pocklington (1905)) demonstrated theoretically that in a media supporting backward wave propagation, the phase velocity can be directed in the direction of the source, in the inverse direction of the group velocity. Forty years later (in 1944), L. I. Mandelshtam studied the properties of NRI media (Mandel'shtam (1944)) and more than twenty years later, V. G. Veselago published an exhaustive study on NRI media. The interest in these media then decreased up to the year 2000.

The actual revival of interest for these media can certainly be explained published (Smith, Padilla, Vier, Nemat-Nasser & Schultz (2000)). This demonstration has been performed at microwaves by assembling a medium of periodic metallic wires (for negative permittivity) (Pendry et al. (1996)) and a medium of split ring resonators presenting a negative permeability (Pendry et al. (1999)). These media can be assimilated to a crystalline structure of artificial molecules hence the term metamaterial.

Different technological solutions have been proposed to synthesize negative refractive index media, such as the use of backward wave transmission lines (Eleftheriades et al. (2003); Lai et al. (2004)) and photonic crystals in negative phase velocity regime (Gadot et al. (2003); Gralak et al. (2000); Qiu et al. (2003)). The approach to be chosen depends mainly on the

applications and the frequency band of interest. All the approaches have the same aim i.e to synthesize NRI metamaterials for the potential applications and considering the industrial and economic potential of such materials.

The synthesis and study of NRI metamaterials is however difficult because of its heterogeneous characteristics. For an easier study of applications of metamaterials in microwave frequency range, homogenization and macroscopic description of these metamaterials can prove to be very helpful. It can specially allow a higher degree of freedom to overcome the fundamental limitations imposed by natural materials on the performances of microwave devices.

In this chapter, the description of NRI resonant metamaterials in terms of a continuous medium will be analyzed. The electrodynamics of NRI materials will first be described. The effective medium theory as applied to NRI resonant metamaterials as well as the calculation methods will then be detailed. Finally numerical results will be presented together with a thorough analysis and interpretation of the effective parameters calculated with respect to the electrodynamics of negative refractive index materials presented for continuous media.

2. Electrodynamics of negative refractive index materials

2.1 Adequate choice of the sign of the refractive index and wave impedance

For backward wave propagation, an adequate choice of the sign of the refractive index $n(\omega)$ given by (1) is necessary.

$$n(\omega) = \pm \sqrt{\varepsilon(\omega)\mu(\omega)}, \quad (1)$$

where $\varepsilon(\omega)$ and $\mu(\omega)$ represent the effective permittivity and permeability respectively.

2.1.1 Refractive index

The determination of the sign in front of the square root of (1) is done thanks to causal properties which the solutions of wave propagation should respect and energy conservation principles. The choice of this sign allows to define, among other parameters, the direction of the outgoing wave with respect to an interface between a NRI and a conventional material.

To demonstrate that for a material with $(\varepsilon(\omega) < 0, \mu(\omega) < 0)$, the sign of the refractive index should be negative, let us consider a current surface in $x = x_0$ (Smith (2000)). The radiation of this surface current in the medium $(\varepsilon(\omega) < 0, \mu(\omega) < 0)$ is then studied as shown on figure 1.

The wave equation in the medium can be written as fol.:

$$\frac{\partial^2}{\partial x^2} E(x) + k^2 E(x) = -j\omega\mu J_0(z), \quad (2)$$

where $E(x)$ is the electric field component along \hat{x} , $\vec{J}_0 = i_0\delta(x - x_0)\hat{z}$ et $\mu = \mu_0\mu_r$. The solution of this equation is given by:

$$E(x) = \alpha \exp(jk|x - x_0|). \quad (3)$$

To determine α , let us first calculate :

$$\frac{\partial^2 E(x)}{\partial x^2} = -\alpha k^2 \exp(jk|x - x_0|) + 2j\alpha k\delta(x - x_0), \quad (4)$$

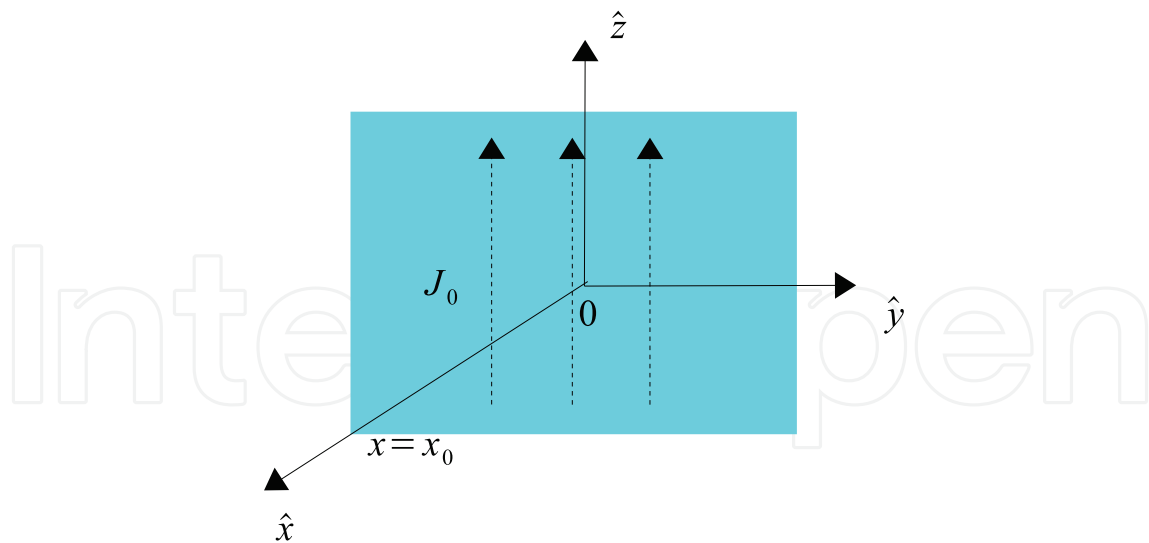


Fig. 1. Surface current J_0 in $x = x_0$ radiating in the medium ($\epsilon(\omega) < 0, \mu(\omega) < 0$). The current distribution is considered uniform and infinite in \hat{y} et \hat{z} .

and substitute the expressions (4) and (3) in equation (2). α is then given by:

$$\alpha = -\frac{\mu\omega i_0}{2k_0 n} = -\frac{i_0 \eta_0 \mu_r}{2n} \quad (5)$$

and the wave equation becomes:

$$E(x) = -\frac{i_0 \eta_0 \mu_r}{2n} \exp(jk|x - x_0|). \quad (6)$$

However, if the power P delivered by the current \vec{J}_0 to the volume V (Balanis (1989)) is calculated, the fol. equation is obtained:

$$P = -\frac{1}{2} \int_V \vec{E} \cdot \vec{J}_0^* dV = \frac{i_0^2 \eta_0 \mu_r}{2n}. \quad (7)$$

This equation represents the work done by the source and it must be positive, which implies that $P > 0$ (Balanis (1989)). The ratio μ_r/n must also be positive. If μ_r is negative, then n must also be negative. An equivalent demonstration can be done for ϵ_r . For a propagative medium, the solution retained for the wave equation verifies backward wave propagation.

To determine the constraints with respect to the sign choice of the imaginary part of the refractive index, let us consider the electric field $\vec{E}(\vec{r}, \omega)$ in a medium with $n = n' - jn''$ for a time dependence in $\exp(j\omega t)$:

$$\vec{E}(\vec{r}, t) = \text{Re} \left[\left| \vec{E}(\vec{r}) \right| \exp(-\vec{k}_0 \cdot \vec{r} n'') \exp[j(\omega t - \vec{k}_0 \cdot \vec{r} n')] \vec{u}_E \right], \quad (8)$$

where \vec{k}_0 is the free space wave vector and \vec{u}_E is the unit vector along the direction of the E-field vector \vec{E} . If a stable propagation is to be ensured, the magnitude of $\text{Re}[\vec{E}(\vec{r}, t)]$ must decrease with time. This implies that the term $\vec{k}_0 \cdot \vec{r} n''$ must be positive and:

$$n'' > 0, \quad (9)$$

irrespective of the sign of n' ¹

2.1.2 Wave impedance

Impedance is a concept generally applied to circuits but is also extended to electromagnetic wave propagation. This extension was developed by Schelkunoff and the analogy between the impedance of a medium for wave propagation and the impedance of a transmission line is fully described in (Stratton (1941)). The physical interpretation of the wave impedance Z given here is based on this analogy.

The complex wave impedance of a medium is strongly related to the flux of energy of the wave propagating in the medium. This is why there are fundamental limitations to the values that Z can admit; one of the limitations is directly linked to the passivity of the medium. These limitations apply to both positive and negative refractive index medium.

The passivity or absence of activity within a medium implies that for a plane progressive electromagnetic wave, the mean energy flux must be directed inside the medium in which the wave propagates (Wohlers (1971)). The directions of the vectors $(\vec{E}, \vec{H}, \vec{k})$ and the energy flux \vec{S} for a plane progressive wave at the interface between a conventional material and an NRI is shown in figure 2.

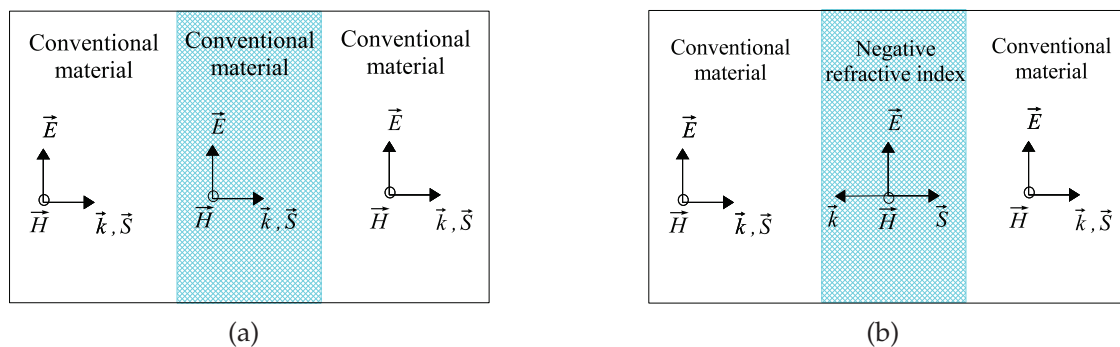


Fig. 2. Direction of the field vectors $(\vec{E}, \vec{H}, \vec{k})$ et \vec{S} for the interaction of a plane wave with at the interface of (a) two conventional material with positive refractive index, and (b) a conventional material and a negative refractive index material.

The wave impedance² is defined as the ration of the electric field to the magnetic field component in the propagation plane; the real part is thus given by:

$$\text{Re}[Z(\omega)] = \text{Re} \left[\frac{\vec{E}(\omega)}{\vec{H}(\omega)} \right] = \frac{|\vec{E}(\omega)|}{|\vec{H}(\omega)|} \cos(\varphi_H - \varphi_E), \quad (10)$$

where $\vec{E}(\omega) = |\vec{E}(\omega)| \exp(-j\varphi_E)$ et $\vec{H}(\omega) = |\vec{H}(\omega)| \exp(-j\varphi_H)$. Equation (10) is verified for both positive and negative refractive indexes. The sign of $\text{Re}[Z(\omega)]$ depends only on the term $\cos(\varphi_H - \varphi_E)$.

¹ It can be shown that for the convention $\exp(-j\omega t)$, n'' is positive also but in this case n should be written as $n = n' + jn''$. This is quite similar for the wave impedance, the permittivity and permeability.

² The wave impedance is generally defined for a *single* plane wave and in the case of a guided or periodic structure, monomodal wave propagation is assumed and an impedance is assigned to each mode.

The mean of Poynting's vector \vec{S}_{av} is calculated, :

$$\vec{S}_{av}(\vec{r}, \omega) = \frac{1}{2} \text{Re}[\vec{E}(\vec{r}, \omega) \times \vec{H}^*(\vec{r}, \omega)] = \frac{1}{2} \left| \vec{E}(\vec{r}, \omega) \right| \left| \vec{H}(\vec{r}, \omega) \right| \cos(\varphi_H - \varphi_E) \vec{u}_S, \quad (11)$$

where $\vec{E}(\vec{r}, \omega) = \left| \vec{E}(\vec{r}, \omega) \right| \exp(-j\varphi_E)$, $\vec{H}(\vec{r}, \omega) = \left| \vec{H}(\vec{r}, \omega) \right| \exp(-j\varphi_H)$ and \vec{u}_S is the unit vector of $\vec{S}_{av}(\vec{r})$.

Knowing that passivity of a medium implies that the energy flux must be directed inside the medium implies that $\vec{S}_{av}(\vec{r}, \omega) > 0$. The term $\cos(\varphi_H - \varphi_E)$ is thus always positive for all medium irrespective of the sign of their refractive index (as it can be verified on figure 2). If we apply this restriction to equation (10), the fol. condition is obtained:

$$\text{Re}[Z(\omega)] > 0, \quad (12)$$

for both conventional and NRI materials³.

There is no particular sign restriction on the imaginary part of the wave impedance. The complex wave impedance provides information non only on wave propagation (as described above) but it also allows physical understanding when there is no wave propagation in a medium (*i.e.* when its imaginary part is much higher than its real part) as to which field component (\vec{E} or \vec{H} fields) is canceled. This information is indeed interesting for the design of artificial magnetic medium such as those based on split-ring resonators. Indeed, if the imaginary part of Z is negative, the medium can be said to be capacitive and there is no wave propagation because of H-field filtering. The response of the medium to an applied magnetic field is thus non-negligible and it can be considered as an artificial magnetic medium.

2.2 Adequate choice of the sign of the effective permittivity and permeability

There are fundamental restrictions limiting the signs that the imaginary part of $\varepsilon(\omega)$ et $\mu(\omega)$ can admit for linear, passive, isotropic homogeneous medium. For conventional material, these restrictions are derived from fundamental theorems of macroscopic electrodynamics (Depine & Lakhtakia (2004); Efron (2004)) and it has been demonstrated in various ways, namely by Callen *et al.* thanks to the fluctuation-dissipation theorems (Callen & Welton (1951)) for arbitrary linear and dissipative systems, and by Landau *et al.* (Landau et al. (1984)) for electromagnetic waves. Based on this last demonstration, we propose to demonstrate the extension of these limitations for NRI materials.

Let us consider a passive, linear, homogeneous, isotropic and dispersive medium of permittivity $\varepsilon(\omega) = \varepsilon'(\omega) - j\varepsilon''(\omega)$ and permeability $\mu(\omega) = \mu'(\omega) - j\mu''(\omega)$. The Poynting vector $\vec{S}(\vec{r}, t)$ provides the definition of the power flux density in a medium with variable fields. It can be written in time-domain for dispersive medium as:

$$\vec{S}(\vec{r}, t) = \vec{E}(\vec{r}, t) \times \vec{H}(\vec{r}, t) \quad (13)$$

Using Maxwell-Faraday et Maxwell-Ampere equations in the absence of sources,

$$\nabla \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t} \vec{B}(\vec{r}, t), \quad (14)$$

³ This restriction is identical in both conventions $\exp(-j\omega t)$ and $\exp(j\omega t)$

and

$$\nabla \times \vec{H}(\vec{r}, t) = \frac{\partial}{\partial t} \vec{D}(\vec{r}, t), \quad (15)$$

the divergence of Poynting vector is given as:

$$-\nabla \cdot \vec{S}(\vec{r}, t) = \vec{E}(\vec{r}, t) \cdot \frac{\partial}{\partial t} \vec{D}(\vec{r}, t) + \vec{H}(\vec{r}, t) \cdot \frac{\partial}{\partial t} \vec{B}(\vec{r}, t). \quad (16)$$

This equation provides an expression of the energy conservation in a dispersive material in time-domain (Balanis (1989)). In frequency domain, the electric and magnetic fields are given, after Fourier transform, by:

$$\vec{E}(\vec{r}, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \vec{E}(\vec{r}, \omega) \exp(j\omega t) d\omega, \quad (17)$$

$$\frac{\partial}{\partial t} \vec{D}(\vec{r}, t) = \frac{j}{2\pi} \int_{-\infty}^{\infty} \omega \varepsilon(\omega) \vec{E}(\vec{r}, \omega) \exp(j\omega t) d\omega. \quad (18)$$

For equation (18), we assume an isotropic material with $\vec{D}(\vec{r}, \omega) = \varepsilon(\omega) \vec{E}(\vec{r}, \omega)$. Integration of the product of Eq. (17) and Eq. (18) with respect to time gives:

$$\int_{-\infty}^{\infty} \vec{E}(\vec{r}, t) \cdot \frac{\partial}{\partial t} \vec{D}(\vec{r}, t) dt = \frac{j}{4\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \omega \varepsilon(\omega) \vec{E}(\vec{r}, \omega) \vec{E}(\vec{r}, \omega') \exp(j(\omega + \omega')t) d\omega d\omega' dt. \quad (19)$$

A first integration with respect to t of the right-hand side of Eq. (19) is done using

$$\int_{-\infty}^{\infty} \exp(j(\omega + \omega')t) dt = 2\pi \delta(\omega + \omega').$$

The Dirac distribution is then eliminated by the second integration with respect to ω' . The principle of causality and reality of fields impose (Good & Nelson (1971)):

$$\vec{E}(\vec{r}, -\omega) = \vec{E}(\vec{r}, \omega)^*,$$

The right-hand side of the equation (19) can finally be written as:

$$\frac{j}{2\pi} \int_{-\infty}^{\infty} \omega \varepsilon(\omega) \left| \vec{E}(\vec{r}, \omega) \right|^2 d\omega. \quad (20)$$

After application of the same procedure for magnetic fields \vec{H} , we obtain:

$$\int_{-\infty}^{\infty} \vec{H}(\vec{r}, t) \cdot \frac{\partial}{\partial t} \vec{B}(\vec{r}, t) dt = \frac{j}{2\pi} \int_{-\infty}^{\infty} \omega \mu(\omega) \left| \vec{H}(\vec{r}, \omega) \right|^2 d\omega. \quad (21)$$

Then substituting $\varepsilon(\omega)$ et $\mu(\omega)$ by their complex expression, the energy dissipated (in the period of field variations) in frequency domain is:

$$\int_{-\infty}^{\infty} Q dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} \omega \left(\varepsilon''(\omega) \left| \vec{E}(\vec{r}, \omega) \right|^2 + \mu''(\omega) \left| \vec{H}(\vec{r}, \omega) \right|^2 \right) d\omega. \quad (22)$$

The divergence of Poynting vector is expressed as the rate of energy transformation to heat: this dissipated energy depends on $\varepsilon''(\omega)$ et $\mu''(\omega)$. The dependence on $\varepsilon'(\omega)$ et $\mu'(\omega)$ is

canceled because the integrand of equation (20) is an odd function of ω ⁴. The two terms of the right-hand side of Eq. (22) represent respectively the dielectric and magnetic losses.

The second law of thermodynamics, stating that the entropy of a isolated macroscopic system never decreases, imposes that $Q > 0$. It is thus necessary according to equation (22) that:

$$\varepsilon''(\omega) \left| \vec{E}(\vec{r}, \omega) \right|^2 + \mu''(\omega) \left| \vec{H}(\vec{r}, \omega) \right|^2 > 0 \quad (23)$$

for positive frequencies ($\omega > 0$). The laws of Thermodynamics also express the irreversible nature of physical processes and the fundamental difference between two types of energy: work and heat (Yavorski & Detlaf (1975)). The energy dissipated by fields into heat is irreversible. In other terms, there can be no exchange between the work done by either the electric field [$\vec{E}(\vec{r}, \omega)$ or magnetic field $\vec{H}(\vec{r}, \omega)$] and the heat dissipated by the other, implying:

$$\varepsilon(\omega)'' > 0 \quad \text{and} \quad \mu(\omega)'' > 0 \quad (24)$$

This demonstration can be very easily extended to NRI materials. Indeed, the starting point of the demonstration is energy conservation through the expression of the divergence of Poynting vector [Eq. (16)] written thanks to Maxwell-Ampère [Eq. (15)] and Maxwell-Faraday [Eq. (14)] equations as well Poynting theorem [Eq. (13)]. For a NRI material, these equations and theorems are valid (Veselago (1968)). Indeed, only the direction of the vector \vec{k} changes in a NRI material thus giving a negative value for the product $\vec{S} \cdot \vec{k}$ (This product is positive for conventional materials). This is easily verified for a monochromatic wave but can actually also be verified for non-monochromatic wave.

Let us consider for instance, the mean of Poynting vector for a dispersive material excited by the superposition of two monochromatic waves of angular frequency ω_1 et ω_2 such that $\omega_1 \neq \omega_2$ (Pacheco-Jr et al. (2002)):

$$\langle \vec{S}(\vec{r}, t) \rangle = \frac{|E|^2}{2} \left(\frac{\vec{k}(\omega_1)}{\omega_1 \mu(\omega_1)} + \frac{\vec{k}(\omega_2)}{\omega_2 \mu(\omega_2)} \right) \quad (25)$$

The relation between the direction of Poynting vector \vec{S} and that of the wave vector \vec{k} is clearly shown by this equation. The direction of \vec{S} is independent of the sign of the refractive index and for any propagative medium, *i.e.* when \vec{k} is real, the ratio k/μ is positive. As shown before, if k takes negative values, then μ will be negative too.

3. Effective parameters of resonant NRI metamaterials

3.1 Effective medium theory as applied to metamaterials

The concept of effective medium for the description of heterogeneous systems by a homogeneous one is very attractive in different field of physics. Homogenization procedures allowing the definition of an effective macroscopic response from physical parameters characterizing the heterogeneous system are generally developed. In our case, from the microscopic parameters (geometrical and physical definitions) of the metamaterial, a macroscopic electromagnetic response can be obtained. If this macroscopic definition

⁴ Principle of causality imposes that (Good & Nelson (1971)): $\varepsilon(-\omega) = \varepsilon(\omega)^*$ and $\mu(-\omega) = \mu(\omega)^*$.

is performed in accordance with the electrodynamics of continuous medium, they can afterwards be used in Maxwell's equations to predict propagation phenomena and provide physical insight into the design of metamaterial-based microwave and optical devices.

In this chapter, the NRI metamaterials considered are assumed periodic and based on resonant inclusions such as the combination of Split Ring Resonator and wire medium. The general definition of the relevant dimensions for the definition of the effective parameters of such periodic medium is depicted on figure 3 (Baker-Jarvis, Janezic, Riddle, Johnk, Kabos, Holloway, Geyer & Grosvenor (2004)).

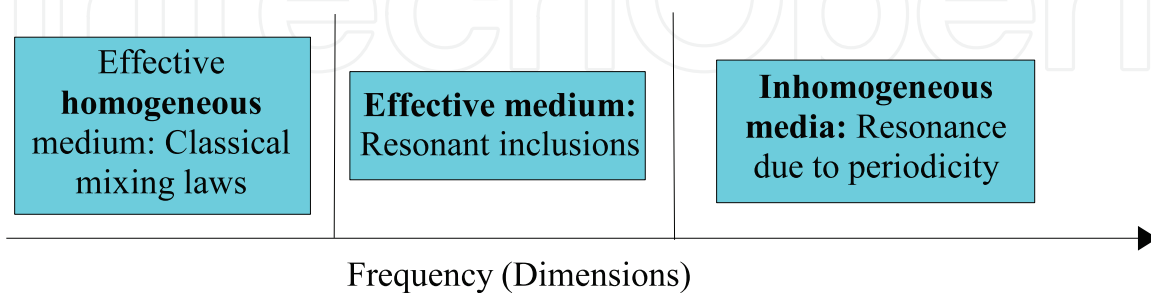


Fig. 3. Dimensions for effective medium of resonant periodic metamaterial.

The left-hand side region represents the quasi-static region where the wavelength is much bigger than the periodicity of the inclusions. The effective parameters of the composite in this zone can be easily calculated using quasi-static solutions or classical mixing rules (Berthier (1993)).

In the right-hand side region, the composite is heterogeneous and the resonances of the medium can be directly linked to the periodicity. Such a composite cannot be considered homogeneous. To study the propagation characteristics of these media, full-wave numerical methods are generally required. The volume under study has to be discretized: a unit-cell is defined and Floquet-Bloch boundary conditions are used. This case is typically the working regime of photonic crystals.

The intermediate region is a region where the inclusions are resonant. The electrical dimensions of the inclusions as well as the periodicity are small compared to the wavelength. Resonant NRI metamaterials belong to this intermediate region. Such a medium is generally considered homogeneous. However, the question which remains to be answered is: how should one study the characteristics of such a medium and how should the associated effective medium be defined?

There is indeed no simple or unique definition to the effective medium concept. The possible approach and definition which will be used in this chapter for NRI metamaterials will be described hereafter.

3.2 Definition of the effective medium concept for composites of the intermediate region

When an EM field is applied to a composite, the fields in the composite result from the interaction between the applied field and the reaction of the inclusions constituting the composite (Baker-Jarvis, Janezic, Riddle, Johnk, Kabos, Holloway, Geyer & Grosvenor (2004); Baker-Jarvis, Kabos & Holloway (2004)). The local field in the composite can be freely propagative, propagative with attenuation or evanescent. The resulting local field is a complicated physical process whereby the applied field polarizes the inclusions which in turn

polarize the neighboring inclusions. The group of inclusions then react by creating a modified local field. The presence of inclusions (or perturbations) in a given environment can make an initially evanescent field propagative (de Fornel (1997)). A common example is the insertion of inclusions in a guide under the cut-off frequency. All these complex interactions are visible at the microscopic or local scale. However, the field in a material as expressed in Maxwell's equations is the macroscopic field, usually defined by constitutive equations.

The definition of constitutive parameters require the determination of a relationship between the local field, the applied field and the macroscopic field. the theory of local field of Lorentz (Berthier (1993); Tretyakov (2003)) can be used but it is not always adequate (Baker-Jarvis, Janezic, Riddle, Johnk, Kabos, Holloway, Geyer & Grosvenor (2004); Baker-Jarvis, Kabos & Holloway (2004)). It has been however applied to certain types of composites. The polarizabilities are calculated analytically and the theory of Lorentz then provides the macroscopic parameters. Numerous examples of such calculations are given in (Tretyakov (2003)) and the papers there cited there. Other methods have also been used in the literature such as those introduced by O. Keller et J. Baker-Jarvis (Baker-Jarvis, Kabos & Holloway (2004); Keller (1996)) but they rely on statistical and quantum approaches. The discussion will be restricted to the context of *classical* electrodynamics.

The definition of effective medium can be mainly performed in two distinct categories of approaches. The first category can be termed *locale* (§ 3.3) and the second one *global* (§ 3.4). In the first case, the effective parameters are defined directly from local fields while the second one allows a definition based on global propagation characteristics of the periodic system, for instance from the model of scattering parameters.

3.3 Local approaches

When they are not based on analytical approaches, the input data are the fields or electric and magnetic induction calculated using full-wave numerical methods. The definition of effective parameters from local fields is not straightforward. Three methodologies can be distinguished. The first one consists in defining an equivalence between the local field calculated and the effective parameters of a corresponding homogeneous medium (Pincemin (1995); Silveirinha & Fernandes (2004a;b; 2005a;b)). The second methodology consists in the calculation of the propagation constant from the phase velocity locally determined using time-domain numerical modeling methods (Moss et al. (2002)). Finally, the third methodology consists in the definition of effective parameters by calculation a linear, surface-based or volume-based mean field values on adequately chosen geometries. Several methods are available in the literature (Acher et al. (2000); Bardi et al. (2002); Lerat et al. (2005); Lubkowski et al. (2005); Pendry et al. (1999); Smith (2005); Smith, Vier, Kroll & Schultz (2000); Weiland et al. (2001)). In the method given by Acher *et al.* (Acher et al. (2000)), it is worth noting that a convergence is demonstrated between effective parameters calculated using this type of numerical approach and those obtained by the Bruggeman extended theory of effective medium (taking into account magnetic polarizability) for the asymptotic case of metal-dielectric slab.

3.4 Global approaches

Global approaches provide effective parameters starting from global responses of the periodic system. These responses such as the scattering matrix, the reflection and transmissions

coefficients, resonant frequencies are observable or measurable quantities which can be either experimentally determined or numerically calculated from fields defined locally in the unit cell of the periodic NRI metamaterial.

The transformation of the local field to the scattering matrix relies on an analogy between propagation in a periodic structure and in waveguides and circuits. It consists in assimilating the periodic structure in a multiple-access system and to study transmission and reflection between the different accesses. The development of such an analogy requires a few assumptions (Hélier (2001); Richalot (1998); Rivier & Sardos (1982)), namely:

- linearity: the vectors \vec{E} et \vec{D} , \vec{B} et \vec{H} are linked to one another by linear relationships,
- stationarity: the properties of the system are invariant with respect to time,
- absence of radiation: the system is closed and energy exchange can only exist between the system accesses,
- existence of pure mode: each access of the system supports a pure mode, i.e. a unique propagation mode characterized by a given propagation constant. If this assumption is not verified, then sufficient supplementary virtual accesses have to be defined to account for higher propagation modes.

Figure 4 depicts an example of a system with three physical accesses modeled using the generalized scattering matrix method described before. Each physical access is artificially decomposed in N virtual accesses, where N represent the number of modes to be taken into account at each physical access.

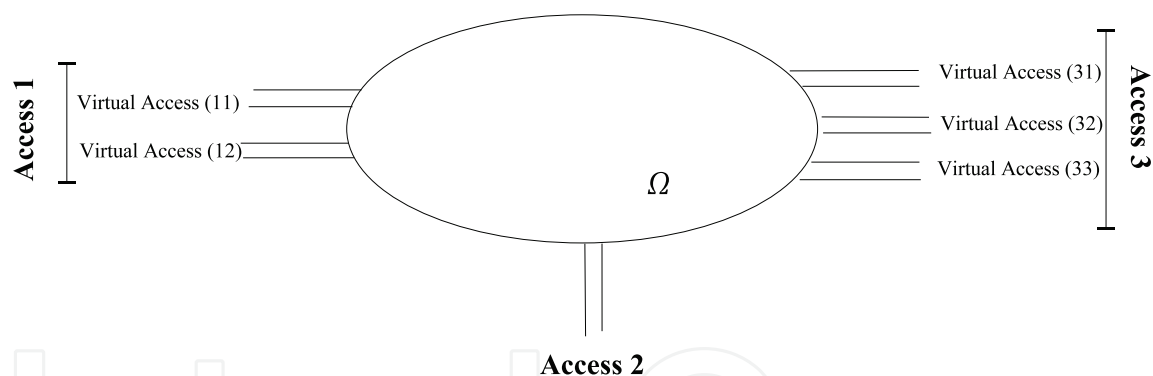


Fig. 4. Example of a system with three physical accesses modeled by a system of N virtual accesses to take into account the number of modes present or excited at each physical access.

Such a scattering matrix allows the complete characterization of the structure both in emitting and receiving modes both in near and far fields. The reflection and transmission matrices can thus be directly determined from this matrix followed by the effective parameters; this procedure is further detailed hereafter.

3.5 Calculation of effective parameters of resonant metamaterials

The calculation method described here belongs to the category of global approaches as defined in section (3.4) and can be divided in two parts, namely for NRI metamaterials structures finite and infinite in the direction of propagation.

3.5.1 NRI metamaterials finite in the propagation direction

For NRI metamaterials finite in the direction of wave propagation, the problem to be solved is the substitution of this periodic structure by a homogeneous slab of same thickness as shown in figure 5.

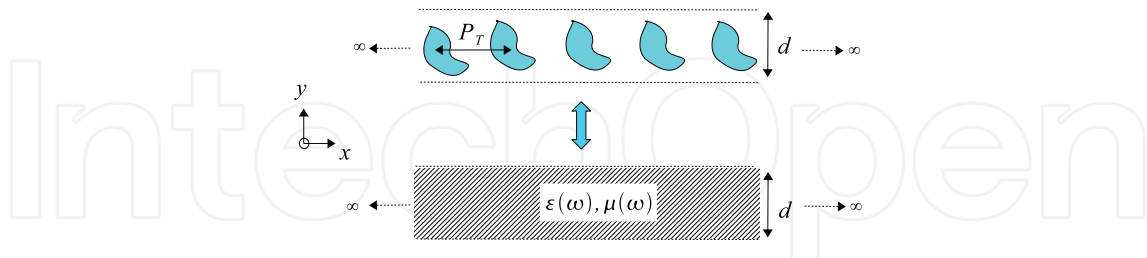


Fig. 5. Equivalence between a periodic composite of transverse periodicity P_T by a homogeneous slab of same thickness d , effective permittivity $\varepsilon(\omega)$ and permeability $\mu(\omega)$.

This substitution or equivalence is only valid under a few assumptions (Lalanne & Hutley (2003); Lalanne & Lalanne (1996)): (i) Only the first mode propagates in the incident medium, transmitted medium and the periodic structure. This condition is given by the fol. equation:

$$|\beta| \leq \frac{\pi}{P_T}. \quad (26)$$

β is the propagation constant in each medium. (ii) Evanescent modes should not be present in the xOy plane. If only the first mode can propagate in the periodic structure with a speed of $c_0/n(\omega)$ where $n(\omega)$ the interference phenomenon is identical to the one which occurs in a homogeneous slab. However, the existence of higher order modes give a much more complex interference phenomenon such that the equivalence with a homogeneous slab is no longer valid.

In the case of a metal-dielectric composite, these equivalence conditions are not automatically satisfied. Indeed, the existing propagation modes and their associated propagation constants depend highly on the nature of the inclusions: their geometry, size and distribution.

The calculation of effective parameters of NRI metamaterials under these assumptions is done in two steps. The first one consists in the determination of the complex reflection and transmission coefficients which can be numerically calculated according to the generalized scattering parameters described in section 3.4. They can also be obtained by experimentally. The second step is then the calculation of the effective permittivity and permeability ($\varepsilon(\omega), \mu(\omega)$) from these reflection and transmission using inversion methods. These methods can either be direct using analytical inversion of Fresnel equations, $(r, t) = f(\varepsilon(\omega), \mu(\omega))$ or performed by an iterative approach. Both approaches are described here.

3.5.1.1 Direct method - Nicholson Ross Weir (NRW) approach

In the NRW method, the wave impedance and refractive index are first calculated. The effective permittivity and permeability are then deduced. The normalized wave impedance of a slab can be described by analogy as the input impedance of a transmission line thus containing information not only on \vec{E}/\vec{H} at the interface of two lines or medium but also of the propagation constant inside the propagating medium. Z is given by:

$$Z = \pm \sqrt{\frac{(1+r)^2 - t^2 e^{-2jk_0 d}}{(1-r)^2 - t^2 e^{-2jk_0 d}'}} \quad (27)$$

where d is the slab thickness, $k_0 = 2\pi/\lambda_0$ is the wave number λ_0 the free-space wavelength. The choice of the sign in front of the square root of Z is done according to the definitions given in section 2.1.

The real part of the refractive index n is given by equation (28):

$$n' = \frac{\arctan(Im(Y)/Re(Y)) \pm m\pi}{k_0 d}, \quad (28)$$

where $m \in \mathbb{Z}$. The variable Y is defined as:

$$Y = e^{-jnk_0 d} = X \pm \sqrt{X^2 - 1}, \quad (29)$$

where

$$X = \frac{e^{jk_0 d}}{2t} (1 - r^2 + t^2 e^{-2jk_0 d}). \quad (30)$$

The choice of the value of m in equation (28) constitute one of the ambiguities of this method which can be solved in different ways, namely (i) by considering various thicknesses and assuming that there is no coupling between different layers of metamaterials in the direction of propagation (Markos & Soukoulis (2001)), (ii) by comparing the measured group arrival time to the calculated one (Baker-Jarvis, Janezic, Riddle, Johnk, Kabos, Holloway, Geyer & Grosvenor (2004)).

The imaginary part of the refractive index n'' is given by:

$$n'' = \frac{\ln|Y|}{k_0 d} \quad (31)$$

n'' is calculated using the fundamental limitation described in 2.1, i.e. $n'' > 0$ for both positive or negative refractive index materials.

Using the two independent equations (32 and 33) the effective permittivity and permeability can be deduced.

$$n = \sqrt{\varepsilon(\omega)}\sqrt{\mu(\omega)} \quad \text{and} \quad Z = \sqrt{\mu(\omega)/\varepsilon(\omega)} \quad (32)$$

$$\varepsilon(\omega) = \frac{n}{Z} \quad \text{and} \quad \mu(\omega) = nZ \quad (33)$$

It should be noted that the refractive index is defined as: $n = \sqrt{\varepsilon_{eff}}\sqrt{\mu_{eff}}$ such that when $\varepsilon(\omega)$ and $\mu(\omega)$ are simultaneously negative, the real part of n is also negative. The common formula $n = \sqrt{\varepsilon_{eff}\mu_{eff}}$ should not be used.

3.5.1.2 Iterative method - Optimization approach

This method consists in the minimization of the difference between the functions $F_1(x)$, $F_2(x)$ and the scattering parameters S_{11} et S_{21} according to the fol. cost function:

$$E(x) = |F_1(x) - S_{11}|^2 + |F_2(x) - S_{21}|^2 \quad \text{with} \quad x = \{\varepsilon(\omega), \mu(\omega)\} \quad (34)$$

The functions $F_1(x)$ et $F_2(x)$ are complex and represent respectively the Fresnel reflection and transmission coefficients defined for a magneto-dielectric slab of thickness d and of infinite

transverse dimensions. For a plane wave having an incident angle of θ_i and a polarization *TE* or *TM*, the reflection coefficient r and transmission t are defined by:

$$r = \frac{A - B}{A + B} \quad \text{et} \quad t = \frac{2A}{A + B}, \quad (35)$$

$$\text{avec} \quad A = \cos qd + \frac{j \sin qd}{Z_0}, \quad B = Z_0 \left(\frac{j \sin qd}{Z} + \frac{\cos qd}{Z_0} \right)$$

$$\text{et} \quad q = k_0 \sqrt{1 - \left(\frac{1}{n} \sin \theta_i \right)^2}.$$

For the TE polarization,

$$Z = \frac{\omega \mu_{eff}}{q} \quad \text{and} \quad Z_0 = \frac{\cos \theta_i}{\epsilon_0 c_0}. \quad (36)$$

For TM polarization,

$$Z = \frac{q}{\omega \epsilon_{eff}} \quad \text{and} \quad Z_0 = \frac{\mu_0 c_0}{\cos \theta_i}. \quad (37)$$

In our case, the functions $F_1(x)$ and $F_2(x)$ of the equation (34) are replaced by r et t equation (35). The cost function (34) is minimized using the non-linear mean square algorithm of Levenberg-Marquardt. To ensure good results, this algorithm needs to start from a feasible point. This is why a large choice of values for the couple $(\epsilon(\omega), \mu(\omega))$ is done for the starting point in frequency. Then if the frequency sampling from the numerical simulations is fine enough and the functions considered to be continuous, the starting point chosen is the one for the previous frequency point.

For a few composites, the algorithm can converge to many solutions for large values of the thickness of the slab. These solutions are not local minima but are solutions to Fresnel equations. To choose the right solutions, two physical criteria have been defined:

- If the scattering parameter S_{21} is close to 1, the structure is propagative. The refractive index, being a parameter representative of propagation⁵, its imaginary part must be close to zero,
- If S_{11} is close to one, there is no propagation in the structure ; the real part of the refractive index must be close to zero.

These criteria are particularly appropriate for NRI resonant metamaterials and may not be adequate for all type of composites. The principal limitation is that the starting point must be far from resonance and the composite should not present high dissipative losses.

3.5.2 Periodic structure infinite in the propagation direction

If the EM wave propagation is considered in a periodic medium such as the one presented on figure 6(a), the solution of the wave equation provides solution for the propagation constant which are given by $k_n = k + 2m\pi/P$ where $m \in \mathbb{Z}$ and $P = P_L$ or P_T .

⁵ The imaginary part of the refractive index does not allow to calculate losses by dissipation of a medium (Landau et al. (1984)). It can only represent the presence or absence of propagation in a medium.

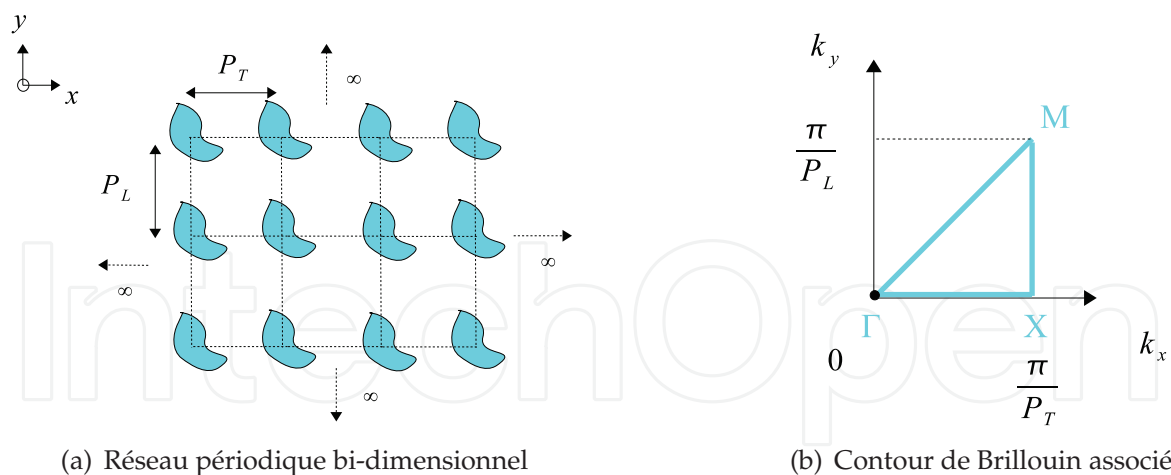


Fig. 6. Réseau périodique bi-dimensionnel et zone irréductible de Brillouin associée.

Because the structure is periodic, the analysis of the propagation in only a unit cell of the constant k is enough : the fundamental analysis domain is defined for $-\pi < kP < \pi$. This fundamental domain consists sufficient information for defining propagation inside the whole structure. Figure 6(b) shows the irreducible Brillouin zone associated to the periodic structure for $P_T = P_L$. This Brillouin zone can be briefly described in terms of the propagation constants (k_x, k_y) in the following way:

1. the ΓX contour corresponds to propagation constants $k_y P = 0$ et $k_x P \in [0; \pi]$. for this contour, only normal incidence is considered.
2. the XM contour corresponds to propagation constants $k_x P = \pi$ et $k_y P \in [0; \pi]$. The incidence angles vary from 0° to 45° .
3. the $M\Gamma$ contour corresponds to propagation constants $k_x P$ et $k_y P \in [0; \pi]$. The only incidence angle considered is 45° .

To calculate the two dimensional dispersion diagram of an arbitrary periodic NRI resonant metamaterial, a source-free eigenmode solver of a numerical modeling tool such as Ansoft HFSS (HFSS (2004)) can be used. The calculation volume is sampled by finite elements in the case of the software HFSS and for specific periodic boundary conditions, the eigenvalues of the "periodic cavity" are searched. A couple of propagation constants (k_x, k_y) belonging to the Brillouin zone is imposed as boundary condition and the eigenfrequency is calculated such that the source-free Maxwell equations with the boundary conditions are satisfied. The calculation of each eigenfrequency is performed in an iterative manner (Chang (2005)). To ensure reasonable calculation time, it is thus necessary to impose two parameters which are the lowest eigenfrequency to be calculated and a limited number of eigen frequencies.

4. Numerical results and interpretation of effective parameters of resonant NRI metamaterials

The first unit cell (figure 7a) considered here as resonant NRI metamaterials is based on the metamaterial edge-side coupled split-ring resonators (EC-SRR) proposed in (Gregor et al. (2003)) because the dissipative losses presented by these metamaterials are relatively low. The second NRI metamaterial unit cell considered are based on broad-side coupled

NRI metamaterials (figure 7b) proposed in (Seetharamdoo et al. (2004)) for the reduced bianisotropic properties they present.



Fig. 7. Unit cell of NRI resonant metamaterials constituted of BC-SRR and EC-SRR and metallic lines. These inclusions are printed on the dielectric teflon substrates ($\epsilon = 2.2$, $\tan \delta = 9 \times 10^{-4}$). The periodicities $P_H=4.5$ mm, $P_T=3.3$ mm, and $d=3.3$ mm.

The unit cell are simulated using Ansoft HFSS and the reflection and transmission coefficients are shown figure 8. A resonance can be observed where the metamaterials are transparent to

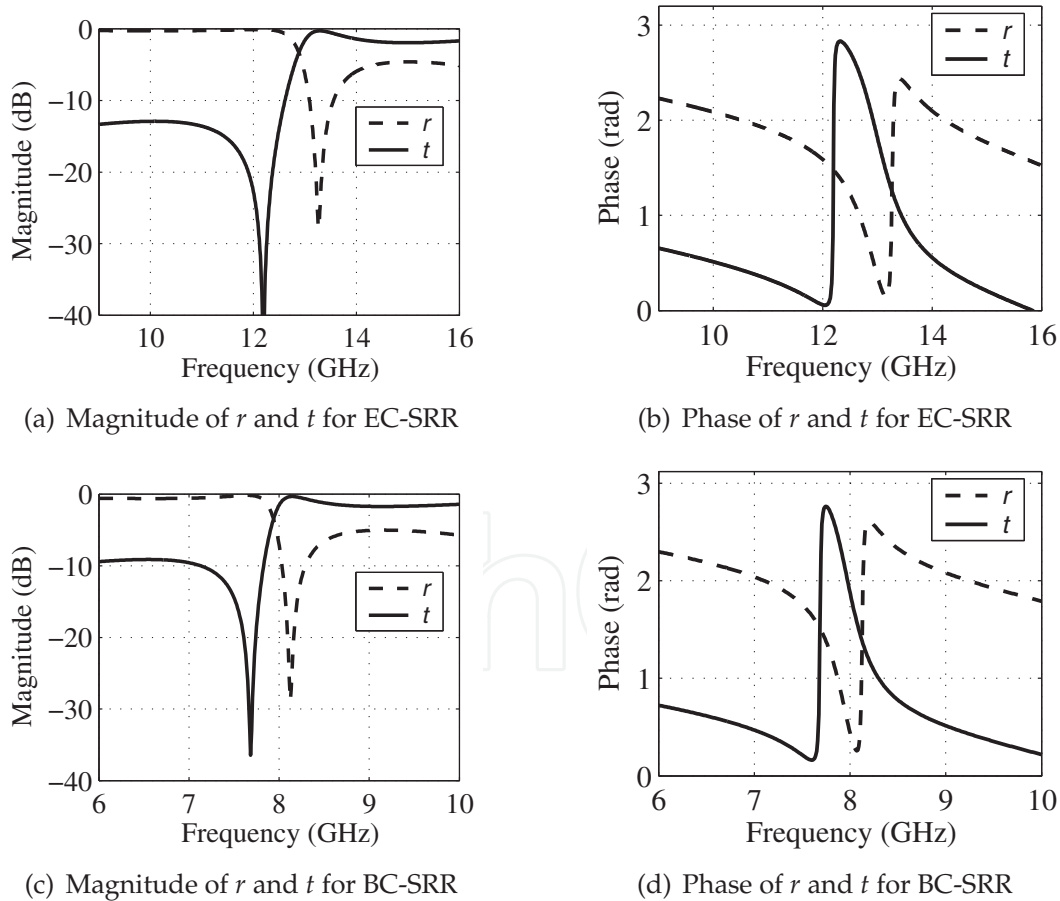


Fig. 8. Reflection and Transmission coefficients of metamaterials constituted of BC-SRR et EC-SRR

the incident wave at the frequencies of 12.3 GHz for the EC-SRR and 8.1 GHz for the BC-SRR respectively.

4.1 Effective parameters calculated by inversion methods

The effective parameters are then calculated by inversion methods presented in the previous section and the refractive index, wave impedance and permittivity and permeability are shown on figure 9.

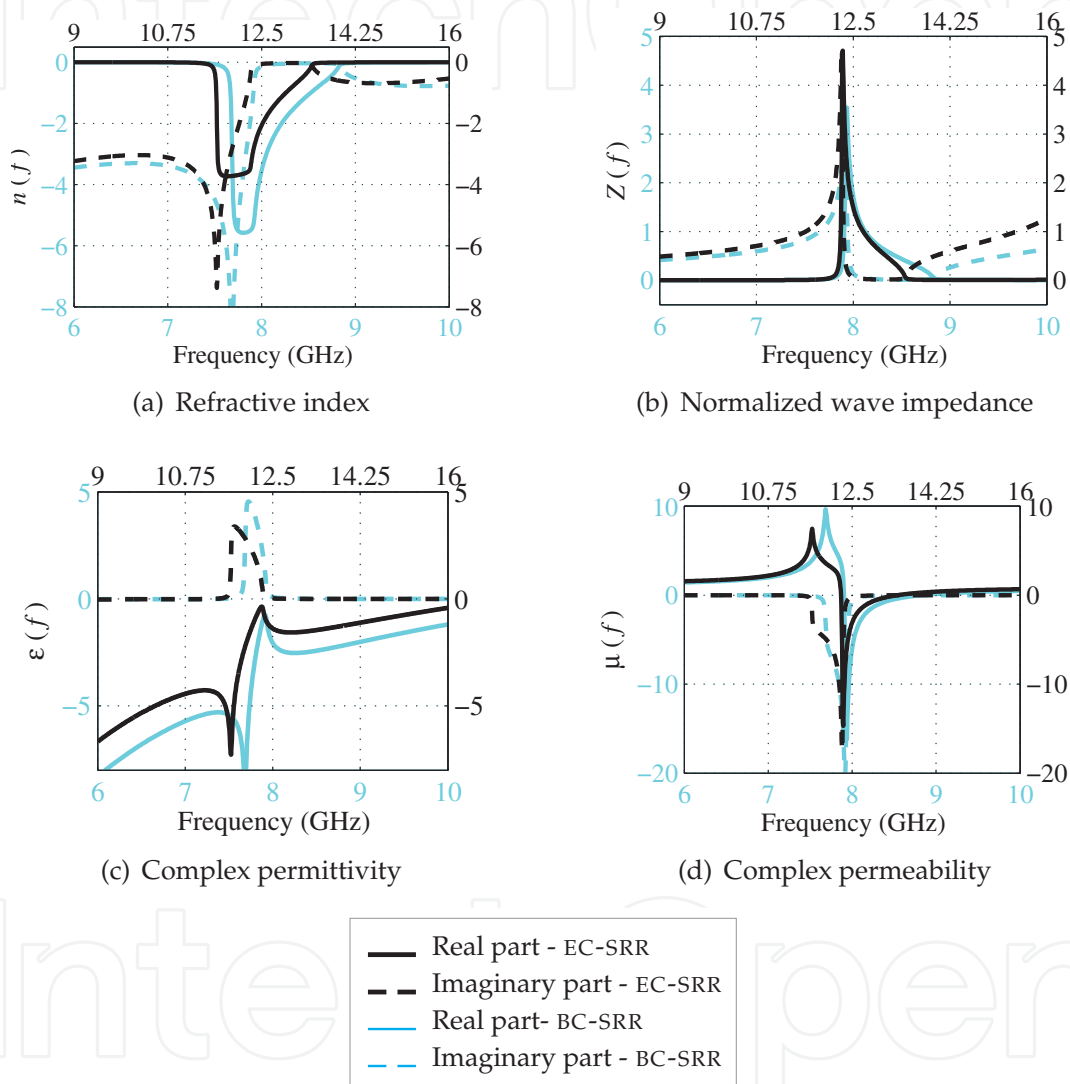


Fig. 9. Effective parameters of NRI metamaterials. The upper frequency scale correspond to EC-SRR structures and lower one to BC-SRR.

The NRI metamaterials constituted of EC-SRR and BC-SRR present respectively a negative refractive index from 11.5 GHz - 13.3 GHz and from 7.7 GHz - 8.7 GHz [figure 9(a)]. It should be noted that the refractive index saturates in both cases ($11.5 \text{ GHz} < f < 12.3 \text{ GHz}$ for the EC-SRR and $7.7 \text{ GHz} < f < 7.9 \text{ GHz}$ for the BC-SRR). This maximum value can be predicted by equation (26). The effective permeability shown on figure 9(d) is resonant and the imaginary part is positive. The effective permittivity shown on figure 9(c) is anti-resonant and presents

also positive values for the imaginary parts. The main frequency bands of interest of these NRI metamaterials are given in table 1.

	BC-SRR	EC-SRR
Negative refractive index	7.7 -8.7 GHz	11.5-13.3 GHz
Negative permeability	7.9 -8.7 GHz	12.3-13.3 GHz
Negative permittivity	6-10 GHz	9-16 GHz
Saturation of the real part of refractive index	7.7-7.9 GHz	11.5-12.3 GHz
$\Im m(\epsilon) > 0$	7.7-7.9 GHz	11.5-12.3 GHz
$\Im m(\mu) > 0$	7.7-7.9 GHz	11.5-12.3 GHz

Table 1. Frequency bands of interest for NRI metamaterials based on BC-SRR and EC-SRR.

A similar behavior can be observed for both metamaterials but with a shift in frequency. This shift as explained in (Seetharamdoo et al. (2004)) is due to higher capacitive coupling in the BC-SRR compared to the EC-SRR. There is indeed a frequency band for which the real part of the refractive index, effective permittivity and permeability are negative. However, in a part of this frequency band the imaginary parts of $\epsilon(\omega)$ and $\mu(\omega)$ are positive which not a physically correct as described in section 2.2. This frequency band deserves further analysis and in the next sections for better understanding of these results, a dispersion diagram as well as a multimodal analysis will be proposed for the BC-SRR NRI metamaterial. The choice of this metamaterial for further analysis is justified by the fact that it has also been shown to be 2D-isotropic (Seetharamdoo (2006)).

4.2 Dispersion diagram of NRI metamaterials

The dispersion diagram is calculated using the method described in section ???. This diagram shown on figure 10(a) gives information on the modes that can propagate in the periodic medium in two dimensions in the irreducible Brillouin zone. The dispersion diagram of the

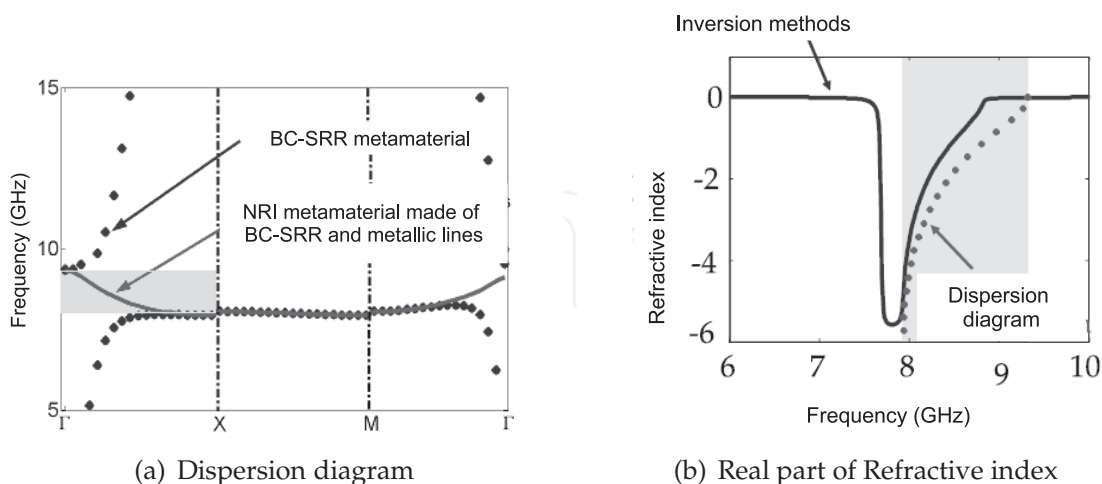


Fig. 10. (a) Two dimensional dispersion diagram of the medium with BC-SRR only and the NRI metamaterial in the irreducible Brillouin zone. (b) Superposition of the refractive index calculated from the dispersion diagram and the one calculated by the inversion methods. The shaded frequency band represents the frequency band where the refractive index is negative and where there is backward propagation.

metamaterial constituted of only BC-SRR (without the metallic line medium) is also shown. In the shaded frequency band, the metamaterial with BC-SRR only presents a forbidden frequency band while in association with the metallic lines, a propagated frequency band is observed. The phase velocity given by the slope of the curve is negative; the propagation is hence a backward wave propagation. The refractive index can be calculated from this phase velocity and it is compared to the one calculated using inversion methods. As it can be observed, there is indeed a frequency band (7.9 - 8.7 GHz) where both results are in good agreement.

However, in the frequency band (7.7 - 7.9 GHz) where the calculation of effective parameters by inversion methods yield unphysical results, the dispersion diagram shows no propagation. This strongly suggests that the results obtained by the inversion method in this frequency band is not correct and is caused by the finite thickness of the structure. If the structure were large enough in the direction of propagation to represent a periodic or a continuous medium, these unphysical results would not have been obtained. Unfortunately, either in measurements or in the design of NRI metamaterials using numerical modeling, it is not always possible to analyze large structures due to the cost or resources required for the calculation.

4.3 Solution proposed: multi-modal analysis

A simple solution to verify the validity of the results given by inversion methods is to make a multimodal analysis of the periodic NRI resonant metamaterial to detect the existence of higher order modes which would definitely result in incorrect effective parameters calculation by inversion methods using a finite-size structure in the direction of propagation. Figure 11 depicts the modal S_{21} parameters and the associated propagation constants for the first two modes of the periodic structure⁶.

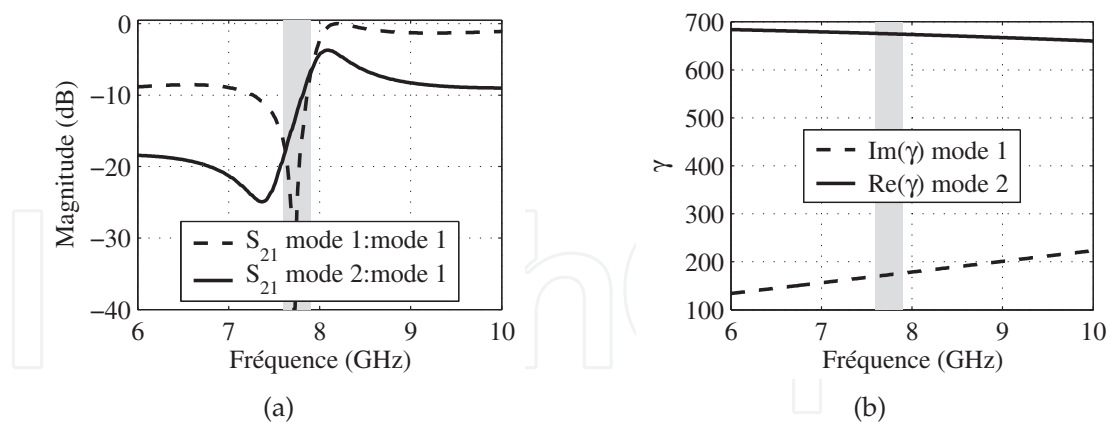


Fig. 11. (a) Modal Scattering parameter S_{21} for the first two modes. (b) Propagation constants of these first two modes. Only $\text{Im}(\gamma)$ is shown for the first mode $\text{Re}(\gamma)$ for the second mode because the corresponding imaginary and real parts are close to zero. The shaded frequency band represents the frequency band where the unphysical results have been observed.

The scattering parameter S_{21} of the fundamental mode presents a resonance at frequency close to 7.8 GHz. Around this frequency and in the shaded frequency band, a second mode can be

⁶ S_{21} Mode2:Mode1 represents for instance what is observed from the profile of the second mode on access 2 when only the first mode is excited on access 1.

observed whose magnitude is higher than that of the fundamental mode. In figure 11(b), this second mode can be seen to be evanescent while the first one is propagative. The value of the propagation constant of the evanescent mode is low enough to show that it can propagate through a few layers of the structure. This implies that the evanescent modes do participate to the interference phenomena in this frequency band and this effect will be more visible with lower dissipative losses in the resonant NRI metamaterial (Seetharamdoo (2006)).

This analysis can prove to be very useful to verify if the assumptions made while using the inversion methods are violated. In this case, one can conclude that the effective parameters calculated in this frequency band are incorrect and non-physical and should thus not be presented or interpreted (Seetharamdoo et al. (2005)).

5. Conclusion

The electrodynamics of NRI materials and the fundamental limitations related to the signs of refractive index, wave impedance, effective permittivity and permeability, both in real and imaginary parts have been fully described. The effective medium theory as it is applied to NRI resonant materials have been detailed with a description of the assumptions linked to this theory for cases of finite thickness in the direction of propagation and infinite dimensions. The methods used for the calculation of effective parameters have been given and applied to numerical models of NRI resonant metamaterials. Unphysical results have been obtained: the imaginary part of the effective permittivity and permeability takes positive values. It has been shown that this is mainly due to the finite size of the structure and that there is a frequency band where the results obtained by the classical inversion methods for the calculation of effective parameters are not correct and this frequency band can be defined thanks to complementary analysis like the calculation of a dispersion diagram and a multimodal analysis.

6. References

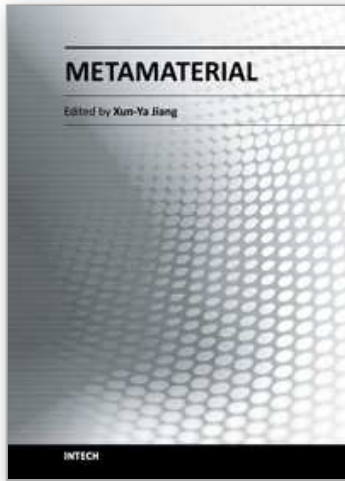
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In-depth analysis of the theory, properties and description of the most potential technological applications of metamaterials for the realization of novel devices such as subwavelength lenses, invisibility cloaks, dipole and reflector antennas, high frequency telecommunications, new designs of bandpass filters, absorbers and concentrators of EM waves etc. In order to create a new devices it is necessary to know the main electrodynamical characteristics of metamaterial structures on the basis of which the device is supposed to be created. The electromagnetic wave scattering surfaces built with metamaterials are primarily based on the ability of metamaterials to control the surrounded electromagnetic fields by varying their permeability and permittivity characteristics. The book covers some solutions for microwave wavelength scales as well as exploitation of nanoscale EM wavelength such as visible specter using recent advances of nanotechnology, for instance in the field of nanowires, nanopolymers, carbon nanotubes and graphene. Metamaterial is suitable for scholars from extremely large scientific domain and therefore given to engineers, scientists, graduates and other interested professionals from photonics to nanoscience and from material science to antenna engineering as a comprehensive reference on this artificial materials of tomorrow.

How to reference

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