Contract No. 218696-ECONAM

Electromagnetic Characterization of NAnostructued Materials

DELIVERABLE D1.1

OVERVIEW OF THREE MAIN APPROACHES TO THE ELECTROMAGNETIC CHARACTERIZATION OF METAMATERIAL LATTICES

Due date of deliverable: T0+3 months

Actual delivery date: 20 of June 2008

Leading contractors: TKK

Surveys on so-called *metamaterials* can be found in books [1, 2, 3] (also see review paper [4]). The history of metamaterials (MTM) starts from paper [5] where the goal to create the so-called *perfect lens* was claimed by J. B. Pendry. The development of MTM showed that composite media with extraordinary material properties are suitable not only for subwavelength focusing and resolution and they found a lot of other applications. Simultaneously the concept of MTM was generalized. Now, transmission line networks with periodical loads and resonant artificial surfaces (metasurfaces) also refer to MM [1, 2, 3]. MTM definitely deserved the special attention paid to them in the modern literature. However, in many papers devoted to them the reader can find mess or wrong results. Especially, it concerns the electromagnetic characterization (EMC) of MTM and, especially, the wrong interpretation of results obtained for so-called effective material parameters (EMP).

In the modern literature MTM are often presented by lattices of resonant scatterers whose characteristic size δ and period a at the resonance is small compared to the wavelength in the host medium λ though comparable with it (practically $(a, \delta)/\lambda = 0.05...0.2$). Notice that the resonance of lattice particles at these comparatively low frequencies is the feature that shares MTM lattices out of photonic crystals, but the resonant wavelength (moreover taking in account its shortening in the lattice compared to free space) shares MTM out of previously known artificial magneto-dielectrics and grants unusual properties. MTM can be also a combination of two (or more) periodic building blocks. One of them can be formed by small magnetic scatterers often called as split-ring resonators (see e.g. [6, 7]), another can be an array of long wires. This combination was first experimentally studied in [8] and later developed in numerous works. Some interesting phenomena in MTM arise namely due to the spatial dispersion in the structure of long metal cylinders. The spatial dispersion corresponds to cases when the wave propagates obliquely to wires or along them. In the present review we do not consider spatially dispersive MTM and do not discuss these effects.

The correct EMC of MTM is very important for their design and optimization. The retrieval of EMP through exact simulations is more accurate than approximate analytical calculation of material parameters through individual particles electric and magnetic polarizabilities which can be are more-or-less accurate only below the resonance band. To measure these polarizabilities is very difficult. It would require very precise and sensitive measurements in a resonator or a waveguide. To calculate them numerically for an individual particle using the HFSS, Microwave CST Studio packages is also very difficult since the polarizability concept implies the separate excitation by the electric and magnetic fields, and one should use sophisticated combinations of waves in order to extract polarizabilities from numerical simaultions of a single particle. And this accurate simulation would be not a worthy task, since all known mixing rules that allow one to find EMP through polarizabilities are approximate.

Meanwhile, the problem of a plane wave incidence to a grid of arbitrary particles is (due to the periodicity in the tangential plane) a standard *cell problem*. Cell problems are as a rule efficiently solvable. As to experimental retrieval, it is much easier to measure the $R-T$ coefficients of a grid than to measure the unit cell electric response for the permittivity and magnetic response for the permeability. In fact, a tool that allows us to relate EMP with $R-T$ coefficients is of prime importance for successful design of MTM.

The present overview refers to lattices of small scatterers (if there are long one like wires we assume that the propagation is normal to their axes). Such MTM can be characterized through EMP. EMC of such MTM is often thought as introducing their EMP, also called as *the homogenization*. The plane-waves in MTM can be also characterized through the scalar or tensor refraction index and scalar or tensor wave impedance, the linear interaction of layers of

MTM with plane-waves can be characterized through the surface impedance, etc. However, the most popular EMC is that in terms of EMP, i.e. the homogenization.

The key point is the insight that there is no unique and mandatory receipt how to define EMP of any electromagnetic lattice beyond the purely static limit. Introducing the material parameters for an array of separate particles at a nonzero frequency is not a unique procedure.

In the modern literature we have found five procedures of the characterization of MTM lattices:

- Procedure 1. EMP obtained by a direct extraction of ε and μ from plane-wave reflection and transmission $(R-T)$ coefficients of the composite slab, assuming a slab to be continuous and uniform medium with such ε and μ and thickness which is equal to the thickness of the host medium.

- Procedure 2. EMP obtained by an indirect extraction of ε and μ from plane-wave reflection and transmission $(R-T)$ coefficients of the composite slab, assuming a slab to be a 3-layer structure, where all 3 layers are continuous and uniform media. The central (thickest) layer is characterized by ε and μ to be found, and the Drude transition layers (thinnest) are characterized by EMP which are averaged between ε and μ and unity (material parameters of free space)[1].

- Procedure 3. EMP for thin MTM layers (1-3 scatterers across the layer) describing the electromagnetic response of the layer per unit area of the surface (i.e. the response of a cell covering the whole layer thickness).

- Procedure 4. EMP are obtained by simulations of the electromagnetic wave propagation in the lattice in all directions. They are extracted as the tensors describing the electromagnetic response of the unit cell to the field averaged in the special way so that in the static limit these non-local EMP would give the correct static material parameters of the lattice. To apply these EMP to boundary problems with MTM layers beyond the static limit one has to deduce the additional boundary conditions, that allows to take in account the effects of spatial dispersion, (such as polaritons excited at the interfaces and exponentially vanishing inside the MTM layer).

- Procedure 5. EMP for infinite (unbounded) MTM lattice introduced through sophisticated line and surface averaging.

We start from Procedure 5, since it seems to us totally useless. It was introduced by J.B. Pendry [6, 9, 10], where these material parameters are obtained as an intermediate result in the modelling of the transfer matrix of the lattice unit cell. In spite of many references to this method of characterization of EMC in the literature there are no examples of extraction of these EMP experimentally or even from numerical simulations. From [9] the reader can deduce the absence of physical meaning of these EMP. The study [10] is devoted to the properties of these EMP but still does not explain how to relate them with $R-T$ coefficients of MTM layers. We think there is no way to associate them with any real boundary problem beyond the static limit.

Procedure 4 developed in works [11, 12, 13] is very accurate and allows one to take in account fine effects. However, it can be hardly applied for the experimental characterization of the MTM

[1] For simplicity it is assumed that the surrounding medium is free space, but this approach can be generalized to arbitrary continuous media.

lattices since we do not know a priori which additional boundary conditions we should apply. Moreover, the EMP are assumed to be non-local i.e. depending on the wave vector explicitly (for the fixed frequency this means the dependence on the angle of propagation and even on the type of the wave – TE, TM or TEM), which makes their experimental extraction very difficult even with known additional boundary conditions. This approach is difficult even for the theoretical characterization of MTM lattices, especially finite ones.

Procedure 1 was first applied for MTM layers in papers [14] and [15], and later in hundreds papers (it is also described in the above cited books devoted to MTM). For example, in [16]-[24] one claims that a composite slabs comprising small number N of monolayers[2] and even the single monolayer has the same EMP as infinite or semi-infinite MTM lattices. Let us discuss how this result becomes possible.

It is clear that in the case $N \to \infty$ the obliquely incident wave refracts and this refraction is affected by lattice particles. On the contrary, in the case when $N = 1$ the electrically small (electric or magnetic dipole) particles do not contribute into refraction. The incident wave meets only one particle across the slab. The interaction of the wave with a monolayer of dipoles leads to the reflection and transmission of the wave without its refraction. What is then the meaning of the refraction coefficient extracted in those works if there is no refraction? The natural reaction of a thinking reader would be to decide that the results of this procedure of extraction are either wrong or senseless.

However, in what concerns papers [16]–[24] and many others this conclusion would be not correct. If the EMP of slabs retrieved in these works turned out to be practically the same for different N this cannot be occasional. There is a certain physics behind these EMP. Which physics? In papers [28, 29, 30] this was explained. These EMP are so-called *Bloch's EMP* introduced and discussed in works [28, 29, 30]. The class of MTM lattices for which these EMP can be introduced was named in these works as Bloch lattices. MTM lattices studied in works [16]-[24] and many others refer to this class.

The Bloch EMP specified for this class of MTM definitely allow one to interpret a finite-thickness lattice as a uniform continuous medium between two interfaces. However, these EMP do not quantitatively describe the electromagnetic response of the unit cell of the medium. Their correct physical meaning is associated with the so-called ABCD matrix of the unit cell of a Bloch lattice which turns out to be fully determined by these ε and μ. The ABCD matrix refers to the transmission-line interpretation of the electromagnetic lattice as a periodically loaded line whole loads are described by this matrix. The values ε and μ in this procedure are scalar and are angularly-dependent. Usually one consider these ε and μ for the normal incidence, only.

In fact, the description of the wave transmission through the unit cell of the MTM lattice is possible:

- in terms of the ABCD matrix (where only 2 terms are independent in the case of reciprocal non-bianisotropic inclusions),
- in terms of the effective refraction index n and the effective wave impedance Z, and, finally,
- in terms of effective (Bloch's) ε and μ.

[2]Monolayer is a single grid of particles placed in the host medium slab of thickness a which is equal to the period of the MTM lattice obtained by the periodic repetition of the monolayer in the normal direction to its interface.

The refraction index n has the physical meaning of the wave phase shift of the wave across one unit cell normalized to the phase shift of the wave over the same distance in free space. The effective wave impedance Z has the physical meaning of the ratio between tangential components of the electric and magnetic fields averaged over the input or the output cross section of the lattice unit cell. For Bloch lattices the effective wave impedance defined as the ratio of transversally averaged E- and H-fields keeps the same for the input plane of the unit cell, for its output plane and even for the central cross section of the cell. This ratio is then the Bloch impedance. For Bloch lattices both Z and n are the same for an infinite lattice and for a finite one, i.e. a stack of N monolayers, including $N = 1$.

The Bloch lattices cannot be photonic crystals, i.e. the unit cell size a must be less (in many cases significantly less) than $\lambda/2$, where λ is the wavelength in the host medium. So, the concept of Bloch lattices physically corresponds to the low frequency region. However this concept can include (at least partially, i.e. except the frequencies where the effects of the lattice spatial dispersion are essential) the range of the inclusion resonance. The electric resonance of inclusions in such lattices should be not overlap with the magnetic one. For Bloch lattices of small inclusions behaving as dipoles (electric ones at the electric resonance of inclusions and magnetic ones at their magnetic resonance) the resonance of effective (Bloch's) ε holds approximately at the frequency of the electric resonance of inclusions and the resonance of effective μ holds at the frequency of the magnetic resonance. This is the only correspondence between the Bloch material parameters and the electromagnetic response of the unit cell.

It is important to notice that the second Bloch material parameters in this situation also experiences the resonance and this resonance is totaly wrong. Namely, at the electric resonance of inclusions not only Bloch's ε resonates, but also Bloch's μ, and vice versa. This simultaneous resonance in a lattice of inclusions whose electric and magnetic resonances do not overlap [16]–[24] once more indicates that the Bloch effective material parameters are fictitious and describe improperly the electromagnetic response of the medium. In hundreds papers devoted to the characterization of MTM (we do not cite them for the sake of space) this wrong resonance is called as the *antiresonance* that produces the terminological mess. The term antiresonance is commonly used in the electrical and radio engineering and means simply the parallel circuit resonance. It has nothing to do with the resonance of the second Bloch parameter which is totally deprived of any physical content.

In fact, the description of the Bloch lattice in terms of the effective Bloch's ε and μ is the alternative to the description of the lattice in terms of the ABCD matrix or in terms of the Bloch impedance Z and the refraction index n. And this alternative gives no new insight compared to Z and n. Moreover, these parameters often lead to the mess because the effective Bloch's ε and μ calculated or extracted from the scattering matrix for a lattice of resonant inclusions:

- violate the locality requirements (see below) that most part of researchers consider as obvious for material parameters. This violation is often interpreted as the signature of the strong spatial dispersion, and one concludes that the lattice cannot be homogenized;

- mistakenly indicate the wrong resonance of the second material parameter.

However, it does not mean that the Bloch material parameters are totally useless. In fact, they indicate the inclusion resonance frequencies and one can distinguish the type of the resonance: is it electric or magnetic. It turns out that only one of two Bloch parameters (either ε or μ) violates the locality requirement, and the resonance of this parameter is wrong. For example, the lowest resonance of lattices of split-ring resonators is magnetic, and Bloch's μ at this resonance looks like as a local material parameter, whereas Bloch's ε violates the locality.

We conclude that the characterization of MTM lattices in terms of Bloch's material parameters can be useful since it can give the correct information on the resonance frequency and on the nature of the resonance (electric or magnetic). The condition of this success is evident: the MTM lattice under characterization should be a Bloch lattice, i.e.

- the resonance of the Bloch's material parameters should obviously hold at low frequencies: $a < \lambda/2$;
- the response of inclusions should be not bianisotropic, i.e. the electric field should not create the magnetic dipoles and vice versa;
- the inclusions should be optically small enough to be described in terms of electric and magnetic dipoles;
- the electric and magnetic resonances should not overlap.

Procedure 2 was developed in works [28, 29] and [31]. It allows to find so-called local (or Lorentz's) EMP of MTM, which were shown in these works to be correct generalizations of well-known static EMP to frequency dependent fields. The procedure was developed only for lattices of reciprocal (non-magnetic) not bianisotropic inclusions, the restriction of the operational frequency is the same as for Bloch material parameters. The artificial magnetism in this case arises as the effect of the inclusion complex shape and disappears in the static limit. These EMP keep the physical meaning of the medium unit volume response to the electric and magnetic fields even in the resonance band of inclusions, except special frequencies where the effects of strong spatial dispersion are essential. In the static limit Lorentz's EMP transit to Bloch EMP and vice versa. The locality of Lorentz's EMP means (see, e.g., in [25]) the system of following conditions:

- Passivity (for the temporal dependence $e^{-i\omega t}$ it implies $\mathrm{Im}(\varepsilon) > 0$ and $\mathrm{Im}(\mu) > 0$ simultaneously at all frequencies, for $e^{j\omega t}$ the sign of both $\mathrm{Im}(\varepsilon)$ and $\mathrm{Im}(\mu)$ should be negative);
- Causality (for media with negligible losses it corresponds to conditions $\partial\left(\omega\varepsilon\right)/\partial\omega > 1$ and $\partial\left(\omega\mu\right))/\partial\omega > 1$. This also means that in the frequency regions where losses are small material parameters obviously grow versus frequency: $\partial\left(\mathrm{Re}(\varepsilon)\right)/\partial\omega > 0$ and $\partial\left(\mathrm{Re}(\mu)\right)/\partial\omega > 0$);
- Absence of radiation losses in arrays with uniform concentration of particles;
- Independence of the material parameters on the wave propagation direction (for given frequency this means the independence of EMP of the slab on the incidence angle of a plane wave).

It was shown that the Bloch material parameters are in this meaning *non-local* within same frequency ranges where the Lorentz EMP are local. This is because the Bloch EMP do not describe properly the electric and magnetic response of the medium.

However, the introduction of Lorentz EMP for lattices of resonant inclusions implies a quite complicated 3-layer representation of any finite-thickness MTM lattice. This leads to the significant complication in the description of MTM compared to the Bloch parameters, since the thickness of Drude layers is still not studied except the special case of the simple cubic lattices of spheres [31]. Probably, this is the reason why this direction advances weakly, and no one attempt to develop it by other authors is known.

Procedure 3 was introduced in [32]. This is an evident alternative to Procedure 2 for very thin layers. Really, the representation of, e.g. a monolayer as a 3-layer structure with Lorentz EMP and Drude transition layers though possible but has no physical meaning. The EMP defined by Procedure 3 were called as mesoscopic EMP. These EMP evidently satisfy to locality requirements together with Lorentz However, in this way one encounetere the following problem: only for very simple inclusions (unloaded short or long wires oriented in parallel to the interface) mesoscopic EMP fit the $R-T$ coefficients. Therefore, it is still not clear how to extract mesoscopic EMP from measurements or simulations of layered structures with complex or tilted inclusions.

To conclude this overview: there are five known methods of the characterization of bulk MTM lattices with finite thickness through effective material parameters, from which we shared out three most prospective ones. One of them (Procedure 2 or direct extraction of EMP) is most popular, however its improper application and wrong interpretation led to the mess and incorrect results in the literature on MTM. Two other procedures are not popular and therefore weakly developed, and it is impossible to judge is it related to their inherent shortcomings or simply with their weak promotion. In this situation it is impossible to definitely make the choice of the best method for the characterization of bulk MTM layers. However, it is obvious to promote the existing insight on the physical meaning of extracted material parameters, since wrongly interpreted results in the literature on MTM are, as a rule, related to the lack of theoretical knowledge.

References

[1] C. Caloz and T. Itoh, *Electromagnetic metamaterials: transmission line theory and microwave applications*. J. Wiley and Sons, NY, 2006.

[2] G. Eleftheriades, K.G Balmain, *Negative-Refraction Metamaterials: Fundamental Principles and Applications*, Wiley: NY, 2006.

[3] N. Engheta, R. Ziolkowski, *Metamaterials Physics and Engineering Explorations*, NY: J. Wiley and Sons, 2006.

[4] S. Anantha Ramakrishna, *Rep. Prog. Phys.* **68** (2005) 449.

[5] J.B. Pendry, *Phys. Rev. Lett.* , **85** (2000) 3966.

[6] J.B. Pendry, A.J. Holden, D.J. Robins, and W.J. Stewart, *IEEE Trans. MTT*, **47** (1999) 2075.

[7] S. Linden, C. Enkrich, M. Wegener et al., *Science*, **306** (2004) 1351.

[8] R.A. Shelby, D.R. Smith, and S. Schultz, *Science*, **292** (2001) 77.

[9] J.B. Pendry, A.J. Holden, D.J. Robins, and W.J. Stewart, *J. Phys. Condens. Matter*, **10** (1998) 4785.

[10] D. Smith and J. B. Pendry, *JOSA B*, **23** (2006) 391.

[11] M.G. Silveirinha, *Physical Review B* **76** (2007) 245117.

[12] M.G. Silveirinha, *Physical Review B* **75** (2007) 115104.

[13] M.G. Silveirinha, *Physical Review E* **73** (2006) 046612.

[14] S. O'Brien and J.B. Pendry, *J. Phys. Condens. Matter*, **14** (2002) 4035.

[15] D.R. Smith, S. Schultz, P. Markos and C. Soukoulis, *Phys. Rev. B.* **65** (2002) 195104.

[16] I. El-Kady, M.M. Sigalas, R. Biswas, K.M. Ho, and C.M. Soukoulis, *Phys. Rev. B* **62** (2000) 15299.

[17] S. O'Brien and J.B. Pendry, *J. Phys.: Condens. Matter*, **14** (2002) 6383.

[18] S. O'Brien, *Artificial Magnetic Structures*, PhD thesis, Imperial College of Science, Technology and Medicine, Department of Physics, available at:
http://www.imperial.ac.uk/research/cmth/research/theses/S.OBrien.pdf.

[19] N. Katsarakis, G. Konstantinidis, A. Kostopoulos et al. *Optics Letters*, **30**, (2005) 1348.

[20] K.C. Huang, M.L. Povinelli, and J.D. Joannopoulos, *Applied Physics Lett.* **85** (2004) 543.

[21] D.R. Smith, P. Kolinko, and D. Schurig, *J. Opt. Soc. Am. B* **21** (2004) 1032.

[22] S. O Brien, D. McPeake, S.A. Ramakrishna, and J.B. Pendry, *Phys. Rev. B*, **69** (2004) 241101.

[23] N. Katsarakis, T. Koschny, M. Kafesaki, E.N. Economou, E. Ozbay, and C. M. Soukoulis, *Phys. Rev. B*, **70** (2004) 201101(R).

[24] N. Katsarakis, T. Koschny, M. Kafesaki, E. N. Economou, C. M. Soukoulis, *Appl. Phys. Lett.* **84**, (2004) 2943.

[25] L.D. Landau and E.M. Lifshitz, *Electrodynamics of continuous media*, Pergamon Press, Oxford, 1960.

[26] N.G. Alexopoulos, C.A. Kyriazidou, and H.F. Contapanagos, *IEEE Trans. Antennas Propag.* **55**, (2007) 254.

[27] D.R. Smith, D. Shurig, *Phys. Rev. Lett.* **90**, (2003) 077405.

[28] C.R. Simovski, S.A. Tretyakov, *Phys. Rev. B* **75**, (2007) 195111(1-9)

[29] C.R. Simovski, *Metamaterials*, **1** (2007) 62.

[30] C.R. Simovski, *Metamaterials*, **2** (2008) in print.

[31] C.R. Simovski, *Journal of Communication Technology and Electronics*, **52**, (2007) 953.

[32] P. Ikonen, E. Saenz, R. Gonzalo, C. Simovski and S. Tretyakov, *Metamaterials*, **1** (2007) 89.