Computation of Effective Surface and Bulk Parameters of Electromagnetic Metamaterials

Xiaoyan Y.Z. Xiong[1], Li Jun Jiang[1], Vadim A. Markel[2], and Igor Tsukerman[3]
[1]Department of Electrical and Electronic Engineering
The University of Hong Kong, Pokfulam, Hong Kong, xyxiong@eee.hku.hk, jianglj@hku.hk
[2]Departments of Radiology and Bioengineering
and the Graduate Group in Applied Math and Computational Science,
University of Pennsylvania, Philadelphia, PA 19104, USA, vmarkel@mail.med.upenn.edu
[3]Department of Electrical and Computer Engineering,
The University of Akron, OH 44325-3904, USA, igor@uakron.edu

***Abstract*—The ideas of div- and curl-conforming approximations of electromagnetic fields have long been established in computational electromagnetics but have so far been confined to edge- and face-element methods. We apply them in a completely different area: effective parameters of electromagnetic metamaterials, periodic dielectric/metal structures whose lattice cell size is smaller than, yet comparable with, the vacuum wavelength. The proposed dual-interpolation methodology allows one to distinguish between surface and bulk parameters. The homogenization procedure involves a basis set of fields that in this paper is computed using finite difference time domain algorithms.**

***Index Terms*—Metamaterials, Effective Material Parameters, Homogenization, Surface Waves, Periodic Structures, Bloch Waves, Finite Difference Time Domain**

I. Introduction

Electromagnetic metamaterials – periodic dielectric/metal structures whose lattice cell size is smaller than, yet comparable with, the vacuum wavelength – have been the subject of extensive research due to remarkable applications proposed in the literature [1]. One critical question is the definition and computation of effective material parameters. In the homogenization limit, i.e. when the lattice cell size a tends to zero relative to the vacuum wavelength, solid mathematical and physical theories are available and can be applied in electromagnetic computation. However, to produce nontrivial physical effects, the lattice cell size must constitute an appreciable fraction of the wavelength [2]. Hence a *non-asymptotic* homogenization theory is called for [3], [4], [5].

Such a theory involves mathematical ideas of div- and curl-conforming interpolations, discrete Hodge operators and Trefftz approximations that are well established in the Compumag community [6], [7], [8], [9] but until recently have not been applied to homogenization. In our methodology [4], [5], one defines the macroscopic **E** and **H** fields by curl-conforming interpolations of a set of basis functions in the material, while the **B** and **D** fields are obtained by div-conforming interpolations.

Among other things, the new methodology allows one to distinguish between the effective material parameters in the bulk and at the surface of a metamaterial sample or, speaking more broadly, to define and compute these parameters as functions of position. This has implications, in particular, for parameter retrieval, a common procedure in design and modeling of metamaterials. This procedure involves analysis of transmission/reflection of plane waves through a slab of several elementary layers. The number of layers can affect the effective parameters (EMPs), but the account of this effect has so far been heuristic.

II. Statement of the Problem

In practice, it is often convenient to work with plane-parallel slabs of identical unit cells arranged on a cubic lattice. The lattice is assumed infinite (or sufficiently wide) in two directions, say, x and y, and finite in the third direction, z. If illumination-independent effective material parameters (EMPs) can be defined for this structure, then (approximate) analytical results for its transmission and reflection coefficients can be easily obtained. The effective medium description of the slab is critical to many proposed applications, e.g. the superlens. In this work, we investigate the effects of the finite width of the slab that in practice often contains only a small number N of elementary cell layers.

For a sufficiently thick slab ($N \gg 1$), EMPs are expected to be independent of N, but for $N \sim 1$ this is not necessarily so. Nevertheless, EMPs are frequently introduced for just a few layers or even for a single layer. This raises the question of finite width effects on homogenization. Recent simulations suggest that these effects are not particularly strong [10], [11]. At the same time, some experiments have demonstrated critical sensitivity to the number of layers [12]. So far, these findings are largely heuristic. It is desirable, therefore, to study the finite width effects mentioned above more systematically.

III. Effective Material Parameters

In the recently developed non-asymptotic homogenization theory [3], [4], [5], the electromagnetic fields inside the sample are approximated by a suitably chosen set of basis functions (modes). The four coarse-grained (macroscopic) EM fields **E**, **H**, **D**, **B** are defined as *curl-conforming* and *div-conforming* interpolations of the microscopic fields **e**, **h**, **d** and **b**, so that

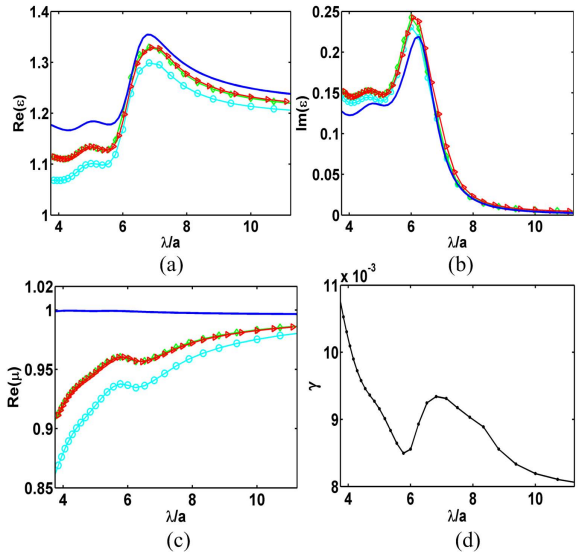

Figure 1: (a)–(c): The diagonal elements of the EMPs for a lattice of gold spheres with the radius of $r_0 = 20\,\text{nm}$ and unit cell size $a = 80\,\text{nm}$. Solid line: the Lewin theory; circles: EMPs for the surface unit cell with $N = 5$; triangles and diamonds: EMPs for the center unit cell with $N = 9$ and $N = 5$ respectively. (d): the in-the-basis error γ.

the former satisfy Maxwell's equations and interface boundary conditions [3], [4], [5]. The material tensor constitutes, by definition, a linear relationship between the $(\mathbf{E}, \mathbf{H})$ and $(\mathbf{D}, \mathbf{B})$.

We have generated the basis set by illuminating the sample with a set of plane waves with different polarizations and traveling in different directions. The simulations made use of the publicly available finite-difference time-domain (FDTD) package MEEP [13]. Perfectly matched layers (PMLs) were introduced at the top and bottom (in the z direction) of the slab, while Bloch-periodic boundary conditions were applied in the x and y directions.

IV. Effective Material Parameters of a Cubic Lattice of Spherical Gold Particles

A cubic lattice of spherical gold particles with the radius of $r_0 = 20$ nm is analyzed; the cell size $a = 80$ nm. The uniform grid size of FDTD is set to $\delta = 2.857\,\text{nm}$ and the simulation time is 8400 $(\delta/2c)$, where c is the speed of light in free space. Fig. 1 compares the EMPs obtained as described above to the results of Lewin's theory [14]. The in-the-basis error γ [4], [5] for the center unit cell at all frequencies is smaller than 1.2% for $N = 5$. However, a large discrepancy between the EMPs calculated for a center cell (diamonds) and a surface cell (circles) can be seen in Fig. 1(a). This result illustrates the influence of surface waves [15]. Moreover, the agreement of the EMPs in the center cell for different numbers of layers, $N = 9$ and $N = 5$, indicates rapid convergence of the EMPs with N.

V. Conclusion

We apply a new homogenization theory of metamaterials based on div- and curl-conforming interpolations of a basis set of fields. This theory provides a rigorous mathematical and physical framework for defining parameters of materials whose lattice cell size is comparable with the wavelength. The methodology also allows one to distinguish between surface and bulk parameters of periodic structures. The basis set was computed via full-wave FDTD simulations. To analyze the dependence of parameters on the thickness of a metamaterial sample and to study theoretically the impact of surface waves, a rigorous coupled-wave analysis was used to disentangle the surface waves from the Bloch waves in the bulk. Details will be provided in the extended paper.

This work was supported in part by the Research Grants Council of Hong Kong (GRF 713011 and 712612), HKU Small Project Funding (201007176196), HKU Seed funding (201102160033), by the University Grants Council of Hong Kong (Contract No. AoE/P-04/08), and by the US National Science Foundation award DMS-1216970 to IT and VM.

References

[1] C. M. Soukoulis and M. Wegener, "Past achievements and future challenges in the development of three-dimensional photonic metamaterials," Nat. Photonics, vol. 5, pp. 523–530, Sep. 2011.

[2] I. Tsukerman, "Negative refraction and the minimum lattice cell size," J. Opt. Soc. Am. B **25**, 927–936, 2008.

[3] A. Pors, I. Tsukerman, and S. I. Bozhevolnyi, "Effective constitutive parameters of plasmonic metamaterials: Homogenization by dual field interpolation," Phys. Rev. E, vol. 84, Jul. 2011.

[4] I. Tsukerman, "Effective parameters of metamaterials: a rigorous homogenization theory via Whitney interpolation," J. Opt. Soc. Am. B, vol. 28, pp. 577–586, Mar. 2011.

[5] I. Tsukerman. "Nonlocal homogenization of metamaterials by dual interpolation of fields," J. Opt. Soc. Am. B, vol. 28, No. 12, pp. 2956-2965, 2011.

[6] Alain Bossavit. "Computational Electromagnetism: Variational Formulations, Complementarity, Edge Elements," San Diego: Academic Press, 1998.

[7] R. Hiptmair. "Discrete Hodge operators," Numer. Math. vol. 90, pp. 265–289, 2001.

[8] T. Tarhasaari, L. Kettunen and A. Bossavit. "Some realizations of a discrete Hodge operator: A reinterpretation of finite element techniques," IEEE Trans. Magn. vol. 35, No. 3, pp. 1494–1497, 1999.

[9] Igor Tsukerman. "Computational Methods for Nanoscale Applications: Particles, Plasmons and Waves," Springer, 2007.

[10] A. Andryieuski, C. Menzel, C. Rockstuhl, R. Malureanu, and A. V. Lavrinenko, "The split cube in a cage: bulk negative-index material for infrared applications," J. Opt. A-Pure Appl. Opt., vol. 11, Nov. 2009.

[11] C. Menzel, T. Paul, C. Rockstuhl, T. Pertsch, S. Tretyakov, and F. Lederer, "Validity of effective material parameters for optical fishnet metamaterials," Phys. Rev. B, vol. 81, Jan. 2010.

[12] G. Dolling, M. Wegener, and S. Linden, "Realization of a three-functional-layer negative-index photonic metamaterial," Opt. Lett., vol. 32, pp. 551–553, Mar. 2007.

[13] Ardavan F. Oskooi, David Roundy, Mihai Ibanescu, Peter Bermel, J. D. Joannopoulos, and Steven G. Johnson, "MEEP: A flexible free-software package for electromagnetic simulations by the FDTD method," Comput. Phys. Commun., vol. 181, pp. 687–702, 2010.

[14] L. Lewin, "The electrical constants of a material loaded with spherical particles" Proc. Inst. Elec. Eng., vol. 94, pp. 65–68, 1947.

[15] V. A. Markel and J. C. Schotland, "Homogenization of Maxwell's equations in periodic composites: Boundary effects and dispersion relations," Phys. Rev. E, vol. 85, 2012.