Homogenization of Thin Dielectric Composite Slabs: Techniques and Limitations

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Abstract – This paper compares different methods for retrieving the transverse effective permittivity of periodic composite slabs whose longitudinal thickness is only a few unit cells. Two computational methods are considered, one based on simulated scattering parameters (S-parameters) and the other one based on fiel averaging by integration. The effect of frequency dispersion is studied by comparing the results with electrostatic estimates given by analytical mixing formulas. Furthermore, the influenc of the slab thickness is studied. We also discuss the boundary effects on the interfaces of the slabs.

Index Terms – Boundary transition layers, effective permittivity, fiel averaging, S-parameters.

I. INTRODUCTION

Heterogeneous media, such as composite materials, are often treated as effectively homogeneous materials [1, 2, 3]. The idea and the benefi of this approximative modeling is that the complex internal microstucture of the material can be forgotten and the material characteristics are averaged into a macroscopic scale. That is, the electromagnetic behavior of the material is described only by two (effective) parameters, the electric permittivity ϵ and the magnetic permeability μ. Such an approximation actually applies to all conventional bulk materials, as well. Naturally, the condition of such homogenization is that the inhomogeneities of the material are very small with respect to the wavelengths of the impinging electromagnetic fields

Once being able to analyze the effective behavior of composite materials, we can go the other way round and see the possibility of synthesizing new artificia materials with desired effective response. In theory, it is possible to create materials even with properties not readily existing in nature. These so called metamaterials have lately been under major interest [4, 5]. However, the homogenization of many proposed materials very seldom goes without problems or doubts [6, 7].

In this paper, we focus on a homogenization of a very simple dielectric structure in order to investigate some fundamental characteristics and limitations of material homogenization. We consider a composite slab consisting of dielectric spheres arranged in a periodic simple cubic lattice in vacuum. The slab is infinit in the transverse plane but in the longitudinal dimension it is only a few layers thick. The slab is excited with a normally incident time-harmonic plane wave (see Fig. 1). The structure is assumed nonmagnetic, *i.e.*, $\mu = \mu_0$, which, for instance, is reasonable when studying polymeric composite materials [8]. Therefore, the only parameter we are retrieving is the effective permittivity ϵ_{eff}, which is a dimensionless number relative to the permittivity of vacuum ϵ_0. Moreover, the spheres are assumed dispersionless and lossless.

In this article, we study the homogenization in a dynamic case in order to see how quickly and strongly the increase of the electrical size of the unit cell makes the effective permittivity estimate deviate from the (quasi)static value. Furthermore, an important objective of this paper is to study how the thickness of the slab, *i.e.*, the number of consecutive unit cell layers, affects the retrieval results.

The simulations are performed using COMSOL

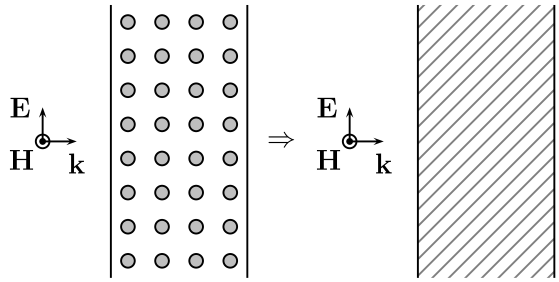

Fig. 1. The original composite medium consisting of a periodic lattice of spherical inclusions is modeled as an effectively homogeneous material.

MULTIPHYSICS 3.5 (3D RF Module, Electromagnetic Waves, Harmonic Propagation), which is a commercial software based on the finite element method (FEM).

In parallel, another related homogenization study is going on, where we more extensively consider the effect of frequency dispersion for a composite slab and an infinite periodic lattice. In those simulations, CST MICROWAVE STUDIO is used. The results of this research are reported in [9]

II. COMPUTATIONAL MODEL OF THE GEOMETRY

The composite slab consists of spheres in a simple cubic lattice, *i.e.*, the unit cell is a cube with a concentric sphere inside (see Fig. 2). The unit cell side length is denoted by a. We consider a composite where the spherical inclusions occupy a volume fraction of $p = 1/4$, *i.e.*, the radii of the spheres become $r = a\sqrt[3]{3/(16\pi)}$. The relative permittivity of the spheres is $\epsilon_{\mathrm{i}} = 10$ and the background material is vacuum with $\epsilon_{\mathrm{e}} = 1$.

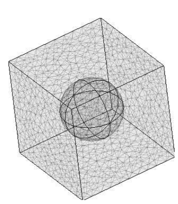

Fig. 2. The unit cell is an $a \times a \times a$ cube with a dielectric sphere inside.

We only consider the case where a linearly polarized transverse electromagnetic (TEM) plane wave is normally incident on the composite slab. In this case, the transverse periodical symmetry of the slab can be modeled using perfect electric conductor (PEC) and perfect magnetic conductor (PMC) boundary conditions. To achieve the desired periodicity, PEC boundaries are placed perpendicularly and PMC boundaries parallel to the chosen direction of the electric field vector. Due to the symmetry of the unit cells, with normal incidence, only one quarter of the unit cells needs to be modeled in the transverse direction, which essentially reduces the computational cost. More general periodic boundary conditions could also be applied, but in that case the whole cells must be modeled. In the longitudinal direction, *i.e.*, the direction of the plane wave propagation, we have to model all the consecutive layers of cells in the slab. We consider three configurations, slabs with thickness of 1, 5, and 9 layers of unit cells. On both sides of the slab, the width of two unit cells of free space is added to ensure sufficient attenuation of possible evanescent higher order modes. The computational domain is terminated with ports, which give rise to the TEM plane wave and allow the computation of the S-parameters. Figure 3 presents the actual modeled geometry in the case of 5 layers.

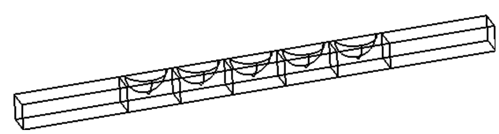

Fig. 3. Example of the modeled geometry with 5 layers.

The geometry is discretized with a tetrahedral mesh. The accuracy of the mesh should remain roughly equal for all geometry configurations, *i.e.*, slabs with a different number of layers. For a certain slab, the same mesh is applied for all frequencies, that is, when we perform a frequency sweep, the mesh needs to be created only once. The field solution is constructed using quadratic vector elements. In our simulations, for slabs with 1, 5, and 9 layers, the meshes consist of 7949, 13997, and 21013 elements, yielding 55148, 97286, and 145626 degrees of freedom, respectively. The simulations are run using a desktop PC with Intel Core 2 Duo CPU 2.66 GHz and 4 GB of RAM. For example, in the case of 5 layers, a sweep of 200 frequency points takes 2141 seconds, which is a little less than 11 seconds per each frequency point.

To validate our simulation results, we also modeled the 5 layered case using the frequence-domain solver of CST MICROWAVE STUDIO (MWS). The geometry setup and the boundary conditions are the same as described above. The unit cell side length was chosen $a = 0.01\,\mathrm{m}$. Figure 4 shows the absolute difference between the obtained S-parameter results, which in the considered frequency range is of the order of 10^{-3}.

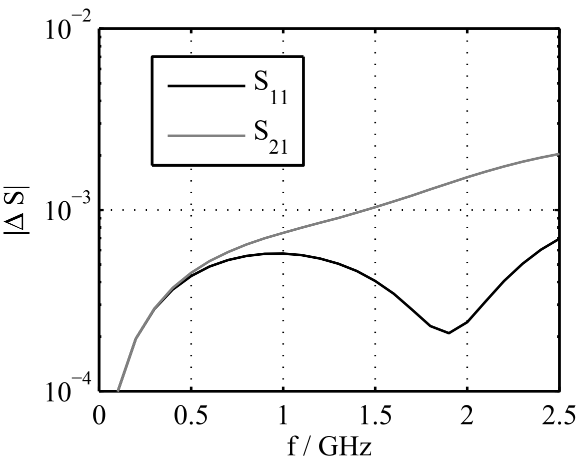

Fig. 4. The difference in simulated S-parameters between COMSOL and CST MWS.

We are considering an electrodynamic case where a propagating wave interacts with the composite material. However, the unit cells must be small enough with respect to the wavelength for the material to behave as homogeneous, so, in that sense, we are near the (quasi)static limit. For convenience, we choose a reference frequency where the edge length of one unit cell equals 1/20 of the wavelength, *i.e.*, $a = \lambda/20$. The wavelength should not, however, be considered the free-space wavelength but the reduced (effective) one inside the material. Therefore, the corresponding reference frequency,

$$f_{20} = \frac{c}{20a\sqrt{\epsilon_{\mathrm{eff}}}}, \tag{1}$$

where c denotes the speed of light in vacuum, depends on the effective permittivity, which is the unknown parameter we are solving. A reasonable a priori estimate is considered in the following.

III. ELECTROSTATIC MIXING RULES

In the electrostatic limit, the effective permittivity of an infinite lattice can be estimated by various analytical mixing formulas [10]. One of the most famous and simplest mixing rules suitable for this case is the Maxwell Garnett (MG) formula, which using the above-mentioned parameter values ($\epsilon_{\mathrm{i}} = 10$, $\epsilon_{\mathrm{e}} = 1$ and $p = 1/4$) gives

$$\epsilon_{\mathrm{eff}} = \epsilon_{\mathrm{e}} + 3p\epsilon_{\mathrm{e}} \frac{\epsilon_{\mathrm{i}} - \epsilon_{\mathrm{e}}}{\epsilon_{\mathrm{i}} + 2\epsilon_{\mathrm{e}} - p(\epsilon_{\mathrm{i}} - \epsilon_{\mathrm{e}})} \approx 1.6923. \tag{2}$$

A more accurate estimate is given by the Lord Rayleigh mixing rule

$$\epsilon_{\mathrm{eff}} = \epsilon_{\mathrm{e}} + \frac{3p\epsilon_{\mathrm{e}}}{\frac{\epsilon_{\mathrm{i}}+2\epsilon_{\mathrm{e}}}{\epsilon_{\mathrm{i}}-\epsilon_{\mathrm{e}}} - p - 1.305\frac{\epsilon_{\mathrm{i}}-\epsilon_{\mathrm{e}}}{\epsilon_{\mathrm{i}}+4\epsilon_{\mathrm{e}}/3}p^{10/3}} \approx 1.6989, \tag{3}$$

and an even more accurate one by the mixing formula derived by McPhedran and McKenzie [11], $\epsilon_{\mathrm{eff}} \approx 1.6990$, which we will use as a static bulk reference value in Eq. (1).

IV. S-PARAMETER RETRIEVAL

The widely applied S-parameter retrieval method is based on measured or simulated reflection and transmission data, namely S_{11} and S_{21}. The method is often referred to as Nicolson–Ross–Weir (NRW) technique named after its originators [12, 13]. Along with the metamaterials research this method has required certain modifications [14, 15].

The normalized impedance z is obtained by

$$z = \pm\sqrt{\frac{(1+S_{11})^2 - S_{21}^2}{(1-S_{11})^2 - S_{21}^2}}, \tag{4}$$

where the sign must be chosen so that the real part of z is positive. The exponent function including the refractive index n is then given by

$$x = e^{-jnk_0 d} = \frac{S_{21}}{1 - S_{11}\frac{z-1}{z+1}}, \tag{5}$$

where $k_0 = \omega\sqrt{\epsilon_0\mu_0}$ is the free-space wave number and d is the thickness of the slab. This method aims at solving both ϵ_{eff} and μ_{eff} by $\epsilon_{\mathrm{eff}} = n/z$ and $\mu_{\mathrm{eff}} = nz$. However, the solution is not unambiguous due to the branches of the logarithm function. The refractive index becomes

$$n = \frac{1}{k_0 d}(j\ln x + 2\pi m), \quad m = 0, 1, 2, \ldots \tag{6}$$

If both ϵ_{eff} and μ_{eff} are unknown, or the material is strongly dispersive, determining the integer m may become diff cult. However, as in our case the composite is assumed non-dispersive and non-magnetic, the correct value for the integer m can simply be adjusted by the condition $\mu_{\text{eff}} = nz \approx 1$.

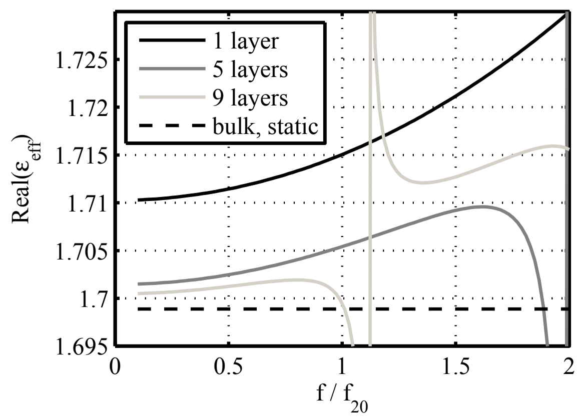

Fig. 5. The retrieved effective permittivity (real part) for different number of layers.

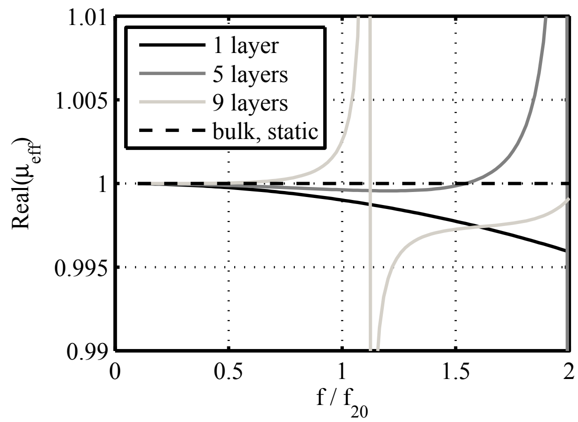

Fig. 6. The retrieved effective permeability (real part) for different number of layers.

Problems appear, when the total effective thickness of the slab becomes $\lambda/2$, or any integer multiple of it. At such frequencies, there occurs a Fabry–Pérot type of resonance where the wave passes through the lossless slab without any ref ection. Although the Fabry–Pérot resonance is a natural response of the slab, it should not affect the material parameter retrieval results. However, as $S_{11} = 0$ and $|S_{21}| = 1$, the impedance z cannot be solved correctly by Eq. (4), which causes the resonances to transfer also to the retrieved parameters ϵ_{eff} and μ_{eff} (see Figs. 5 and 6, respectively). Naturally, these resonances in permittivity and permeability are not physical properties of the studied material but a characteristic of the retrieval method. Moreover, the behavior of ϵ_{eff} is anti-resonant, *i.e.*, near the resonance the permittivity decreases with increasing frequency, which violates the principle of causality (see Fig. 5).

The retrieval also yields very small imaginary parts for ϵ_{eff} and μ_{eff} (not plotted herein). At the resonance, their maximum level is of the order of 10^{-4}, *i.e.*, they are not numerically zero, but compared with the real part they become negligible. However, the imaginary parts may appear with incorrect sign, which indicates a violation of passivity. Especially for metamaterials, where the inclusions often are resonant and lossy, the NRW technique tends to give unphysical material parameters. This problem is discussed more extensively in [7].

However, the refractive index n is not affected by the Fabry–Pérot resonances remaining smooth over all frequencies. This allows us to f ght the problem by demanding $\mu_{\text{eff}} = 1$ and solving the permittivity directly by $\epsilon_{\text{eff}} = n^2$. This modif ed retrieval yields smooth and physically reasonable estimates for ϵ_{eff} (see Fig. 7).

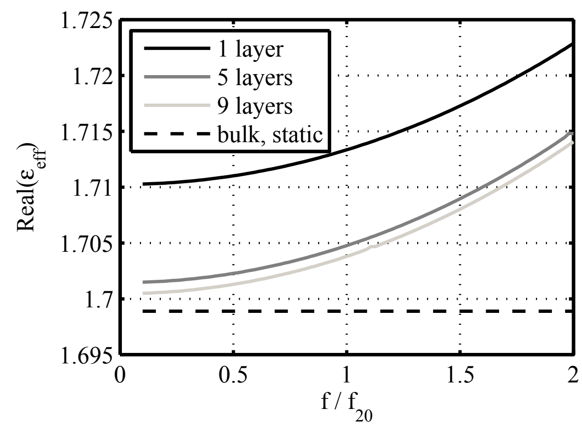

Fig. 7. The effective permittivity (real part) retrieved by $\epsilon_{\text{eff}} = n^2$ for different number of layers.

As a general observation, it can be seen that as the frequency increases, the obtained permittivity starts to notably deviate from the static reference. Also, the number of layers affects the permittivity. The increase of the number of layers makes the permittivity tend to the bulk value at the static limit. With only one layer, the retrieved permittivity is clearly higher.

V. FIELD AVERAGING BY INTEGRATION

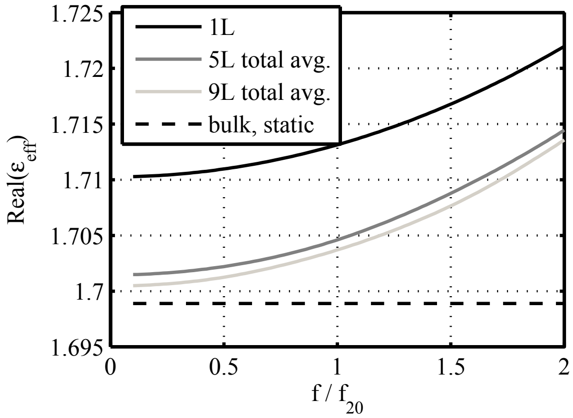

Fig. 8. The effective permittivity (real part) retrieved by f eld integration.

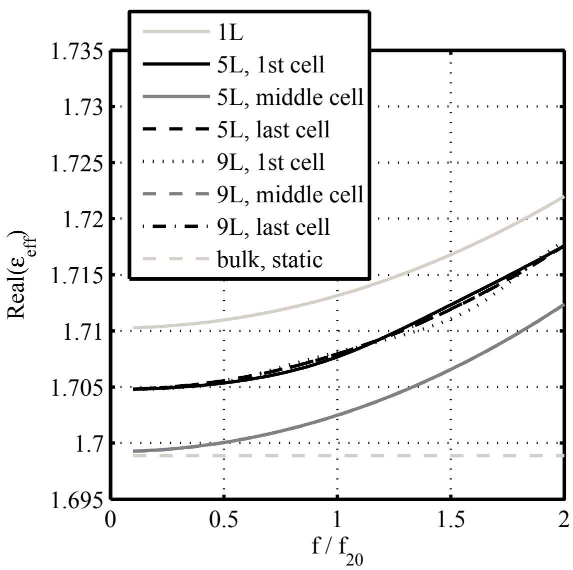

Fig. 9. The effective permittivity values retrieved by f eld integration in different unit cells.

Whereas the previous method observed the material from the outside, another approach is to consider the constitutive relation within the material. In each individual point $\mathbf{D}(\mathbf{r}) = \epsilon(\mathbf{r})\mathbf{E}(\mathbf{r})$. Then, if averaged over the whole material, the relation between the displacement current $\mathbf{D}$ and the electric f eld $\mathbf{E}$ is def ned by the effective permittivity, $\langle\mathbf{D}\rangle = \epsilon_{\text{eff}}\epsilon_0\langle\mathbf{E}\rangle$.

Field averaging is studied, for instance, in [16]. We, however, choose a very simple and straightforward procedure where the f elds are averaged by volume integration over each unit cell. Actually, due to the symmetry and linearly polarized normally incident plane wave excitation, one quarter of a cell is needed. The effective permittivity of a unit cell is obtained by

$$\epsilon_{\text{eff}} = \frac{\langle D_t\rangle}{\epsilon_0\langle E_t\rangle} = \frac{\int D_t dV}{\epsilon_0 \int E_t dV}, \tag{7}$$

where subscript t refers to the component transverse to the wave propagation. Finally, for the whole slab, the permittivities of separate cells are averaged once more over all consecutive layers. Figure 8 presents the retrieved permittivities for different slabs.

This method allows us to investigate the permittivity separately in each cell. It turns out that there are only three different kinds of cells, as can be seen in Fig. 9. In a one-layered case, the unit cells do not have any neighboring cells around them. This situation yields the highest permittivity value. Another case are the layers on the boundary that have neighbors on one side and the third group are the cells inside the slabs with neighbors on both sides. All the interior cells give the same permittivity, although only the values of the midmost cells are plotted in Fig. 9. The boundary permittivity is higher than the interior permittivity. At the static limit, the interior permittivity tends to the bulk value given by static mixing formulas. The values of the boundary and interior permittivities do not depend on the number of layers.

These results support the theory of boundary transition layers, which suggests that the effective model of the homogenized material should include separate boundary layers with permittivity different from the interior material [7]. This boundary permittivity becomes higher than the bulk value and the suff cient thickness of the transition layer would be one unit cell, which is in agreement with previous literature [17, 18]. Also, [18] suggests a modif cation to the Maxwell Garnett formula for computing the static transverse boundary permittivity. Unfortunately, the volume fraction $p = 1/4$ considered in our study is too large for the MG formula, Eq. (2), to give accurate results. Nonetheless, the predicted difference between the boundary and the bulk permittivities becomes 0.006, which quantitatively agrees with the difference seen in Fig. 9 very well.

VI. COMPARISON BETWEEN THE METHODS

Figure 10 presents the effective permittivities retrieved by different methods. The original S-parameter method (NRW) is suffering from the

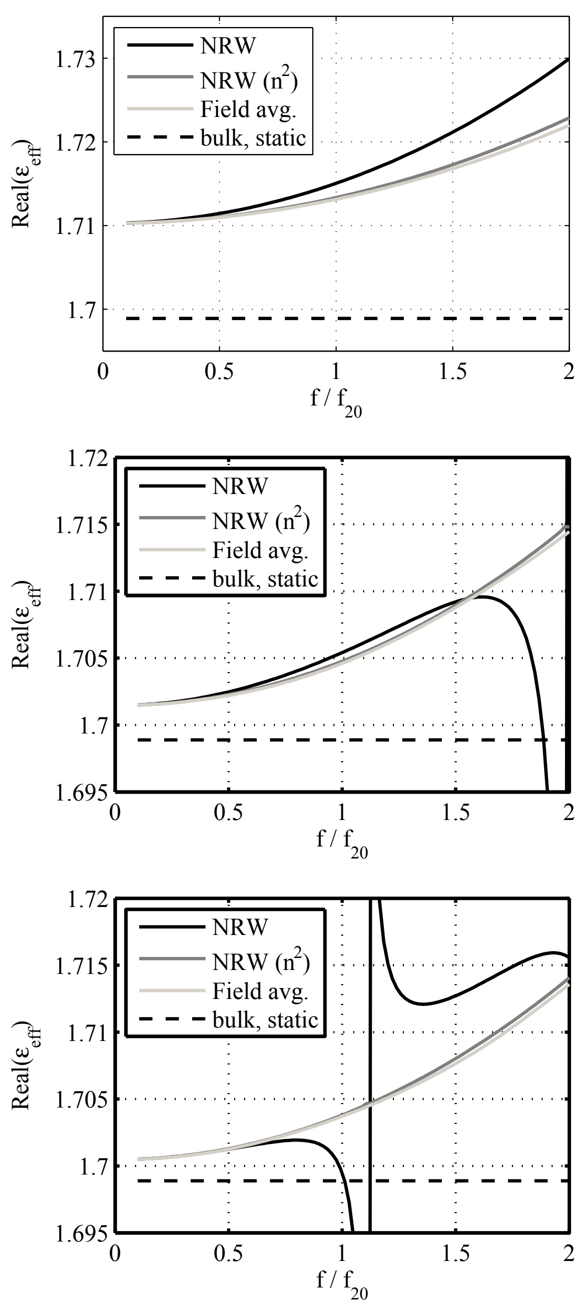

Fig. 10. Comparison of the retrieval methods for a slab with 1 layer (top), 5 layers (middle), and 9 layers (bottom).

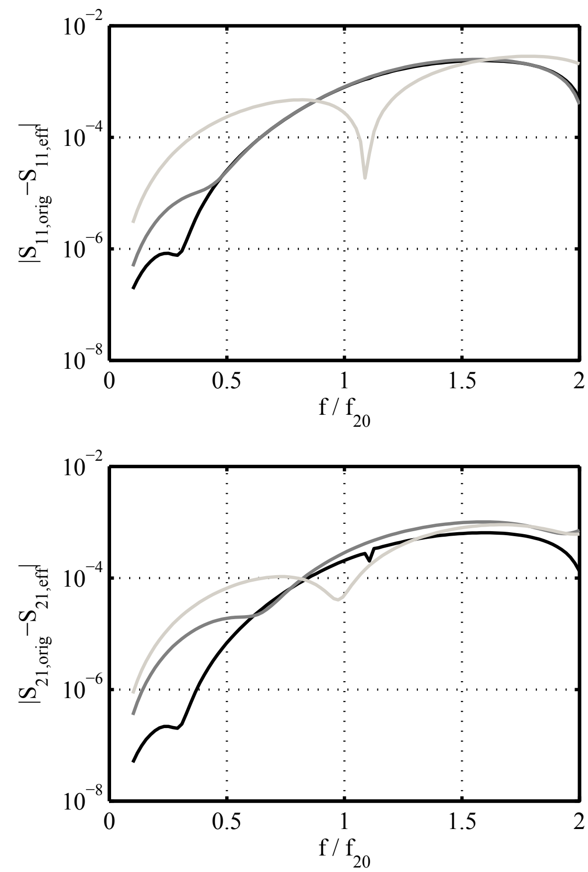

Fig. 11. The absolute error between the S_{11} (top) and S_{21} (bottom) of the original 9-layered composite slab and the homogenized model. The used models: modified NRW with $\epsilon_{\text{eff}} = n^2$ (black), field averaging method (grey), and boundary transition layer model (light grey).

Fabry–Pérot resonances that also contaminate the retrieval results. Increasing the slab thickess makes the resonances shift lower in frequency. Despite the nonmagnetic nature of the original composite, the method also yields effective permeability μ_{eff}, which, with increasing frequency, starts to deviate from unity. Moreover, the retrieved parameters show unphysical behavior. Instead, assuming $\mu_{\text{eff}} = 1$ and computing ϵ_{eff} as the square of the refractive index n gives smooth results that are very similar to the ones given by the field averaging method. In the static limit, all methods tend to the same value. This value depends on the number of layers.

Altogether, based on two different methods, we have four ways to build the homogenized model for the composite slab: the original NRW approach with both $\epsilon_{\text{eff}} = n/z$ and $\mu_{\text{eff}} = nz$, the modified NRW with $\mu_{\text{eff}} = 1$ and $\epsilon_{\text{eff}} = n^2$, the field averaging method with homogeneous ϵ_{eff} for the whole slab, and the piecewise homogeneous model with separate transition layers with different permittivity. If the effective model is correct, it should also have the same scattering properties as the original composite. It turns out that the other models but the original NRW do not exactly reproduce the original S-parameters.

Figure 11 presents the absolute differences between the simulated S-parameters of the original slab and the different homogenized models in the case of 9 layers. The errors are anyway relatively small, yet not numerically negligible, and they start to grow with increasing frequency. Also, there are no significant differences between the models.

VII. CONCLUSIONS AND DISCUSSION

Two different computational methods for homogenization of thin composite slabs were considered and compared, namely the S-parameter (NRW) method and the field averaging method. Both techniques also offered modified ways to model the effective permittivity, in S-parameter method by the non-magnetic material assumption and in the averaging method by using the boundary transition layers. The original NRW method yielded both ϵ_{eff} and μ_{eff} resonant and unphysical violating the principles of causality and passivity. When $\mu_{\text{eff}} = 1$ was assumed and the permittivity computed as $\epsilon_{\text{eff}} = n^2$, the result was smooth and similar to the one obtained by field averaging. The field averaging method, however, suggested a piecewise homogeneous model where the boundary layers are modeled separately using slightly higher permittivity.

When the frequency, *i.e.*, the electrical size of the unit cells, was increased, neither of the methods proved superior. However, important fundamental conclusions can be drawn.

Firstly, for homogenization purposes, the electrical size of the unit cell should be very small. As seen in Fig. 11, with increasing frequency, the homogenized models fail to produce the same scattering parameters with the original composite slab. Our results suggest that the unit cell size $a \approx \lambda/20$, where λ is the reduced wavelength inside the material, is a limit, after which the material cannot safely be considered perfectly homogeneous. Futhermore, from Figs. 5–10 we see that the cells must be extremely small, $a \approx \lambda/100$, before the (quasi)static state is reached. Naturally, in practical experiments a certain tolerance for an acceptable error must be defined. In our case, the absolute differences are small numbers and in many cases they may seem negligible. The focus of this paper is, however, to find fundamental limitations of material homogenization approach in general, and to discuss the characteristics of different homogenization methods.

Secondly, the value of material parameters should not depend on the amount of the material. A sufficient amount of layers is required for the slab to behave as a bulk material. From Fig. 10, it is seen that not even the 9-layered slab exactly converges to the bulk value. This is explained by the effect of the boundary layers, which have higher permittivity than the interior layers increasing the total average permittivity of the slab. That is, a homogeneous material should include enough layers in order to make the boundary effect negligible. A slab with only one or two layers cannot be considered a material at all.

Moreover, considering the applicability of the original NRW method, we see from Fig. 10 that we must operate with frequencies where the electrical thickness of the slab remains below $\lambda/2$. However, at the same time, the thickness must be large enough in terms of unit cell layers for the slab to resemble bulk material. These two limitations roughly imply that for reliable usage of the NRW technique, the slab thickness should be at least 10 layers or more, which means that the maximum unit cell size should be of the order of $\lambda/50$.

Furthermore, the current study is still restricted focusing only on dielectric composite and the normal incidence. By considering oblique incidence from different angles, possible effects of anisotropy and spatial dispersion could be studied. Also, assuming the composite non-magnetic, non-dispersive, and lossless is quite an idealization. Moreover, especially in metamaterials research, the inclusions are assumed strongly dispersive and resonant having also negative material parameter values. In these more complex cases, extra care must be taken that the assumption of effective homogeneity holds. Therefore, futher fundamental study is needed.

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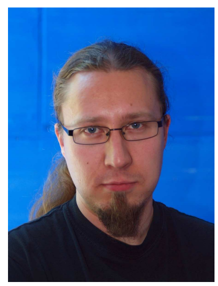

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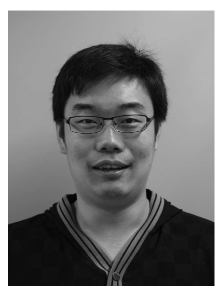

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