On the Homogenization of Thin Isotropic Layers

Sergei A. Tretyakov and Ari Henrik Sihvola

***Abstract*—Homogenization of extremely thin dielectric or composite layers is considered. Special attention is focused on the fact that the permittivity near the surface of the slab is affected by the presence of the boundary. This makes the effective permittivity inhomogeneous, and the slab becomes effectively anisotropic. The anisotropy effect cannot be neglected for slabs whose thickness is on the order of the depth of one molecular or inclusion layer. The analysis results in approximate second-order boundary conditions, which describe electromagnetic properties of the layer. Numerical examples show that the effect in reflection coefficient cannot be neglected if the depth of the boundary layer is a quarter of the slab thickness. Also, the magnitude of the boundary effect increases for higher slab permittivities.**

***Index Terms*—Material modeling, surface effect, thin layers.**

I. Introduction

COMPOSITE materials carry an important role in present-day high-technology applications. By mixing different materials in a clever manner, one may be able to manufacture synthetic materials with desired electric, magnetic, and even magnetoelectric properties. Mixing rules to homogenize bulk materials are available, and the literature is extremely rich in papers that discuss effective medium properties of heterogeneous materials.

In many practical applications, however, a composite cannot be treated as a sample of uniform bulk medium. For example, in thin-film technology, the material samples have extremely large surface area and the surface effect has to be given attention. In solid-state studies, surface phenomena have been studied: for example, analyses of the polariton modes show the surface effect on the dispersion of the polarization [1]. Although surface science is a large discipline in its own right, not much discussion on the surface effects appears in the literature of mixing models. Two-dimensional mixtures, i.e., thin layers as result from the homogenization in the plane, have been analyzed [2]; however, there the surface-to-bulk transition is not considered. Numerical simulations of this transition based on summation of quasi-static dipole fields [1] and on the planar percolation model [3] are available in the literature.

Our aim in this paper is to give a simple analytical model for the surface effect for thin-layer composites. The fact that the layer to be analyzed is thin means that it is considerably smaller than the wavelength of the incident electromagnetic field, and in the extreme case the thickness of the slab to be treated can be only a few layers of molecules or other inclusions that are the building blocks of the composite. The transverse plane is considered infinite, and the composite is homogeneous along the transverse directions. Inclusions or molecules are assumed to be randomly distributed. For consideration of the surface effect in regular lattices, we refer to [4] and the references therein.

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II. Theory

When considering interaction of electromagnetic fields with thin composite layers, two distinct length scales should be taken into account. One of them is the inclusion or molecular size as compared to the layer thickness. We assume that the layer is *thin* in the sense that its thickness is comparable with the molecular size. As will be shown in Section II-B, this means that the permittivity and permeability are inhomogeneous across the slab although the inclusion concentration is uniform. The other scale is the wavelength as compared to the layer thickness. Here we study *thin* layers also in the sense that the thickness is small compared to the wavelength. This means that in calculations of reflection and transmission coefficients, effectively inhomogeneous permittivity and permeability can be averaged across the slab, as is done in Section II-A. For thin (in the first sense) layers, the surface effect is important and can be seen even from the reflection and transmission of waves of large wavelength.

A. Averaging the Field Equations

Assume that a thin slab can be modeled as a layer whose permittivity and permeability depend on the distance to the layer boundary. The reason for this model of a homogeneous slab is that the local field needed in the homogenization process inside the layer is different from that close to the layer boundary. Furthermore, the way the surface polarizability affects the overall permittivity is different for field excitation parallel and perpendicular to the plane of the slab. Thus, the effective material parameters of the slab are symmetric uniaxial dyadics whose axis is normal to the interfaces.

The averaging can be done extending the approach of [5, Section 6.2] to uniaxial slabs. That method is based on the assumption that for thin slabs[1] the distribution of the tangential components of the fields inside the slab can be approximately found from the quasi-static equations; see details in [6] and [8]. For that purpose

$$\nabla \cdot [\epsilon(z) \nabla \phi(x, y, z)] = 0 \tag{1}$$

for the scalar potential ϕ is solved; see [5]. Here the coordinate z is normal to the slab boundaries. This determines the tangential field distribution in the slab and the relation between the averaged field values and that just on the slab boundaries. Wave propagation along the slab (that is, dependence on the x and y

[1]More precisely, for slabs whose thickness d satisfies $|\beta| d \ll 1$, where β is the normal component of the wavevectors in the slab.

coordinates) is governed by the usual time-dependent Maxwell equations.

The final result can be expressed in terms of generalized second-order boundary conditions for the slab [5], [7], [8]. Simple generalization for the case when the material is uniaxial with the axis normal to the interfaces leads to the following conditions:

$$\mathbf{E}_{t+} = \mathbf{E}_{t-} + j\omega\hat{\mu}_t d \left(\overline{\overline{I}}_t + \frac{1}{\omega^2 \hat{\mu}_t \breve{\epsilon}_n} \nabla_t \nabla_t \right) \cdot \mathbf{n} \times \mathbf{H}_{t-} \tag{2}$$

$$\mathbf{n} \times \mathbf{H}_{t+} = \mathbf{n} \times \mathbf{H}_{t-} + j\omega\hat{\epsilon}_t d \left(\overline{\overline{I}}_t + \frac{1}{\omega^2 \hat{\epsilon}_t \breve{\mu}_n} \mathbf{n} \times \nabla_t \, \mathbf{n} \times \nabla_t \right) \cdot \mathbf{E}_{t-} \tag{3}$$

where $\mathbf{n}$ is the unit vector normal to the interfaces and $\mathbf{E}_{t\pm}$ and $\mathbf{H}_{t\pm}$ are the tangential fields on the interfaces between the layer and the surrounding space. Indexes $\pm$ refer to the opposite sides of the layer. $\overline{\overline{I}}_t$ is the two-dimensional unit dyadic defined in the interface plane, and ∇_t is the two-dimensional gradient operator. The averaged material parameters that appear in these equations can be interpreted as the normal and transversal components of permittivity and permeability,[2] which read

$$\hat{\epsilon}_t = \frac{1}{d} \int_0^d \epsilon_t(z)\, dz \tag{4}$$

$$\breve{\epsilon}_n = d \left(\int_0^d \frac{dz}{\epsilon_n(z)} \right)^{-1} \tag{5}$$

$$\hat{\mu}_t = \frac{1}{d} \int_0^d \mu_t(z)\, dz \tag{6}$$

$$\breve{\mu}_n = d \left(\int_0^d \frac{dz}{\mu_n(z)} \right)^{-1}. \tag{7}$$

Here, d is the thickness of the slab and the subindexes t and n refer to the tangential (parallel to the interface) and normal (perpendicular to the interface) components of the permittivity and permeability dyadics.

There is a simple physical interpretation for the averaging rules (4)–(7). Indeed, because of the stratified one-dimensional geometry of the slab, the averaging is equal to calculating the effective permittivity and permeability of a stack of disks. This is tantamount to solving the problem of the total capacitance of capacitors in series (for the field direction normal to the interface) and in parallel (for tangential field). In the first case the capacitances are additive, and in the latter case their inverses are additive.

The next step is to calculate the averaged parameters in (2) and (3). We consider nonmagnetic slabs for simplicity; hence there is no magnetic polarization and both the normal and tangential averaged components of the permeability are equal to that of free space: $\hat{\mu}_t = \breve{\mu}_n = \mu_0$. The permittivity averaging, on the other hand, needs a more careful treatment.

[2]This interpretation is based on the fact that these averaged quantities appear in the boundary conditions on place of the constant parameters of uniform layers. The averaged fields and displacements are connected in a more complicated manner [5].

B. Local Fields and Local Permittivity

Consider a thin dielectric layer with electric field incident on it. If the permittivity of the layer is modeled as a homogenized medium property along the lines as is done in ordinary material homogenization [9, pp. 366–368], the effective permittivity is different in the part close to the surface from that inside the medium. This is due to the fact that if the layer is so thin that there are only a few layers of molecules across it, we have to take into account that the local field that acts on a given molecule is different for molecules inside the layer and just on its surface.

Consider first the case of an inclusion, or a molecule that is located well inside the layer, such that the surface effects can be ignored. As is well known, the local field $\mathbf{E}_{\text{loc}}$ that is responsible for the dipole moment induced in the particle is the external field $\mathbf{E}_{\text{eff}}$ amplified by the "Lorentzian" contribution from the surrounding polarization $\mathbf{P}$ [10]

$$\mathbf{E}_{\text{loc}} = \mathbf{E}_{\text{eff}} + \frac{1}{3\epsilon_0}\mathbf{P} \tag{8}$$

where the factor of one-third comes from the symmetric assumption for the shape of the inclusion [11]. The permittivity of free space is denoted by ϵ_0.

However, for the molecules just on the surface of the layer, the situation is different. The polarization $\mathbf{P}$ surrounds the inclusion only on one side, and therefore the Lorentzian contribution must be halved

$$\mathbf{E}_{\text{loc}} = \mathbf{E}_{\text{eff}} + \frac{1}{6\epsilon_0}\mathbf{P}. \tag{9}$$

Thus, assuming that the molecules are evenly distributed in the medium with inclusion concentration n, their dipole moments add up to the average electric polarization

$$\mathbf{P} = n\alpha\mathbf{E}_{\text{loc}}. \tag{10}$$

Here, α is the single molecule polarizability, the relation between the exciting field and the dipole moment. Using all these relations, we can write for the permittivity of the layer, depending on the position z

$$\epsilon_t(z) = \epsilon_n(z) = \epsilon_0 + \frac{n\alpha}{1 - n\alpha\gamma(z)/\epsilon_0}. \tag{11}$$

Here, $\gamma(z) = 1/3$ for molecules inside the layer and $\gamma(z) = 1/6$ for the molecules located near the layer surfaces.

It is to be noted that with the molecules near the surface, we mean particles that are very close to the surface but just inside the boundary. Then the effect of the surface polarization is included in the effective field on the same basis as for the molecules well inside the bulk layer.

Regarding the depth of the boundary layer, we assume that it is equal to the width of one layer of molecules. For a cubic lattice, the boundary layer thickness is around the characteristic distance between the particles: $c = n^{-3}$. This assumption is supported by the numerical results of [1], where it has been found that only a few nearest to the surface molecule layers see a different local field from that in the bulk.

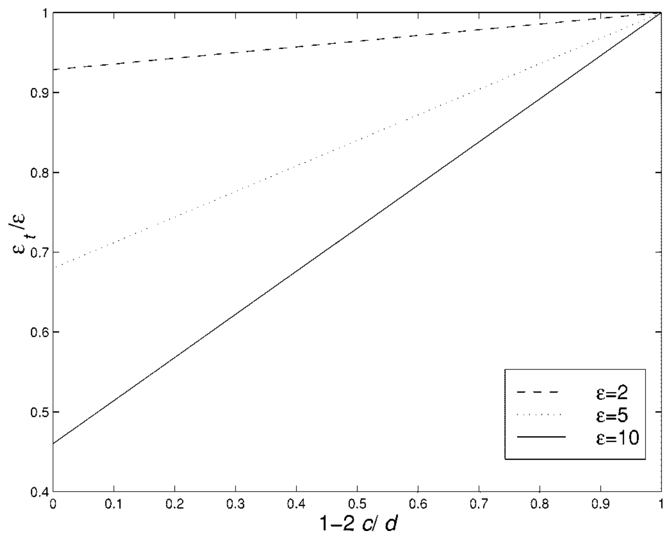

Fig. 1. The averaged transverse permittivity $\hat{\epsilon}_t$ of the slab as a function of the relative fraction of the surface layer within the slab.

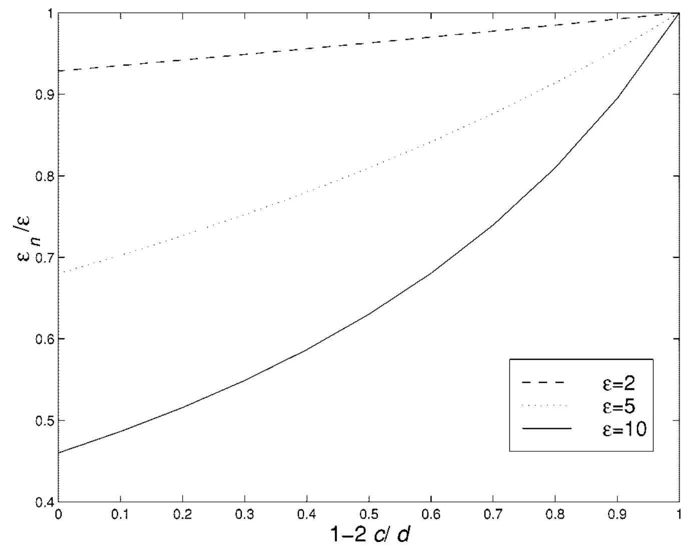

Fig. 2. Averaged normal permittivity $\breve{\epsilon}_n$ of the slab as a function of the relative fraction of the surface layer within the slab.

C. Averaged Permittivity

Now that the permittivity dependence is known as a function of the position within the slab, the normal and tangential components of the permittivity dyadic can be calculated. The boundary layers occupy a volume fraction $2c/d$ of the layer, and the fraction of the internal volume is $1-2c/d$. Evaluation of the integrals in (4)–(7) gives

$$\hat{\epsilon}_t = \epsilon_0 + \frac{n\alpha}{1-\frac{n\alpha}{3\epsilon_0}}\left(1-\frac{2c}{d}\frac{\frac{n\alpha}{6\epsilon_0}}{1-\frac{n\alpha}{6\epsilon_0}}\right) \tag{12}$$

$$\breve{\epsilon}_n = \epsilon_0\frac{1+\frac{2n\alpha}{3\epsilon_0}}{1-\frac{n\alpha}{3\epsilon_0}+\frac{2c}{d}\frac{3\left(\frac{n\alpha}{3\epsilon_0}\right)^2}{2+5\frac{n\alpha}{3\epsilon_0}}}. \tag{13}$$

The latter relation can be approximated for small values of $n\alpha$

$$\breve{\epsilon}_n \approx \epsilon_0 + \frac{n\alpha}{1-\frac{n\alpha}{3\epsilon_0}} - \frac{2c}{d}3\epsilon_0\frac{\left(\frac{n\alpha}{3\epsilon_0}\right)^2\left(1+\frac{2n\alpha}{3\epsilon_0}\right)}{\left(1-\frac{n\alpha}{3\epsilon_0}\right)^2\left(2+\frac{5n\alpha}{3\epsilon_0}\right)}. \tag{14}$$

Using the relation between the relative bulk permittivity ϵ_r and inclusion polarizability α

$$\frac{n\alpha}{3\epsilon_0} = \frac{\epsilon_r-1}{\epsilon_r+2} \tag{15}$$

we can express the above result in another form

$$\frac{\hat{\epsilon}_t}{\epsilon_0} = \epsilon_r - \frac{2c}{d}\frac{(\epsilon_r-1)^2}{\epsilon_r+5} \tag{16}$$

$$\frac{\breve{\epsilon}_n}{\epsilon_0} = \frac{\epsilon_r}{1+\frac{2c}{d}\frac{(\epsilon_r-1)^2}{7\epsilon_r-1}}. \tag{17}$$

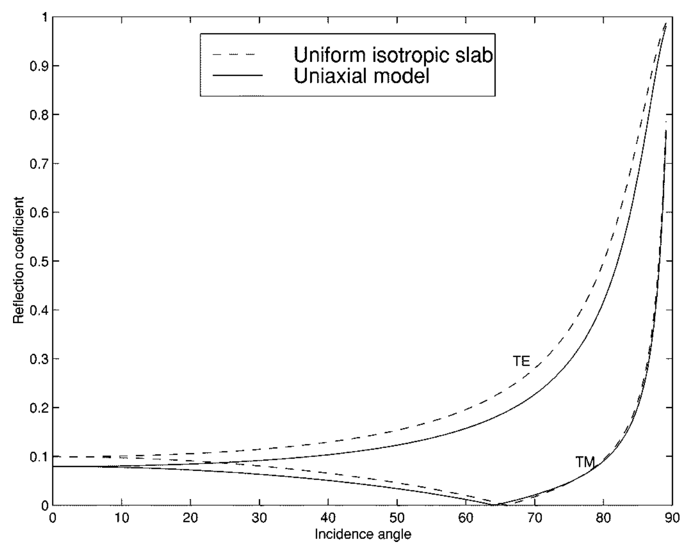

Fig. 3. Absolute values of the reflection coefficient from a thin slab in air. The relative bulk permittivity value is 5. One surface layer occupies a quarter of the slab thickness.

III. Numerical Examples

Figs. 1 and 2 show the dependence of the effective averaged permittivities (transverse and normal components) as functions of the relative thickness of the boundary layer. The natural limit case is when the layer becomes thick enough: both components tend to the bulk values of the permittivity because the boundary effect loses its significance. The surface effect is more pronounced for media with high permittivity values. These theoretical results are in qualitative agreement with the numerical simulations for the effective conductivity of thin films that are reported in [3]. Unfortunately, the quantitative comparison is not possible because polarizabilities of single inclusions are not specified in [3]. It is interesting to note that when the slab gets extremely thin (zero value of $1-2c/d$), both the transverse and normal components take equal values and the slab is effectively isotropic. This is because the local permittivities (11) are indeed isotropic. Also, the bulk values (corresponding to $1-2c/d=1$)

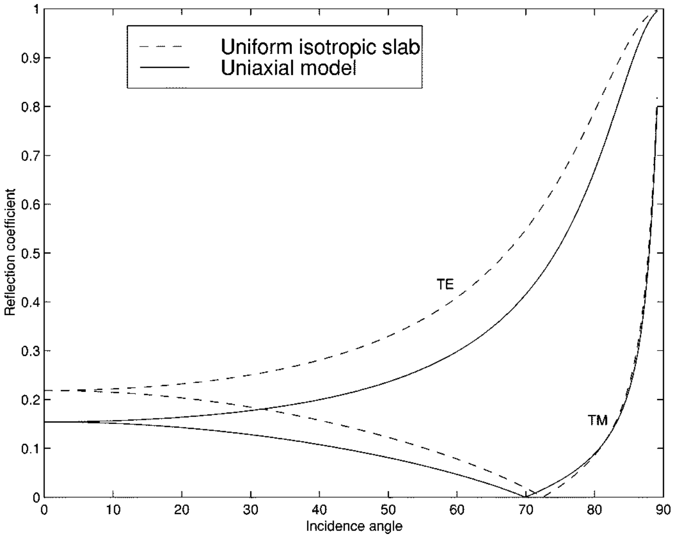

Fig. 4. Absolute values of the reflection coefficient from a thin slab in air. The relative bulk permittivity value is ten. One surface layer occupies a quarter of the slab thickness.

are isotropic. In the general case when the surface effect is essential, the slab is effectively uniaxial.

Numerical examples showing the reflection coefficient from a thin dielectric layer in air are given in Figs. 3 and 4. The relative permittivity of the slab material (as defined for bulk samples) is taken to be five or ten. The normalized layer thickness is $k_0 d = 0.05$ ($k_0 = \omega\sqrt{\epsilon_0\mu_0}$ is the free-space wave number). The ratio $c/d = 0.25$. For the slab with the bulk relative permittivity equal to five, we have $\hat{\epsilon}_t = 4.2\epsilon_0$ and $\check{\epsilon}_n = 4.05\epsilon_0$; the other case, $\epsilon_r = 10$, corresponds to numbers $\hat{\epsilon}_t = 7.3\epsilon_0$ and $\check{\epsilon}_n = 6.3\epsilon_0$.

To illustrate the strength of the surface effect, the reflection curves for a slab of the uniform permittivity are also shown in these figures. These are slabs with isotropic and homogeneous permittivity $\epsilon_r = 5$ and 10, respectively. We observe that the reflection coefficient is smaller if the nonuniform nature of the local field is taken into account. This is because the surface effect decreases the averaged permittivity, both components of it. The figures show that the effect of the nonhomogeneity of the local field is quite essential for the present examples.

IV. Conclusion

This paper has given a simple physical model for the dielectric surface effect in slabs that are thin with respect to the wavelength of the field, such that the surface-wave effects can be neglected. The fact that the local field acting on the furthermost molecules or inclusions at the surface is smaller than those well inside the material leads to inhomogeneity of the effective permittivity across the slab. Therefore the slab is anisotropic because of the different averaging principle for the parallel and perpendicular polarizations of the incident electromagnetic wave. This effect is solely due to the presence of the boundary since homogenization of bulk samples leads to isotropic material relations. The numerical results show a visible surface effect in the homogenized permittivity values when one surface layer occupies a quarter of the slab thickness.

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