Modeling of Effective Dielectric Properties of Composites using Expansion into Fourier Series and Finite Element Model

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1. INTRODUCTION

Composite materials consist of two or more constituents which differ in physical properties. They can be prepared in many ways leading to a large variety of morphologies. The morphology of a composite has a big influence on its macroscopic behaviour. Therefore, the relation between the morphology and resulting physical (e.g., dielectric, thermal, elastic etc.) properties is of a great practical importance.

With a big progress in computer technology in recent years, morphology of composites and prediction of their macroscopic behaviour have become an attractive object for computer modelling [3, 4]. Space distribution of the dielectric constant in a periodic composite can be prescribed in two ways:

1. explicitly, i.e. $\epsilon(x,y) = \epsilon_a$ in the matrix and $\epsilon(x,y) = \epsilon_b$ in the inclusion,
2. and using an expansion into Fourier series.

While the former method is straightforward for composites of simple morphologies (spherical, cylindrical inclusions), the latter one can be useful in case of complex morphologies (e.g. gyroidal). The objective of this study is an investigation of the Fourier series method for using in Finite Element Method (FEM).

2. ELECTROSTATIC

Introducing	the scalar electric potential	Φ
	the electric field intensity	$E = \nabla\Phi$
	the material permittivity	ε
	the polarization vector	P
	the electric displacement	$D = \varepsilon.E + P$
	the electric space charge density	ρ
and	the Maxwell's equation	$\nabla.D = \rho$

the problem of electrostatic results in solving the differential equation

$$-\nabla.\ (\varepsilon.\nabla\Phi - P) = \rho \quad \text{in } \Omega, \tag{1}$$

associated with boundaries conditions that can be written as a Neuman condition, $-n.D = \rho_S$, where ρ_S is the surface charge, or a Dirichlet condition, $\Phi = U$, where U is a fixed potential.

Finite Element Model

Starting by converting the differential problem to its weak form, the Finite Element Method consists on approximating the problem (1) on finite space, meshing its geometry using simple geometric elements associated with a finite number of linear forms L_i. For instance linear forms in *Lagrangian elements* associate any function to its values at the geometric elements' vertexes. Hence, instead of looking for the exact solution Φ of the problem (1), we look for a finite number of potential's values (the ones at the mesh's nodes). Moreover the definition of finite elements is coupled with the definition of *shape functions* s_i fulfilling the conditions $L_i(s_j) = \delta_{ij}$. Since shape functions form a base for the finite dimensional space in which approximated solution is looked for, we can substitute them for test functions occuring in the variational form. Calculations in the present work were performed using FEM software package FEMLAB of company COMSOL [5].

Homogeneisation

We consider a biphasic material constituted of matrix and inclusions with respective permittivities ε^a and ε^b. Homogeneisation consists on finding the permittivity ε^{eff} of an 'equivalent' homogeneous material, i.e. a material which would need the same among of energy as the considered biphasic one when they undergo the same test:

$$W^{hom}(\varepsilon^{eff}) = W^{biph}(\varepsilon^a, \varepsilon^b), \tag{2}$$

where W is the total stored electric energy defined as

$$W = \frac{1}{2}\int_\Omega (\varepsilon.\nabla\Phi).\nabla\Phi\ dx, \tag{3}$$

with Φ solution of the problem (1) respectively applied to the biphasic or homogeneous body.

Identification method

Effective permittivity ε^{eff} is a matrix whose components can be determined providing following computering testes.

• The diagonal component ε^{eff}_{kk} ($k \in \{1..d\}$, d=1,2 or 3 is the space dimension) is determined imposing a constant difference of potential U between the capacitor plates on the k-direction while assuming periodic conditions in all other directions as shown on the figure Fig. 1. Indeed, because of symmetries, $\Phi = \Phi(x_k)$ and (3) leads to

$$\varepsilon^{eff}_{kk} = \frac{2\ h_k\ W}{S_k\ U^2} \tag{4}$$

where $h_k = x_k^{max} - x_k^{min}$, S_k is the surface normal to the k-direction and $W = W^{biph}$ has to be previously calculated for the exact composite material using the Finite Element Method. Such a test is repeated changing the preferential direction $k \in \{1..d\}$ to determine all diagonal components.

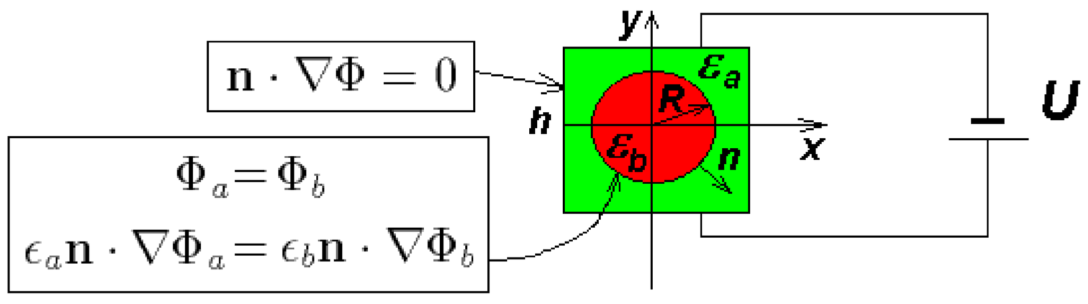

Fig. 1: Unidirectional model capacitor as a periodic biphasic material.

• The extra-diagonal component ε^{eff}_{kp} is determined making the difference of potential U on the k-direction dependent on the space variable x_p ($p \in \{1..d\}$, $p \neq k$), i.e. $U = U(x_p)$. Indeed, because of the symmetries, $\Phi = \Phi(x_k, x_p)$ and (3) leads to

$$\varepsilon^{eff}_{kp} = \frac{1}{2}\left(2W - \varepsilon^{eff}_{kk}\int\left(\frac{\partial\Phi}{\partial x_k}\right)^2 dx - \varepsilon^{eff}_{pp}\int\left(\frac{\partial\Phi}{\partial x_p}\right)^2 dx\right)\left(\int\frac{\partial\Phi}{\partial x_k}\frac{\partial\Phi}{\partial x_g}dx\right)^{-1} \tag{5}$$

since the permittivity matrix is symmetric, i.e. $\epsilon^H_{kp} = \epsilon^H_{pk}$. This test is done only once if $d = 2$. If $d = 3$, it has to be repeated changing the values of k and p in $\{1,3\}$, $k \neq p$.

3. EXPANSION INTO FOURIER SERIES

Let us consider a periodic function f of the d-dimensional orthogonal space with period h_p in the p-direction, $p \in \{1, d\}$, having real values in [0,1], i.e.

$$f : [-h_1/2, h_1/2] \times .. \times [-h_d/2, h_d/2] \to [0,1]$$

This function can be approximated by its expansion into **Fourier series** $\mathcal{F}$, i.e.

$$\lim_{N_p\to\infty,\ \forall p\in\{1,d\}} \mathcal{F} = f, \tag{6}$$

with

$$\mathcal{F}(x_1,..,x_d) = \sum_{n_1=-N_1}^{+N_1} .. \sum_{n_d=-N_d}^{+N_d} e(n_1,..,n_3) S(n_1,..,n_d) \exp\left(2\pi\ i\ \sum_{p=1}^{d}\frac{n_p\ x_p}{h_p}\right), \tag{7}$$

where N_p, n_p are integers, $e(n_1,..,n_3)$ are filters defined as

$$e(n_1,..,n_3) = \exp\left(-2\pi^2\ \sigma_0^2\ \sum_{p=1}^{d} n_p^2\right), \tag{8}$$

where $\sigma_0 < 1$ is the so-called sharpness of the interface, and the Fourier coefficients $S(n_1,..,n_3)$ are defined as

$$S(n_1,..,n_3) = \frac{1}{\prod_{p=1}^d h_p}\int_{-h_1/2}^{h_1/2} .. \int_{-h_d/2}^{h_d/2} f(x_1,..,x_d)\exp\left(-2\pi i\sum_{p=1}^{d}\frac{n_p x_p}{h_p}\right)dx_1..dx_d, \tag{9}$$

It can be noticed that even if the coefficients $S(n_1,..,n_3)$ are complex, the series $\mathcal{F}(x_1,..,x_d)$ is a real number because the coefficients are conjugate one to an other. For instance

$$S(n_1,..,n_d) = \overline{S(-n_1,..,-n_d)},$$
$$S(-n_1,..,-n_p,n_{p+1},..,n_d) = \overline{S(n_1,..,n_p,-n_{p+1},..,-n_d)},$$

and so on.

General biphasic material

Considering a composite body constituted of two isotropic materials, the space distribution of permittivity $\varepsilon(x) = \epsilon\ \mathbf{Id}$ can be approximated using the Fourier series

$$\frac{\epsilon}{\epsilon^a} = 1 + \left(\frac{\epsilon^b}{\epsilon^a} - 1\right)\mathcal{F}(x_1,..,x_p), \quad x_p \in [-h_p/2, h_p/2], \quad p \in \{1,d\}. \tag{10}$$

with $\mathcal{F}$ defined in (7). In general case, the coefficients $S(n_1,..,n_d)$ do not have analytic expressions. However they can always be numerically approached. Numerical integration consists on summing areas being calculated on $M_p - 1$ intervals $[x_p^{j-1}, x_p^j]$, $j \in \{2, M_p\}$, obtained from a discretisation of $[-h_p/2, h_p/2]$, i.e.

$$S(n_1,n_2,n_3) = \frac{1}{2^d}\sum_{j_1=2}^{M_1} .. \sum_{j_d=2}^{M_d}\left(\prod_{p=1}^{d}\frac{x_p^{j_p} - x_1^{j_p-1}}{h_p}\right)\sum_{\delta_1=0}^{1} .. \sum_{\delta_d=0}^{1} g(x_1^{j_1-\delta_1}, .., x_d^{j_d-\delta_d}), \tag{11}$$

with

$$g = f\ \exp\left(-\pi\ i\ \sum_{p=1}^{d}\frac{2\ n_p\ x_p}{h_p}\right). \tag{12}$$

With $d = 2$ the expression (11) becomes

$$S(n_1,n_2) = \sum_{j_1=2}^{M_1}\sum_{j_2\geq 2}^{M_2}\frac{(x_1^{j_1} - x_1^{j_1-1})(x_2^{j_2} - x_2^{j_2-1})}{4h_1h_2}\ [g(x_1^{j_1}, x_2^{j_2}) + g(x_1^{j_1-1}, x_2^{j_2})$$
$$+ g(x_1^{j_1}, x_2^{j_2-1}) + g(x_1^{j_1-1}, x_2^{j_2-1})].$$

4. RESULTS

We illustrate the effective dielectric behaviour of periodic composites by a model 2D capacitor of the size of square elementary composite cell with edges of the length h filled by matrix and inclusion of circular shape with radius R - see Fig. 2.

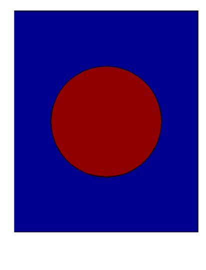

Fig. 2: Single circular inclusion in matrix.

Such a geometry leads a to isotropic effective permittivity which value is determined applying unidirectional gradient of external potential and assuming periodic conditions along the perpendicular direction as given in equation (4). Nevertheless dielectric constant of periodic composites with such morphology is known and given by the asymptotic formula [1, 2]

$$\frac{\epsilon^{eff}}{\epsilon^a} = 1 + \frac{2\beta\ v^b}{1 - \beta\ v^b - 0.305827\ \beta^2\ {v^b}^4 + ...}, \qquad \beta = \frac{\epsilon^a - \epsilon^b}{\epsilon^a + \epsilon^b} \tag{13}$$

where v^b is the volume fraction of inclusions, i.e. $v^b = \pi R^2$.

Result of the homogeneisation is illustrated on the figure Fig. 3 as the evolution of the relative effective permittivity $\epsilon^{eff}/\epsilon_a$ with the inclusion radius R for various values of the relative inclusion permittivity ϵ_b/ϵ_a. Analytic solution (13) is plotted as solid lines while the numerical result (4) is marked with triangles, circles and stars. The energy W entering is the latter expression is calculated solving the Maxwell equation on composite body using the Finite Element Method. It is worth noticed that both analytical and numerical results exactly coincide.

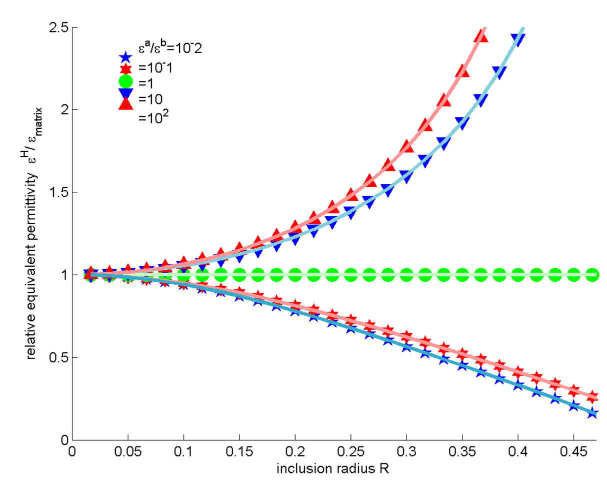

Fig. 3: Relative effective permittivity $\epsilon^{eff}/\epsilon_a$ v.s. inclusion's radius with $\epsilon_b/\epsilon_a = 4$.

Five inclusions model

The method can be generalized in modeling effective properties of periodic composites with more complex morphologies, as for example a square element filled by matrix and 5 circular inclusions at center and corners - see Fig. 4. Comparison of space distribution of dielectric constant simulated by the above methods is given in Fig. 4 and Fig. 5. The including of the smoothness parameter leads to more realistic space distribution except the proximity of interphase. Fig. 6 shows the dependence of the effective dielectric constant obtained by FEM using two ways of the simulation of the space distribution of dielectric constant. A systematic error is obtained when smoothness parameter is used.

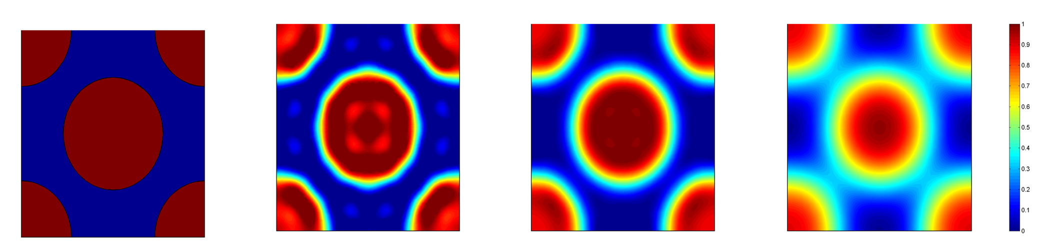

Fig. 4: Space distribution of the dielectric constant (left figure) and its expansion into Fourier series (from the right to the left: without filter, and filtered with smoothness parameter $\sigma_0 = 0.05$ and $\sigma_0 = 0.1$)

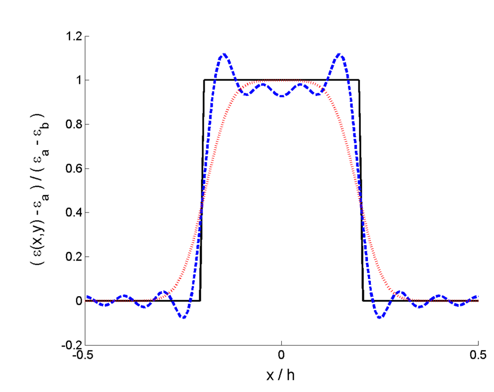

Fig. 5: Space distribution of the relative dielectric constant $\frac{\epsilon(x,y)-\epsilon_a}{\epsilon_b-\epsilon_a}$ in cross-section $y = 0$ (black full line) with $R/h = 0.2$, and its expansion into Fourier series without filter (blue dash line) and filtered with smoothness parameter $\sigma_0 = 0.05$ (red dot line).

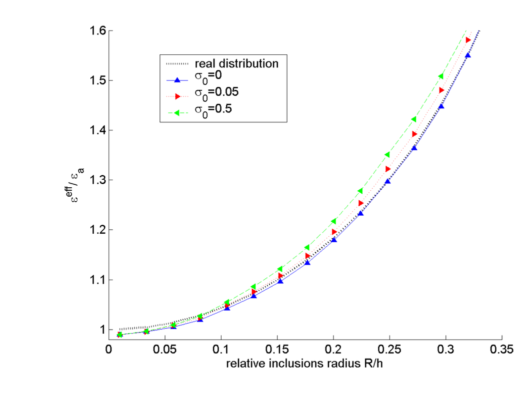

Fig. 6: Relative effective permittivity $\epsilon^{eff}/\epsilon_a$ v.s. inclusion's radius with $\epsilon_b/\epsilon_a = 4$ using the real permittivity distribution (black full line) and its expansion into Fourier series without filter (marked with blue triangles) and filtered with smoothness parameter $\sigma_0 = 0.05$ (marked with red triangles) and $\sigma_0 = 0.1$ (marked with green triangles)

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