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NUMERICAL COMPUTATION OF DIELECTRIC PERMITTIVITY OF MIXTURES

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Statistic and matrix mixtures were modelled using a FEM based software from the ANSOFT Corporation and their static permittivity was computed. The study presented in this paper emphasizes the influence that shapes, dimensions, distances between particles, filling factor and space distribution of inclusions have upon the static average permittivity of the composite dielectrics. The results of the computations are compared with analytical solution obtained from well-known formulas.

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1. Introduction

Considering the rising importance of composite materials for insulating systems, a precise study of their dielectric properties is required. [1]

An often requirement of engineering consists in manufacturing new materials, with improved properties, for specific applications. This goal can be achieved by designing some dielectric mixtures specially fitted for the desired application. The main problems that need to be studied regard: finding the average permittivity of the mixture when the permittivities and concentrations of the homogenous components are known; studying the relaxation phenomenon that appear in mixtures in order to locate the peaks of dielectric losses. Therefore, the possibility of numerical model composites can be a very useful tool.

The model that we used is called MAXWELL 2(3)D, and it's based on the Finite Element Method. The static permittivity of mixtures (statistical and matrix mixtures, with different shapes, space distribution, sizes and concentrations of the inclusions) was computed using two different methods. Where analytical solution is available, a comparison is done with the numerical results.

2. Theoretical approach

Dielectric properties of mixtures depend on the properties of the components. This section presents the computational methods that we used.

2.1 Numerical approach

The key parameter, which should be obtained for calculation of the dielectric properties of a mixture, is the electric field distribution $E(x,y)$ within a domain. Once this one is known, it can be used in different ways. The equation to be solved in order to obtain this parameter is known as Gauss' law [1, 4]: $\nabla \cdot (\varepsilon_r \varepsilon_0 E(x,y)) = \rho(x,y)$, where $\rho(x,y)$ represents the charge density on the domain. This equation was solved using a FEM based software from the ANSOFT Corporation named *Maxwell 2D*. The average permittivity of the composite can now be computed using one of

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the following two methods:

1. The first method (M1) requires the calculation of the average electric field $\tilde{E}$ and electric flux density $\tilde{D}$ over the entire computational domain, with:

$$\tilde{E} = \frac{1}{\Omega}\int_{\Omega} E d\Omega \qquad \text{and} \qquad \tilde{D} = \frac{1}{\Omega}\int_{\Omega} D d\Omega \tag{1}$$

The average permittivity can now be calculated with the formula:

$$\varepsilon_m = \tilde{D}/\tilde{E} \tag{2}$$

2. The second method (M2) requires the calculation of the electrostatic energy over the computational domain, and the permittivity is obtained from:

$$\frac{1}{2}\varepsilon_m \frac{1}{\Omega}\int_{\Omega} E^2 d\Omega = \frac{1}{\Omega}\int_{\Omega} \frac{1}{2} ED d\Omega \tag{3}$$

The two methods mentioned above led to the results that will be presented in a following section of the paper.

2.2 Analytical approach

In order to compute the average permittivity of mixtures, some formulas are available, formulas based on different models of non-homogenous dielectric. The analytical solutions, obtained with the following formulas, were compared with the numerical ones.

For statistical mixtures, the following formulas are available [1, 5]:

- $\log \varepsilon_m = \sum_i y_i \log \varepsilon_i$ (Lichtenecker – Rother or the logarithmical law of mixtures) (4)
- $\sqrt[3]{\varepsilon_m} = \sum_i y_i \sqrt[3]{\varepsilon_i}$ Landau Lifshitz (5)
- $\varepsilon_m = \frac{1}{2}\left[y_1\varepsilon_1 + y_2\varepsilon_2 + \frac{\varepsilon_1\varepsilon_2}{y_1\varepsilon_2 + y_2\varepsilon_1} \right]$ (Samaharaze), (6)

and for matrix mixtures:

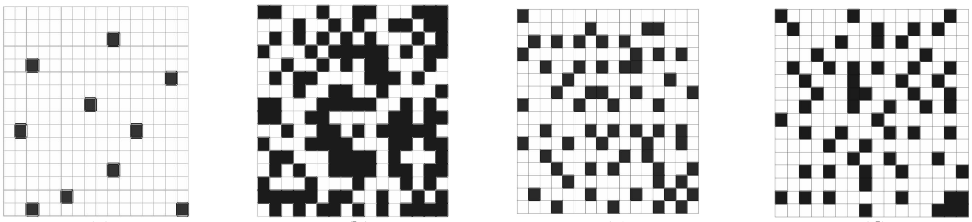
- $\varepsilon_m = \varepsilon_1 \frac{2\varepsilon_1 + \varepsilon_2 + 2y(\varepsilon_2 - \varepsilon_1)}{2\varepsilon_1 + \varepsilon_2 - y(\varepsilon_2 - \varepsilon_1)}$ (Maxwell-Wagner) (7)
- $(1-y)\frac{\varepsilon_1 - \varepsilon_m}{\varepsilon_1 + (d-1)\varepsilon_m} + y\frac{\varepsilon_2 - \varepsilon_m}{\varepsilon_2 + (d-1)\varepsilon_m} = 0$ (Ralph-Landauer) (8)

with *d* being the dimension of the space (*d=2 or 3*).

3. Geometrical model

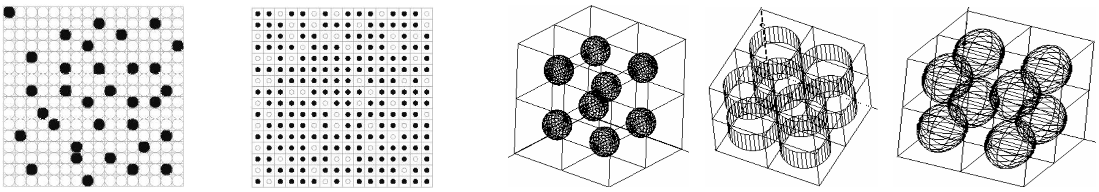
First, statistical mixtures were considered. The disordered media was considered to be a crossword puzzle-like structure. The networks were composed of 16 X 16 cells, and the variation of the permittivity was studied as a function of the number (filling factor) and distribution of inclusions. Fig. 1 displays the considered structures for the lowest and largest filling factor, and also some examples of random structures having the same filling factor.

In order to establish the influence of size and shape of the inclusions, we considered structures with the same filling factor (y_i =0,1) bat with quite different cylinder radius (Fig. 2,a) and structures with spherical, elliptical or cylindrical inclusions (Fig. 2,b). For the last case, the modelling was three-dimensional.



(a) (b) (c) (d)

Fig. 1. Structures with minimum (a) and maximum (b) number of inclusions. Structures with random distribution of the inclusions (c) and (d).



a b

Fig. 2. Structures with: a – cylindrical inclusions of different size for the same filling factor; b – spherical, elliptical and cylindrical inclusions.

Afterwards, ordered structures were considered, the mixture being composed of spatially distributed spherical inclusions in a host media. The host media forms a matrix (16 X 16 elements) with square lattice, a fragment being plotted in Fig. 3.

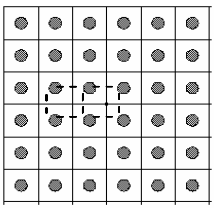


Fig. 3. Square lattice structure. Grey circles represent the inclusions distributed in the host media.

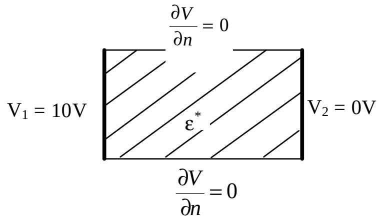


Fig. 4. Boundary conditions assigned to the model.

The filling factor of this structure, *y*, varies from 0,1 up to the maximum possible value 0,785 (when the diameter of the inclusion equals the side of the square cell).

The boundary conditions assigned to the models are presented in Fig. 4 (the material was considered to form the dielectric of a plane capacitor, with constant and uniform internal electric field). The host material has the permittivity $\varepsilon_{r1} = 4$ and the inclusions $\varepsilon_{r2} = 6{,}5$.

4. Results and discussions

The goals of this paper consist in evaluating the average permittivity of mixtures and analysing the influence of various factors. The values obtained for statistical and matrix mixtures – computed analytically and numerically for different concentration of the filler– are emphasized in Table 1.

One can realize that values computed with M1 are larger, and also closer to the analytical solution, than those obtained with M2. For statistical mixtures, the minimum error is established with respect to Lichtenecker formula (0,03% for y_i = 0,039 and 0,36% for y_i = 0,5) and the maximum error with respect to Landau - Lifshitz formula (0,12% respectively 0,62%). For matrix mixtures, the errors with respect to Maxwell–Wagner formula are 0,38% for y_i=0,1 and 1,1% for y_i=0,5.

Table 1. Values of ε_m for statistical and matrix mixtures and different concentration of the filler.

Statistical mixtures					
Lichtenecker	Landau - Lifshitz	Samahadze	M1	M2	Concentration of inclusions
4.076584519	4,082902	4,079335	4.0778179	4.062402	0.0390625
4.234180523	4,252145	4,240883	4.2352363	4.188535	0.1171875
4.482071175	4,514677	4,491119	4.4846462	4.39797	0.234375
4.65534282	4,69557	4,663849	4.6659871	4.554538	0.3125
5.099019514	5,149284	5,10119	5.1173728	4.978366	0.5
Matrix mixtures					
Maxwell - Wagner	Error Landauer– M1	Error Landauer–M2	M1	M2	Concentration of inclusions
4.210526	0.001342	0.004819	4.19467	4.151041	0.1
4.888889	0.004415	0.015104	4.83679	4.683629	0.4
5.132075	0.004792	0.016453	5.075234	4.900267	0.5
5.384615	0.004716	0.016324	5.328452	5.14572	0.6
5.878365	0.002883	0.01022	5.846789	5.719308	0.785

The results of the study regarding the influence of shape and sizes of the inclusions are given in Table 2.

Table 2. Values of ε_m for different shapes and sizes of the inclusions.

Method	Inclusions' shape			Nr. of cylindrical inclusions in a structure for y_i = 0,1				
	sphere	cylinder	ellipsoid	33	80	100	130	200
M1	4.6297	4.59880	4.61337	4.1942	4.19521	4.19441	4.19464	4.1943
M2	4.5332	4.46465	4.53556	4.1506	4.15217	4.15082	4.15112	4.1505

One can notice that lower values for ε_m are obtained for the cylindrical shape of the inclusions, whereas the higher values belong to the spherical shape. Meanwhile, the size of the cylinder radius has little or no influence on the values of ε_m (the error between the maximum and minimum values is about 0.0023% for M1 and 0.0024% for M2).

Finally, we considered 8 different distribution of the inclusions, for y_i = 0,1. The results are given in Table 3. One can see that the influence of space distribution is not significant.

Table 3. Variation of ε_m for different space distributions of inclusions (numerical results).

Structure's number	1	2	3	4	5	6	7	8
M1	4.484646	4.480265	4.482976	4.480672	4.490875	4.490211	4.571502	4.413095
M2	4.397970	4.389486	4.395266	4.390189	4.407595	4.408347	4.556962	4.285807

5. Conclusions

The numerical computation indicates that Lichtenecker's formula (for statistical mixture) and Maxwell – Wagner's formula (for matrix mixtures) are the most appropriate for evaluating the average permittivity. The numerical method M1 is more accurate that M2. The error increases along with the increase of concentration. For the same value of the filling factor (y_i = 0.5) the static permittivity of statistical mixtures is larger than that of matrix mixtures (relative error 0.82%). The influence of shape, size and space distribution of the inclusions is not significant (errors below 6%).

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