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2D Study of Inclusion Shape Effect on the Effective Permittivity of Random Inhomogeneous Media

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ABSTRACT

The effective properties of composite materials are closely related to the shape and arrangement of its constituent phases. In the quasi-static limit, we use the finite element method as a numerical tool to evaluate the effective permittivity of loss-less random composite materials with small grains and short fibers as fillers. The effect of the inclusion shapes as a function of surface fraction is highlighted. The numerical tool used to extract the exact value of the effective permittivity takes into account all internal multipolar interactions which contribute to the polarization of the material medium. The Maxwell-Garnett theory fails to predict the effective permittivity of the studied hetero structures for high permittivity contrast, but, Looyenga and Böttcher mixing rules predict more accurately the short fiber and granular fillers of the composite materials respectively.
KEYWORDS: Random Composite Materials, Finite Element Method, Effective Permittivity, Mixing Rules.

INTRODUCTION

Modeling of composite materials by the empirical mixturerules allowsa universal analysis with saving time and cost, which is of immense importance of viewpoints scientifically and industrial.But the inability of these mixing rules to describe completely the macroscopic behavior of heterogeneous structures which depend strongly on the components parameters makes their application more limited.Numerous fast and efficient numerical methods have been developed. Numerical modeling of composite materials, the computation of their effective permittivity, the accuracy of these methods, time and memory required for calculations are the topics discussed in many works [1-3]. The success of compositematerials is derived from the ability to obtain wide range properties (e. g. electrical, thermal and mechanical) depending on the intrinsic properties of the constituent phases. The macroscopic or effective permittivity is an average property binding the internal topology of the shape and the spatial arrangement of the fillers and their volume or surface fraction. But, the classical mixture rules are unable to predict accurately the dielectric behavior of heterogeneous systems, especially for high contrast permittivity between different phases and for complex shape of inclusions. In contrast, different computational approaches are used to study the dielectric composite materials with complex topology. The Finite-Difference Time-Domain [4-5], Boundary Integral [6-7] and the Finite Element [8-9] are the popular methods employed to analyse random and periodic filler arrangements in heterogeneous structures.

Classical mixing rules, like as Maxwell Garnet, Bruggmann, Böttcher and Looyenga are widely used to evaluate the effective permittivity of such mixtures. These formulae work very well when the contrast between the permittivities of the various phases of the inhomogeneous media is not very large. However, in the case of applications of material engineering, sometimes the composite needs to be constructed with an extremely large electrical contrast and the choice of the mixing theory is problematic. In addition, the inclusion shape is another parameter which has a considerable effect on the effective permittivity.

The aim of this study is to highlight by numerical simulation the impact of the inclusion shape in random composite and to choose what mixture rule is suitable for the case of high contrast within dilute limit. The outline of the paper is as follows: in section I, a brief review of some properties of effective medium approaches and some empirical mixing formulas. Section II, describes the finite-element computational aspects. Section III, reports the results of simulations and comments the effect of filler shapes on the effective permittivity of composite materials and the simulation data are compared with Looyenga and Böttcher mixing rules. Closure is provided in section IV.

I. EFFECTIVE PERMITTIVITY PROPERTY OF HETEROGENEOUS MEDIA

One long-standing issue and rich area of research in the theory of composite materials is the determination of their effective transport coefficients. A principal question with these materials is how the effective permittivity can be evaluated as a function of inclusion shape, their arrangement from the external electric field,

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their volume fraction and the contrast between the permittivities of different phases. Abundant theoretical and computational descriptions of the effective permittivity of two component random or periodic materials do exist. But, in the absence of detailed microstructure characterization, evaluating the effective permittivity is a difficult task with different descriptions, and consequently, to serious errors in interpreting experimental results.

The mixture under study consists of 2D-two dielectric components, of which one is treated as host medium (continuous matrix), and the other inclusion phase with respective permittivities ε_1 and ε_2. The mixture rules and effective permittivity ε_{eff} equations most widely used by practitioners for calculating the bulk permittivity ε_{eff} of inhomogeneous materials are these of Maxwell Garnett [2]

$$\varepsilon_{eff} = \varepsilon_1 \frac{\varepsilon_1 f_1(1-A) + \varepsilon_2(f_2 + Af_1)}{\varepsilon_1 + Af_1(\varepsilon_2 - \varepsilon_1)} \tag{1}$$

derived based on the polarization induced by external applied, uniform electric field on isolated spherical inclusions located within a host material, Böttcher (also called symmetric Bruggmann equation) [10]

$$\frac{f_1(\varepsilon_1 - \varepsilon_{eff})}{\varepsilon_{eff} + A(\varepsilon_1 - \varepsilon_{eff})} + \frac{f_2(\varepsilon_2 - \varepsilon_{eff})}{\varepsilon_{eff} + A(\varepsilon_2 - \varepsilon_{eff})} = 0 \tag{2}$$

and Looyenga [11]

$$\varepsilon_{eff}^{1-2A} = f_1\varepsilon_1^{1-2A} + f_2\varepsilon_2^{1-2A} \tag{3}$$

With f_1 and f_2 are the surface fractions of host media and inclusions respectively. A ($0 \le A \le 1$) is the polarization factor which depends on the shape of inclusions. It should also be noted that these formulas give poor approximations at high concentrations of inclusions and at high contrast permittivity. But, we can adjust each formula for grain and short fiber inclusion shapes, with the aim to help the practitioners to approximate the real effective permittivity more accurately.

II. FINITE-ELEMENT COMPUTATIONAL APPROACH

Here, we are interested of extracting ensemble-average (effective) permittivity of random composite materials using the Finite-Element FE numerical tool. The detailed description of the method for determining the effective permittivity in the quasi-static limit can be found elsewhere [9]. As both computing power and the efficiency of the FE computational method, it is becoming possible to investigate new composite materials through computer simulations before they have even been synthesized. FE tool is used to compute the solution of Laplace equation by determining the electric field and potential distribution from the physical properties of different phases of the composite material. Recent works have shown that the FE method could be successfully applied to compute the effective permittivity of periodic composite materials [12]. The basic scheme of the FE method is now briefly recalled.

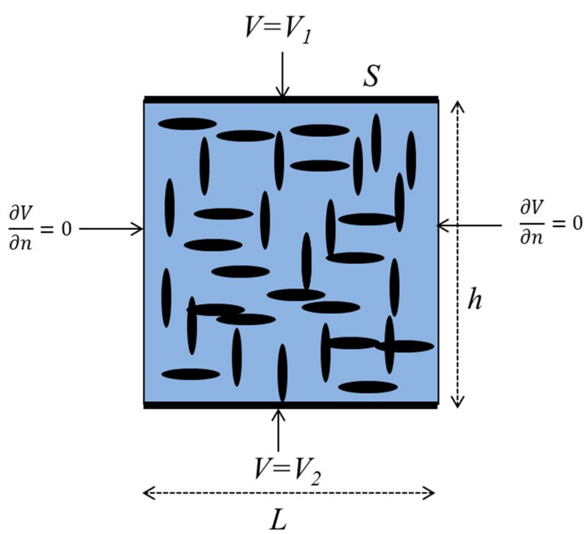

Figure 1: Illustration of the numerical computation of the effective permittivity of random inhomogeneous media. The black inclusions with permittivity ε_2 are immersed in the background host matrix with permittivity ε_1.

We consider a parallel plate capacitor shown in figure1 formed by two metal plates of area S and separated by height h. The two plates are submitted to a potential difference V_1-V_2=$1V$. Solving the problem at hand means finding the local potential distribution inside the computational domain by solving Laplace's equation (first principal of electrostatic):

$$\nabla(\varepsilon_0 \varepsilon(r) \nabla V) = 0 \tag{4}$$

Where $\varepsilon(r)$ and V are the local relative permittivity and the potential distribution inside the material domain respectively with zero charge density. ε_0=8.85.10^{-12}F/m is the permittivity of the vacuum. The electrostatic energy W can be written in terms of potential derivatives by:

$$W = \frac{1}{2}\varepsilon_0 \iint \varepsilon(x,y)\left[\left(\frac{\partial V}{\partial x}\right)^2 + \left(\frac{\partial V}{\partial y}\right)^2\right]dxdy \tag{5}$$

Periodic boundary conditions $\partial V/\partial n$=0 are enforced on the edges perpendicular to the parallel plates, thus, the edge fringing effects can be eliminated. The effective permittivity ε_{eff} can be computed from the energy W stored in the capacitor as

$$\mathrm{W} = \frac{1}{2}\varepsilon_0 \varepsilon_{eff} \frac{S}{h}(V_1 - V_2)^2 \tag{5}$$

In this equation $S=dL$ stands for the surface of the plates (for the 2D domain structure considered below, d is set equal to 1 unit length).

III. SIMULATION MODELS, RESULTS AND DISCUSSION

A series of simulations were performed on random composites with granular and short fiberinclusions. Examples of simulated composites are shown in figure 2.The computational domain is a square of 1*cm²* surface, granular inclusions are represented by small squares which the side is equal to 0.1*mm*(figures 2a and 2b), and in figures 2c and 2d, inclusions of short fibers are modeled by rectangles (2x0.08) *mm²* surface each one. The upper and lower boundaries of the computational domain are subjected to a difference potential of 1*V* whichthe two-dimensional distribution of the electric field is solved by the finite element method. During all simulations, we shall only consider the case where the different phasesof the studied composite materials are initially discharged and do not contain free charges. The relative permittivity of the fillers and the host medium are equal to ε_2=114 and ε_1=3.7 respectively, where the permittivity contrast $k=\varepsilon_2/\varepsilon_1$=30.81. By increasing the number of inclusions, randomly dispersed into computational domain, the surface fraction increases too. For short fibers case, (figures 2a and 2b), the orientation angle, a random parameter comprised between 0° and 180°, is added to the random position parameter. It should be noted that the inclusions can overlap. The materials being loss-less and their permittivities are real numbers. Two series of different numerical experiments were performed. The results of our simulations on the effective permittivity of dielectric mixtures are compared with the Maxwell Garnett, Looyenga and Böttcher analytical equations. The data obtained on the effect of filler shapes at high permittivity contrast (k=30.81) are given.

To investigate the effect of mixture-components geometry on the effective permittivity, simulations with randomly oriented and dispersed inclusions of different shapes, such as small squares and rectangular wires (short fibers) were carried out. The results obtained by the FE method are presented in figure 3.

It shows first that the effective permittivity curve of short fiber-filled composite is higher than the curve obtained for granular composite over the studied range [0-30%]. However, the polarizability of 2D- short fibers is greater than the squares or quasi-discoidal inclusions. Moreover, figure 3 exhibits a divergent prediction behavior between Maxwell Garnett, Looyenga and Böttcher models in the investigated range of surface fraction. The Maxwell Garnett model is inappropriate to predict the effective permittivity of random composite materials and its curve is too lower (figure 3); because its formulation is based on isolated spherical inclusions immersed in homogeneous host media. In random heterogeneous media, the multipolar interactions between fillers contribute to the polarization of the material medium. We can see that the Looyenga curve is more suitable to predict more accurately the effective permittivity of short fiber-filled composites for A=0.32 in the [0-15%] surface fraction range. Böttcher curve with A=0.5 is suitable to predict the granular composite only in the dilute limit less than 15% too. This limit increases when k decreases [13].

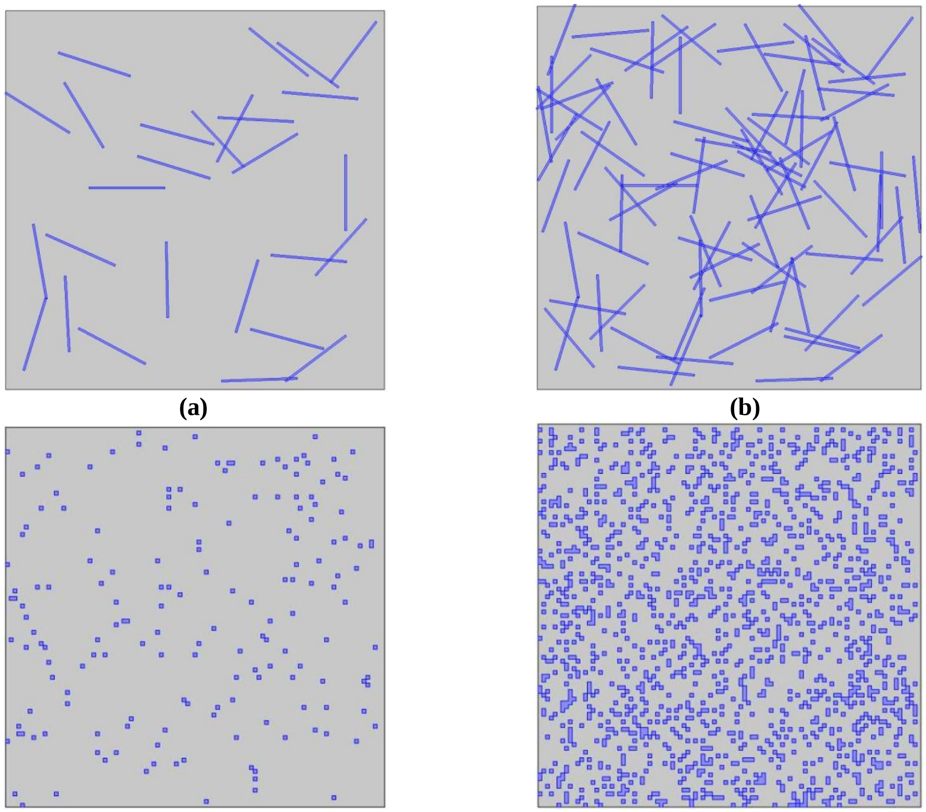

Figure 2: The short fibers ((a) and (b)) and the small squares ((c) and (d)) inclusions of permittivity ε_i=114 and surface fraction $f$are embedded randomlyintobackground media of permittivity ε_e=3.7. Specimens of virtual composites with different surface fractions of inclusions:f=2.68% for (a), f=8.83% for (b), f=1.7% for (c), and f=15.6% for (d) are presented for examples.

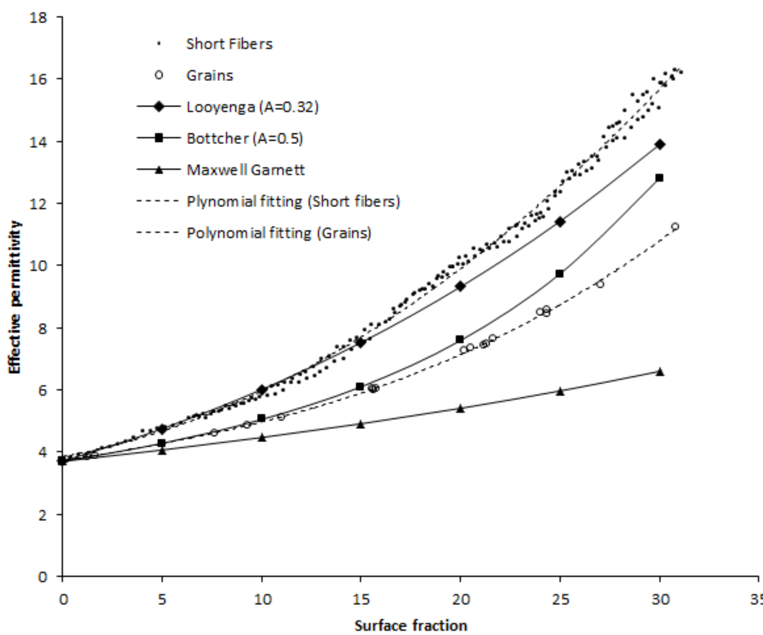

Figure 3: Simulations and analytical data of effective permittivity of the virtual composites shown in figure 2 as a function of the surface fraction. The numerical data predict more accurately the effective permittivity taking into count the shapes of the fillers and theremultipolar interactions. The dashed plots are the polynomial fitting of the numerical results.

Collectively, all of the presented numerical results assess the accuracy of the computed data of the effective permittivity for 2D loss-less heterogeneous materials which is of great importance in acceptance or rejection of specific mixing rule. Our computations confirm that the effective permittivity become progressively accurate than the empirical rules as more microstructure is incorporated. The methodology presented here is useful to investigate the dielectric condensed matter which is important in many technological applications, e. g., characterization of geophysical media, medical applications of microwaves and materials science. It can be generalized to multicomponent mixtures with arbitrary shapes of the fillers. By mathematical analogy, the results are also valid for magnetic composites materials. To keep the concept of effective permittivity valid, the spatial variation of the external field must be very large compared to the typical size of the inclusions.

IV. CONCLUSION

In conclusion, we have established a series of 2D-simulations by the finite element method of dielectric random composite materials. The inclusions are uniformly and randomly distributed into background host media. The numerical results are performed on loss-less heterogeneous media with granular and short fiber inclusions, and the effect of the filler shapes is highlighted. Maxwell Garnett model is inadequate to predict the effective permittivity of random composites, but Looyenga and Böttcher equations are suitable to anticipate the effective permittivity values of composite materials based on short-fiber and granular fillers respectively. This study, with the great simplicity and versatility, helps to compare the effective properties of different material combinations with changing the electrical properties of constituents and inclusion shapes, and can be extended to multiphase structures containing arbitrary shaped components. However, it is a very useful starting point for any material engineering application.

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