Paper Reference: COM2-01011-2005

The effective permittivity of lossless granular composites: From periodic to random distributions

J. Martín-Herrero*, J. Peón-Fernández, T. P. Iglesias****

**** Dpt. Theory of the Signal. University of Vigo. Spain***

julio@uvigo.es

***** Dpt. Applied Physics. University of Vigo. Spain***

jpeon@uvigo.es

tpigles@uvigo.es

Abstract

In this paper, we apply some well known results derived from the theory of homogenization for the Maxwel's equations to obtain the effective permittivity of periodical and non periodical arrangements for spherical particles. The analysis is restricted to lossless and non magnetic media at Long Wave Approach –LWA. Random arrangement of particles is modelled as a "super crystal" with a "big" unit cell where the statistical parameters of the whole distribution are preserved. That allows us to make an unified treatement for periodic and random distributions, from diluted to opaline structures

1. Introduction

Many natural geophysical media could be modelled as discrete heterogeneous random distributions of different scatters [1,2]. Also, the new materials known as Photonic Band Gap (PBG) materials – more appropriately called Electromagnetic Band Gap (EBG) materials- are composed by periodic distributions of single scatters embedded into a continuous background medium [3]. Understanding how e.m. waves and fields interact with such kinds of media will supply information about the composition and spatial distribution of the scatters in the system. This is very relevant for applications in remote sensing, non destructive analysis and tailoring the e.m. properties of artificial EBG materials. The starting point in the research on EGB materials is that the propagating e.m. waves in a periodic dielectric lattice may present a set of forbidden frequency bands, depending on the dielectric contrast, the size and the spacing of the components. But usually this is not the case for LWA: at low frequency, the dispersion relation. $\omega(\vec{k})$ is a continuous function, and from its derivative the effective permittivity of the system (for non-magnetic media) can be obtained for every frequency . In the following, we present briefly some basic results of the behaviour of e.m. waves propagating in a periodic structure and the asymptotic behaviour for LWA. The results would be valid for random macroscopically homogeneous media, provided that the wavelength is higher than the characteristic length of homogeneity. In this case, the system can be simulated as a periodic arrangement of an elementary unit cell, inside which the statistical parameters of the whole system are preserved. In order to simplify the calculations, we only consider spherical inclusions

2. LWA for the effective permittivity in a periodic dielectric structure

In a transparent, lossless, non magnetic and source free medium, a monochromatic wave satisfies

$$\vec{\nabla} \times \frac{1}{\varepsilon(\vec{r})} \vec{\nabla} \times \vec{H}_\omega(\vec{r}) = \frac{\omega^2}{c^2} \vec{H}_\omega(\vec{r}) \qquad (1)$$

for the magnetic field $\vec{H}_\omega$. Here, ω is the angular frequency, c is the velocity of light in the vacuum, and $\nabla \vec{H}_\omega(\vec{r}) = 0$.

For a periodic medium, the inverse of the permittivity could be expanded as a Fourier series:

$$\varepsilon^{-1}(\vec{r}) = \sum_{\vec{R}} \varepsilon_{K-K'} e^{-i(\vec{K}-\vec{K}')\cdot\vec{r}} \qquad (2a)$$

where

$$\varepsilon_{\vec{K}-\vec{K}'} = \frac{1}{V_\Omega}\int_\Omega d^3r\,\varepsilon^{-1}(\vec{r})e^{i(\vec{K}-\vec{K}')\cdot\vec{r}} \qquad (2b)$$

Ω is the unit cell of the distribution (with volume V_Ω) and $\vec{K}$ and $\vec{K}'$ are generic vectors of the reciprocal lattice.

Developing the field $\vec{H}_\omega$ into Bloch modes:

$$\vec{H}_\omega(\vec{r}) = \sum_{i=1}^{2}\sum_{\vec{K}} h_i(\vec{k}+\vec{K})\vec{u}_i e^{i(\vec{k}+\vec{K})\cdot\vec{r}} \qquad (3)$$

In this expression, the unit vectors $\vec{u}_i$ form an orthonormal triad with the unit vector along the direction of propagation of the mode $\vec{k}+\vec{K}$, $\vec{k}$ lying in the first Brillouin zone, and h_i are the projections of $\vec{H}_\omega$ on $\vec{u}_i(\vec{k}+\vec{K})$ (i=1,2). By introducing the equations(2-3) into the equation.(1), tedious, but simple algebra leads to [4,5]

$$\sum_{\vec{K}'}\left|\vec{k}+\vec{K}\right|\left|\vec{k}+\vec{K}'\right|\varepsilon_{\vec{K}-\vec{K}'}\begin{pmatrix}\vec{u}_2\cdot\vec{u}_2' & -\vec{u}_2\cdot\vec{u}_1' \\ -\vec{u}_1'\cdot\vec{u}_2 & \vec{u}_1\cdot\vec{u}_1'\end{pmatrix}\begin{pmatrix}h_1(\vec{k}+\vec{K}') \\ h_2(\vec{k}+\vec{K}')\end{pmatrix} = \frac{\omega^2}{c^2}\begin{pmatrix}h_1(\vec{k}+\vec{K}) \\ h_2(\vec{k}+\vec{K})\end{pmatrix} \qquad (4)$$

This equation gives a way to obtain the dispersion relationship $\omega(\vec{k})$ for the allowed modes, and from which, it is able to obtain the group velocity of the wave by differentiation. This eigenvalue problem will give an exact solution only when is solved all the possible (infinite!) $\vec{K}$ values, and extending the sum to the infinite $\vec{K}'$ vectors. In the limit of Long Wave Approach (LWA), by considering the inverse problem of the equation (4), it is obtained [6]

$$\sum_{\vec{K}'}\frac{k^2}{k\left|\vec{k}+\vec{K}'\right|}\Psi^{-1}_{\vec{k},\vec{K}'}\begin{pmatrix}g_1(\vec{k}+\vec{K}') \\ g_2(\vec{k}+\vec{K}')\end{pmatrix} = \frac{c^2k^2}{\omega^2}\begin{pmatrix}g_1(\vec{k}) \\ g_2(\vec{k})\end{pmatrix} \qquad (5)$$

where the operator $\Psi^{-1}_{\vec{k},\vec{K}'}$ is the inverse of

$$\Psi_{\vec{k},\vec{K}'} = \varepsilon_{\vec{K}-\vec{K}'}\begin{pmatrix}\vec{u}_2\cdot\vec{u}_2' & -\vec{u}_2\cdot\vec{u}_1' \\ -\vec{u}_1'\cdot\vec{u}_2 & \vec{u}_1\cdot\vec{u}_1'\end{pmatrix} \text{ for } \vec{K}=0 \qquad (6)$$

Now, taking the limits $\omega \to 0$ and $\vec{k} \to 0$ in equation (5), the only non vanishing term in the left hand side correspondsto $\vec{K}'=0$. Also $(c^2k^2/\omega^2)_{k\to 0} = \varepsilon_{eff}$, so finally

$$\varepsilon_{eff} = \Psi^{-1}_{0,0} \qquad (6)$$

The resulting effective permittivity is a (2x2)-matrix, and so, for each wave direction there are generally two possible values for the wave velocity $v^g_{eff} = c/\sqrt{\varepsilon_{eff}}$

It must be noticed that the effective permittivity resulting from this process tends to the scalar wave result if the limits are taken before the inversion of the matrix Ψ, loosing all the structural influences over the homogenized permittivity. All these influences are introduced by the whole set of values for $\varepsilon_{\vec{K}-\vec{K}'}$. In general, the Fourier transforms of the permittivity distribution on the unit cell are

$$\varepsilon_{\vec{K}-\vec{K}'} = \sum_i f_i^a(\vec{K}-\vec{K}')f_i^g(\vec{K}-\vec{K}') \qquad (7)$$

adding over all the "i" scatters lying in the cell, and where f_i^a is the "atomic" factor of the "i" scatter, containing the size and shape information, and f_i^g is the geometric factor of the distribution. For spherical scatters centred at $\vec{r}_i$ with radius R_i

$$f_i^a(\vec{G}) = \frac{3p_i}{R_i^3}\left(\varepsilon_i^{-1}-\varepsilon_m^{-1}\right)\frac{\sin(GR_i - GR_i\cos(GR_i)}{G^3} \qquad (8a)$$

and $f_i^g(\vec{G}) = e^{i\vec{G}\cdot\vec{r}_i}$

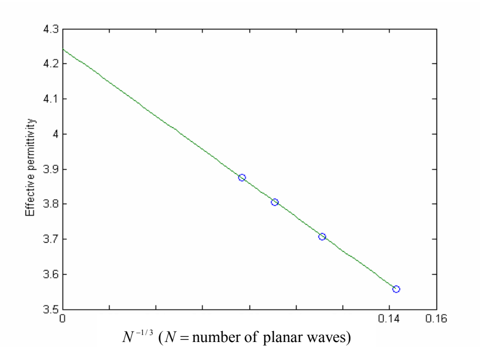

Figure 1. Convergence test for the effective permittivity of SC spheres (ε=10) into air. Fractional concentration of spheres p=0.4

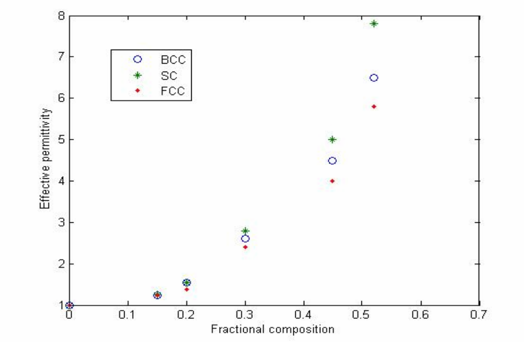

Figure 2. Effective permittivity of sphere cubic distributions (SCC, BCC, FCC) with ε=10 into air

3. Numerical results.

We calculate the effective permittivity for different arrangements of spherical particles embedded into a continuous matrix. The selected configurations are cubic lattices with different number n of identical scatters arranged as SCC (n=1), BCC (n=2), FCC (n=4), and randomly distributed (n=5, 10 and 15). Calculations where performed using a standard Matlab™ package.

Inversion of the matrix Ψ was carried out by taking the N reciprocal $\vec{K}$ vectors with the smaller norms. (N=number of planar waves to superpose in the equation (5)).

Figure 1 is a test of convergence for the obtained effective permittivity for a SC lattice. The scatter permittivity is ε_i=10 , placed into air ε_m=1: The volume fraction of the inclusion is *p*=0.4. Results were obtained for N=7^3, 9^3, 11^3 and 13^3 . The plot of ε_{eff} versus $N^{-1/3}$ is almost linear, and we obtain the extrapolated value as N→∞ by least-squares adjust. Figure 2 shows the achieved results for the spherical scatters into air, arranged as BCC, FCC and SCC for different fractional compositions (below the minimum percolation threshold). In figure 3 we plot the evolution of the effective permittivity for five, ten and fifteen identical spheres with permittivity ε=10 randomly distributed into air. The random distributions were generated using a Random Sequential Adsorption algorithm [6].. Figure [4] shows an illustration of an achieved result for ten closed pack spheres. In figure 3, the broken line corresponds to the theoretical result achieved from the Quasi Crystalline approach with Coherent Potential and Percus-Yevick pair distribution (QC-CP-PY)- see reference [1]. This result matches perfectly with the simulated results for the fifteen spheres (circles). Deviation of the simulations with respect to the QC-CP-PY expected values increases as the number of scatters decreases. The asterisks and the points correspond to the simulations for ten and five spheres respectively.

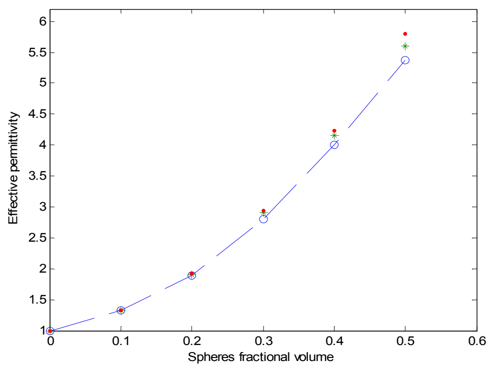

Fig. 3. Evolution of the ε_{eff} for fifteen (o), ten (*) and seven (·) dielectric spheres (ε=10) into air. The broken line corresponds to the expected values from QP-CP-PY approach.

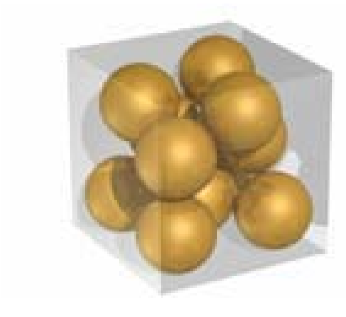

Fig. 4. An illustration of the ten closed pack spheres randomly distributed

5. Comments

An exact solution for equation (6) can be achieved only by taking the whole set of the reciprocal vectors. Convergence will not be achieved unless a high enough number of planar waves is considered into matrix Ψ. We carried out our calculations up to 13^3 contributions, although it required considerable computation time (from 20 s for $N=7^3$ to 4500 s for $N=13^3$ for every single calculation).
Our calculations were performed in Matlab™, using its standard libraries and commands. So our code is far from being optimized, and most of the computation time is devoted to inverting the matrix (equation (5b)). Careful analysis of the symmetries for every lattice would help selecting a more accurate algorithm for matrix inversion, thus minimising the computing time. The proposed method is "exact" for the calculation of the effective permittivity of periodic composites. For random homogeneous composites, the method would work properly as long as the wavelength is higher than the scale of homogeneity of the system. In this case, the composite could be modelled as a single cubic arrangement of a big point group. We limit our treatment to spherical inclusions, in order to avoid the calculation of the "atomic" and "geometric" form factors (equation (7)), by using their analytic expressions. The generalization of the presented results, excluding some other simple scatter shapes, would require the use of some of the available Fast Fourier Transform algorithms in order to calculate these parameters. The computing time would be increased in this case.

References

1. L.Tsang, J.A. Kong and K-H Ding, '*Scattering of electromagnetic waves:Theories and applications*'. Wiley Interscience (N.Y. 2000)
2. M.I. Mishchenko, '*Scattering, Absorption and Emission of Light by Small Particles*'. Cambridge U.P. (2002). Also available in http://giss.nasa.gov/~crmim/books.html
3. J. Joannopoulous, R. Meade and J. Win, '*Photonic crystals: moulding the flow of light'.* Princeton U.P.(1995).
4. S.G. Johnson and J.D. Joannopoulos, '*Block-iterative frequency domain methods for Maxwell's equations in a planewave basis*'. Optic Express, vol. 8, n. 3, pp 173-190 (2001).
5. S. Guo and S. Albin, '*A simple plane wave implementation method for photonic crystal calculations*'. Optic Express , vol. 11, n. 2, pp 167-175 (2003).
6. S. Datta, C.T. Chan, K.M. Ho and C.M. Soukoulis, '*Effective dielectric constant of periodic composites*'. Phys. Rev. B, vol 48, n. 8, pp. 14936-14943 (1993).
7. M.D. Rintoul and S. Torquato, *'Reconstruction of the structure of dispersions'*. J. Colloid Inter. Sci. 186, pp.467-76 (1997)