

# Extended T-matrix method to study the electromagnetic properties of 3D or 2D heterogeneous structures

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## Abstract

The goal of our work is to study the electromagnetic response of complex heterogeneous structures made with inclusions dispersed into a dielectric matrix. These structures can be photonic band gap structures (PBG) or metamaterials whose specific properties can be used in many domains in optical or microwave frequency range. A code of multiple-scattering had been developed at the laboratory to calculate the scattered fields in heterogeneous structures made up of N spheres, whatever their size and nature may be, dispersed in a matrix to form three-dimensional structures. This model can be extended to two-dimensional structures and to spheroid inclusions.

## 1 - Introduction

The use Photonic Band Gap structures (PBG) in the conception of materials with specific electromagnetic properties in microwave frequency range: absorbing, scattering or transparent materials, is very interesting because of the specificities of these materials. The main domains of applications are Electromagnetic Compatibility or uperstrates of antennas.

There is not general empirical law to model PBG. To be able to build such structures with specific properties, it is necessary to simulate them. Many methods exist to simulate PBG. The methods derived from solid state physics provide us the band structure [1, 2]. They enable us to locate the band gaps but not their level. Other methods get possible to visualize the transmission and the reflection of these PBGs. They are classified in two categories: time-domain and frequency methods. One can quote for the time-domain methods Finite Difference Time Domain Method, Finite Integration Method [3, 4] with Perfect Boundary Approximation [5]. Their main disadvantage is a lack of precision. Among the frequency methods, the Finite Element Method has not this problem. The memory reserved for the calculations is a function of the size of the studied structure.

Analysis of infinite structure is treated easily by these traditional methods by using periodic boundary conditions. On the other hand for the study of finished structure and defects, the duration and the memory reserved for the calculation become toolarge.

A code of multiple-scattering has been developed at the laboratory to avoid these limitations. It calculates the scattered fields in heterogeneous structures made up of inclusions dispersed in a matrix [6, 7]. In the case of the three-dimensional structures studied here, inclusions have a spherical shape, infinite cylinders allow ones to build two-dimensional structures. A recall of the broad outline of the theory of multiple-scattering and a study of the simple cubic PBG will enable us to understand the influence of the defects in these PBGs. The possibility of the extension of the code to non-spherical inclusions is presented.

## 2 – Multiple scattering modeling

The multiple-scattering method is separated in two parts. Fig. 1 describes this method. The first step is the calculation of the scattered wave by an object, sphere or infinite cylinder, by using the extended Mie scattering theory. Incident and scattered fields are developed on a basis of spherical or cylindrical harmonics, given by the geometry of the object and its optical properties. One writes the transfer matrix between the incident field and the scattered field. This matrix contains all the information about nature, size and shape of the object.

The second part of method is an iterative algorithm, that makes to pass the calculation of the scattered field from a single object to N ones. For the first order, one calculates the diffraction of the incident field for each sphere or

cylinder. For the second order, the scattered field of first order for one sphere or cylinder becomes the incident field for the N-1 other ones. With this new incident field, the scattered field is calculated as for the first order and so on for higher orders. This iterative process stops when an energetic criteria is satisfied. The total scattered field is the sum of the contributions of all objects for all orders .

The nature and the size of these N spheres can be different. Moreover, spheres may be put in a random way, it doesn't have there conditions of symmetries in the spheres positions. These two last remarks show all the interest of this method in calculation of PBG with defects and random structures. The method was developed for cylindrical and spherical objects. It can be extended to other objects. The computing time relatively weak is compared with other methods. As an example, for a structure of 180 spheres, it takes approximately 2 hours of calculation on a supercomputer. One obtains for this duration the coefficients of transmission and reflection on 100 points of frequencies and 1800 angles of observation. This speed of calculation allows us to do a parametric study of the simple cubic structure.

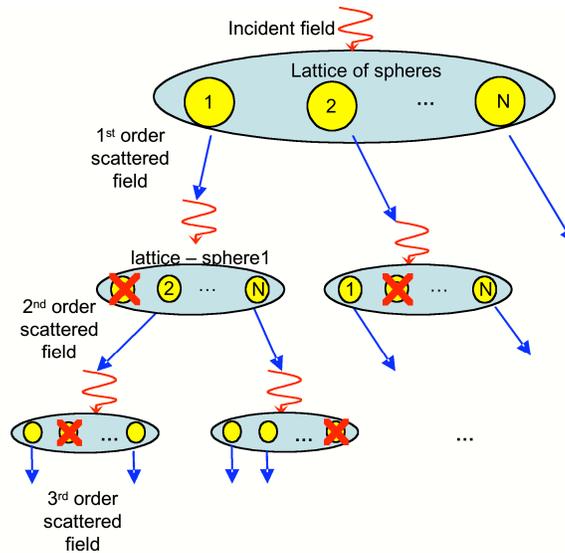


Fig.1. Block diagram of multiple-scattering method

### 3 – Study of 3D structures

#### 3.1 – Preliminary study of simple cubic PBG without defect

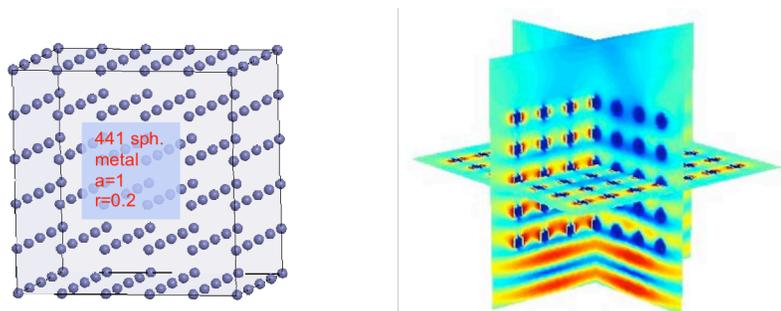


Fig.2.: Near field into a PBG made with 5 layers of conducting spheres

Initially, we studied a simple cubic lattice without defect with metal inclusions of spherical form (Fig.2). This PBG is composed of 5 layers according to the axis of propagation and 36 spheres by layer. A study of the transmission of the PBG in function of the spheres radius or the lattice constant gave us a better understanding of this

structure. On the right of Fig.2, we represented the local field transmitted through this cubic PBG of the lattice constant 30 mm for various radii.

### 3.2 – Random variations of radii and spheres positions

We studied the influence of random variations of radii and spheres positions. We kept the same PBG structure as previously. On Fig.3.a, we operate a random variation of spheres radii around the initial value. We keep constant the average and the standard deviation of radii. The first forbidden band goes up gradually by increasing the percentage of random variation of the lattice constant. This band gap has a traditional behaviour. The lattice is disorganized as the random variation increases. On the other hand the second band almost does not vary. The first two bands have a radically different behaviour. By modifying the lattice gradually, the first forbidden band will become complete whereas it is not the case for the second. The second band does not result from constructive or destructive interferences between all the layers.

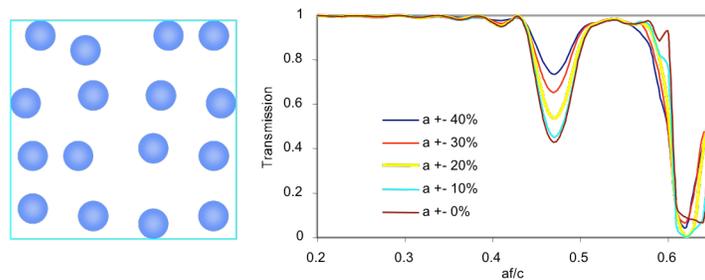


Fig.3.a. Random variation of radii

In the second time, we make a random variation on the spheres positions (Fig.3.b). Here also, the average and the standard deviation of spheres positions are constant. A random variation of spheres positions has a weak influence until  $\pm 10\%$ . Beyond this percentage, the two forbidden bands disappear rather quickly. There is almost a percentage threshold where the lattice does not behave any more out of photonic crystals. The cubic structure is more sensitive to the variations of spheres sizes than the variations of positions. For small random variations preserving the average parameters of the initial lattice, the physical characteristics of the PBG remain the same ones.

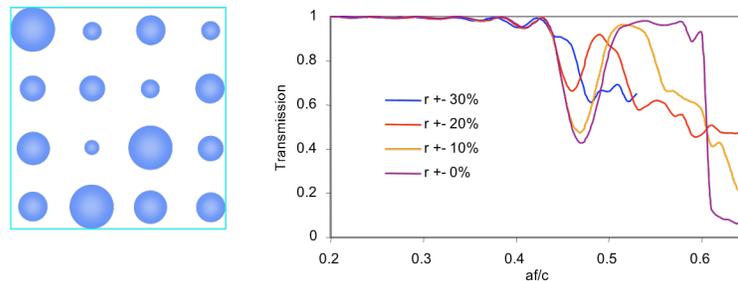


Fig 3.b. Random variation of spheres positions

## 4 – Extension of the method

### 4.1 – Local defect in a two-dimensional PBG

This method, was applied to 2D structures made with infinite parallel cylinders. The figure 4 present the effect of resonance of the electric field due to a local defect in a material made with infinite conducting cylinders placed along a triangular network

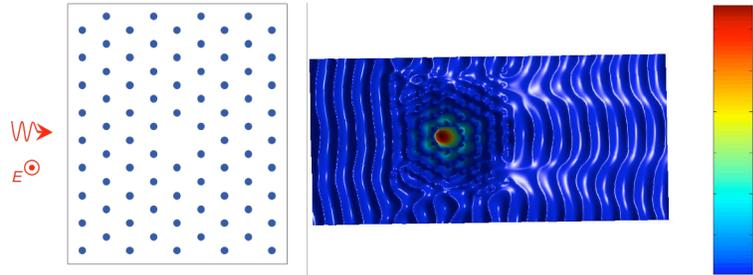


Fig 4 : local defect due to a missing cylinder in a 2D structure made with perfectly conducting infinite cylinders

## 4.2 – Other shapes of inclusions

To apply the multiple scattering model to non spherical objects, the analytical extended Mie theory applied to spheres or cylinders is replaced by the numerical extended boundary conditions method (EBCM) which allows to express the relation between scattered and incident field through a scattering matrix (non-diagonal in this case). Figure 5 presents two examples of scattered field in the cases of oblate and prolate spheroids.

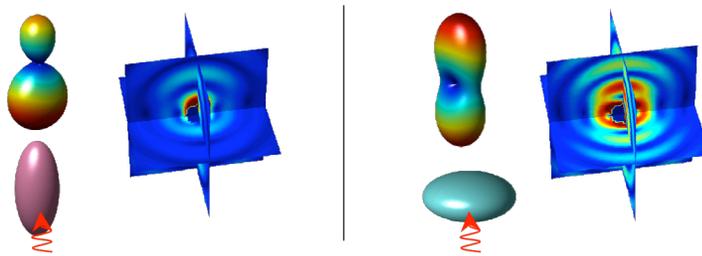


Fig 5 : mapping of the electrical scattered field and intensity of diffraction in the case of two dielectric spheroids : left a prolate spheroid whose refractive index is 7, right an oblate spheroid whose refractive index is 7

## 5 - Conclusion

The code of multiple-scattering of electromagnetic waves we first developed for spherical inclusions[10] is actually extended to other shapes. After the study of networks of cylinders, we are actually applying this model to other shapes of inclusions

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