Efficiency of 2D homogenization formulas for magnetic nanocomposite materials

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Abstract. Magnetic nanocomposite materials are used in a large area of applications. In many cases the solution of homogenizing these materials could make work easier. This paper studies the efficiency of two homogenization formulas (Maxwell-Garnett and Bruggeman) for different situations: varying the number of particles for the same volume ratio, varying the dispersion of inclusions in the material. The investigations were made for 5 different volume ratios (approximate 10%, 20%, 30%, 40% and 50%) and 4 different ratios for the magnetic permeability of the inclusions and of the domain. The discussions were referred to the response of the composite and homogenized materials through two curves on the exterior of the domain.

1 Introduction
Magnetic composite materials were used in various applications ranging from magnetic sensors and micro electrical machines to electromagnetic shielding and biomedical applications (such as magnetic drug delivery into the human body or enhancing the contrast image in magnetic resonance) [1] ÷ [3]. Some of the composite materials had very complex structure and thus sometimes the study of their properties is difficult. One solution for this problem is to make some simplifying assumptions. For example, we can consider that all the material inclusions have exactly the same form and geometric size and that they are perfectly embedded in the matrix. Other common assumption is the homogenization technique. The idea behind this technique is to replace the complex structure of the real material with a homogeneous one which is able to describe correctly all the material properties. Using the homogenization technique it was determined that the medium has the same properties in each point and the macroscopic rules and formulas can be applied with success. One of the immediate results of using homogenization is that the time needed to obtain the desired solutions is reduced [4].

Homogenization techniques are based on analytical formulas (such as Maxwell Garnett, Bruggeman, Clausius-Mossotti) or different computational methods (finite difference method, finite element method, boundary element method) [5] ÷ [7]. The aim of this paper is to analyze the numerical 2D results of the homogenization process, using two analytical formulas (Maxwell-Garnett and Bruggeman) for several situations involving different volume ratios between inclusions and matrix, different magnetic permeability ratios and, also, observing how the number and position on the inclusions into the material influences the homogenization process.

The initial Maxwell-Garnett formula was used for the dielectric permittivity of a material, but it was successfully applied to magnetic material as follows [8]:

\[
\frac{\mu_o - \mu_m}{\mu_o + 2\mu_m} = f \cdot \frac{\mu_i - \mu_m}{\mu_i + 2\mu_m}
\]

where the indexes are indicated as: homogenous (o), matrix (m), respectively the inclusions (i), \( \mu \) is the magnetic permeability, and \( f \) is the ratio volume between the inclusions and the domain. The Bruggeman formula (using the same notations) is a bit more elaborated, by taking into account the interaction between the particles in the composite material [8]:
\[
(1 - f) \cdot \frac{\mu_m - \mu_o}{\mu_m + 2\mu_o} + f \cdot \frac{\mu_i - \mu_o}{\mu_i + 2\mu_o} = 0
\]  

(2)

The following study was based on these formulas to calculate the homogenous magnetic permeability of the material.

2 Numerically Investigated Situations

The sample studied is a discus of 50 nm radius. The inclusions are discuses with different radiuses arranged symmetrically in the matrix. The investigation focused on the median relative errors (relation (3)) between the magnetic flux density obtained in the homogeneous and the inhomogeneous cases on two exterior curves (one of 52.5 nm radius, named \(C_1\) and the other of 60 nm radius named \(C_2\)).

\[
\varepsilon_r = \frac{\sum_{k=1}^{n} (B_{incl}^{(k)} - B_{hom}^{(k)})}{n},
\]

where \(n\) is the number of points determined by the software (FEMM plots 300 points for each curve). The domain is placed in uniform magnetic flux density of about 22 mT from the bottom of the investigated domain for each case studied.

The study uses different variables to present the importance of each parameter in the numerical simulation. Different values for the matrix and inclusions permeability were used, following four ratios between them as follows:

**Table 1. Situation simulated for magnetic permeability**

<table>
<thead>
<tr>
<th>(\mu)</th>
<th>(\mu_m)</th>
<th>(\mu_i)</th>
<th>(\mu_m / \mu_i)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Situation</td>
<td>S(_1)</td>
<td>S(_2)</td>
<td>S(_3)</td>
</tr>
<tr>
<td>(\mu_m)</td>
<td>10</td>
<td>5</td>
<td>100</td>
</tr>
<tr>
<td>(\mu_i)</td>
<td>1000</td>
<td>50</td>
<td>10</td>
</tr>
<tr>
<td>ratio ((\mu_m / \mu_i))</td>
<td>0.01</td>
<td>0.1</td>
<td>10</td>
</tr>
</tbody>
</table>

Another important aspect is the influence of the volume ration between the inclusions and the matrix and 5 concentrations are simulated: 10%, 20%, 30%, 40%, respectively 50%.

The last two aspects included in this study were the influences of the number of inclusions (there were simulations for 4 inclusions, named “few - f” and 10 inclusions – “many – m”) and the placement of these inclusions in the matrix (simulations for the situation of “center – c” or “peripheral – p” dispersions of the inclusions in the matrix).

3 Results and discussion

For the first comparison, the magnetic flux density spectrum was presented (figure 1) in the cases of central, respectively peripheral dispersion of 4 inclusions. For these situations the relative errors were presented on the closest curve on the graph (\(C_1\)) using equation (3), for two concentrations of inclusions (20%, respectively 50%) using both formulas (Maxwell-Garnett - MG and Bruggeman - B). The ratio of the magnetic permeabilities for the horizontal axis corresponds to the values from table 1.
Fig. 1. Magnetic flux density for central and peripheral dispersion of 4 inclusions

Fig. 2. Relative errors for considered situations on curve $C_1$ for a concentration of 20% (a), respectively 50% (b) of the inclusions in the matrix.

In figure 3 and 4, are presented the same situations for central and peripheral dispersions of 10 inclusions into the matrix.

Fig. 3. Magnetic flux density for central and peripheral dispersion of 10 inclusions
Fig.4. Relative errors for considered situations on curve $C_1$ for a concentration of 20% (a), respectively 50% (b) of the inclusions in the matrix.

To study the influence of the position of the inclusions into the matrix, in figure 5 and 6 are presented the relative errors using equation (3) for 4 and 10 central and peripheral inclusions.

Fig.5. Relative errors for considered situations on curve $C_1$ for central (4 and 10) (a) and peripheral (4 and 10) (b) inclusions (concentration 20%)

Fig.6. Relative errors for considered situations on curve $C_1$ for central (4 and 10) (a) and peripheral (4 and 10) (b) inclusions (concentration 50%)

In the previous graphs concentrations of 50% were selected because this situation produces the highest relative errors, as it can be seen in the figure 7, for 4 and 10 central inclusions.
In the last part of the study the objective was to emphasize the variation of the relative errors for all inclusion concentrations (10% to 50%), for the four situations presented in table 1, using Maxwell-Garnet formula only.

4 Conclusions

The aim of this study was to establish the influence of different parameters to the analytical homogenization techniques involving Maxwell-Garnett and Bruggeman formulas. First of all, Maxwell-Garnett formula gave more accurate results than Bruggeman ones for most of the investigated situations. Although, in the cases of 10 inclusions it was observed that the relative errors for both formulas were close. This aspect can be regarded to the fact that Bruggeman formula is taking into account the interaction between the particles which is more intense for 10 inclusions. Also, for a ratio of 100 between the matrix permeability and the inclusions permeability the relative errors for both formulas are also very close independent of the other parameters taken into account in this study. On the other hand, the most disadvantageous situation is the one with ratio 0.1.

The influence of inclusion position into the matrix was showed in figure 2 for 4 inclusions and in figure 4 for 10 inclusions. For lower concentrations (such as 20%) it was obvious that, for both formulas, central dispersion is more accurate than the peripheral one. In the case of 50% particle concentration, the relative errors for central and peripheral dispersion become closer,
especially when Maxwell-Garnett formula is used. One can conclude in this case that the position of the inclusions into the matrix is important only in a dilute composite material. Both formulas considered in this study do not explicit take into account the number of inclusions for the same inclusion concentrations in the material. The relative errors shown in figure 5 marked out that Maxwell-Garnett formula provides more accurate results for 4 then 10 inclusions, but for higher concentrations the relative errors were similar with the two previous cases. All cases studied on the second curve $C_2$, gave smaller relative errors, as it was expected. The study might be continued with investigation of 3D inclusions, with different shapes of the particles and even considering inclusions of different magnetic permeabilities.

References