MICRO-SCALE MODELLING OF THE COMPOSITE MATERIAL MAGNETIZATION

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Lucrarea analizează rezultatele numerice ale micro-modelării magnetizării, bazată pe ecuațiile Landau-Lifshitz-Gilbert, pentru un eşantion din material compozit având dimensiuni geometrice şi proprietăți magnetice diferite ale componentelor sale: matrice din Fe, Ni sau Co cu incluziuni (particule sau fibre) din $SmCo_5$ *sau* CrO_2. *Simularea tridimensională a procesului de magnetizare se realizează folosind programul comercial Magsimus. Este studiată dependența valorilor obținute pentru magnetizația remanentă de proprietățile magnetice ale componentelor materialului (matrice şi incluziuni). Rezultatele demonstrează la scară microscopică faptul că un material compozit are proprietăți magnetice superioare față de materialul magnetic omogen corespunzător (fara incluziuni).*

The paper analyses the numerical results of the magnetization micro-modelling, based on Landau-Lifshitz-Gilbert equations, of a composite material sample with different geometric dimensions and magnetic properties of its components: matrix of Fe, Ni or Co with inclusions (particles or fibres) made from $SmCo_5$ *or* CrO_2. *The three-dimensional simulation of the magnetization process is made using Magsimus software. The dependence of the obtained remanent magnetization values on the geometric structure and magnetic properties of the material components (matrix and inclusions) is studied. The results prove at microscopic level that a composite material has better properties than the homogeneous one (without inclusions).*

Keywords: composite magnetic materials, numerical analysis, micro-scale magnetic characterisation

1. Introduction

In order to satisfy the continuous demands for an industry which is developing day by day, researchers seek to create new materials which respond to these expectations. One of the easiest way is taking existing materials and, by changing their composition or properties, obtaining new ones.

Composite materials can be described as a combination of two or more different materials designed to satisfy certain technical requirements, providing

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advanced features and properties. At the macroscopic level, the constituent materials keep their separate identity within the composite, but the newly obtained material has different characteristics altogether from those of its components [1], [2]. The simplest composite is made from two different materials. One constituent is called the reinforcing phase (inclusions). The other one in which the first material is embedded is called the matrix [3]. The reinforcing phase material may come in the form of fibres, particles, or flakes and is added to the matrix to improve or modify its properties. The matrix phase materials are generally continuous [4], [5]. Because there are many types of matrices and reinforcement techniques, they can be combined in so many ways that the potential for development and implementation of new materials is very high.

The composite material industry expands the possibilities of using hard and soft magnetic materials. Metal, ceramic or polymer matrices can be used for magnetic applications. In general, polymer-matrix composites are useful for transformer cores and related applications or as magneto-optical media for optical devices and integrated optics [6]; ceramic-matrix composites are desirable in high temperature applications, but also have a high cost of fabrication. For this reason, they are used more in high-tech applications such as for military, airspace or medicine. Metal-matrix composite materials are taken into consideration for the analysis presented in this paper.

Metals are among the most common ferromagnetic materials. Because of this reason, metal-matrix composite combinations are often found through the composite magnetic materials. Generally this type of composite can be divided into three categories: magnetic metal-matrix composite materials (ferromagnetic or ferrimagnetic) and magnetic reinforcements; composites with metal-matrix and nonmagnetic reinforcements (antiferromagnetic, paramagnetic or diamagnetic); and composites with non-magnetic matrix, but with magnetic reinforcements.

One important objective of the Electrical Engineering technical community is to obtain more compact and efficient electrical machines, using composite magnetic materials [7]. The starting point of this optimization is the analysis of the electromagnetic properties of the composite material. The scientists invested enormous effort in trying to find the mixtures of components that have the needed properties (e.g. high values of the saturation and remanent magnetization, strong coercive fields). The best results were obtained using composite materials with ferromagnetic metal-matrix (e.g., Fe, Ni or Co) and inclusions from hard magnetic materials (e.g. materials used for rare-earth permanent magnets) [6], [7]. The numerical simulations presented in this paper use this kind of composite materials.

This paper presents the 3D numerical simulation for the micromagnetization (magnetization process at microscopic scale) of different composite materials having ferromagnetic matrix and magnetic reinforcements.

The magnetic material behaviour is modelled at microscopic level by Landau-Lifshitz-Gilbert (LLG) equation [8] and an accurate simulation of the magnetization process is presented. The presented numerical tests use material data for the components that correspond to real magnetic materials. This kind of analysis is very useful because the magnetic properties of the composite material can be improved by numerical design and optimization, starting from the value of the remanent magnetization, which is obtained by changing the shape and the dimension of the inclusions or the material used for the matrix or for the reinforcements. Some results of the comparison between the micro- and macroscopic approaches of the magnetization process were presented in [14], but only for homogeneous materials and for thin-layers composite magnetic structures.

The novelty of this paper consists in the complexity of the geometrical structure of the analyzed composite and in the correlation between the micro-scale analysis of the magnetization process and the macro-scale magnetic properties of the materials used for matrix and for inclusions. Indeed, the scientific literature present separately the two approaches (microscopic and macroscopic), due to the different scientific background and the numerical treatment of LLG equation requires large computing resources, the existing results being obtained for simple geometric configurations.

2. Micro-scale analysis

In the micromagnetic approach, the evolution of the magnetization vector **M** around the effective magnetic field vector **H** is governed by the Landau-Lifshitz (LL) equation, a time-dependent differential equation that expresses the damped-precession motion of the magnetization vector under the influence of an applied field [8]:

$$\frac{d\mathbf{M}}{dt} = -\gamma \mathbf{M} \times \mathbf{H} - \frac{\lambda}{M} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}) \quad , \quad \text{in } \boldsymbol{\Omega} \tag{1}$$

where $\boldsymbol{\Omega}$ is a bounded domain. The LL equation is accompanied by the Neumann boundary condition on the borders of $\boldsymbol{\Omega}$ [9], [10]. The total effective magnetic field **H** models the contributions of various components – the anisotropy, demagnetization, applied and exchange magnetic fields. The damped-precession motion of **M** around **H** is characterized [9] by the damping factor λ (the speed of attenuation of the magnetization value during the transient evolution described by (1)) and the precession parameter γ (the rate of precession for the vector **M** around the vector **H**). In general the damping factor λ is a positive phenomenological constant characterizing the magnetic material [11], [12].

The LL equation was modified by Gilbert in 1955 [8]:

$$\frac{d\boldsymbol{M}}{dt} = -\gamma_G \boldsymbol{M} \times \boldsymbol{H} + \frac{\alpha_G}{M}(\boldsymbol{M} \times \frac{d\boldsymbol{M}}{dt}) \tag{2}$$

where α_G is the Gilbert damping factor and γ_G is the Gilbert precession factor; γ_G can be computed as $\gamma_G = 1.105*10^5 g$, where g is the gyromagnetic ratio.

There is a significant difference between the Landau-Lifshitz and Landau-Lifshitz-Gilbert (LLG) equations even though they are very similar from the mathematical point of view [13]. Indeed, if one considers $t\rightarrow\infty$, the solution value is ∞ for the LL equation (1) and it is 0 for the LLG equation (2). The numerical result obtained from the equation (2) is in agreement with the experimental observation that a very large damping should produce a slow motion and this is why the Landau-Lifshitz-Gilbert equation is preferred.

For the micro-scale analysis of the magnetization process presented in this paper, a commercial software program Magsimus© was used. This software is very useful for the design and analysis of three-dimensional micro-magnetic systems and was used by the authors in [14] for homogeneous materials and for thin-layers composite magnetic structures. The modelling techniques are based on the micro-magnetic theory for calculating the equilibrium magnetic states of a system [8]. The solver computes the solution of the LL or LLG equation and one equation is written for each magnetic element of the simulated system.

The analysis of the magnetization process was made for several examples of composite materials with periodic structure. There are two main reasons behind the choice of this kind of materials: this periodicity is found often in the usual composite materials and this hypothesis makes the problem easier to be solved using numerical computations.

3. Modelling approach

The study is focused on the influence of various external magnetic fields on the remanent magnetization of different composite materials for quasi-static regime. The purpose of this analysis is to highlight the performances of these materials by comparing the results with the classical properties of materials without inclusions (homogeneous materials), and to show how the composite material properties and structure influence the remanent magnetization.

The analysis is split into three cases. The first two cases present the micromagnetization of two samples (500nm×500nm×500nm and 300μm×300μm×300μm) that have cubic particles as inclusions; the last case analyses a sample (5 μm × 5 μm area and 1 μm thickness) with fibre-type reinforcements. The numerical analysis allows the representation of the magnetization vector distribution inside the composite material; for example, Fig. 1 presents the results for the third case, where the three reinforcements are represented with thick lines. Ferromagnetic metal-matrix (Fe, Ni and Co) and inclusions (reinforcements) from magnetic materials (CrO_2 and $SmCo_5$) were considered in all cases. The simulations for each case of composite samples include the particular configuration of the homogeneous material (the matrix and the inclusions are made from the same material), the remanent magnetization values, which are obtained for the homogeneous material and for the composite material, being compared.

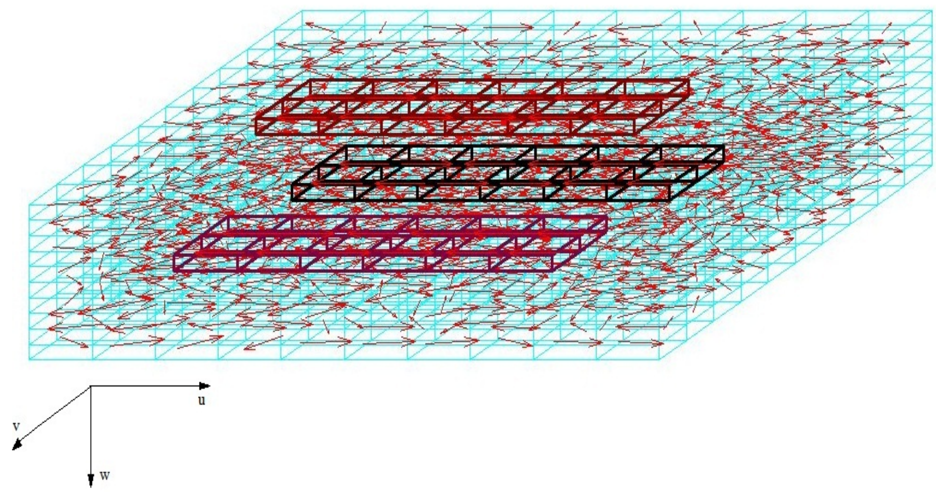

Fig. 1. Distribution of the magnetization vector **M** inside a composite material with three fibre-type reinforcements (represented by thick line contours).

The geometric model consists of two main parts: the matrix and the inclusions (reinforcements). The matrix was defined in the software model as a "pseudo-soft magnet" where the magnetization vector is not fixed in magnitude and can rotate freely in three dimensions under the influence of an external field. It is characterized by the relative magnetic permeability tensor and the saturation magnetization [8]. The reinforcements were defined as "normal magnet" – the magnetization vector has a fixed magnitude and it is free to rotate in all three dimensions under the influence of an external field. The sample volume is divided (meshed) by elements (cells) having the shape of rectangular prisms, each element being characterized by the magnitude and the angular orientation of its magnetization vector [14].

The magnetization process is due to different pulses of external magnetic field that are applied along the normal direction of the sample section (direction *u* in Fig. 1). The mesh size (cell dimensions) and the parameters of Landau-Lifshitz-Gilbert equation were adapted, according to the simulation demands - mesh fitted on the geometrical configuration, high computation convergence rate, limited hardware resources and an average time to solve the magnetic field problem. The time-dependent magnetic field problem is decomposed by Magsimus software in a sequence of quasi-static problems [8]. The software uses the error-correcting Runge-Kutta method for the integration of the differential equations written for each sample cell.

The user interface of the Magsimus software imposes, for each magnetic material involved in the problem, to specify the following data: the magnitude of magnetization vector at saturation M_s, the exchange stiffness constant A, anisotropy constant K, gyromagnetic ratio, damping factor α and electrical conductivity σ. These properties, extracted from [13] and [15], are listed in Table 1 for the magnetic materials involved in our simulations. For matrix materials the relative permeability is also provided ($\mu_{r\_Fe} = 5000$, $\mu_{r\_Co} = 250$, $\mu_{r\_Ni} = 600$).

Table 1

Magnetic material properties (from [13], [15])

Material	$\mu_0 M_s$ [T]	A 10^{-11} [J/m]	K 10^5 [J/m^3]	σ 10^6 [S/m]	$(\gamma M_s)^{-1}$ [ps]
Fe	2,16	1,5	0,48	0,112	2,6
Co	1,82	1,5	5	0,157	3,1
Ni	0,62	1,5	-0,06	0,146	9,2
CrO_2	0,5	0,1	0,22	0,004	11,4
$SmCo_5$	1,05	2,4	170	0,2	5,4

4. Results and discussion

The simulation starts from an initial magnetization state represented by a distribution of the magnetization vector inside the meshed domain; for each cell, the vector **M** is oriented, randomly (non-magnetized material) or in a given direction (the material is initially magnetized). The samples were considered to have uniaxial magnetic anisotropy, the easy magnetization axis being the long axis (e.g. the *u* axis in Fig. 1). An external magnetic field having the amplitude H = 80 kA/m is applied along the easy magnetization axis; the shape of this pulse is presented in Fig. 2. For each step of the applied field evolution, the simulation goes on until reaching the equilibrium state. Our numerical tests show that the number of the mesh cells, the geometry sample, the number of field steps and the damping factor can affect the duration of the simulation and the determination of the equilibrium states. For example, the computation time is more than 100 times bigger (the computer performances influence the value of this last number) if the number of cells becomes 10 times bigger (the mesh is refined). Also, the damping factor value imposes the magnitude of the damping term in the LLG formula (the second term in the right-hand part of the equation (2), which models the energy loss mechanisms in real materials); consequently, the damping factor value imposes how the magnetization vector tends to become aligned with the applied magnetic field vector). The applied magnetic field profile (see Fig. 2) is determined by three intervals – the first interval when the field is rising, the second one, where the field value is maintained constant, and the third one, where the field values decrease to zero. Each interval is divided in a number of time steps (this number is at user's choice) and each step represents the time during the magnetic equilibrium state is reached; for example, the case from Fig. 2 corresponds to 30 equilibrium states.

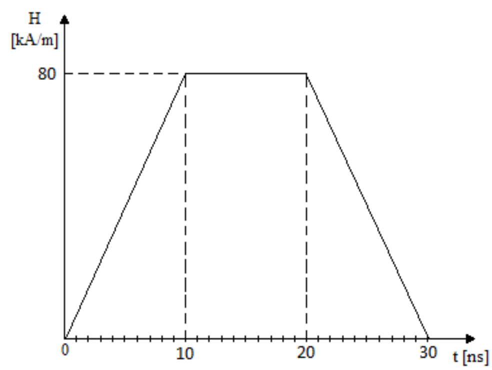

Fig. 2. The applied magnetic field evolution in time.

The first case presents the comparison between a homogeneous material (Fe, Cu or Ni) and a composite material having the same matrix material but with $SmCo_5$ or CrO_2 particle-type inclusions; the considered domain has 500 nm × 500 nm × 500 nm. The applied magnetic field has the profile presented in Fig. 2, and it was applied along the *u* axis (easy magnetization axis).

The macroscopic magnetization of the sample results by the superposition of the contributions (local / microscopic magnetization vectors) of all mesh cells. Its *u*-component (along the applied magnetic field direction) depends on the field magnitude as it is presented in Fig. 3 for a sample with Fe matrix and different inclusions ($SmCo_5$ or/and CrO_2). The initial magnetization state and the remanence state correspond to the points H=0 on the lower curve and on the upper curve of each magnetization cycle. Each point on the computed curves M = f(H) from Fig.3 corresponds to an equilibrium magnetization state, which is obtained by solving the LLG equation. The irregularity in the M = f(H) curve is due to the magnetization jumps between the equilibrium states and to the errors associated to the discretization of the LLG equation using a limited mesh (small number of cells).

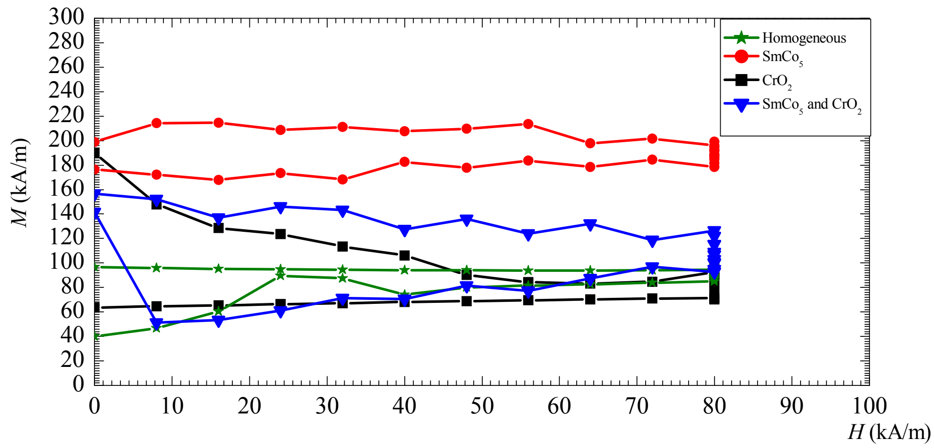

Fig. 3. Magnetization vs. applied magnetic field strength on the easy magnetization axis, for different inclusions materials in Fe matrix.

The magnetization curves presented in Fig. 3 were obtained for a Fe sample and for three composite samples having Fe matrix and inclusions from $SmCo_5$ and CrO_2; the applied field has the profile presented in Fig. 2. These numerical results show that the material of the inclusions have a big influence in the final results: the remanent magnetization is smaller in the homogeneous case (96 kA/m) than in the other cases; for example, the remanent magnetization for the composite material with a mixture of $SmCo_5$ and CrO_2 inclusions equals 156.57 kA/m. It can be also observed that the remanent magnetization values obtained for $SmCo_5$ inclusions and for CrO_2 inclusions are comparable (198.96 kA/m v.s. 190.01 kA/m), but the evolutions are different. However, the remanent magnetization state must be correlated with the initial state; the magnetization gain (difference between the values corresponding to the remanent and to the initial magnetization states) is 22 kA/m, for $SmCo_5$ inclusions, and 112 kA/m, for CrO_2 inclusions. One explanation could be the significant influence that the anisotropy constant K (see Table 1) has on the magnetization component along the easy axis. The composite having strong anisotropic inclusions ($SmCo_5$) has the same high value for the magnetizations computed for successive states during the magnetic field applying, but it is hardly to increase this magnetization level by applying an external field. Contrary, the CrO_2 inclusions (having weak anisotropy) allows the easy magnetization of the corresponding composite material.

The choice of the matrix material is also important for a desired application. The effect of the matrix material on the magnetic behaviour of the composite material was studied by comparing a homogeneous sample (made by Fe, Cu or Ni) with a composite material sample having the same matrix material with inclusions of $SmCo_5$ particles; the samples have 500nm×500nm×500nm. Fig.

4 presents the computed magnetization values for three homogeneous samples and the corresponding composite samples with $SmCo_5$ inclusions. The values of the remanent magnetization are higher for a composite than for a homogeneous magnetic material (see Table 2).

Table 2

Remanent magnetization M_r [kA/m]

Matrix material	No inclusions (homogeneous material)	$SmCo_5$ inclusions
Fe	96.51	198.46
Co	173.13	217.36
Ni	51.43	62.5

The improvement given by adding $SmCo_5$ inclusions on the remanent magnetization values is better for Fe and Co matrices. For example, it can be easily observed from Table 2 that the remanent magnetization is double for the composite material made by Fe matrix and $SmCo_5$ inclusions than for the homogeneous sample made by Fe.

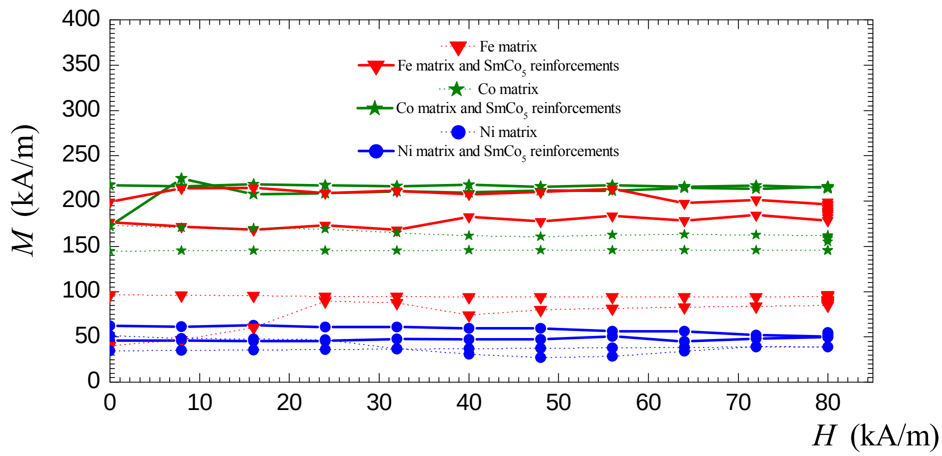

Fig. 4. Magnetization curve for different matrix material (Fe, Co, Ni) for homogeneous and composite materials having $SmCo_5$ inclusions

The same effect of the magnetic materials used for the matrix and for the inclusions (reinforcements) of a composite material were also observed for a smaller sample (300μm×300μm×300μm).

The second class of tests considers composite materials having Fe matrix and CrO_2 reinforcements or isolated CrO_2 inclusions. The effect of the inclusions type (isolated or not) on the magnetization process is presented in Fig. 5: the isolated inclusions have a stronger effect, the remanent magnetization being higher in this case. This result is confirmed by the experimental data (e.g. in medicine), the non-agglomerated inclusions giving better magnetic properties of the composite material.

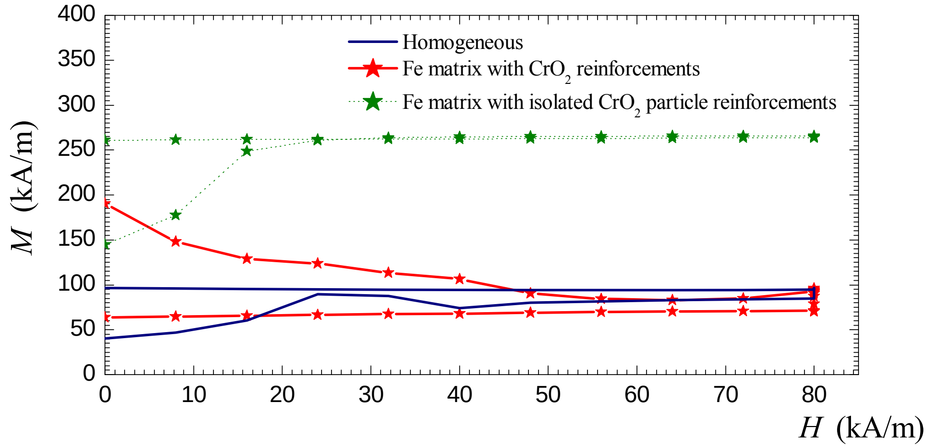

Fig. 5. Magnetization vs. applied magnetic field strength on the easy magnetization axis, for different types of CrO_2 inclusions, in Fe matrix.

The remanent magnetization state at microscopic level, after applying the pulsed external magnetic field, can be analyzed in Fig. 6 for two composite materials having Fe matrix with CrO_2 inclusions. The difference between the two composite materials is the interaction of the inclusions: each inclusion (reinforcement) is surrounded by the matrix (Fig.6.a.) or it is isolated from the neighbours (Fig.6.b). The last material model could be used for modelling core-shell inclusions or for an easier modelling of composite materials with distributed electrical contacts. For example, some soft magnetic composite materials can be modelled [16] by considering a periodic model obtained by the repetition of a structure as the one presented in Fig. 6.b.

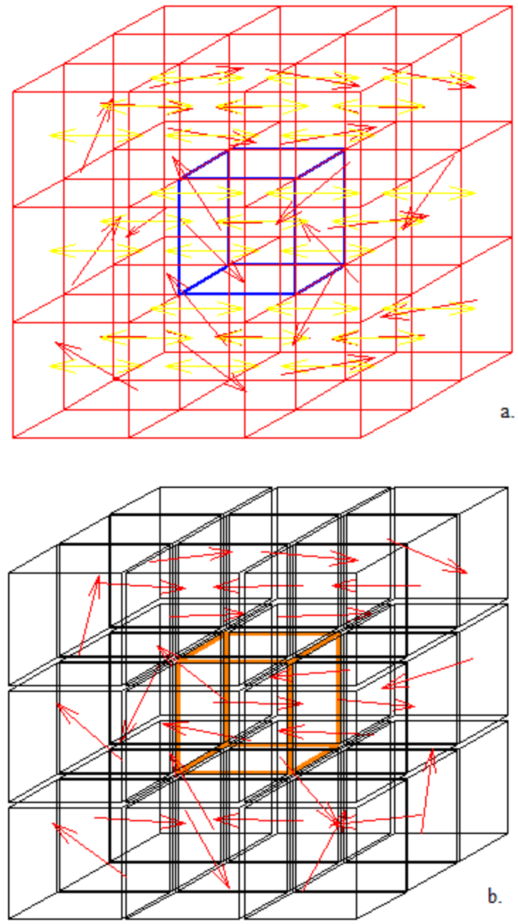

Fig. 6. Modelling of CrO_2 reinforcement in a Fe matrix: a) in contact; b) isolated

The third set of simulations analyses a composite with fibre-type reinforcements. The use of fibres as reinforcements for composite materials is important because the mechanical properties (e.g. stiffness and strength) of the material are improved, as the technical literature [4] reports: the number of fibres and their positioning (horizontal, vertical or at a certain angle) influence the material strength. Our numerical tests are dedicated to the correlations between the density of fibres, their positioning in the matrix, and the magnetic properties of the composite material, especially the remanent magnetization. Unfortunately, the hardware and software constraints limited the numerical model and only 2 or 3 fibres can be considered, the obtained results being more qualitative. For example, two fibres in different positions were considered, but no significant differences were found, so one can not study the influence of the fibres orientation on the macroscopic magnetic properties.

Table 3 presents the remanent magnetization values for a homogeneous material and for the corresponding composites having three different matrix materials (Fe, Co or Ni) and a different number of $SmCo_5$ fibres as inclusions. The increasing of the fibres number improves the remanent magnetization of the composite for any matrix material, because the density of inclusion material ($SmCo_5$) increases and the composite magnetic material has better properties than the matrix material. It must notice that this effect (increasing of M_r with the increasing of the fibres number) is more pronounced for Ni matrix. Of course, a complete study must also consider the shape and the orientation of fibres, not only their density.

Table 3

Remanent magnetization M_r [kA/m] for composite materials with $SmCo_5$ fibres

Matrix material	0 fibres (homogeneous material)	2 fibres	3 fibres
Fe	24.297	55.751	89.650
Co	23.197	61.376	89.750
Ni	17.674	24.736	50.618

6. Conclusions

The behaviour of the composite magnetic materials placed in an external magnetic field was simulated at microscopic scale using a 3D software.

The purpose of the analysis was to show how the composite material properties and structure influence the remanent magnetization values. The paper highlights the superiority of these composite magnetic materials in comparison with the similar homogeneous materials (materials as the composite matrix, but without inclusions).

The presented research shows that the remanent magnetization depends on the geometry of the material components (matrix and inclusions) and their magnetic properties, giving a few design guidelines. For each different application it is important to carefully analyze, by numerical simulation, the effect on the composite magnetic properties of the combination between the matrix and the reinforcements, especially regarding the shape and the dispersion of the inclusions and the magnetic properties of the components. In all analyzed cases, higher values for the remanent magnetization were obtained for the composite materials by comparison with the values for the homogeneous materials.

The study shows the utility of a micromagnetic simulation software, as Magsimus, to approximate the magnetic material behaviour during the magnetization process, in order to optimize the structure of a composite magnetic material for a desired application, where the profile of the applied magnetic field could be predicted.

The analysis will continue considering other magnetic composite materials (e.g. soft magnetic composite materials) and taking into account the coupling between the magnetic properties and the electrical properties.

Acknowledgment

The work has been funded by the Sectorial Operational Programme Human Resources Development 2007-2013 of the Romanian Ministry of Labour, Family and Social Protection through the Financial Agreement POSDRU/88/1.5/S/60203.

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