HOMOGENIZATION OF RANDOM ANISOTROPY PROPERTIES IN POLYCRYSTALLINE MAGNETIC MATERIALS

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Abstract. This paper is devoted to the determination of the equivalent anisotropy properties of polycrystalline magnetic materials, modelled by an assembly of monocrystalline grains with a stochastic spatial distribution of easy axes. The mathematical theory of Γ-convergence is applied to homogenize the anisotropic term in the Gibbs free energy. The procedure is validated focusing on the micromagnetic computation of reversal processes in polycrystalline magnetic thin films.

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1. Introduction

In the last years, much effort has been devoted to the development of theoretical models and advanced micromagnetic computational codes to study magnetization processes at micrometric and submicrometric scale [1, 2]. Criticalities can appear in the treatment of the spatial distribution of heterogeneous physical parameters when polycrystalline magnetic materials are modelled. Usually, they are described as an array of grains, geometrically constructed using Voronoi diagrams [3]. We employ an alternative approach, where the sample is modelled by an assembly of monocrystalline grains, assuming a stochastic spatial distribution of easy axes, and the mathematical theory of Γ-convergence (for multiple-scale problems in micromagnetism, see for instance [4]) is applied to homogenize the anisotropic term in the Gibbs free energy. The proof of convergence is detailed in [5]. Here, the homogenization result is used to study precessional switching in polycrystalline magnetic thin films, comparing the results obtained by considering heterogeneous and homogenized media.

2. Setting of the problem and homogenization result

We deal with a polycrystalline magnetic sample, which occupies a bounded region D in $\mathbb{R}^3$. We introduce the magnetic spatial distribution $\mathbf{M}\colon \mathbb{R}^3 \to \mathbb{R}^3$, with $|\mathbf{M}| = M_{\mathrm{S}}\chi_D$, where $M_{\mathrm{S}} > 0$ is a fixed constant (saturation magnetization), and the rescaled magnetization $\mathbf{m} := \mathbf{M}/M_{\mathrm{S}}$.

The total energy associated to the system is the sum of the exchange energy $E_{\mathrm{exc}}(\mathbf{m})$, the anisotropy energy $E_{\mathrm{an}}(\mathbf{m}, \omega)$, the magnetostatic energy $E_{\mathrm{magn}}(\mathbf{m})$ and the Zeeman energy

$E_{\rm ext}(\mathbf{m})$, namely

$$\begin{aligned} E(\mathbf{m},\omega) \quad := \quad & \int_D A|\nabla \mathbf{m}|^2 \,\mathrm{d}\mathbf{x} + \int_D f_{\rm an}(\mathbf{m},\mathbf{x},\omega)\,\mathrm{d}\mathbf{x} \\ & -\frac{\mu_0}{2}\int_D M_{\rm S}\mathbf{H}_{\rm m}\cdot \mathbf{m}\,\mathrm{d}\mathbf{x} - \mu_0 \int_D M_{\rm S}\mathbf{H}_{\rm a}\cdot\mathbf{m}\,\mathrm{d}\mathbf{x}. \end{aligned} \tag{2.1}$$

In (2.1) $A > 0$ is the exchange constant; $f_{\rm an}$ represents the anisotropy energy density given by $f_{\rm an}(\mathbf{m},\mathbf{x},\omega) := k_{\rm an}[1-(\mathbf{m}\cdot\mathbf{u}_{\rm an}(T_{\mathbf{x}}\omega))^2]$, where $k_{\rm an} > 0$ is the magnetocrystalline anisotropy constant and $\mathbf{u}_{\rm an}\colon \Omega \to \{|\mathbf{x}| = 1\}$ is a random distribution of easy axes: (Ω,μ) is a probability space and T is a 3-dimensional ergodic dynamical system on Ω. Moreover, μ_0 is the magnetic permeability of vacuum; $\mathbf{H}_{\rm m} := \nabla u$ is the magnetostatic field, and the scalar potential u is the solution of the Poisson equation $\nabla^2 u + \nabla\cdot\mathbf{M} = 0$.

In [5] the spatial homogenization of the anisotropy energy $E_{\rm an}$ is investigated. More precisely, if $E^{\varepsilon}_{\rm an}(\mathbf{m},\omega) := \int_D f_{\rm an}\left(\mathbf{m},\frac{\mathbf{x}}{\varepsilon},\omega\right)\mathrm{d}\mathbf{x}$, then the family $E_\varepsilon(\mathbf{m},\omega) := E_{\rm exc}(\mathbf{m}) + E^{\varepsilon}_{\rm an}(\mathbf{m},\omega) + E_{\rm magn}(\mathbf{m}) + E_{\rm ext}(\mathbf{m})$ Γ-converges, as $\varepsilon \to 0^+$, a.s. in Ω, to

$$\bar{E}(\mathbf{m}) = E_{\rm exc}(\mathbf{m}) + k_{\rm an}\int_D\int_\Omega [1-(\mathbf{m}\cdot\mathbf{u}_{\rm an}(\omega))^2]\,\mathrm{d}\mu\,\mathrm{d}\mathbf{x} + E_{\rm magn}(\mathbf{m}) + E_{\rm ext}(\mathbf{m}). \tag{2.2}$$

The homogenization result, defined by Eq. (2.2), is applied to determine the equivalent anisotropy properties of a polycrystalline magnetic medium. By considering a spherical coordinate system with angular coordinates θ $(0 \le \theta \le \pi)$ and ϕ $(0 \le \phi \le 2\pi)$, $\mathbf{u}_{\rm an}$ is assumed to be a Gaussian random variable $\mathbf{u}_{\rm an} : \Omega \to \mathbb{R}^3$, with a probability density function $P(\theta,\phi) = \rho(\theta)\rho(\phi)$ where $\rho(\nu) = \frac{1}{s_\nu\sqrt{2\pi}}e^{-\frac{|\nu-\eta_\nu|^2}{2s_\nu^2}}$, being $\nu = \theta$ (or $\nu = \phi$), s_ν the standard deviation and η_ν the expected value. In order to derive equivalent anisotropy parameters, $\bar{f}_{\rm an}(\mathbf{m})$ is numerically interpolated by an equivalent anisotropy function having the expression: $f^*_{\rm an}(\mathbf{m}) = k^*_{\rm an}[1-\gamma(\mathbf{m}\cdot\mathbf{u}_{\rm an}(\eta_\theta,\eta_\phi))^2]$, where $k^*_{\rm an}$ is the equivalent anisotropy constant and γ is a dimensionless interpolating coefficient. As an example, the plots of the equivalent anisotropy functions and the corresponding energy surfaces are shown in Fig. 1 for two values of the standard deviation s (having assumed $s = s_\theta = s_\phi$), with $\eta_\theta = \pi/2$ and $\eta_\phi = \pi$. At the increase of s, the equivalent anisotropy energy surface tends to a sphere, since there is an asymptotic behaviour towards isotropy.

3. Numerical analysis

The homogenization procedure has been validated by simulating the precessional switching of a $4\,\mu$m $\times 4\,\mu$m polycrystalline magnetic film, with thickness equal to 20 nm. In the film plane the grains are assumed to have a square shape with size of 20 nm; in each grain a given anisotropy direction $\mathbf{u}_{\rm an}$ is assumed. The micromagnetic simulations are performed by integrating the Landau-Lifshitz-Gilbert (LLG) equation:

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_{\rm G}}{(1+\alpha^2)}\left[\left((\mathbf{M}\times\mathbf{H}_{\rm eff}) + \frac{\alpha}{M_{\rm S}}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\rm eff})\right)\right], \text{ with } |\mathbf{M}| = M_{\rm S} \tag{3.1}$$

where $\gamma_{\rm G} = 2.21\cdot 10^5\,\mathrm{mA}^{-1}\mathrm{s}^{-1}$ is the absolute value of the gyromagnetic ratio and α is the damping constant [1]. The effective field $\mathbf{H}_{\rm eff}$ is the sum of applied field $\mathbf{H}_{\rm a}$, anisotropy field $\mathbf{H}_{\rm an}$, exchange field $\mathbf{H}_{\rm ex}$ and magnetostatic field $\mathbf{H}_{\rm m}$. In particular, $\mathbf{H}_{\rm an}$ is deduced by the anisotropy energy function $f_{\rm an}$ as $\mathbf{H}_{\rm an} = -\frac{1}{\mu_0}\frac{\partial f_{\rm an}(\mathbf{M})}{\partial \mathbf{M}}$. The spatial discretization of the LLG equation is performed by using the finite element method with linear basis functions,

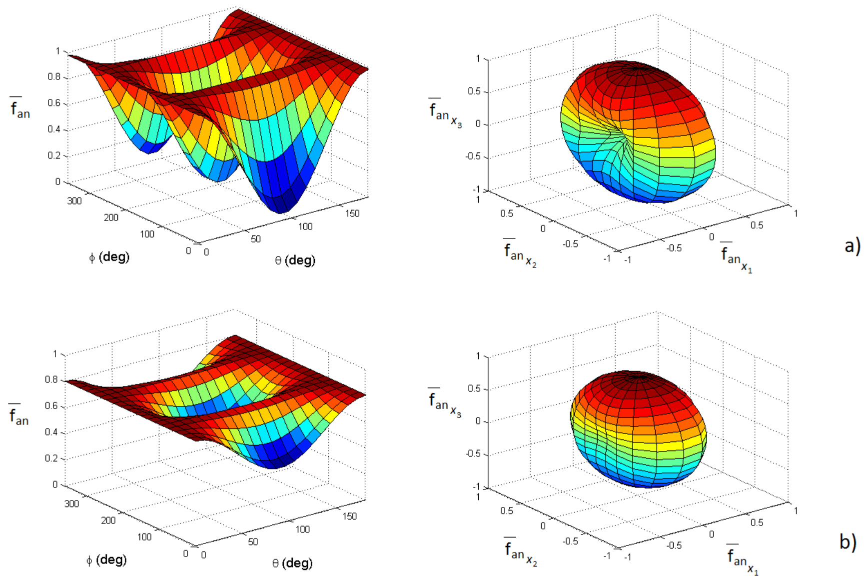

FIGURE 1. Equivalent anisotropy function $\bar{f}_{\mathrm{an}}(\mathbf{m})$ and corresponding energy surfaces, for $s = \pi/20$ (a) and $s = \pi/5$ (b), having assumed $\eta_\theta = \pi/2$ and $\eta_\phi = \pi$.

assuming the components of $\mathbf{H}_{\mathrm{eff}}$ as nodal unknowns [6]. Then, the magnetization update is performed via a norm-conserving scheme based on the Cayley transform [7]. To accelerate the computation, the magnetostatic field due to "far" dipoles is evaluated by a multipole expansion technique [8].

In the simulations the following physical parameters have been considered: $M_{\mathrm{S}} = 800\,\mathrm{kA/m}$, $A = 15$ pJ/m and $\alpha = 0.02$. The thin film is discretized into volume elements with size $\sim 6.6\,\mathrm{nm}$. We assume that $k_{\mathrm{an}} = 50$ kJ/m^3 and vector $\mathbf{u}_{\mathrm{an}}$ is randomly distributed over the film plane (i.e. angle θ is fixed to $\pi/2$), while angle ϕ has a Gaussian distribution with standard deviation s_ϕ and expected value η_ϕ. The precessional switching is simulated starting from a uniform spatial distribution of the magnetization along the x_1-axis and applying a constant field $\mathbf{H}_{\mathrm{a}}$, with amplitude equal to 100 kA/m, along the x_2-axis (see Fig. 2a). In particular, Figs. 2b and 2c show the results obtained for a standard deviation s_ϕ of $\pi/6$ and π, respectively. The fitting parameters $k^*_{\mathrm{an}}/k_{\mathrm{an}}$ and γ are equal to 0.977 and 0.921 for $s = \pi/6$, while they are equal to 0.88 and 0.567 for $s_\phi = \pi$. The results are validated by comparison to the ones obtained for the heterogeneous structure, putting in evidence a good agreement, also when considering grains having bigger size. Some discrepancies arise at the increase of the standard deviation, since the heterogeneities in the anisotropy term become more important. To highlight the effect of grains on anisotropy properties, we have also computed the magnetization time evolutions obtained in the absence of anisotropy ($k_{\mathrm{an}} = 0$) or assuming a uniform uniaxial anisotropy along x_1-axis (see Fig. 2d).

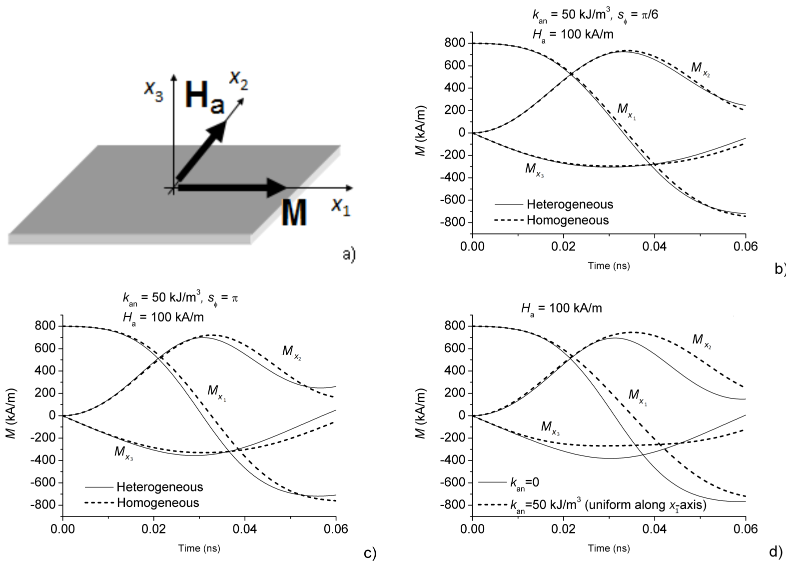

FIGURE 2. (a) Scheme of the precessional switching. Time evolution of the magnetization components assuming an anisotropy constant k_{an} equal to 50 kJ/m^3 and a variable standard deviation s_ϕ: (b) $s_\phi = \pi/6$ and (c) $s_\phi = \pi$. The results obtained with the heterogeneous structure are compared with those given by considering homogenized parameters. (d) Time evolution of the magnetization components disregarding anisotropy or assuming a uniform uniaxial anisotropy along x_1-axis with k_{an} equal to $50\,\text{kJ/m}$.

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