Determination of the equivalent anisotropy properties of polycrystalline magnetic materials: theoretical aspects and numerical analysis

Michela Eleuteri

University of Verona (Italy)

Supported by: GNAMPA 2010 “Problemi variazionali in micromagnetismo” (resp. M. Eleuteri)

Joint project with...

- **Variational problems in micromagnetism**
  - I. Fonseca, G. Leoni, (2000); G. Pisante (2004); E. Acerbi, I. Fonseca, G. Mingione (2006), A. De Simone, R.V. Kohn, S. Müller, and F. Otto (2006).
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Task of the research project

- Development of theoretical formulations based on the classical tools of Mathematical Analysis, in particular the methods of the Calculus of Variations and of the analysis of Partial Differential Equations, for studying magnetization processes in complex magnetic nanostructures
- Strong connection between PoliTO and INRIM, between mathematics and numerics, with the aim of giving the necessary mathematical support for developing advanced computational models for the micromagnetic calculus and the analysis of the nanostructures produced the INRIM research team
- The relevance of such activity is underlined by the more and more growing attention which has been dedicated, during the last decade, to the study of micromagnetic problems with the methods of the Calculus of Variations and, more generally, of the Mathematical Analysis
- The basic aim is the comprehension of the connections between the material properties on the microscopic level and the behavior on the macroscopic scale, with the idea of giving a modeling interpretation of the experimental data

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- The attention is focused on the study of the Landau-Lifschitz-Gilbert (LLG) equation, universally adopted in the prediction of the nonlinear dynamic of magnetic materials on micron- and submicron-scale
- Great importance to the analysis of the minima of the Gibbs free energy functional, strictly connected to the LLG equation, with the aim of determining the equilibrium configurations in complex magnetic systems
- The development of mathematical models for the analysis of magnetic nanostructures may present criticalities concerned with the treatment of the spatial distribution of the physical and structural parameters, whose combination gives origin to phenomena characterized by a strongly multiscale nature
- In particular, the energy functional is characterized by the simultaneous presence of energetic terms that deal with very different length scales, whose interaction must be treated in a very accurate way, in order to have a correct interpretation of the evolution of magnetic domains
- To this end, a first aim will be concerned with the development of multiscale formulations based on homogenization techniques and on the Gamma-convergence theory

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Plan of the talk

- Nanostructures and nanotechnology
- Magnetic nanostructures (examples and polycrystalline magnetic materials)
- Criticalities from the strongly multiscale nature of the magnetization processes (numerical treatment difficult task)
- Our approach and our results

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Nanostructures and nanotecnology

- General agreement of the fact that the first person who had intuition about the potentialities of nanotecnologies was R. Feyman (Nobel Prize in Physics, in 1965)
- In a well known conference in 1959 at the Californian Institute of Technology said a sentence that became famous: “There is plenty of room at the bottom” (meaning “at the atomic dimension”)
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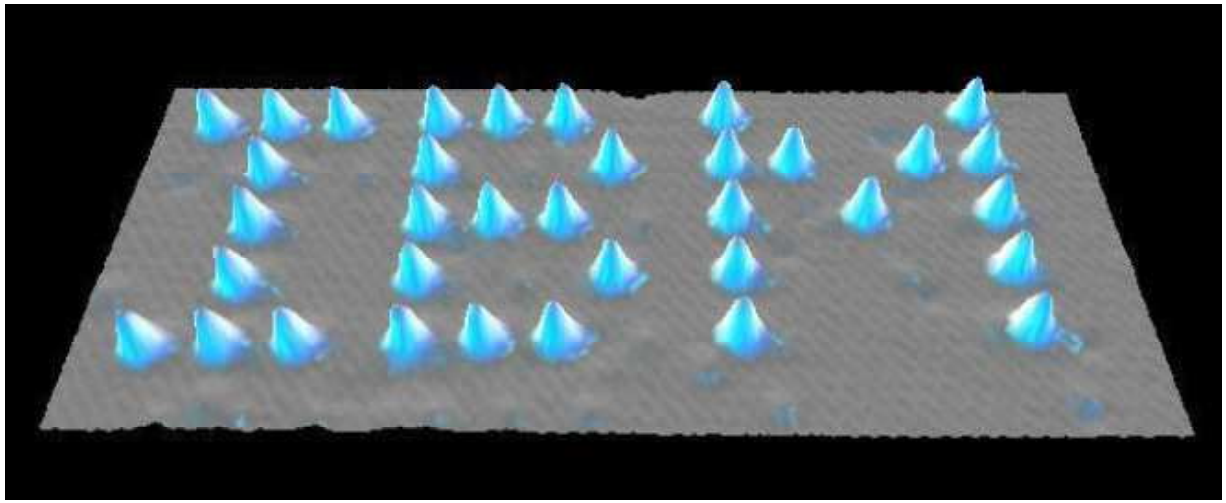

Figure 1: A nickel sheet where there have been posed atoms singularly manipulated (From: Marco Bettinelli “Nanostrutture e nano-tecnologie”(2008))

- **Nanotechnology:** to modify intentionally matter, at the atomic or subatomic scale (interdisciplinary)

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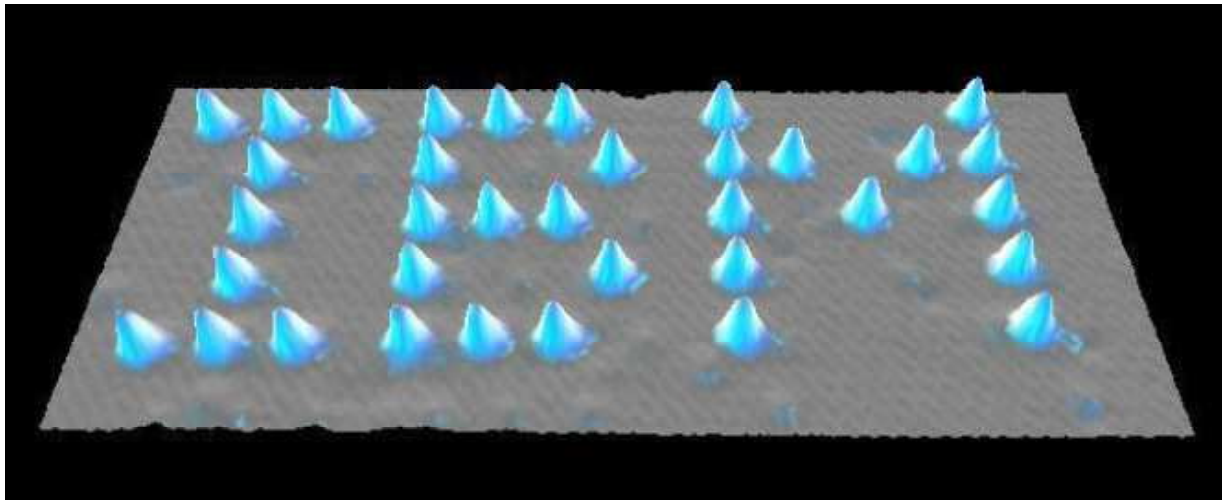

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Magnetic nanostructures

R. Skomski “Nanomagnetis” J. Phys.: Condens. Matter, **15** (2003) R841-R896.

- Thousands of years of human curiosity have led to the discovery of magnetism, and for many centuries magnetism has stimulated progress in science and technology
- For a long time, the focus had been on macroscopic magnetism, as exemplified by the compass needle, by the geomagnetic field and by the ability of electromagnets and permanent magnets to do mechanical work
- Atomic-scale magnetic phenomena, such as quantum-mechanical exchange, crystal-field interaction or relativistic spin-orbit coupling were discovered in the first half of the last century and are now exploited, for example, in advanced permanent- magnet intermetallics
- However, only in recent decades it became clear that solid-state magnetism is, to a large extent, a nanostructural phenomenon

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Magnetic nanostructures

- The scientific and technological importance of magnetic nanostructures has different reasons (overwhelming variety of structures with interesting physical propertiesc - from naturally occurring nanomagnets and comparatively easy-to-produce bulk nanocomposites to demanding artificial nanostructures; involvement of nanoscale effects in the explanation and improvement of the properties of advanced magnetic materials; the fact that nanomagnetism opened the door for completely new technologies)
- A naturally occurring biomagnetic phenomenon is magnetite (Fe3O4) nanoparticles precipitated in bacteria, molluscs, insects and higher animals
- Magnetostatic bacteria live in dark environments and contain chains of 40-100 nm magnetite particles used for vertical orientation

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- Similar magnetite particles have been found in the brains of bees, pigeons and tuna, and it is being investigated whether and how the particles serve as field sensors for migration
- Magnetite and other oxide particles are also responsible for rock magnetism, exploited for example in archaeomagnetic dating and for monitoring changes in the Earth's magnetic field
- A fascinating approach is artificial nanostructuring to create completely new materials and technologies
- Advanced magnetic nanostructures are characterized by a fascinating diversity of geometries, ranging from complex bulk structures to a broad variety of low-dimensional systems - Figure 2 shows some examples

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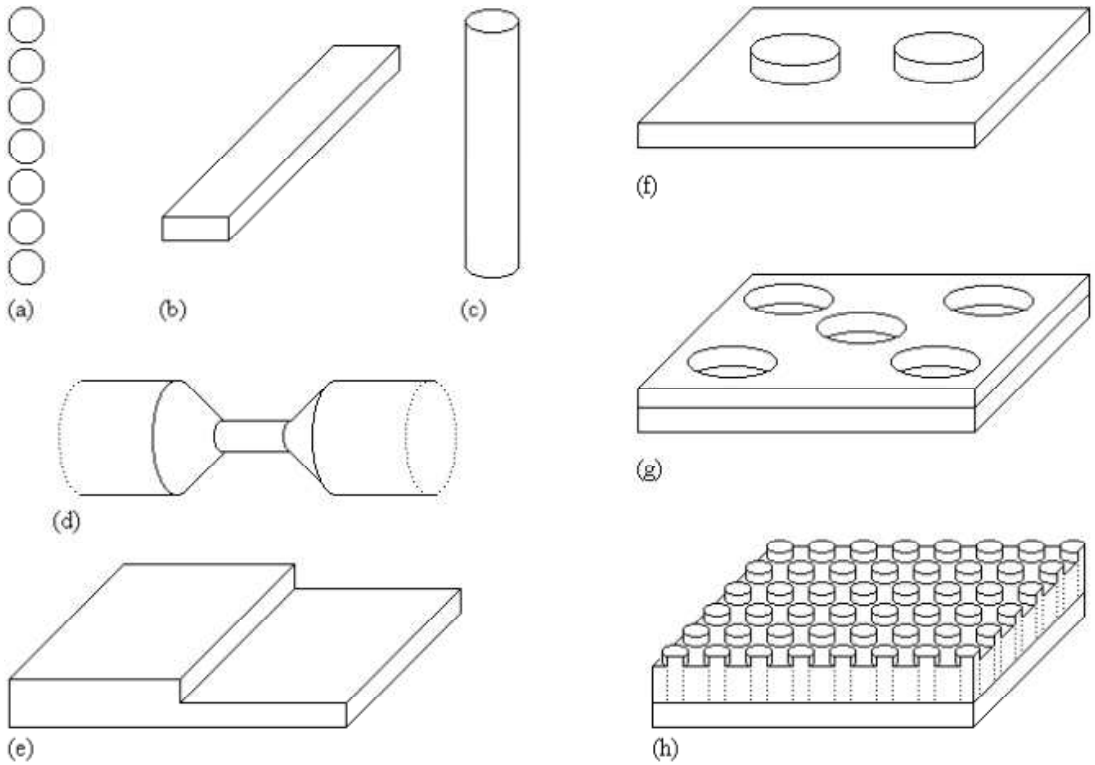

Figure 2: Typical nanostructure geometries: (a) chain of fine particles, (b) striped nanowire, (c) cylindrical nanowire, (d) nanojunction, (e) vicinal surface step, (f) nanodots, (g) antidots and (h) particulate medium.

Micromagnetic numerical models: difficulties

- Micromagnetic numerical models common tool for evaluating the magnetization processes in magnetic nanostructures
- Deep understanding of the relationship between structural properties and magnetic domain formation - outcomes in technological applications
- Micromagnetics theory based on a continuum approximation of the magnetization spatial distribution - different energy contributions compete to determine magnetic domain configuration
- Most important contributions: exchange, magnetostatic, anisotropy and Zeeman energies whose accurate approximation is essential to correctly evaluate time and spatial evolution of magnetization within the sample
- Energy terms act at different spatial scales (nanometric resolution: exchange term; sample dim.: long-range magnetostatic interactions)
- Magnetic anisotropy expresses the tendency of the magnetization to lie along certain crystallographic directions - intermediate spatial scale
- Magnetic properties are influenced by the size, shape, boundary properties and orientation distribution of grains
- Micromagnetic simulations complex task - simulations often performed under the hypothesis of single crystal

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Micromagnetic numerical models: difficulties

- Micromagnetic numerical models common tool for evaluating the magnetization processes in magnetic nanostructures
- Deep understanding of the relationship between structural properties and magnetic domain formation - outcomes in technological applications
- Micromagnetics theory based on a continuum approximation of the magnetization spatial distribution - different energy contributions compete to determine magnetic domain configuration
- Most important contributions: exchange, magnetostatic, anisotropy and Zeeman energies whose accurate approximation is essential to correctly evaluate time and spatial evolution of magnetization within the sample
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Micromagnetic numerical models: difficulties

- Assumption of uniaxial or cubic anisotropy (valid for samples having dimensions comparable than grain size)
- Assumption inadequate in presence of polycrystalline materials (grain orientation and distribution affect the behaviour of the system)
- Polycrystalline materials usually modelled within micromagnetic numerical codes as an array of grains, geometrically constructed using Voronoi diagrams - each single-crystal grain is assumed to have a randomly oriented uniaxial anisotropy
- Strong impact on the geometry building and meshing, making the pre-processing phase very complex
- We propose an alternative procedure, based on the replacement of the polycrystalline magnetic material with an homogenized sample having equivalent anisotropy properties
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First results obtained

O. BOTTAUSCIO, V. CHIADÒ PIAT, M. ELEUTERI, L. LUSSARDI, A. MANZIN: *"Determination of the equivalent anisotropy properties of polycrystalline magnetic materials: theoretical aspects and numerical analysis"*, submitted.

- The $\Gamma-$convergence theory is here adopted to homogenize the anisotropic contribution in the energy functional and derive the equivalent anisotropy properties
- The reliability of this approach is investigating focusing on the computation of the static hysteresis loops of polycrystalline magnetic thin films, starting from the numerical integration of the LLG equation

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Setting of the problem

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- $\mathbf{M} \in L^2(\mathbb{R}^3;\mathbb{R}^3)$ magnetization vector field, with $\mathbf{M} = M_S \chi_D$ in $\mathbb{R}^3$, M_S being the saturation magnetization; $\mathbf{m} \in L^2(\mathbb{R}^3;\mathbb{R}^3)$ $\mathbf{m} = \mathbf{M}/M_S$ rescaled magnetization
- magnetic energy behaviour described by the following functional

$$F(\mathbf{m}, \mathbf{H}_a) = \int_D A|\nabla \mathbf{m}|^2 \, dx + \int_D f_{an}(\mathbf{m}, \mathbf{u}_{an}) \, dx - \frac{\mu_0}{2} \int_D M_S \mathbf{H}_\mathbf{m} \cdot \mathbf{m} \, dx - \mu_0 \int_D M_S \mathbf{H}_a \cdot \mathbf{m} \, dx$$

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The $\Gamma-$convergence result

- $K := \left\{ \mathbf{m} \in L^2(\mathbb{R}^3;\mathbb{R}^3) : \mathbf{m}_{|_D} \in H^1(D;\mathbb{R}^3),\ |\mathbf{m}| = \chi_D \text{ a.e. in } \mathbb{R}^3 \right\}$
- For any $\mathbf{m}$, let $v \in H^1(\mathbb{R}^3)$ be the unique solution of the equation

$$\nabla^2 v + \nabla \cdot \mathbf{m} = 0, \text{ in } \mathscr{D}'(\mathbb{R}^3)$$

- $(\Omega, \mathscr{F}, \mu)$ probability space; T 3-dimensional ergodic dynamical system
- Let $\varphi : \mathbb{R}^3 \times \mathbb{R}^3 \times \Omega \to [0, +\infty)$ be a measurable map such that $\varphi(0,0,\cdot) \in L^1(\Omega)$ and

$$|\varphi(\mathbf{m}_1, \mathbf{x}, \omega) - \varphi(\mathbf{m}_2, \mathbf{x}, \omega)| \leq L|\mathbf{m}_1 - \mathbf{m}_2|$$

- We assume that for any $\mathbf{m} \in \mathbb{R}^3$, the random field $\varphi(\mathbf{m}, \cdot, \cdot)$ is stationary and ergodic: therefore $\varphi(\mathbf{m}, \mathbf{x}, \omega) = f(\mathbf{m}, T_{\mathbf{x}}\omega)$ for a suitable map $f : \mathbb{R}^3 \times \Omega \to [0, +\infty)$.

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- We assume that for any $\mathbf{m} \in \mathbb{R}^3$, the random field $\varphi(\mathbf{m}, \cdot, \cdot)$ is stationary and ergodic: therefore $\varphi(\mathbf{m}, \mathbf{x}, \omega) = f(\mathbf{m}, T_x\omega)$ for a suitable map $f : \mathbb{R}^3 \times \Omega \to [0, +\infty)$.

The $\Gamma-$convergence result

- $K := \left\{ \mathbf{m} \in L^2(\mathbb{R}^3;\mathbb{R}^3) : \mathbf{m}_{|_D} \in H^1(D;\mathbb{R}^3),\ |\mathbf{m}| = \chi_D \text{ a.e. in } \mathbb{R}^3 \right\}$
- For any $\mathbf{m}$, let $v \in H^1(\mathbb{R}^3)$ be the unique solution of the equation

$$\nabla^2 v + \nabla \cdot \mathbf{m} = 0, \text{ in } \mathscr{D}'(\mathbb{R}^3)$$

- $(\Omega, \mathscr{F}, \mu)$ probability space; T 3-dimensional ergodic dynamical system
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if $\mathbf{m} \in K$, and $+\infty$ otherwise.

Theorem

The family $(E_\varepsilon(\cdot,\omega))_{\varepsilon>0}$ Γ-converges, a.s. in Ω as $\varepsilon \to 0^+$, with respect to the strong topology of $L^2(\mathbb{R}^3;\mathbb{R}^3)$, to the functional $\bar{E}\colon L^2(\mathbb{R}^3;\mathbb{R}^3) \to [0,+\infty]$ given by

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Application to polycrystalline magnetic materials

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$$\bar F(\mathbf{m}) := A\int_D |\nabla \mathbf{m}|^2\,d\mathbf{x} + \int_D \bar f_{\rm an}(\mathbf{m}(\mathbf{x}))\,d\mathbf{x} - \frac{\mu_0}{2}\int_D M_S\mathbf{H}_{\rm m}\,d\mathbf{x} - \mu_0\int_D M_S\mathbf{H}_{\rm a}\cdot\mathbf{m}\,d\mathbf{x}$$

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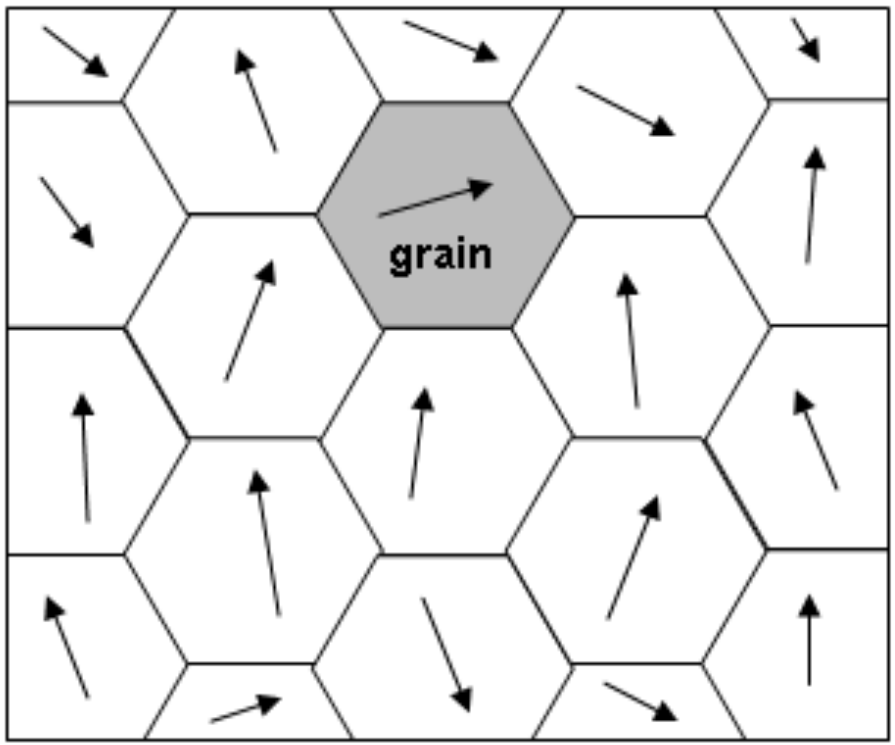
Determination of equivalent anisotropy properties

- The result of the asymptotic problem is applied to the calculation of the equivalent anisotropy properties of a polycrystalline magnetic sample, considering a uniform spatial distribution of the magnetization vector: such a sample is represented as an assembly of grains characterized by a random distribution of easy axes - Fig. a)



a)

Determination of equivalent anisotropy properties

- $\mathbf{u}_{\text{an}}$ Gaussian random variable with a probability density function $P(y) = P(\theta, \phi) = \rho(\theta)\rho(\phi)$ where $\rho(\nu) = \frac{1}{s_\nu \sqrt{2\pi}} \exp\left(\frac{-|\nu - \eta_\nu|^2}{2s_\nu^2}\right)$
- Spherical coordinate system with angular coordinates θ and ϕ $\mathbf{u}_{\text{an}} = \sin\theta\cos\phi\mathbf{i} + \sin\theta\sin\phi\mathbf{j} + \cos\theta\mathbf{k}$
- having assigned to $\mathbf{m}$ a specific direction described by angles α_1 and α_2 the equivalent anisotropy function $\bar{f}_{\text{an}}$ is numerically computed as

$$\bar{f}_{\text{an}}(\mathbf{m}) = \frac{1}{\int_0^\pi \int_0^{2\pi} P(\theta,\phi)\sin\theta d\theta d\phi} \int_0^\pi \int_0^{2\pi} f_{\text{an}}(\mathbf{m}, \mathbf{u}_{\text{an}}) P(\theta,\phi)\sin\theta d\theta d\phi$$

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- To derive equivalent anisotropy parameters, $\bar{f}_{\text{an}}(\mathbf{m})$ numerically interpolated by an **equivalent uniaxial anisotropy function** of the form $f^*_{\text{an}}(\mathbf{m}) = k^*_{\text{an}}[1 - \gamma(\mathbf{m} \cdot \mathbf{u}_{\text{an}}(\eta_\theta, \eta_\phi)^2)]$ with k^*_{an} equivalent anisotropy constant and γ a dimensionless interpolating coefficient

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where
$f_{\text{an}}(\mathbf{m}, \mathbf{u}_{\text{an}}) = f_{\text{an}}(\alpha_1, \alpha_2, \theta, \phi) = k_{\text{an}}[1 - (\mathbf{m}(\alpha_1, \alpha_2) \cdot \mathbf{u}_{\text{an}}(\theta, \phi))^2]$.

- In the case of uniform distribution of vector $\mathbf{u}_{\text{an}}$ in the (x_1, x_2)-plane, the following **equivalent planar anisotropy function** is used as interpolator $f^*_{\text{an}}(\mathbf{m}) = k^*_{\text{an}}[1 - \gamma(\mathbf{m}_{x_1}\, \mathbf{u}_{\text{an},\mathbf{x_1}}(\eta_\theta + \mathbf{m}_{x_2}\, \mathbf{u}_{\text{an},\mathbf{x_2}}(\eta_\phi)^2)]$

Determination of equivalent anisotropy properties

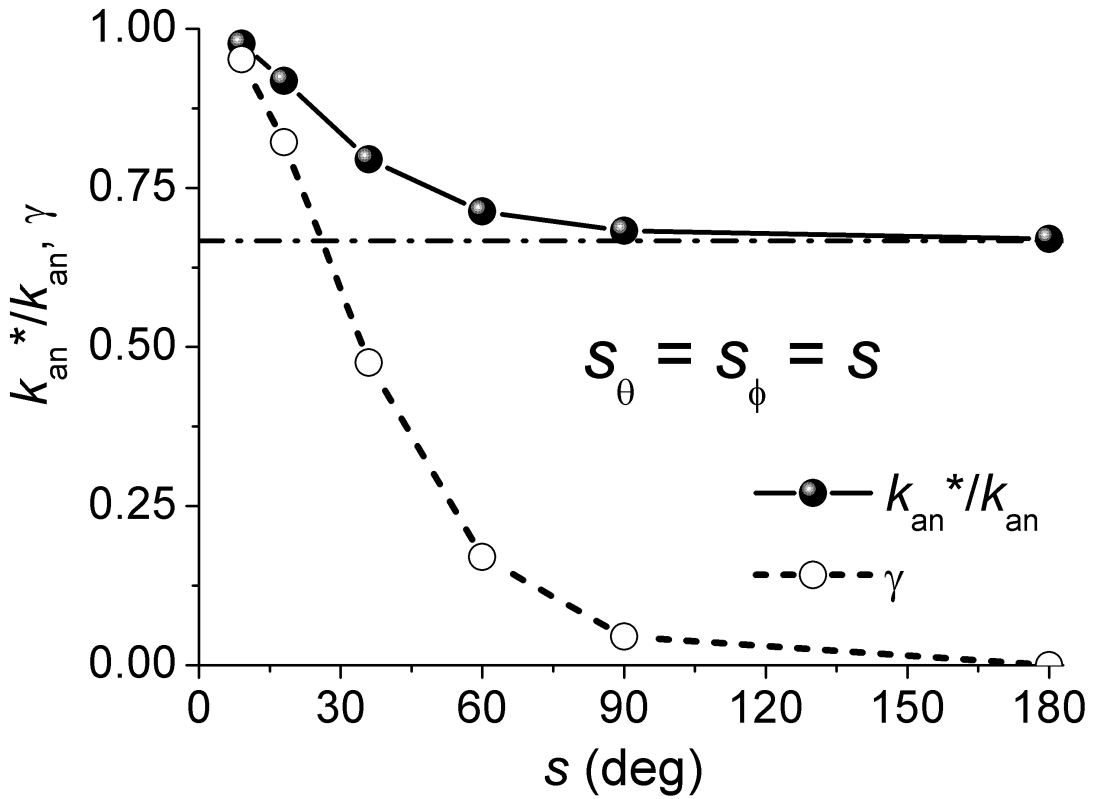

Figure 3: Asymptotic behaviour of the equivalent parameters k_{an}^* and γ at the increase of the standard deviation s, here assumed identical for the two angular coordinates (that is $s = s_\theta = s_\phi$), having also assumed $\eta_\theta = \pi/2$ and $\eta_\phi = 0$. The interpolation is made under the hypothesis of equivalent unidirectional anisotropy

Determination of equivalent anisotropy properties

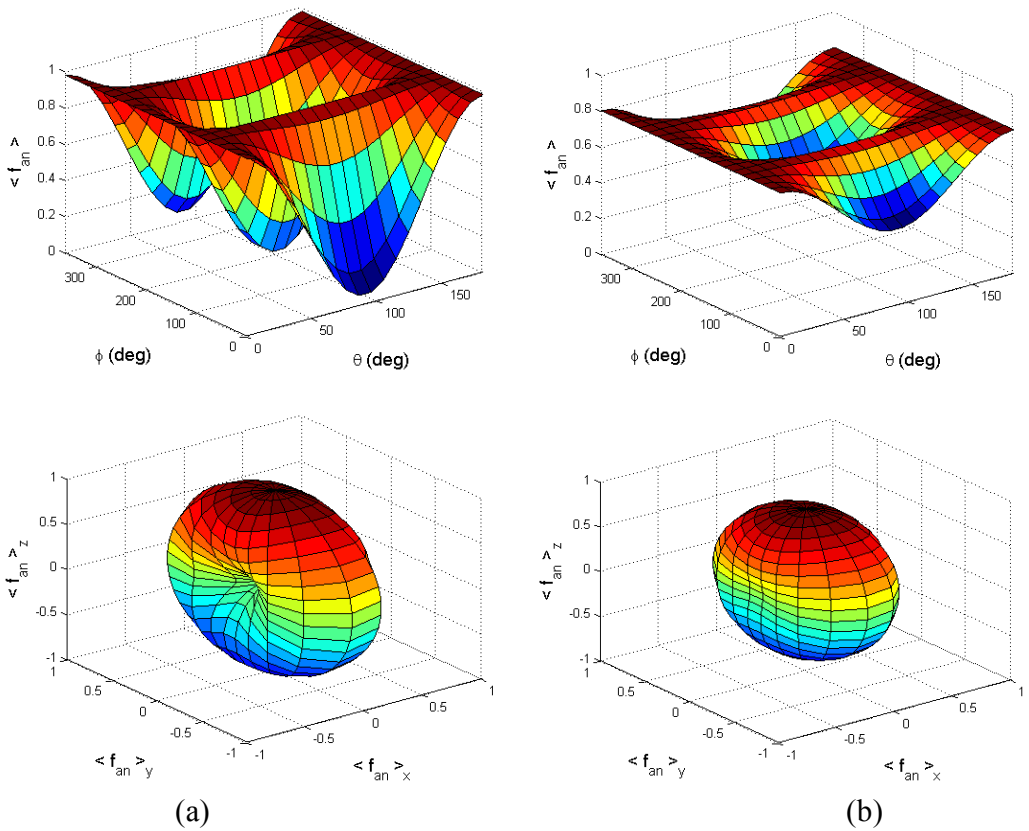

Figure 4: Equivalent anisotropy function and corresponding energy surfaces for the Gaussian distribution, for $s = 0.16$ rad (a) and $s = 0.63$ rad (b), where $\eta_\theta = \pi/2$ and $\eta_\phi = \pi$. At the increase of s, the equivalent anisotropy energy surface tends to a sphere, since there is asymptotic behavior towards isotropy.

Determination of equivalent anisotropy properties

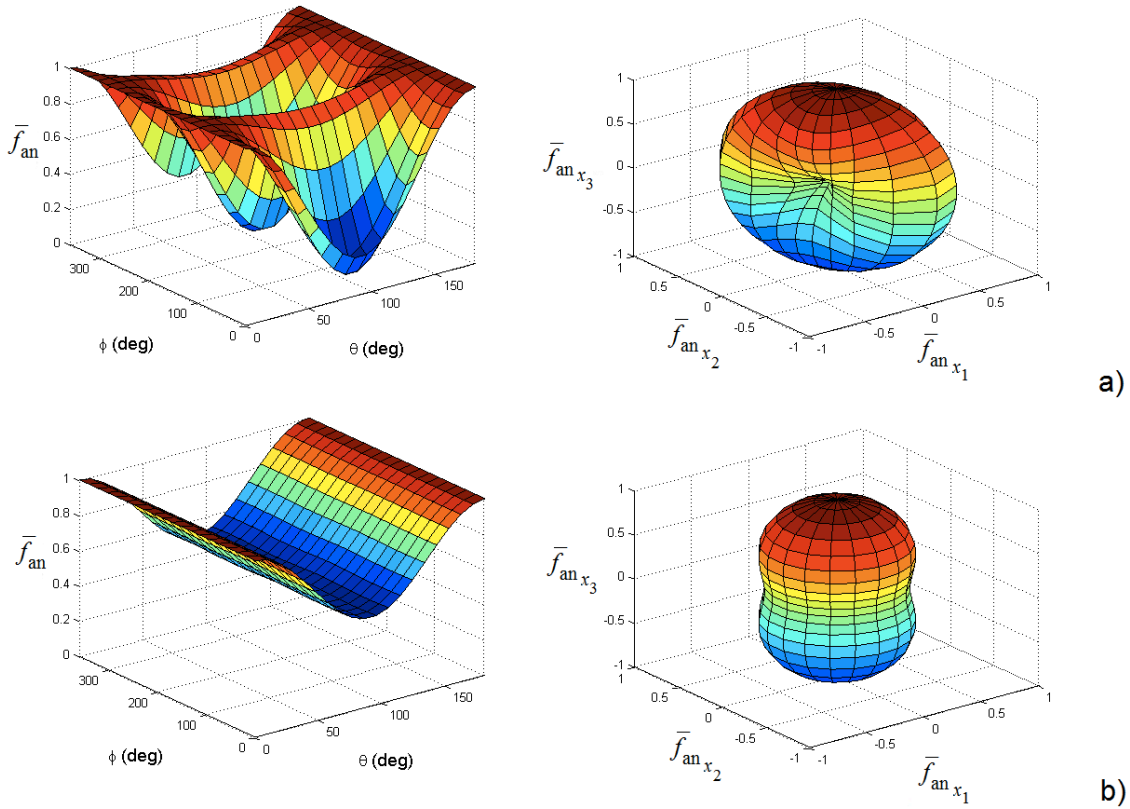

Figure 5: Equivalent anisotropy function and corresponding energy surfaces, for Gaussian distribution with $s = \pi/6$ (a) and for the uniform distribution (b)

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) has been validated by simulating a precessional switching of a polycrystalline magnetic film
- A film with size and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with ; in each grain a given anisotropy direction $\mathbf{u}_{an}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[(\mathbf{M}\times\mathbf{H}_{\text{eff}}) + \frac{\alpha}{M_S}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_a + \mathbf{H}_{an} + \mathbf{H}_{ex} + \mathbf{H}_m$ and

$$\mathbf{H}_{ex} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u, \ \nabla^2 u = -M_S\nabla\cdot\mathbf{m}; \quad \mathbf{H}_{an} = -\frac{1}{\mu_0}\frac{\partial f_{an}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 2) is applied to the computation of the static hysteresis loop of a thin film made of a polycrystalline magnetic material
- A film with size and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with ; in each grain a given anisotropy direction $\mathbf{u}_{\text{an}}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left(\mathbf{M}\times\mathbf{H}_{\text{eff}}\right)+\frac{\alpha}{M_S}\mathbf{M}\times\left(\mathbf{M}\times\mathbf{H}_{\text{eff}}\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{an}} + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{m}}$ and

$$\mathbf{H}_{\text{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u,\ \nabla^2 u = -M_S\nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\text{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\text{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with ; in each grain a given anisotropy direction $\mathbf{u}_{\mathrm{an}}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}\right)+\frac{\alpha}{M_S}\mathbf{M}\times\left(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\mathrm{eff}} = \mathbf{H}_{\mathrm{a}} + \mathbf{H}_{\mathrm{an}} + \mathbf{H}_{\mathrm{ex}} + \mathbf{H}_{\mathrm{m}}$ and

$$\mathbf{H}_{\mathrm{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u, \ \nabla^2 u = -M_S \nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\mathrm{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\mathrm{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with ; in each grain a given anisotropy direction $\mathbf{u}_{\mathrm{an}}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}) + \frac{\alpha}{M_S}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}})\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\mathrm{eff}} = \mathbf{H}_{\mathrm{a}} + \mathbf{H}_{\mathrm{an}} + \mathbf{H}_{\mathrm{ex}} + \mathbf{H}_{\mathrm{m}}$ and

$$\mathbf{H}_{ex} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u, \ \nabla^2 u = -M_S \nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\mathrm{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\mathrm{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ /$2\mu m \times 2\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with ; in each grain a given anisotropy direction $\mathbf{u}_{\text{an}}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left(\mathbf{M}\times\mathbf{H}_{\text{eff}}\right)+\frac{\alpha}{M_S}\mathbf{M}\times\left(\mathbf{M}\times\mathbf{H}_{\text{eff}}\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{an}} + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{m}}$ and

$$\mathbf{H}_{\text{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u,\ \nabla^2 u = -M_S\nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\text{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\text{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ /$2\mu m \times 2\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with size of $20nm$; in each grain a given anisotropy direction $\mathbf{u}_{\mathrm{an}}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}\right)+\frac{\alpha}{M_S}\mathbf{M}\times\left(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\mathrm{eff}} = \mathbf{H}_{\mathrm{a}} + \mathbf{H}_{\mathrm{an}} + \mathbf{H}_{\mathrm{ex}} + \mathbf{H}_{\mathrm{m}}$ and

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Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ /$2\mu m \times 2\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with size of $20nm$ /dimension ranging from $20nm$ to $100nm$; in each grain a given anisotropy direction $\mathbf{u}_{\text{an}}$ is assumed, randomly distributed over the entire sample
- by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left(\mathbf{M}\times\mathbf{H}_{\text{eff}}\right) + \frac{\alpha}{M_S}\mathbf{M}\times\left(\mathbf{M}\times\mathbf{H}_{\text{eff}}\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{an}} + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{m}}$ and

$$\mathbf{H}_{\text{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u,\ \nabla^2 u = -M_S \nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\text{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\text{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ /$2\mu m \times 2\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with size of $20nm$ /dimension ranging from $20nm$ to $100nm$; in each grain a given anisotropy direction $\mathbf{u}_{\text{an}}$ is assumed, randomly distributed over the entire sample
- Micromagnetic simulations are performed by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left((\mathbf{M}\times\mathbf{H}_{\text{eff}}) + \frac{\alpha}{M_S}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{an}} + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{m}}$ and

$$\mathbf{H}_{\text{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u,\ \nabla^2 u = -M_S \nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\text{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\text{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ /$2\mu m \times 2\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with size of $20nm$ /dimension ranging from $20nm$ to $100nm$; in each grain a given anisotropy direction $\mathbf{u}_{\text{an}}$ is assumed, randomly distributed over the entire sample
- Micromagnetic simulations are performed /The time evolution towards equilibrium states in the computation of the static hysteresis loop is calculated by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left((\mathbf{M}\times\mathbf{H}_{\text{eff}}) + \frac{\alpha}{M_S}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{an}} + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{m}}$ and

$$\mathbf{H}_{\text{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u,\ \nabla^2 u = -M_S\nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\text{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\text{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results

- The homogenization procedure described so far 1) simulating a precessional switching 2) computation of the static hysteresis loop
- A film with size $4\mu m \times 4\mu m$ /$2\mu m \times 2\mu m$ and thickness equal to $20nm$ is considered
- In the film plane (xy-plane) the grains have a square shape with size of $20nm$ /dimension ranging from $20nm$ to $100nm$; in each grain a given anisotropy direction $\mathbf{u}_{\text{an}}$ is assumed, randomly distributed over the entire sample
- Micromagnetic simulations are performed /The time evolution towards equilibrium states in the computation of the static hysteresis loop is calculated by integrating the Landau-Lifschitz-Gilbert equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\frac{\gamma_G}{(1+\alpha)^2}\left[\left((\mathbf{M}\times\mathbf{H}_{\text{eff}}) + \frac{\alpha}{M_S}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})\right)\right],$$

with $|\mathbf{M}| = M_S$; $\mathbf{H}_{\text{eff}} = \mathbf{H}_{\text{a}} + \mathbf{H}_{\text{an}} + \mathbf{H}_{\text{ex}} + \mathbf{H}_{\text{m}}$ and

$$\mathbf{H}_{\text{ex}} = \frac{2k_{ex}}{\mu_0 M_S^2}\nabla^2\mathbf{M}; \quad \mathbf{H}_m = \nabla u,\ \nabla^2 u = -M_S\nabla\cdot\mathbf{m}; \quad \mathbf{H}_{\text{an}} = -\frac{1}{\mu_0}\frac{\partial f_{\text{an}}(\mathbf{M})}{\partial \mathbf{M}}$$

Numerical validation of the homogenization results: simulating a precessional switching

- The spatial discretization of the LLG equation is performed by using the finite element method with linear basis functions, assuming the Cartesian components of $\mathbf{H}_{\text{eff}}$ as nodal unknowns
- Then, the magnetization update is performed via a norm-conserving scheme based on the Cayley transform
- To accelerate the computation, the magnetostatic field due to "far" dipoles is evaluated by a multipole expansion technique
- In the simulations the following physical parameters have been considered: $M_S = 800kA/m$, $A = 15pJ/m$ and $\alpha = 0.02$
- The thin film is discretized into volume elements with size $\sim 6.6nm$. We assume that $k_{\text{an}} = 50kJ/m^3$ and vector $\mathbf{u}_{\text{an}}$ is randomly distributed over the film plane (i.e. angle θ is fixed to $\pi/2$), while angle ϕ has a Gaussian distributionwith 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 $\mathbf{H}_{\text{a}}$, with amplitude equal to $100kA/m$, along the x_2-axis

Numerical validation of the homogenization results: simulating a precessional switching

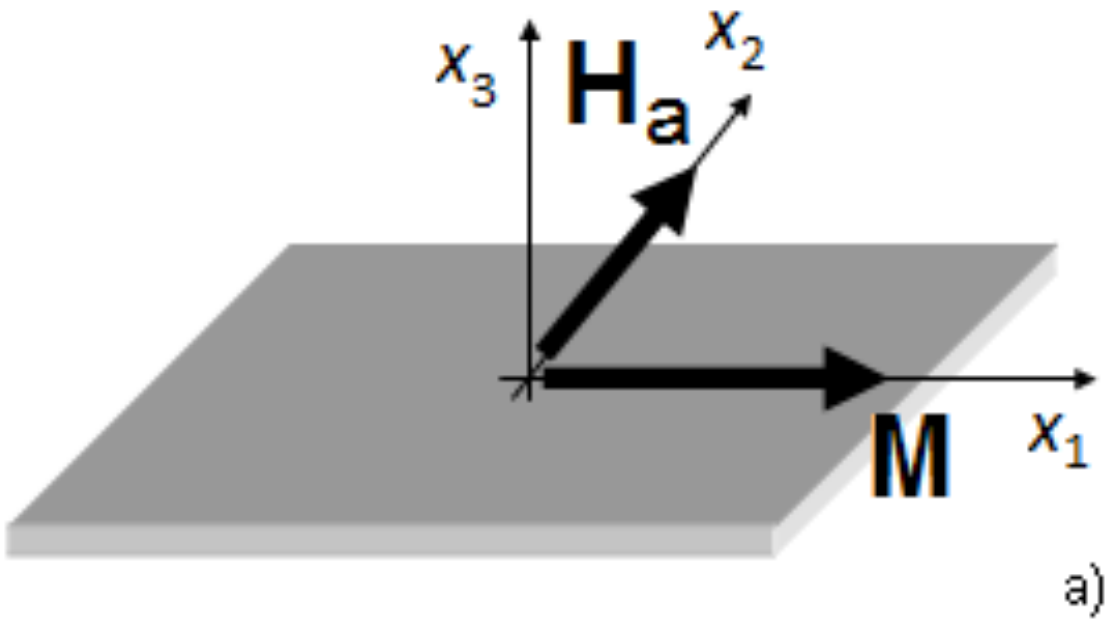
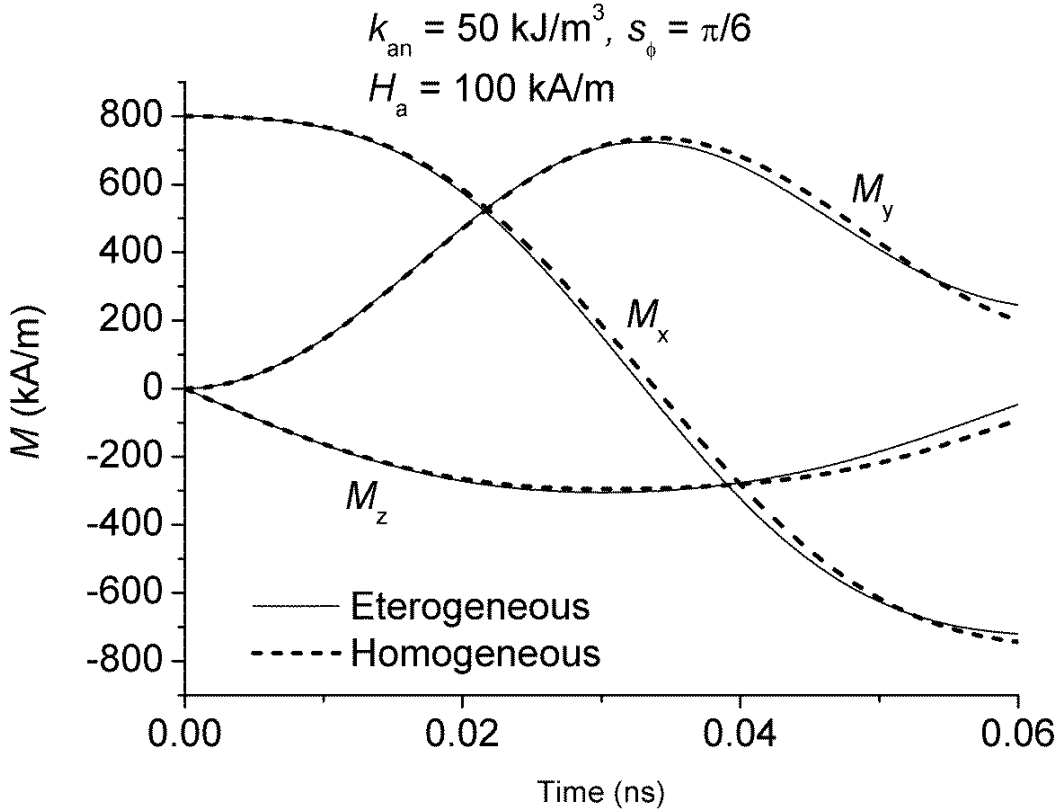


Figure 6: The precessional switching is simulated starting from a uniform spatial distribution of the magnetization along the x_1-axis and applying a constant field $\mathbf{H}_{\mathrm{a}}$, with amplitude equal to $100kA/m$, along the x_2-axis

Numerical validation of the homogenization results: simulating a precessional switching

- In the next pictures we show the results obtained for a standard deviation s_ϕ of $\pi/6$, $\pi/2$ and π respectively
- The fitting parameters $k^*_{\text{an}}/k_{\text{an}}$ and γ are equal to 0.977 and 0.921 for $s_\phi = \pi/6$, 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 becomes 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 ($k_{\text{an}} = 0$) or assuming a uniform uniaxial anisotropy along x_1-axis

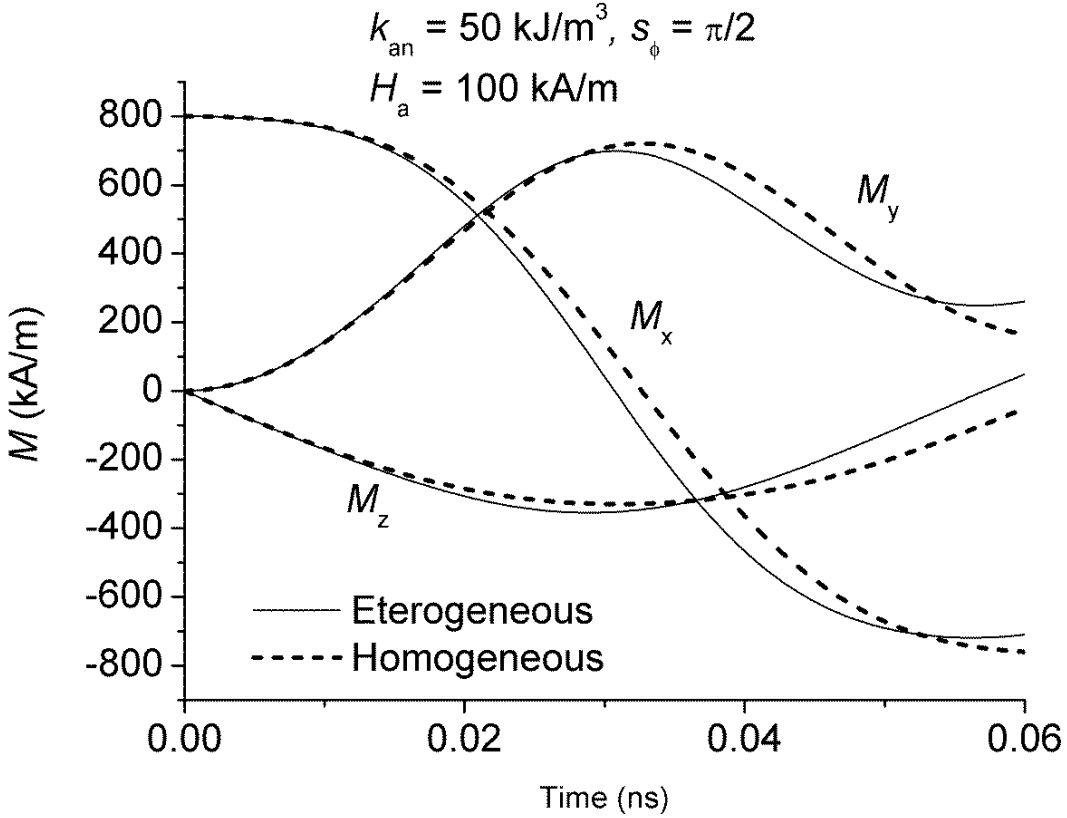
Scheme of the precessional switching 1/5



(a)

Figure 7: Time evolution of magnetization components assuming an anisotropy constant k_{an} equal to $50kJ/m^3$ and a variable standard deviation s_ϕ. The grain size is equal to $20nm$. The results obtained with the heterogeneous structure are compared with those given by considering homogenized parameters $s_\phi = \pi/6$.

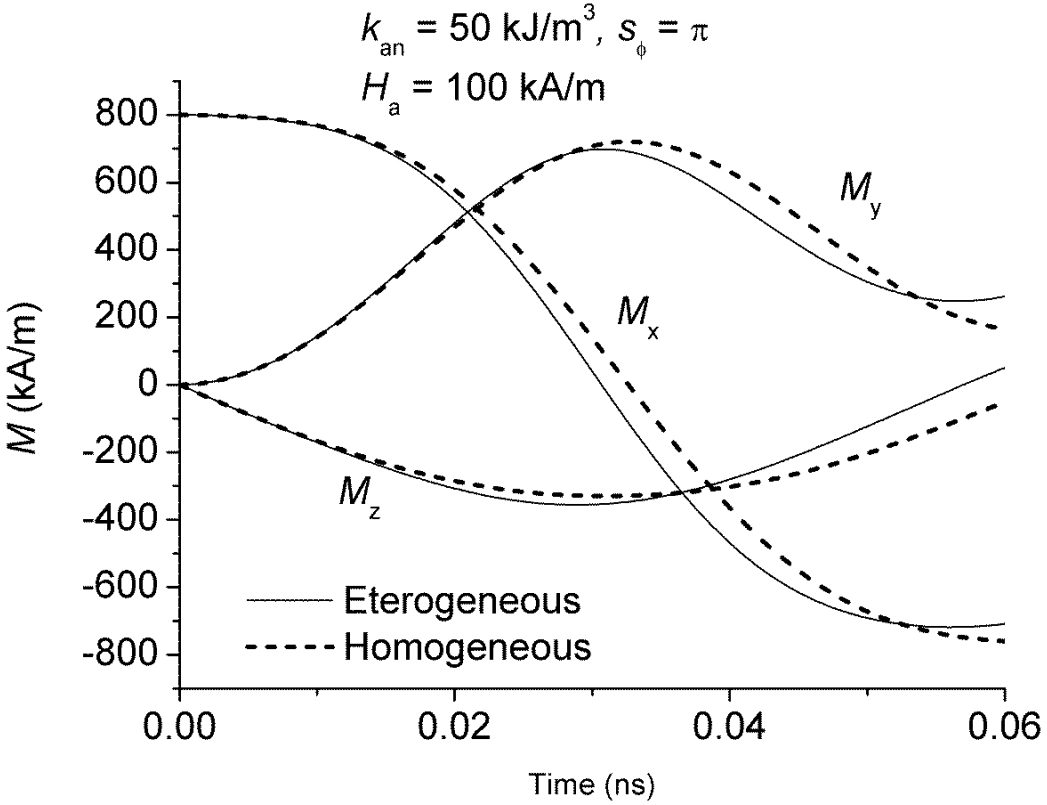
Scheme of the precessional switching 2/5



(b)

Figure 8: Time evolution of magnetization components assuming an anisotropy constant k_{an} equal to $50kJ/m^3$ and a variable standard deviation s_ϕ. The grain size is equal to $20nm$. The results obtained with the heterogeneous structure are compared with those given by considering homogenized parameters $s_\phi = \pi/2$.

Scheme of the precessional switching 3/5



(c)

Figure 9: Time evolution of magnetization components assuming an anisotropy constant k_{an} equal to $50kJ/m^3$ and a variable standard deviation s_ϕ. The grain size is equal to $20nm$. The results obtained with the heterogeneous structure are compared with those given by considering homogenized parameters $s_\phi = \pi$.

Scheme of the precessional switching 4/5

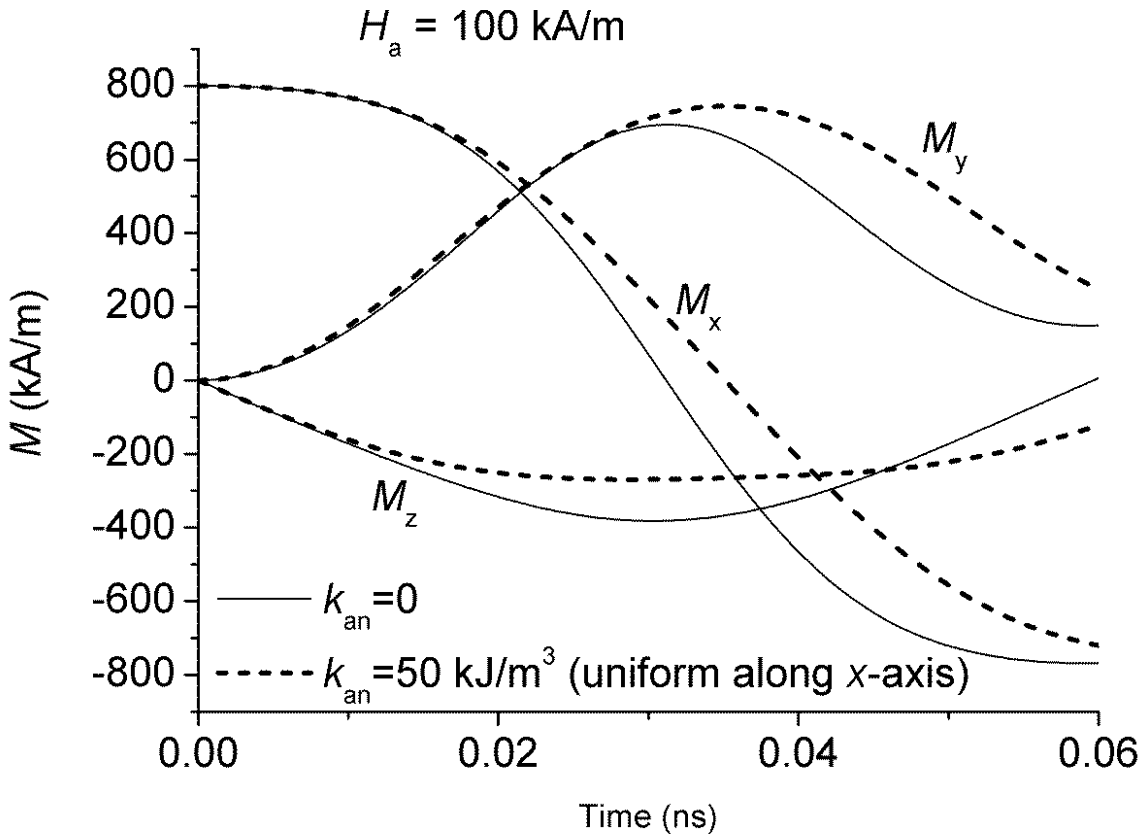


Figure 10: Time evolution of magnetization components disregarding anisotropy or assuming an anisotropy constant k_{an} equal to $50kJ/m^3$ uniformly distributed along $x-$axis.

Scheme of the precessional switching 5/5

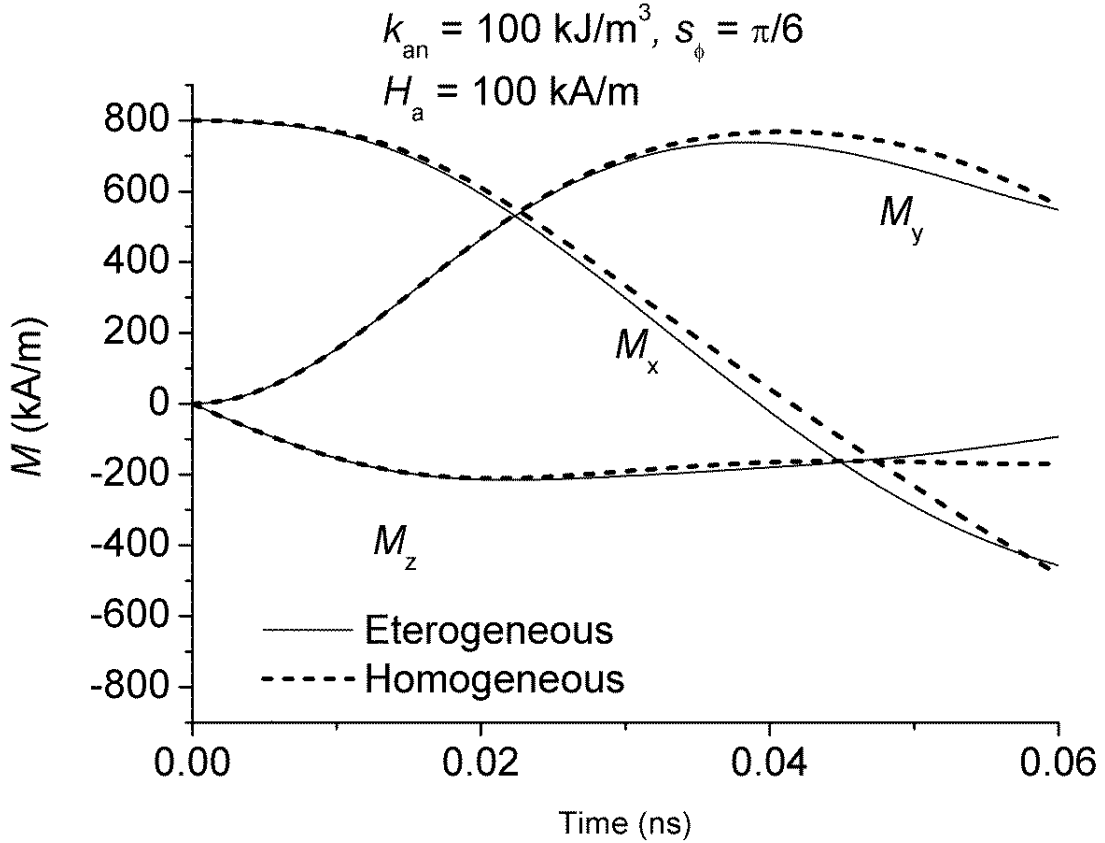


Figure 11: Time evolution of magnetization components assuming an anisotropy constant k_{an} equal to $100kJ/m^3$ and a standard deviation $s_\phi = \pi/6$. The grain size is equal to $20nm$. The results obtained with the heterogeneous structure are compared with those given by considering homogenized parameters.

Numerical validation of the homogenization results: computation of the static hysteresis loop

- The spatial discretization of the LLG equation is performed by using the finite element shape functions, assuming the Cartesian components of $\mathbf{m}$ as nodal unknowns
- To speed-up the computation and limit the memory requirements, the magnetostatic field due to “far” dipoles is evaluated by a multipole expansion technique
- A norm-conserving scheme, based on the Cayley transform is adopted to time integrating the LLG equation, so that the magnitude of $\mathbf{m}$ is preserved during the time evolution towards equilibrium states
- To compute the descending branch of the static hysteresis loop, the simulation starts from a uniform magnetization in the direction x_1, then an external field of $200kA/m$ is applied along the same direction and reduced in steps of 4 kA/m until the magnetization is reversed
- For each step of the applied field, the magnetization time evolution is computed until the equilibrium state, assumed to be reached when the maximum nodal value of the misalignment between magnetization and effective field, $|\mathbf{m} \times \mathbf{H_{eff}}|$, is lower than a fixed threshold Θ

Numerical validation of the homogenization results: computation of the static hysteresis loop

- In the simulations here reported, the following physical parameters are considered: $M_S = 800\,\mathrm{kA/m}$ and $A = 15\,\mathrm{pJ/m}$
- The magnetic film is discretized into a 2-D mesh with element size $\sim 6.6\,\mathrm{nm}$, comparable with the exchange length ($\sim 6.1\,\mathrm{nm}$)
- We assume that $k_{\mathrm{an}} = 100\,\mathrm{kA/m}$ and anisotropy vector $\mathbf{u}_{\mathrm{an}}$ is randomly distributed over the film plane $(x_1 x_2)$, that is $\theta = \pi/2$
- In the following table, the values of the fitting parameter $k^*_{\mathrm{an}}/k_{\mathrm{an}}$ and γ, derived from the homogenization process, are reported, with reference to two limit cases of random distribution

Case	$k^*_{\mathrm{an}}/k_{\mathrm{an}}$	γ
$s_\phi = \pi/6$	0.993	0.796
Uniform distribution	0.5	-1

- In the first case, we consider a narrow Gaussian distribution ($s_\phi = \pi/6$), i.e. the easy axis is mainly oriented towards the expected value ($\eta_\phi = 0$); in the second case a uniform distribution in the film plane is imposed.

Numerical validation of the homogenization results: computation of the static hysteresis loop

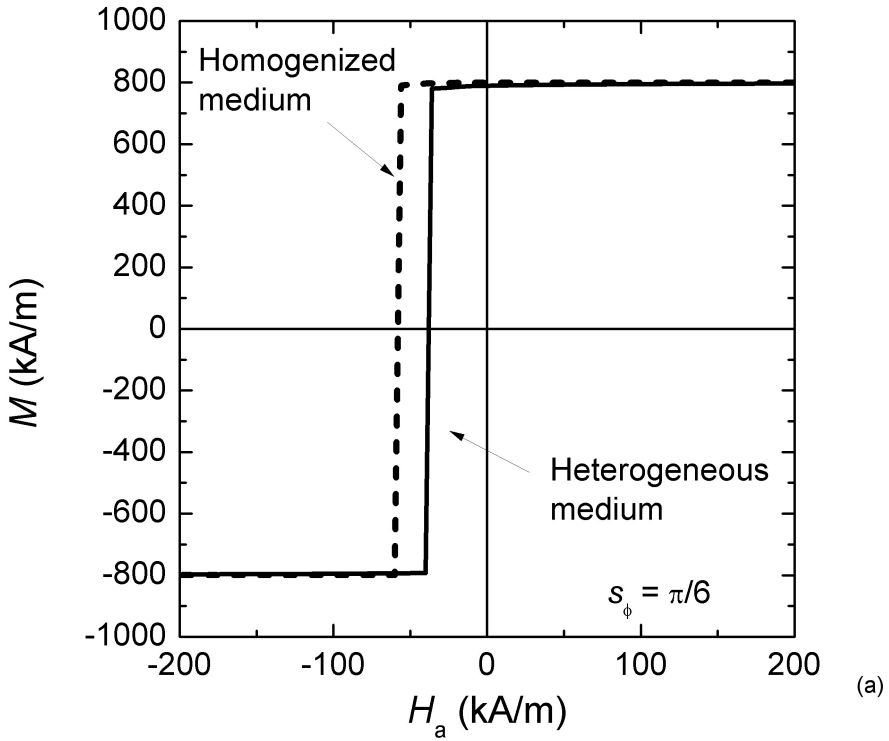


Figure 12: Comparison between the descending branches of the static hysteresis loops with randomly distributed anisotropy direction (heterogeneous medium) and with equivalent properties (homogenized medium). We assume a Gaussian distribution with standard deviation $s_\phi = \pi/6$ in the film plane. The grain dimension is 20 nm.

Numerical validation of the homogenization results: computation of the static hysteresis loop

- In the following figure instead we compare the results of the micromagnetic simulations performed on the magnetic film effectively composed of grains with randomly distributed anisotropy direction $\mathbf{u}_{\mathrm{an}}$, with those obtained by considering equivalent homogenized properties
- The grain dimension is here fixed to $20\,\mathrm{nm}$. The approximation given by the homogenization approach provides qualitatively good results, leading to hysteresis loops having similar shapes
- Anyway, some discrepancies arise in the prediction of the coercive field and of the remanent magnetization. The approximation is strongly influenced by the type of anisotropy random distribution: in particular, with the narrow Gaussian distribution a larger value of the coercive field is found, since the magnetization results much more pinned along the preferential direction
- The opposite behavior occurs with a uniform distribution in the film plane, as a consequence of the strong reduction of the equivalent anisotropy constant. Similar results have been found when considering grains having bigger size $(100\,\mathrm{nm})$.

Numerical validation of the homogenization results: computation of the static hysteresis loop

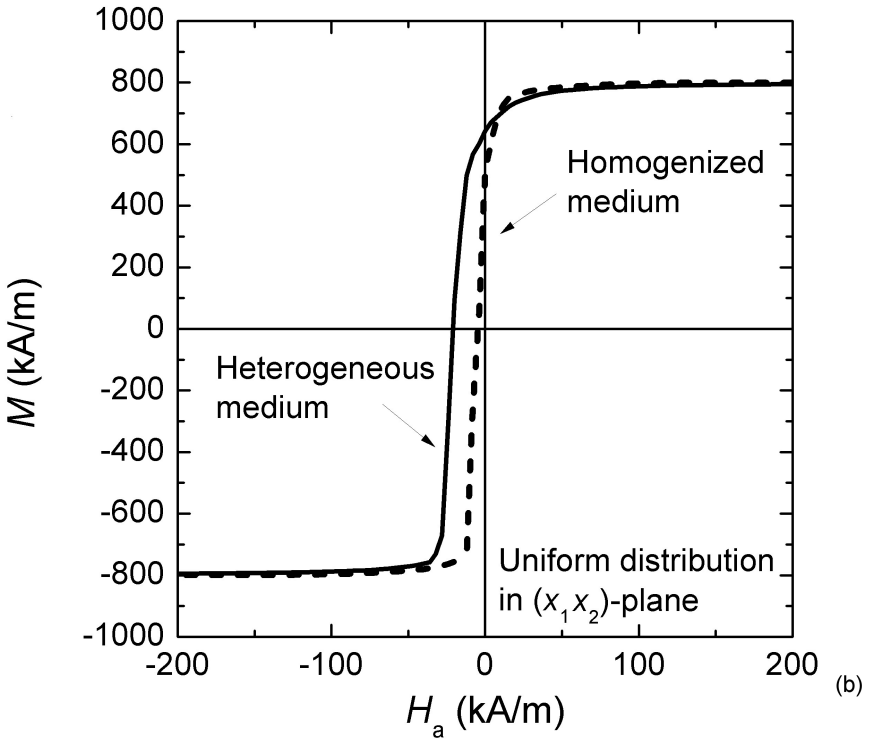


Figure 13: Comparison between the descending branches of the static hysteresis loops computed with randomly distributed anisotropy direction (i.e. heterogeneous medium) and with equivalent properties (i.e. homogenized medium). Here we assume a uniform distribution in the film plane. The grain dimension is assumed to be equal to 20 nm.