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Numerical evaluation of energy barriers in nano-sized magnetic elements with Lagrange multiplier technique

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Abstract

In the present paper we apply the method of the Lagrangian multiplier, previously proposed to evaluate energy barriers in small magnetic particles as multispin systems, for different nanosized magnetic elements, such as magnetic grains, dots and nanowires. We show that the method is capable to determine the energy barriers corresponding to highly non-homogeneous magnetization states. Three examples: a micromagnetically discretized Fe cylindrical dot/nanowire, FePt atomistic grain and a nanocomposite grain with different exchange coupling strengths are considered.

Keywords: Micromagnetic modelling; Energy barrier; Magnetic recording

Evaluation of energy barriers in nano-sized magnetic elements is important from the point of view of determination of long-time thermal stability of their magnetization. This is especially relevant in our days for magnetic recording applications, for example, to determine the energy barriers of high-anisotropy magnetic grains for recording media of the next generation [1]. Numerical evaluation of the energy barrier should be done in a multidimensional space and is a difficult problem, especially when collective reversal modes are involved. Up to now, only the use of the elastic nudged band method has been extensively studied in nano-sized magnetic systems on the basis of the micromagnetic description [1,2]. Here, we report the use of the method of the Lagrangian multiplier to determine energy barriers of simple magnetic elements such as nano-sized magnetic grains, particles, dots, wires, etc.

In systems mentioned above the occurrence of only one or several reversal modes could be expected. Consequently, the multidimensional space could be parameterized as a function of one "reaction coordinate", as, for example, average magnetization vector. This is done by minimizing the energy of the system with an additional constraint. Previously, this method has been proposed and successfully applied to determine the effective energy landscape and energy barriers of small magnetic particles with surface anisotropy [3]. It should be noted here that the implementation of the method on the basis of existing codes with energy minimization, using, for example the Landau–Lifshitz–Gilbert (LLG) equation integration is much simpler than that of the previously reported calculations of energy barriers using the nudged elastic band method. We have implemented the method on the basis of both micromagnetic and atomistic formalisms.

The method consists in projection of multidimensional energy landscape on one or several coordinates by guessing the character of the possible reversal mode and, therefore, choosing an appropriate constraint. For example, in the case of small particles with surface anisotropy, dominated by the exchange interactions [3], one can expect the type of the behavior corresponding to the rotation of the particle macrospin as the whole, so that the multidimensional space is "projected" into one unit magnetization vector $\vec{m}_0(\theta_0, \varphi_0)$. This is done by adding to the total energy one more term, $-N\vec{\lambda}(\vec{m} - \vec{m}_0)$, where $\vec{\lambda}$ is the Lagrangian multiplier, $\vec{m}$ is the particle magnetization direction: $\vec{m} = \sum \vec{s}_i / |\sum \vec{s}_i|$, $\vec{s}_i$ is the individual local magnetic

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spins and N is the number of spins inside the particle. This term produces an additional field and, therefore, the total magnetization is biased in the direction $\vec{m}_0(\theta_0, \varphi_0)$. To find the conditional minimum, the LLG equation of motion without the precessional term is solved.

$$\frac{d\vec{s}_i}{dt} = -\alpha[\vec{s}_i \times [\vec{s}_i \times \vec{h}_i]], \quad (1)$$

where α is the formal damping parameter, $\vec{h}_i = -\partial E/\partial \vec{s}_i$ is the local field and E is the total system magnetic energy augmented with the Lagrangian multiplier term. To this equations one should add also three equations for the Lagrangian multiplier components: $\dot{\vec{\lambda}} = \partial E/\partial \vec{\lambda}$. The stationary points found in this approach are also the stationary points of the original Hamiltonian. However, if the system has many metastable states, only part of these points compatible with the behavior assumed by the biased direction would be found. The method can produce highly non-collinear multidimensional stationary points.

The method allows to calculate the effective energy landscape for nanoelements in terms of the biased direction $\vec{m}_0(\theta_0, \varphi_0)$ which provides a useful illustration of the configurational anisotropy governed by the shape of the nanoelement. In the following we present several examples of energy barrier calculation in magnetic grains (dots, wires).

The saddle point could be found as the one of the effective energy landscape. Alternatively, we notice that the stationary points coincide with the condition: $[\vec{\lambda} \times \vec{m}_0] = 0$, and, therefore, they can be found by minimizing the functional $F(\theta_0, \varphi_0) = |[\vec{\lambda}(\theta_0, \varphi_0) \times \vec{m}(\theta_0, \varphi_0)]|$, where $\vec{\lambda}(\theta_0, \varphi_0)$ is found as a result of the conditional minimization procedure, described above. The gradients of this functional, which are necessary for the minimization procedure, should be evaluated numerically. If a direct minimization procedure (instead of the LLG equation integration) is used, the stationary point would satisfy directly $\vec{\lambda} = 0$ condition.

To illustrate the performance of the method, we have calculated the energy barriers of rectangular magnetic grains as a function of their elongation. The general idea of this calculations is the same as in Ref. [4], however, the high-anisotropy grain was implemented on the basis of atomistic calculations with correct lattice structure and the Heisenberg exchange rather than finite element micromagnetic simulations. The parameters used for calculations were that corresponding to doped FePt: the anisotropy value $K = 2 \times 10^7\,\mathrm{erg/cm^3}$ and the saturation magnetization $M_s = 1100\,\mathrm{emu/cm^3}$, the Heisenberg exchange constant $J = 7.7 \times 10^{-14}\,\mathrm{erg}$, the fct lattice parameters $a = b = 0.272\,\mathrm{nm}$ and $c = 0.385\,\mathrm{nm}$. Fig. 1 represents energy barriers of an isolated grain with basis size $S = 6\,\mathrm{nm} \times 6\,\mathrm{nm}$ as a function of elongation L. The configurations of the saddle points are presented in Fig. 2(a and b). Varying the grain height, we have observed how the configuration of the saddle point changes from that

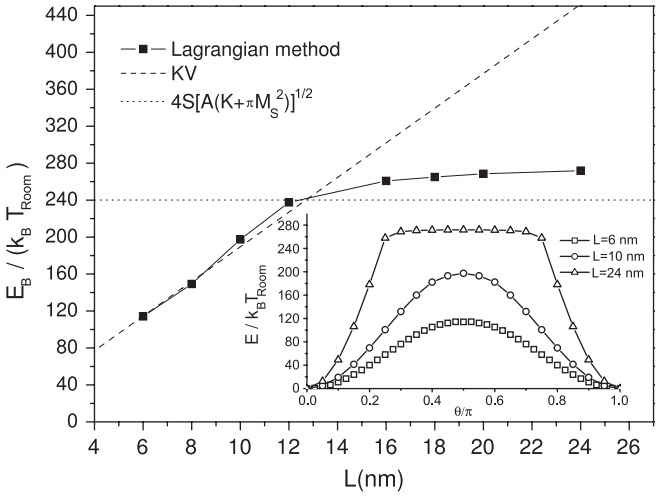

Fig. 1. Energy barriers vs elongation of an isolated grain of FePt with a basis size of $S = 6\,\mathrm{nm} \times 6\,\mathrm{nm}$. Inset shows the effective energy as a function of the polar coordinate θ.

corresponding to coherent rotation (the energy barrier value proportional to system volume) to the one related to the domain wall propagation (the energy barrier value independent of the system volume), which energy barrier is approximately the domain wall energy $E_{DW} = 4S[A(K + \pi M_s^2)]^{1/2}$ including the ideal shape anisotropy term of an infinite wire. The critical system size for which the propagation rather than that rotation mode occurs was determined in this case as 12 nm.

The second example (Fig. 3) represents a cylindrical magnetic grain (dot or wire), implemented on a basis of full micromagnetic model (discretization size 1 nm) with parameters corresponding to Fe and with cubic anisotropy (two of the easy axes in XY plane), $K = 50\,000\,\mathrm{J/m^3}$, the exchange parameter $A = 8.3 \times 10^{-12}\,\mathrm{J/m}$ and the saturation magnetization value $M_s = 2.15\,T$. The number of values of θ and φ used in the calculation was 51×51. To evaluate the magnetostatic energy, the DADI method [5] has been used. It is clearly seen that in this case there is a competition between magnetocrystalline and shape anisotropies: the shape anisotropy is responsible for the increment of the energy barrier for the magnetization switching along z-direction. The value of this barrier is plotted in Fig. 4 as a function of the particle elongation. It is normalized to the effective anisotropy value K_{eff} multiplied by the volume V. The effective anisotropy value has been evaluated for a single-domain particle with intrinsic cubic anisotropy and uniaxial shape anisotropy

$$E_{SD} = -\tfrac{1}{2}\mu_0 M_s^2 m_z^2 - \tfrac{1}{2}K(m_x^4 + m_y^4 + m_z^4), \quad (2)$$

calculating analytically the energy barrier $K^*_{eff} = \Delta E_{SD}/V$. This gives the maximum possible energy barrier corresponding to the coherent reversal as $4.7 \times 10^5\,\mathrm{J/m^3}$. In longer wires energy barriers corresponds to that of the domain wall nucleation and, therefore, its value saturates as a function of the wire length.