A path method for finding energy barriers and minimum energy paths in complex micromagnetic systems

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Abstract

Minimum energy paths and energy barriers are calculated for complex micromagnetic systems. The method is based on the nudged elastic band method and uses finite element techniques to represent granular structures. The method was found to be robust and fast for both simple test problems as well as for large sytems such as patterned granular media. The method is used to estimated the energy barries in CoCr based perpendicular recording media.

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1. Introduction

The thermal stability of magnetic media and magnetic storage elements becomes important with decreasing size of the magnetic structures [1]. The calculation of the thermal stability requires the estimation of transition rates between stable equilibrium states of the magnet. The calculation of transition rates needs a detailed characterization of the energy landscape along the most probable path which is taken by the system from its initial state to a final state. The energy landscapes of micromagnetic systems drastically depends on

the microstructure of the magnet and may contain many local minima. Using the finite element method it is possible to represent complex geometries and grain structures. The combination of the finite element method and an algorithm for finding the minimium energy path provides a tool to calculate the energy barriers in large scale micromagnetic systems.

Berkov [2] calculated the transition path of interacting single domain particles, minimizing the action along the path. He showed that a direct minimization of the action may also give paths through local maxima which have to be excluded. In theoretical chemistry, path integral Monte Carlo methods are applied to calculate the rate of transitions in chemical reactions of diffusion events [3]. The Monte Carlo method is used to sample the most probable transition paths. Another family of methods for the calculation of transition paths are the elastic band methods. Starting from an initial guess for the path which connects two local minima of the system, a highly probable path is found moving the points along the path according to an algorithm which resembles tensioning an elastic band accross a mountain. A common feature of all methods is the discrete representation of the path connecting the inital state of the system with its final state.

In micromagnetics we represent the magnetic states of a system by a set of magnetic moments. This corresponds to the magnetization at the nodes of the finite element mesh, which is used to model the geometry and grain structure of the magnet. A sequence of magnetic states can be constructed in such a way as to form a discrete representation of a path from the initial magnetization state $\mathbf{M}_\mathrm{i}$ to the final magnetization state $\mathbf{M}_\mathrm{f}$. The most simple case of the initial path is just a straight line interpolation in the configuration space between $\mathbf{M}_\mathrm{i}$ and $\mathbf{M}_\mathrm{f}$. For the configuration space we use polar coordinates of dimension $2N$, where N is the number of magnetization vectors (nodes). An optimization algorithm is then applied until at any point along the path the gradient of the energy is only pointing along the path. This path is called minimum energy path (MEP) and means that the energy is stationary for any degree of freedom perpedicular to the path.

The method thus does not just give the saddle point, but also gives a more global view of the energy landscape, for example, if more local minima and saddle points are found along the minimum energy path. The minimum energy path typically represents the path with the greatest statistical weight. From this path statistical quantities as for example rate con-

stants for the thermally induced magnetization reversal can be calculated. In magnetic recording applications the knowledge of rate constants is crucial since they determine termal stability of the recorded data.

Section 2 of this paper describes the micromagnetic background and the numerical details of the algorithm for finding the minimum energy path. Section 3.1 illustrates the method showing the calculation of the transition path of two magnetostatically interacting particles. Section 3.2 presents examples for small particles where the magnetization reversal mode is homogeneous rotation. In Section 3.3 the method is applied to estimate the energy barrier for the nucleation and expansion of domains in a columnar grain as used in perpendicular magnetic recording. In Section 3.4 the minimum energy barrier of a submicron, granular thin film is calculated. Section 4 summarizes the results.

2. A path finding method using finite elements

The micromagnetic description of the system starts from the total magnetic Gibbs' free energy [4]

$$E(\boldsymbol{u}) = \int_{\Omega} \left(A \left[\sum_{k}^{x,y,z} (\nabla u_k)^2 \right] + K_1[1 - (\boldsymbol{u}\boldsymbol{a})^2] - \frac{1}{2} J_s \boldsymbol{u}\boldsymbol{H}_s - J_s \boldsymbol{u}\boldsymbol{H}_{ext} \right) dV. \qquad (1)$$

E is the sum of the exchange energy, the anisotropy energy, the stray field energy, and the Zeeman energy. $\boldsymbol{u}$ denotes the unit vector parallel to the magnetization direction. A is the exchange constant, K_1 ist the magnetocrystalline anisotropy constant, and J_s is the spontaneous magnetic polarization. $\boldsymbol{a}$ is the unit vector along the magnetocrystalline anisotropy direction. $\boldsymbol{H}_s$ is the magnetic stray field and $\boldsymbol{H}_{ext}$ is the external field. The integral (1) is over the total volume of the magnetic particles. In a stationary state the magnetic system occupies a local mimimum of (1). Owing to thermal activation, the system may overcome an energy barrier and spontaneously moves towards a different local minimum of the energy.

We use the finite element method to calculate E for complex magnetic systems. The direction components of the magnetic polarization, u_k, are interpolated by piecewice linear functions on a tetrahedral grid. The integral in (1) breaks into a sum of integrals over tetrahedral elements. In order to evaluate the stray field, $\boldsymbol{H}_s$, we use a hybrid finite element / boundary element method [5]. Using the finite element method it is possible to represent irregularly shaped grains and boundary phases.

Henkelman and Jónsson proposed the nugded elastic band method to calculate minimum energy paths [6]. We use a slightly modified variant of this method to evaluate transition paths in micromagnetics. An intitial path is assumed which connects the initial magnetization state $\mathbf{M}_\mathrm{i} = \mathbf{M}_1$ with the final magnetization state $\mathbf{M}_\mathrm{f} = \mathbf{M}_n$. A path is represented by a sequence of n images, $\mathbf{M}_k$, where the index k runs from 1 to n. The path is optimal, if for any image $\mathbf{M}_k$ the gradient of the energy is only pointing along the path. Therefore the images of the optimal path have the following property

$$\boldsymbol{D} = -\{\nabla E(\mathbf{M}_k) - (\nabla E(\mathbf{M}_k) \cdot \boldsymbol{t})\boldsymbol{t}\} = 0 \quad \text{for } k = 1, n. \tag{2}$$

Here $\boldsymbol{t}$ denotes the unit tangent vector along the path. For an optimal path the component of the energy gradient that is normal to the path is zero. The optimal path can be found using an iterative scheme. In each iteration step the images are moved in a direction parallel to the negative gradient of the energy and normal to the current path. So $\mathbf{M}_k$ is moved in a direction parallel to

$$\boldsymbol{D} = -\{\nabla E(\mathbf{M}_k) - (\nabla E(\mathbf{M}_k) \cdot \boldsymbol{t})\boldsymbol{t}\}. \tag{3}$$

To keep an equal distance between successive images, Henkelman and Jónsson [6] introduce a spring froce in addition to $\boldsymbol{D}$. E and co-workers apply a reparametrization after a few iterations to ensure equal distance between the images [7]. We obtained good results without the spring force and without reparametrization, using a variable order, variable time step method to relax the inital path towards a mimimum energy path. We represent the path finding scheme with a system of ordinary differential equations

$$\frac{\partial \mathbf{M}_k}{\partial t} = \boldsymbol{D}(\mathbf{M}_k) \qquad \text{for } k = 2, n\text{-}1. \tag{4}$$

We solve (4) numerically, using the software package CVODE [8].

We use polar coordinates to represent the magnetization configuration of an image, $\mathbf{M}_k$. The dimension of the configuration space is $2N$, where N is the number of nodes of the finite element mesh. This gives a total number of variables in equation (4) of $2N \times (n-2)$, as the initial and the final magnetization state do not move. The direction $\boldsymbol{D}$ is calcuated in the configuration space. In order to calculate the gradient of the energy in polar coordinates, we use the following equations [9]:

$$\frac{\partial E}{\partial \vartheta_i} = \frac{\partial E}{\partial u_{1,i}}\frac{\partial u_{1,i}}{\partial \vartheta_i} + \frac{\partial E}{\partial u_{2,i}}\frac{\partial u_{2,i}}{\partial \vartheta_i} + \frac{\partial E}{\partial u_{3,i}}\frac{\partial u_{3,i}}{\partial \vartheta_i}, \tag{5}$$

$$\frac{\partial E}{\partial \varphi_i} = \frac{\partial E}{\partial u_{1,i}}\frac{\partial u_{1,i}}{\partial \varphi_i} + \frac{\partial E}{\partial u_{2,i}}\frac{\partial u_{2,i}}{\partial \varphi_i} + \frac{\partial E}{\partial u_{3,i}}\frac{\partial u_{3,i}}{\partial \varphi_i}, \tag{6}$$

where i runs over all nodes of the finite element mesh. Care has to be taken, calculating the local tangent at an image k. The single use of either a forward difference approximation, backward difference approximation, or a central difference approximation develops kinks in the path [6]. The kinks prevent the string from converging to the minimum energy path. The optimal choice of the appropriate difference approximation depends on the energy difference between successive magnetization states. We use forward differences climbing up a hill, backward differences going down a hill, and second-order central differences when crossing a saddle or a local minimum:

$$\boldsymbol{t} = \frac{\mathbf{M}_{k+1} - \mathbf{M}_k}{|\mathbf{M}_{k+1} - \mathbf{M}_k|} \qquad \text{if } E(\mathbf{M}_{k-1}) < E(\mathbf{M}_k) < E_t(\mathbf{M}_{k+1}), \tag{7}$$

$$\boldsymbol{t} = \frac{\mathbf{M}_k - \mathbf{M}_{k-1}}{|\mathbf{M}_k - \mathbf{M}_{k-1}|} \qquad \text{if } E(\mathbf{M}_{k-1}) > E(\mathbf{M}_k) > E(\mathbf{M}_{k+1}), \tag{8}$$

$$\boldsymbol{t} = \frac{\mathbf{M}_{k+1} - \mathbf{M}_{k-1}}{|\mathbf{M}_{k+1} - \mathbf{M}_{k-1}|} \qquad \text{if } E(\mathbf{M}_{k-1}) < E(\mathbf{M}_k) > E(\mathbf{M}_{k+1}) \text{ or}$$

$$E(\mathbf{M}_{k-1}) > E(\mathbf{M}_k) < E(\mathbf{M}_{k+1}). \tag{9}$$

3. Examples

3.1 Interacting single domain particles

In order to test our path finding method we start with a simple test case. We study two single domain particles with saturation polarization J_s, uniaxial anisotropy (K_1) and identical volumes (V). The line connecting the particles is parallel to the uniaxial anisotropy direction. The distance between the particles is R. In polar cordinates the magnetization of this two particle system is described by four angles $(\theta_1,\phi_1,\theta_2,\phi_2)$. Although there are four independent variables only cases where the magnetizations of the two particles are in the same plane describe equilibrium states. It is therefore sufficient to study cases where only θ_1 and θ_2 vary. The total energy then becomes [10]

$$E/(K_1V) = sin^2\theta_1 + sin^2\theta_2 + k_{\mathbf{int}}[sin\theta_1 sin\theta_2 - 2cos\theta_1 cos\theta_2] \tag{10}$$

$$k_{\mathbf{int}} = J_s^2 V/(2\mu_0 R^3 K) \quad \text{reduced interaction constant} \tag{11}$$

Thus ∇E can be calculated analytically in this case. With this reduction to two dimensions the energy lanscape with paths can be plotted which helps us to verify our method and results. Figure 1 shows one possible case of the energy landscape where no external field is applied. In the initial state the magnetization of both particles is parallel ("up up"). We then connect the initial state with the final state ("down down") with a straight line. This initial path describes the coherent rotation of the magnetizations where the two magnetic moments rotate from the initial state to the final state in opposite direction (asymmetric fanning $\delta\theta_1 = -\delta\theta_2$). The energy landscape with the initial path and the minimum energy path are shown in figure 1. The inital path (black line) moves over the top of the hill. Applying the algorithm described in section 2 we obtain a minimum energy path as given by the white line in figure 1. In the minimum energy path one particle starts rotating. The system passes the first saddle point and reaches a local minimum. The moments are antiparallel. Then the second particle rotates. The system crosses a second saddle point and ends in the final state where the magnetic moments are parallel. It becomes obvious from the energy landscape that there is a second possible minimum energy path which can be reached from the same initial path. Both paths describe the same process. The particles

start to switch in the opposite order in the two paths. Figure 2 shows the energy as a function of the arclength of the initial path and the minimum energy path. During the solution of equation (4), the path relaxes to the minimum energy path. The path becomes longer and the maximum develops to two saddle points and a local mimimum.

Testing more complex problems with the 2D energy landscape, we found that the tangent estimate is crucial for the convergence of the method [6] and has to be evaluated as described in section 2.

3.2 Small quadratic magnet

As another simple problem, we study a small quadratic thin magnet of CoCr which has high uniaxial anisotropy (K_1 = 0.3MJ/m^3, J_s = 0.5 T, A = 10 pJ/m). The particle size is 5 nm x 5 nm x 1 nm and is meshed with a finite element grid with 16 nodes. The particle lies in the yz-plane (see figure 3). The dimension is of the configuration space is 32 and a visualization of the energy landscape is no more possible. The magnetocrystalline anisotropy axis, $\boldsymbol{a}$, is parallel to one long edge. In the initial state the magnetization is parallel to the easy axis and therefore in a local minimum. In the final state the magnetization has opposite direction to the initial state and is also in a local minimum. For testing our method we assume an initial path in which the magnetization rotates coherently out of the plane. In the minimum energy path the magnetization still rotates coherently since the particle is small and thus behaves like a single domain particle. However, the rotation now takes place in plane since here the magnetostatic contribution to the total energy is lowest (see figure 3).

3.3 Elongated magnetic grain

A more complicated problem is one elongated magnetic particle with uniaxial magnetocrystalline anisotropy parallel to the long axes. This model represents one magnetic grain of a perpendicular recording media such as CoCr [11]. The grain diameter is 13 nm. As before we start with a straight line in polar coordinates for the initial path increasing the angle of the magnetization with the long axis of the particle on every node by a constant step from one image to the next (coherent rotation). It was found that above a certain criti-

cal lenght, l_c, of the particle the minimum energy path changes from coherent rotation to nucleation followed by domain wall motion until the whole magnetization is reversed. This can also be understood by an analytical estimate. In the following F denotes the area of the basal plane of the elongated grain. The domain wall energy is $E_{wall} = 4F\sqrt{AK_1}$ while the energy for coherent rotation is $E_{rot} = K_1 V$. Now if the particle length is increased only V increases while F remains constant. Thus there will be a critical length where $E_{wall} < E_{rot}$ and the nucleation and expansion of a domain wall becomes energetically favorable.

Figure 4 shows images along the initial path and the minimum energy path for a particle with a length $l > l_c$. Clearly, the algorithm detects the minimum energy path, which is given by the nucleation of a reversed domain at one end of the particle. The wall moves through the particle and the reversed domain expands. A nucleation of reversed domains at both ends will require twice the wall energy, E_{wall}, and this is no minimum energy path. Figure 5 shows the energy as a function of the arclength along the initial path and the minimum energy path. The energy increases as the reversed domain is formed and remains constant during the motion of the domain wall.

3.4 Patterned granular media

Patterned media [12] show great potential for future ultra-high density magnetic recording. In patterned media, each discrete element is exchange isolated from other elements, but inside each element polycrystalline grains are strongly exchange-coupled, behaving more like a larger single magnetic grain.

We apply the path method to one island of such patterned media. The edge length is 70 nm, the grain diameter is about 10 nm and the film thickness is 21 nm. The island consists of 49 grains. The grains are in direct contact and perfectly exchange coupled. The easy axes of the grains are perpendicular to the film plane with a random deviation of the direction from the plane normal within cone of about 8° for each grain.

Again we start with the coherent rotation for the initial path. The minimum energy path is shown in figure 6. The reversal starts with a nucleation in one corner. The domain expands and the length of the domain wall increases. At the first saddle the length of the domain

wall reaches a maximum. A minimum state is also found where about half of the magnetization is reversed. This two domain state has a straight (short) domain wall (see figure 6) which reduces the total wall energy. In addition, the two domain state is magnetostatically favorable. Therefore the two-domain state is a local minimum. Figure 7 shows the energy as a function of the arclength along the initial and the minimum energy path. The energy barrier for crossing the second saddle from the local minimum (two domain state is about 200 $k_B T$, for T = 300 K. Thus the intermediate two domain state is quite stable. The high energy barriers between the initial and the final state are due to the perfect coupling between the grains. As the grains cannot reverse independently, the energy barrier is much larger than $K_1 V$, where V is the average grain volume. Further investigations of the effect of the intergrain exchange constant on the minimum energy path showed that the intergrain exchange constant can be reduced to only 10 % of its bulk value without a drastic decrease of the energy barrier.

4. Conclusion

A numerical algorithm to compute the minimum energy path in micromagnetic sytems was implemented. The minimum energy path may be used to calculate transition probabilities using the reversible work formulation of classical transition state theory [13]. The method combines a string method for finding rare events with the finite element method for modeling complex geometries and structures:

- Saddle points and local minima along the minimum energy path can be identified.
- The computation time of the path finding algorithm has the same order of magnitude as the computation for the solution of the Landau-Lifshitz-Gilbert equation for the very same microstructure.
- In discrete media for perpendicular recording with an island size of 70 nm, the minimum energy path starts with the nucleation of reversed domains at the corners followed by domain wall motion.

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5. References

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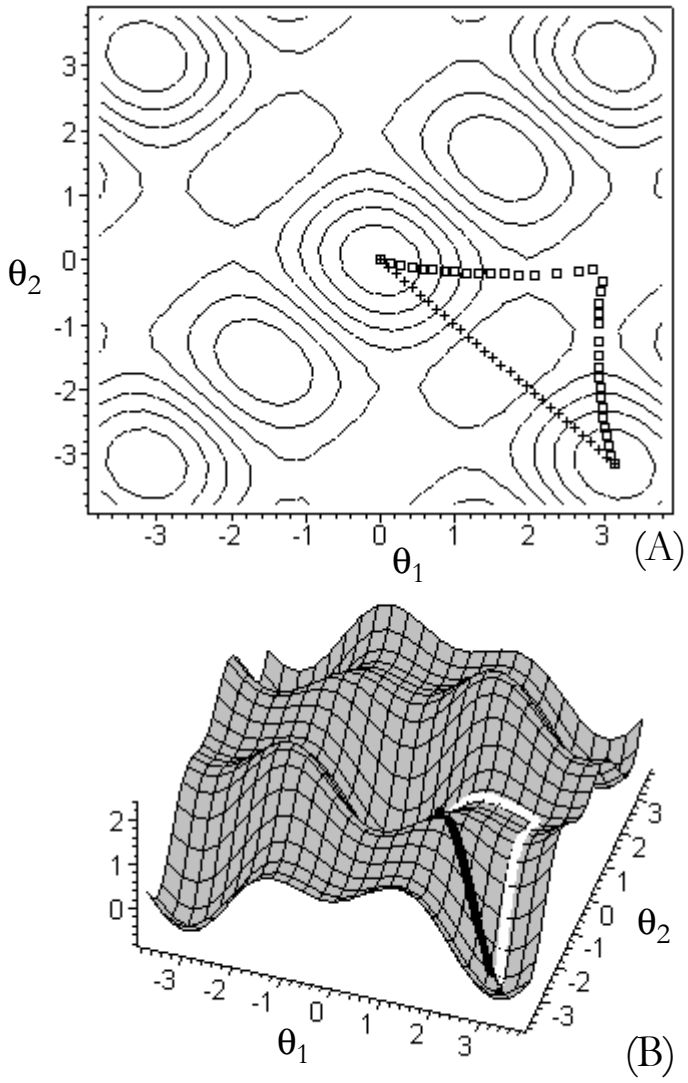

Figure 1: (A) Contour plot with initial path (crosses) and minimu energy path (boxes). (B) energy surface with initial path (black) and minimum energy path (white) for a system of two interacting magnetic particles. k_{int}=0.2

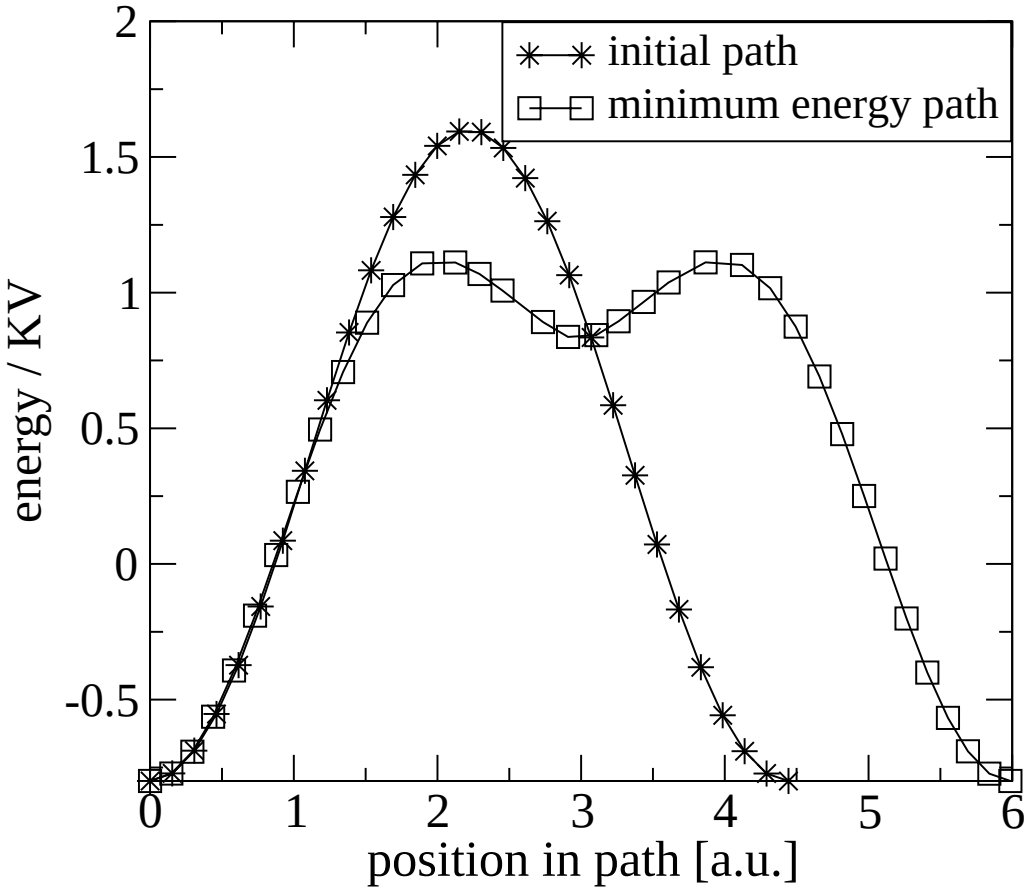

Figure 2 Energy along the initial path and the minimum energy path for a system of two interacting magnetic moments.

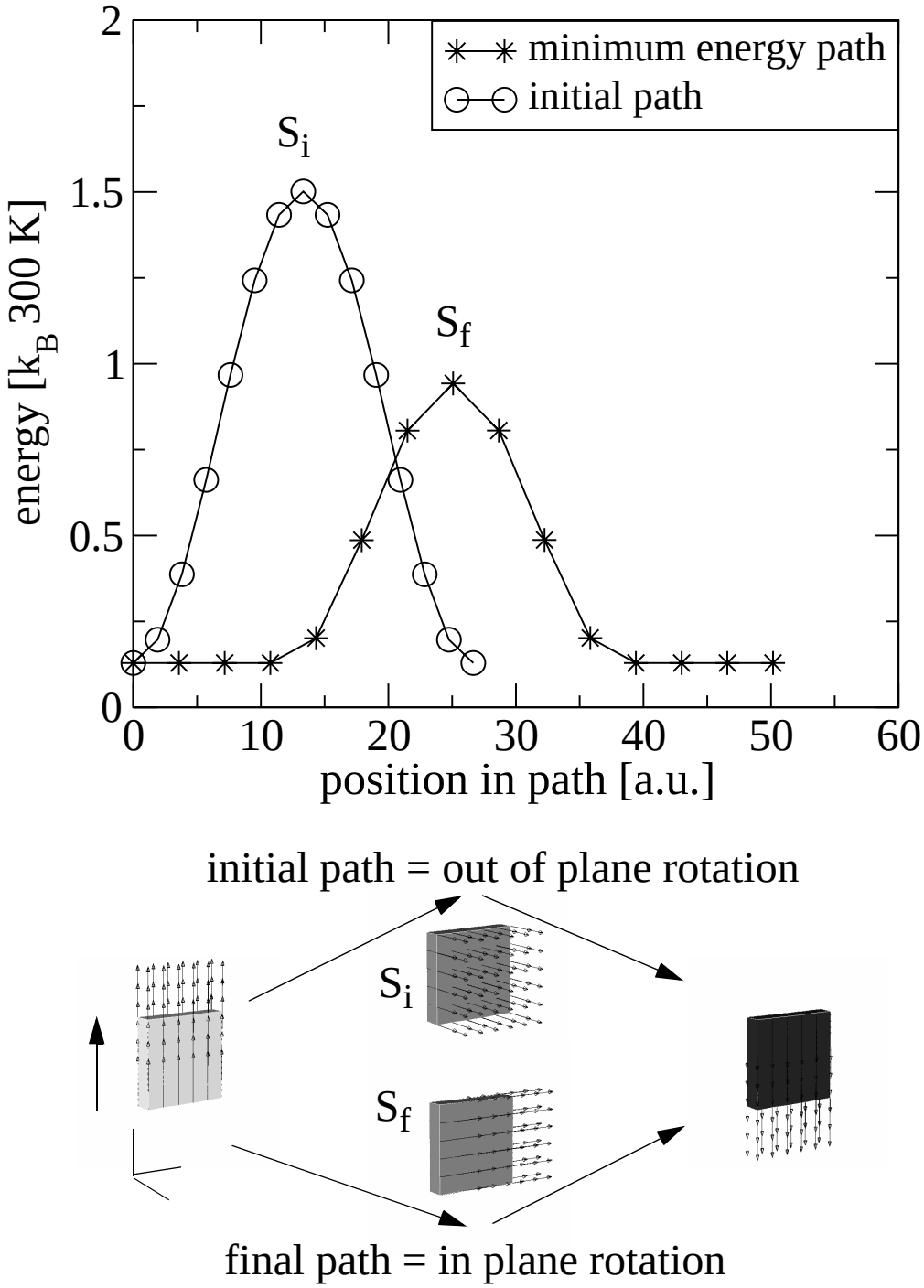

Figure 3 Energy along the initial path and minimum energy path with illustration of the magnetization along the paths. The particle has a size of 5x5x1 nm and a high uniaxial anisotropy parallel to the edge. In the minimum energy path the magnetization reverses by rotation in plane since this lowers the magnetostatic energy. (S_i....energy barrier of initial path, S_f.....energy barrier of minimum energy path = saddle point.)

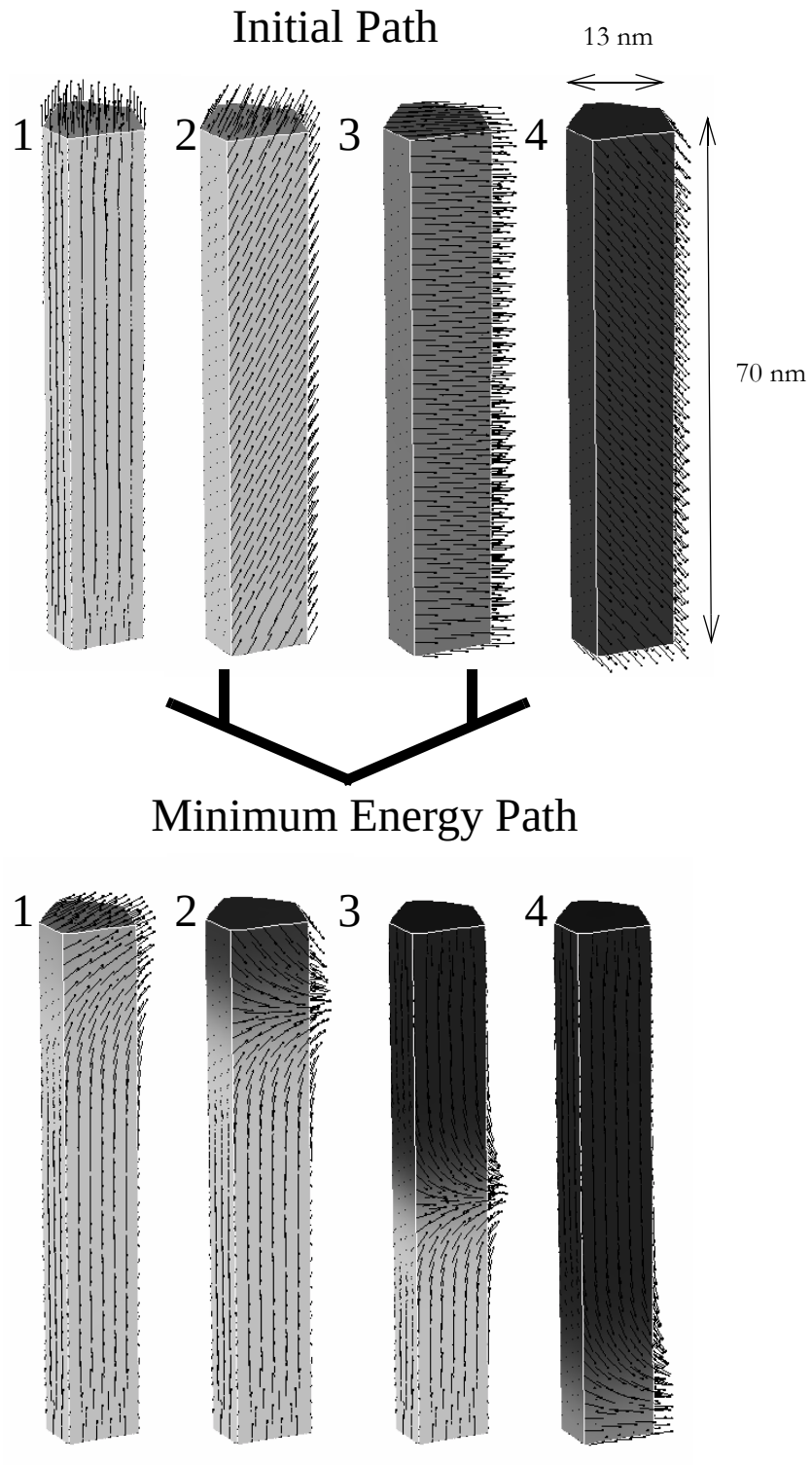

Figure 4 Magnetization states along the initial path and the minimum energy path for an elongated CoCr particle with the easy paralell to the long axis. Grey: magnetization up; black: magnetization down.

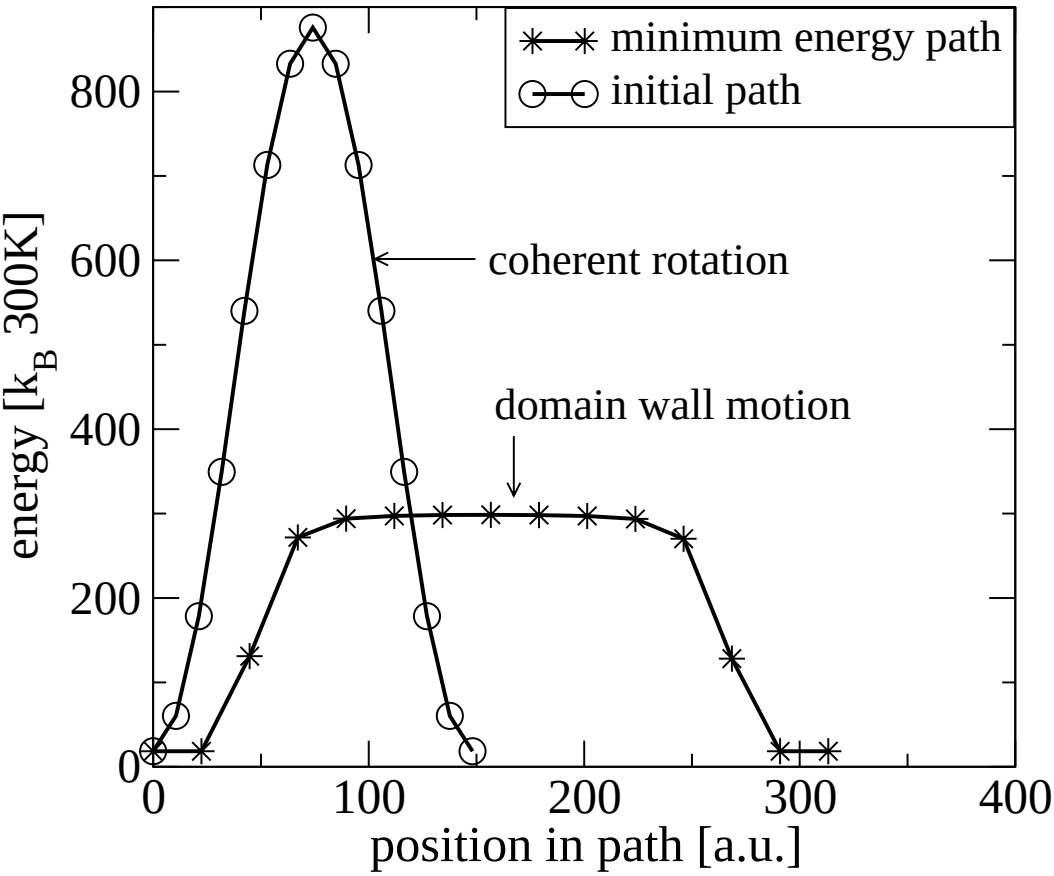

Figure 5 Energy along the initial path and the minimum energy path for an elongated CoCr particle with the easy axis parallel to the long axes. In the minimum energy path the magnetization reverses by nucleation followed by domain wall motion.

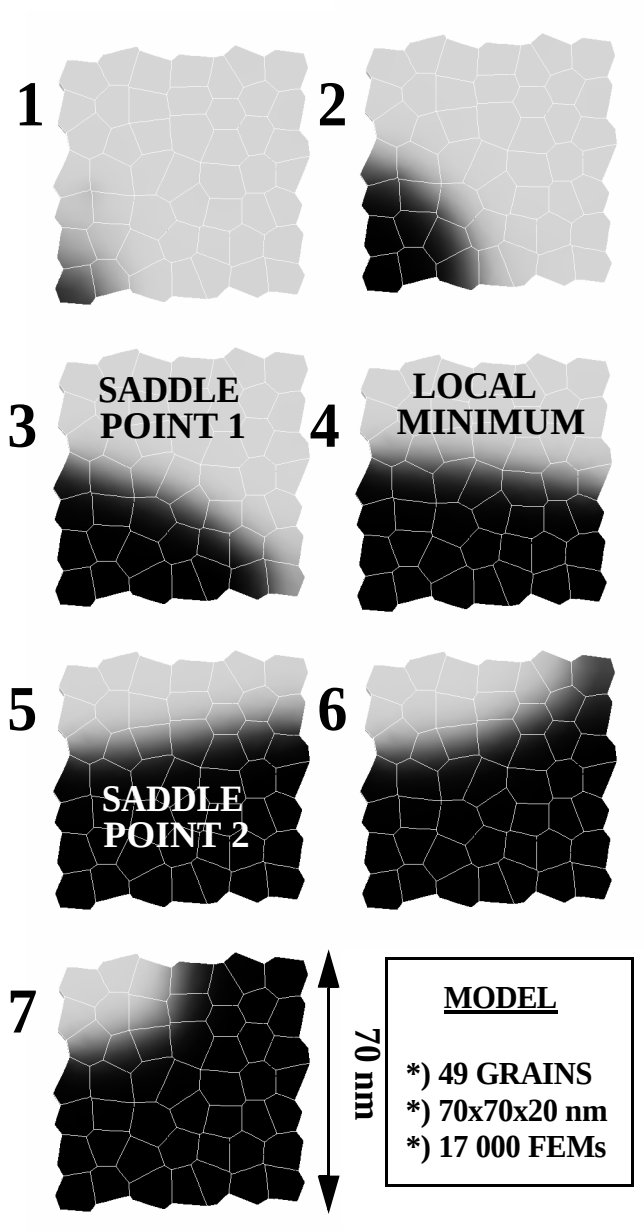

Figure 6 Magnetization states along the initial path and the minimum energy path for an island of a patterned CoCrPt media with granular structure. The easy axes is perpedicular to the plane. Grey: magnetization up: black: magnetization down.

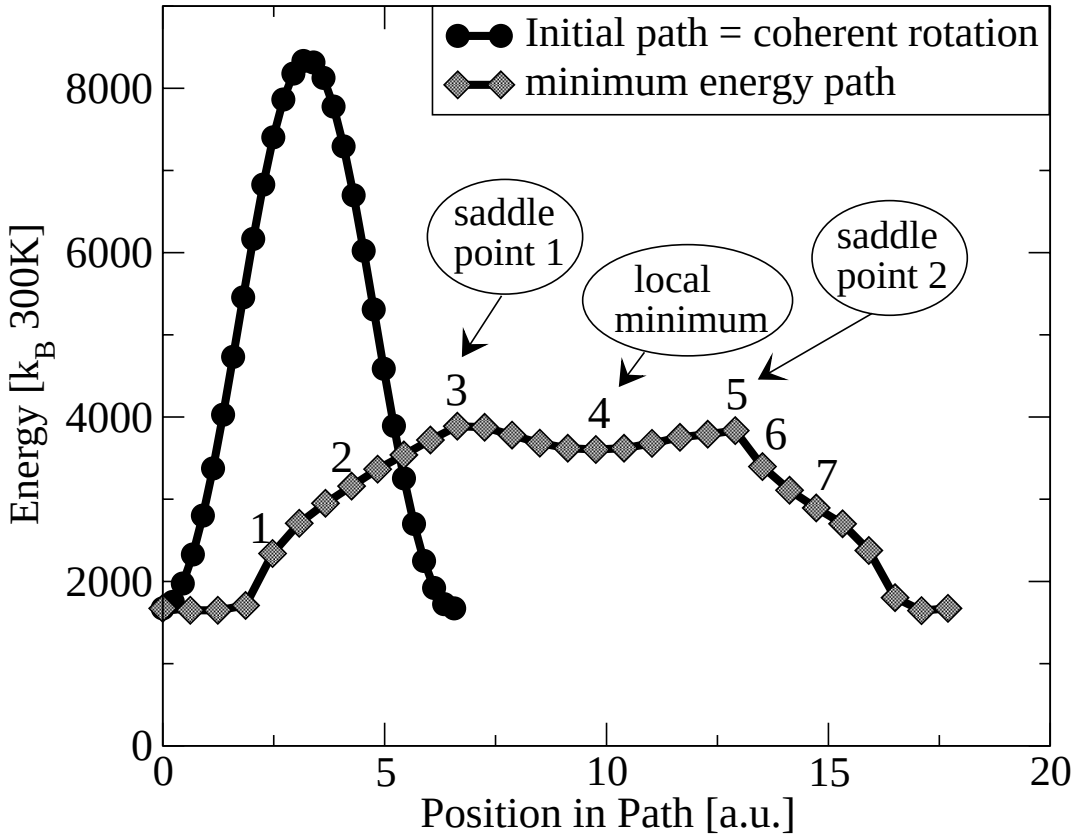

Figure 7 Energy along the initial path and the minimum energy path for a element of a patterned CoCrPt media with granular structure. The easy axis is perpedicular to the plane.