Energetics of domain wall in magnetic nanowire

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Abstract. Micromagnetic modeling is used to study the energetics of magnetic switching of single-layer permalloy nanowire. The energy landscape of the system is studied using Nudged Elastic Band method. It has been shown that presence of rectangular shape defects on long side and inside nanowire leads to the appearance of local maxima and minima on the energy profile. Thus artificially created imperfections can be used for effective DW pinning.

1. Introduction
Magnetic nanowires (MN) have attracted new interest in recent years due to rich physics related to the nucleation and propagation of domain walls (DW) in them. Such systems represent a good framework for studies of magnetic phenomena at nanoscale [1]. From the other side MN is of perspective object for the development of new generation of spintronic devices. One of the possible perspectives is the racetrack memory widely discussed in recent years [2]. Another interesting direction for applied research in this field is associated with the development of different types of magnetic logic devices based on domain wall motion in nanowires [3]. Modern progress in the nanolithography of metallic films made it possible to create experimentally MN with nanometer size dimensions. Besides that there is a wide spectrum of experimental techniques available to study micromagnetic states of such system with high resolution. While a lot of works have already been published devoted to the studies of DW dynamics, not so much is known about the energetics of those processes.

Physics of DW nucleation and motion can be described using micromagnetic theory. This theory assumes a phenomenological description of the magnetic system where the total energy of the system is a functional of a continuous magnetization function. Numerical implementation of the model assumes spatial discretization of the system using fine grid. We considered here only magnetic nanowires with in plane magnetization. It is mostly the case for thin magnetic films. It is well understood now that there might exist two possible domain wall types in magnetic nanowire with in plane magnetization: Transverse Domain Wall (TDW) and Vortex Domain Wall (VDW) depending on the geometry of system [4,5]. TDW are typical for narrow and thin nanowires, while VDW dominate for wide and thick systems. From application point of view narrow nanowires are more promising for using in high density information storage devices. Therefore we limit this study to the case of very narrow magnetic nanowires where only TDW exist.

It is well known that imperfections of nanowire shape can create pinning sites for DW. In particular creating microscopic defects (notches) made on the MN through precise lithographic process let one to create artificial pinning sites to control DW motion in nanowire[6]. Estimating of depinning field for such defects is an important problem. This is related to the energy barrier for DW passing through the pinning site. Theoretical estimates of energy barriers can be done using Nudged Elastic Band method...
within micromagnetic model [7]. In this work we used this method to explore energy landscape of magnetic nanowires with different artificially created imperfections, finding local energy minima and estimating energy barriers between them. Main goal of this work is a systematic study of the effect of different types of rectangular shape defects on the energetics of DW moving through the nanowire.

2. Method
Our model system consists of a single layer permalloy nanowire of rectangular shape with different defects located on its long side and inside it. The nanowire has the following dimensions: length 200 nm, width 20 nm and thickness 5 nm. The energetics of that system is calculated using standard micromagnetic model. According to this model the total energy of magnetic is a functional of magnetization and might be expressed as a sum of four terms:

$$E_{tot} = E_{exch} + E_{anis} + E_{ext} + E_{demag}$$

(1)

where $E_{exch}$ represents the energy of quantum exchange interaction, $E_{anis}$ - the energy of magnetic crystallographic anisotropy, $E_{ext}$ - the energy of interaction with external field (Zeeman energy) and $E_{demag}$ - magnetostatic energy due to the long range magnetostatic interaction (demagnetization field energy). Competition of those contributions to the total energy is responsible for all variety of magnetic phenomena, including magnetic domain formation and magnetic hysteresis. Micromagnetic model itself allows us to explore stability of different magnetic states. Solving Landau-Lifshitz-Gilbert (LLG) equation allows to minimize the total energy of the system and to find possible stable states. It also allows the study of magnetization reversal of the system when changing external magnetic field.

However in many cases it is of interest exploring energy landscape of the system and finding energy barriers for transition between different local minima. To solve this task it is necessary to find Minimal Energy Path (MEP) in multidimensional space corresponding to energy surface of the system. This is highly nontrivial task when taking into account huge dimensionality of the space. One possible solution of this problem is using Nudged Elastic Band method in the framework of micromagnetic theory. Within this method the chain of images of the system corresponding to its different states is created along possible transition path. Those images of the system are connected by elastic springs, thus forming elastic band stretched between initial and final energy minima. Such procedure provides elastic band passing through saddle point and makes it possible to find Minimal Energy Path (MEP) between initial and final states. Recently this method was also used in studies of magnetic systems. There is complete description of the application of the NEB method within micromagnetic theory given in the paper[7]. In the case of magnetic systems components of magnetization vectors taken at different spatial locations of the grid are used as coordinates of multidimensional space. In this work we adopted existing algorithm[7] for micromagnetic modeling of magnetic nanowires.

This formalism has been implemented on the base of our program code MICROMAG [8] written in Intel Visual Fortran language with the use of elements of object oriented programming. As a result, the program code NEB_MICROMAG has been created and debugged. All details of the algorithm and its program realization are given in the paper [9]. Verification of the code NEB_MICROMAG was performed by comparing the results obtained for standard square shaped single layer permalloy nanosland with the data published by other group earlier. Such comparison showed good agreement of the minimal energy path and corresponding energy profile with the results of the paper [10]. The following parameters for permalloy film were used in this work: exchange constant $A=13.0*10^{-12}$ J/m, uniaxial anisotropy constant $K1=0.0$ J/m$^3$, saturation magnetization $Ms=8.0*10^5$ A/m, damping constant $\alpha=0.5$. Zero value of anisotropy constant was used to simplify analysis. It is known that thin permalloy films obtained using sputtering deposition can have very low anisotropy. Mesh sizes of the spatial grid were 2*2*5 nm. We also used the following parameters of the numerical scheme in the calculations. Time step for integration of LLG equation is set to be equal to 0.01 ps, spring constant value for NEB chain is equal to 1.0. Criterion for the convergence of NEB minimization is set in such a way that calculation stops whenever maximal change of the magnetization direction at given time step $dm<10^{-5}$. 


3. Results
To start calculation of the Minimal Energy Path for particular transition in the system under study one needs to generate preliminary initial guess transition path. Inherited property of the NEB method is that it converges to the nearest MEP to the initial guess trajectory. Traditionally simple linear interpolation is used for generating the chain of images representing initial guess trajectory. It is usually obtained through different schemes of linear interpolation between initial and final state. Unfortunately the nature of the magnetization vector does not allow using simple algorithm of linear interpolation because the norm of the magnetization vectors should be conserved. In that case what can be done is just using different forms of gradual rotations of the magnetization from initial to final state. However it is not the only option. There might be numerous possibilities for creating initial guess trajectory using different artificial construction schemes (“manually”). It is reasonable to assume that there might be several alternative transition paths for magnetization switching in the nanowire. In our recent work we found that there might be few alternative scenarios for DW nucleation and motion through the nanowire [11].

In this work we generated initial guess trajectory for NEB by artificially moving transverse DW through the nanowire. In such a way the sequence of configuration of the system with different positions of the DW inside the nanowire creates chain of states. After minimization of the total energy of such chain with NEB micromagnetics we obtained Minimal Energy Path. Energy profile shows the dependence of the total energy of the system on the reaction coordinate along MEP. Corresponding energy profiles along MEP for different cases of nanowire with or without defects are shown in figures 1-5. There are 5 possible configurations of the nanowire which we have studied: 1) nanowire without defects (figure 1), 2) nanowire with hole inside (figure 2), 3) nanowire with rectangular shape bump on the long side (figures 3, 4) nanowire with the rectangular shape notch on the long side (figure 4), and 5) nanowire with the combination of bump and notch on the long side (figure 5).

The first case is the nanowire of ideal rectangular shape without defects. In that case the energy profile has a shape of extended plateau (figure 1). Energy of the system is increased at the beginning of the transition path as the result of single DW nucleation. When DW is propagating along the nanowire total energy does not change, until it drops when DW disappeared on the opposite end.

![Figure 1. Energy profile for DW propagation through nanowire without defects. Schematic picture of nanowire is shown under the plot.](image1)

![Figure 2. Energy profile for DW propagation through nanowire with rectangular hole inside. Schematic picture of the nanowire with hole is shown under the plot.](image2)

It is well known fact that imperfections on the nanowire can work as pinning centers. This effect might be used in applications to control DW motion. Here we consider several possible cases. Introducing the defect in a form of rectangular shape hole (width of 40 nm and height of 10 nm) inside nanowire center leads to the appearance of an extended local minimum on the energy profile (figure 2). This is due to reducing energy of the system when DW length is decreased.
When adding small rectangular shape bump (width of 40 nm and height of 10 nm) on the long side of the nanowire we observe the appearance of additional maximum on the energy profile (figure 3). This is due to increasing energy of the system when DW length is increased.

**Figure 3.** Energy profile for DW propagation through nanowire with bump on the long side. Schematic picture of the nanowire with bump is shown under the plot.

Another kind of defect considered here is the rectangular shape notch (width of 40 nm and depth of 10 nm) located in the middle of the long side of the nanowire. This kind of defect is widely discussed in literature as an effective way for DW pinning. As it was expected the energy profile shown in figure 4 contains local minimum in the middle of the transition path, corresponding to the DW passing through the notch. Again we can say that this effect is due to reducing energy of the system when DW length is decreased.

Finally, we consider the case of the combination of two defects together: the bump and the notch. Corresponding energy profile is shown in figure 5. From analysis of this picture we see that maximum and minimum are joined together that leads to the enhancement of DW pinning effect.

**Figure 4.** Energy profile for DW propagation through nanowire with notch on the long side. Schematic picture of the nanowire with notch is shown under the plot.

**Figure 5** Energy profile for DW propagation through the nanowire with bump and notch on the long side. Schematic picture of the nanowire with bump and notch is shown under the plot.

Thus, our results show how different defects in the nanowire can modify its energetics of DW motion. By combining defects and varying their sizes one can obtain pinning site with required properties.
4. Conclusions
In summary using NEB micromagnetics we have studied the energetics of magnetization switching in nanowires. This numerical technique let us to explore minimal energy paths for DW nucleation and motion in the magnetic nanowire. For single DW nucleation path we studied the dependence of the energy barrier on the nanowire geometry. We explored the effect of nanowire imperfections on the energetics of magnetization switching. From analysis of the results we may conclude that creating different imperfections on the nanowire allows modifying energy profile for DW propagation though the nanowire. This information may help in design of DW pinning sites.

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