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A numerical approach to incorporate intrinsic material defects in micromagnetic simulations

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Spintronics devices like racetrack memory rely on the controlled movement of domain walls in magnetic nanowires. The effects of distributed disorder on this movement have not yet been studied extensively. Defects give rise to a pinning potential that can be characterized in terms of a depth and an interaction range. We investigate how the effects of defects can be realistically introduced in micromagnetic simulations by comparing the properties of the pinning potential to experimental results in the literature. We show that the full 3-dimensional simulations can be replaced by equivalent 2-dimensional ones and propose two approaches to include defects.

I. INTRODUCTION

Many future spintronics devices are based on the controlled movement of domain walls in magnetic nanowires. Consequently, it is important to have a complete understanding of the dynamics governing this motion. Domain wall mobility is extensively described in the literature for perfect nanowires or nanowires with edge roughness. However, real wires always contain a large number of intrinsic material defects. Recently, it has been observed that this distributed disorder throughout the whole wire has an important effect on the domain wall mobility, e.g., domain walls can get pinned to trapping sites. Several experiments have been conducted to characterize the nature of these trapping sites and quantify their properties. It is found that defects give rise to potential wells in the micromagnetic energy landscape. These potentials can be characterized in terms of their depth and interaction range. In this contribution, we numerically investigate the properties of defects implemented in different ways and propose a method to realistically include the influence of intrinsic defects in 2-dimensional (2D) numerical simulations.

Polycrystalline magnetic materials are built up out of grains with possibly varying lattice orientations and imperfect grain boundaries. Despite some controversy, there are indications that mainly the grains influence the magnetic processes in Permalloy (Py) because the measured trapping site density is correlated with the grain density. Experiments are able to characterize the resulting pinning potential. The depth of the well is found to be 1–5 eV, while its interaction range is of the same size as the vortex core diameter used to probe the defect, i.e., approximately 20 nm.

In numerical simulations, the energy of the system is accessible which makes measuring the properties of the potential well a much less challenging task than for experiments, where only macroscopic quantities are measurable. This advantage is used to perform a systematic study of different possibilities to include trapping sites in numerical simulations. Because of the suspected link, we investigate two different implementations that are reminiscent of the grains.

II. METHODS

To determine the properties of the potential well in micromagnetic simulations, we simulate a disk (diameter: 750 nm, thickness: 10 nm) in which a defect is introduced in the central region, see Fig. 1(a). A magnetic vortex is inserted 200 nm from the center. From that point, the vortex relaxes, following a spiralling trajectory towards the disk center. During this slow relaxation (over 400 ns), the energy of the system is probed, see Fig. 1. The depth of the potential well is extracted from the difference between the energy with and without defect. The interaction range is measured from the center of the defect and is determined by the radius over which the potential is deeper than 10% of its maximum, as shown in Fig. 1.

One way to simulate a grain is to focus on its physical size: not every grain has the same thickness. We perform 3-dimensional (3D) simulations in which we simulate the grain as a region with a different thickness. A disk is simulated in which the thickness of the center region is reduced by 2.5, 5, or 7.5 nm, corresponding with 1, 2, or 3 finite difference (FD) cells. We also investigated if we can replace these simulations by performing an equivalent and faster 2D simulation in

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which the saturation magnetization is changed. This method has been used before to investigate the effects of disorder on domain wall motion. A second way to simulate a grain is to introduce a grain boundary by defining a region with a reduced exchange stiffness constant at the boundaries.

All micromagnetic simulations were performed using the GPU-based micromagnetic software package MuMax. Typical material parameters for Py are used: saturation magnetization $860 \times 10^3$ A/m, Gilbert damping parameter $\alpha = 0.02$, and exchange stiffness constant $13 \times 10^{-12}$ J/m. In the 2D simulations, the disks are discretized using cells of $3.125 \times 3.125 \times 10$ nm$^3$. In the 3D simulations, the thickness of the disk is further discretized using cells with a thickness of 2.5 nm. Simulations were performed for defect regions of different sizes of $1 \times 1$ up to $4 \times 4$ FD cells with a reduction in the saturation magnetization/exchange stiffness constant at the boundaries ranging from 10% to 100%. In the simulations in which the saturation magnetization is reduced, the exchange length at the boundary of the defect region is reset to its original value.

### III. RESULTS AND DISCUSSION

#### A. Grain thickness

The grain thickness reduction was simulated by removing FD cells from the top layer. The results are shown as green points in Fig. 2(a). It is observed that the depth of the potential well rises as a function of reduction in thickness, and is larger for larger defect regions.

An effort is made to investigate if these 3D simulations can be reduced to equivalent 2D simulations in which defects are simulated as regions with a reduced saturation magnetization. The depth of the resulting potential well is linearly dependent on the reduction in saturation magnetization and is larger for larger defects, see Fig. 2(a). For sizes larger than $1 \times 1$ FD cells, a jump is observed for defects with the saturation magnetization set to 0. This jump is caused by the disappearance of the vortex core in the defect. To make the 2D simulations equivalent to the 3D ones, it is not sufficient to reduce the saturation magnetization the same amount as the reduction in thickness. There are two different approaches possible to make the simulations equivalent. A first approach is to include regions with larger sizes in the 2D simulations, e.g., in Fig. 2(a), it can be seen that the $2 \times 2$ FD cell sized defects in the 3D simulations lie on the same curve as the $3 \times 3$ FD cell sized defects in the 2D simulations. A second approach is to reduce the saturation magnetization more than the corresponding reduction in thickness. To estimate the size of this reduction Fig. 2(a) can be used as a guide.

The interaction range is weakly dependent on the thickness reduction and seems to be dependent on the size of the defect. However, this dependency arises mainly because the interaction range is measured from the center of the defect. If the size of the defect is deducted from the interaction range, it is found that the resulting distance is almost constant and equal to the vortex core diameter. This observation is supported by Refs. 10 and 11, where it is stated that the measured energy is convolved with the energy profile of the vortex core, resulting in an interaction range of approximately the same size as the diameter of the vortex core. The interaction
ranges for the 3D simulations are not shown and are approximately 20 nm, which is a factor two larger than in the 2D simulations. This can be explained by the fact that the vortex core is larger in 3D simulations.

B. Grain boundary

In the simulations with defects implemented as regions with a reduced exchange stiffness constant at the boundaries, it is found that the depth of the potential well slowly rises as a function of the reduction in the exchange stiffness constant. It is observed that larger defects give rise to deeper potential wells. See Fig. 2(b).

The interaction range is weakly dependent on the reduction in the exchange stiffness constant and rises for larger defects. This dependency is just as in the previous case caused by the method, i.e., the interaction range is measured from the centre of the defect region and not from the edge.

Based on these results, the following methods to realistically include defects in micromagnetic simulations are proposed. First, defects can be included as regions with a size of approximately 10 by 10 nm (similar to the film thickness) with their saturation magnetization reduced by 50%. Alternatively, defects can be defined as regions with the exchange constant reduced by 70% at the boundaries. The potential well caused by such defects is shown in Fig. 1 and has a depth close to the average of the experimentally measured values. For both approaches, the interaction range is approximately the same as the vortex core diameter.

IV. CONCLUSION

In conclusion, we investigated two different ways to include material defects in micromagnetic simulations, both based on the crystal structure in Permalloy. One way to simulate a grain is defining a region with reduced thickness in 3D simulations, or equivalently, an appropriately chosen defect size or reduction in saturation magnetization in 2D simulations. A second way consists in reducing the exchange stiffness constant at the boundaries of the defect region. The interaction range and depth of the potential well are determined by the size of the defect and the reduction of the micromagnetic parameter. Based on this characterization, we propose two ways to realistically include the influence of defects in micromagnetic simulations.

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