Micromagnetic study of soft magnetic nanowires

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In this paper, micromagnetic analysis of an array of long magnetic nanowires (NWs) embedded in a nonmagnetic matrix is performed. It is found that for NWs with diameters on the order of a hundred nanometers, the anisotropy and exchange energies are negligible, so the total free energy is a sum of the Zeeman and magnetostatic energies. The minimum magnetostatic energy corresponds to the maximum Zeeman energy, whereby half of the NWs are magnetized parallel to the external field, while the rest of the NWs are magnetized antiparallel to the external field, while the rest of the NWs are magnetization reversal process. Additionally, the hysteresis loop area of the nanocomposite is inversely proportional to the NW diameter in the range from 20 to 200 nm. The results pave the way for designing of NW-based devices such as optimized magnetic sensors for biomedical applications with a trade-off between miniaturization and energy loss.

Keywords: micromagnetic simulation, soft magnetic nanowires, array of nanowires, hysteresis of nanowires

I. INTRODUCTION

NWs have vast applications in novel logic devices, data storage, permanent magnets, sensors, and biomedicine^{1–5}. The higher shape anisotropy of NWs compared to their thin film and nanoparticle counterparts make them promising nanostructures for soft and hard magnetic materials. For instance, permanent magnets need to exhibit a high coercivity and energy product³, while magnetic sensors require a low coercivity and hysteresis loss⁶. Such large-scale applications can be obtained by tuning the diameter, aspect ratio, and structure of the NWs.

The coercivity changes strongly with the average grain size for different nanocrystalline alloys. In a single domain ferromagnetic region the coercivity is proportional to d^6 , where dis the diameter of the grain⁷. At a critical size the exchange energy starts to balance the anisotropy energy (i.e. when the grain switches from single-domain to multi-domain structures). However, the coercivity of multi-domain grain size is inversely proportional to the diameter. Correspondingly, the thickness of NW determines the coercivity and type of reversal modes. Depending on the wires' diameter, either transverse wall or vortex wall can be formed during the magnetization reversal process of homogeneous NWs^{8–11}. Helicoidal vortex wall and transverse mode have been observed in the magnetization reversal process of isolated and first-neighbors arrays of diameter-modulated NWs¹¹.

This work presents a micromagnetic analysis of high-aspect ratio (length>>diameter and interwire distance) NWs embedded in a nonmagnetic matrix. The hysteresis loss of a highly packed array of NWs is presented to obtain a trade-off between the diameter of the NWs and the hysteresis loss of the composite. In the simulations reported in the paper, we considered the influence of the number of nanowires and their diameter on the magnetization process. The separation distance between the wires is also a significant factor whose influence will be analyzed in future research. The paper is organized as follows. The magnetization reversal process of a single NW and an array of NWs are demonstrated in sections II and III. The dependency of hysteresis loss on the diameter of wire is discussed in section IV. Finally, a conclusion is given.

II. MAGNETIZATION REVERSAL PROCESS OF AN ISOLATED NW

A rigorous way of studying the magnetic properties of nanoscale assemblies is micromagnetic simulation, either static or dynamic. Static approaches typically involve the minimization of free energy (exchange, anisotropy, magnetostatic, and external field interaction energies combined), while the dynamic approaches are based on the Landau-Lifshitz-Gilbert equation. Several free micromagnetic software packages have been introduced by different research groups worldwide: OOMMF¹², MuMax¹³, MagPar¹⁴, Nmag¹⁵, etc. In particular, OOMMF¹² is a well-known completely functional micromagnetics package. Since 3D numerical analysis of an infinite array of NWs is computationally an intensive task, the Ohio Supercomputer Center (OSC) resources¹⁶ are utilized for OOMMF simulations. For the purposes of this work the energy minimization¹⁷ is utilized to study the magnetization reversal process of the NWs.

To understand the magnetization reversal process of an array of NWs, first, a long single NW embedded in a nonmagnetic matrix is analyzed. To obtain the magnetization distribution, the total free energy is minimized to reach the equilibrium condition. In OOMMF, the mesh is comprised of lattices of rectangular prisms. In the simulation, the mesh size, and the diameter, and the length of the NW are 2 nm, 124 nm, and 3200 nm, respectively. The saturation magnetization, exchange coefficient, and anisotropy coefficient of the Iron based NW are 2.1 T, 10 pJ/m and 47000 J/m, respectively. Cubic anisotropy with easy directions is aligned with the co-

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ordinate axes. Our numerical analysis has shown that, if the length to diameter ratio is higher than 25, they can for practical purposes be assumed infinitely long. An external magnetic field is applied along the NW long axis. The hysteresis of the single NW is shown in Figure 1, while the inset shows the top view of the unit cell.

To elucidate the magnetization reversal mechanism, the 2D plane of magnetization states at four different points of the hysteresis curve (points a, b, c, and d in Figure 1) are shown in Figure 2. As represented in the inset of Figure 1, the plane is located in the middle of the unit cell; this is highlighted with a purple dashed line. Since the NW is very long, the right half end of the NW is presented, where the applied field direction for all cases is from right to the left. At point a, all magnetic moments are already aligned antiparallel to the applied field. At point b, the magnetic moments from both ends of the NW start to rotate and align parallel to the applied field and move toward the middle of the NW. Then, at point c, the NW magnetic moments are divided into three sections. First, part of the NW is totally magnetized in the direction of the applied field. Second, at some part of NW (the very right end and middle of the NW), the magnetic moments exhibit a vortex behavior, as discussed below. Third, part of the NW is still anti-parallel to the external field (the very left end of the Figure 1(c)). In fact, magnetization reversal nucleates at both ends of the NW via a localized vortex mode and propagates toward the NW center, where this whole process occurs in an abrupt switch in the hysteresis curve. Finally, at point d, the NW is entirely magnetized in the direction of the applied field. The cross section of the magnetization process of Figure 1(b) at two different locations along the NW is exhibited in Figure 3. The cross section close to the NW end shows a vortex-like propagation where the vortex core is in the center of the NW. During the domain wall propagation, the vortex core approximately follows a spiral pattern and moves toward the edge of the NW. Similar results are presented in Ref. 11.

The points b and c refer to transitory states in a reversal process that changes the magnetization immediately from nearly



FIG. 1. Hysteresis curve of a single NW. The coercivity is $H_c = 40$ mT. Top view of the NW is shown in the inset. In the simulation, the diameter and length of the NW are 124 nm and 3200 nm, respectively. The mesh size is 2 nm. Public domain micromagnetic software OOMMF is used for the simulation.

fully magnetized in one direction to nearly fully magnetized in the other. The transitory case also brings into question the scenario of domain walls nucleating simultaneously at both ends of the wire and then moving together to annihilate in the center. Generally, elongated systems have a nucleation field and a wall propagation field¹⁸. If the propagation field is higher than the nucleation field, then domains may nucleate at both ends of the wire, and then, as the field is increased, the walls begin to move. Depending on the specifics of pinning sites in the wire, a similar scenario can be obtained for the wall annihilation. On the other hand, if the propagation field is lower than the nucleation field, then, once a wall nucleates at either end, it will immediately sweep through the wire. The exact value of the nucleation field at an end depends sensitively on the local part geometry, material variation, defects, and even random thermal processes. Domain nucleation in a physical sample (as opposed to a simulation) will unlikely occur at exactly the same time at both ends.

III. MAGNETIZATION REVERSAL PROCESS OF AN ARRAY OF NANOWIRES

In this work, our goal is to study an infinite array of NWs. OOMMF supports periodic boundary conditions (PBC) only in one axis direction. Therefore, to reduce the computational domain, the magnetization reversal mechanism of nine NWs is investigated here as shown in Figure 4(a) (each NW is labeled with a number). The PBC in the y-axis improves the accuracy of the model compared to defining a finite number of NWs along the y-axis. Figure 4(b) illustrates the magnetization. Zeeman energy, demagnetization energy, and total energy in terms of an external magnetic field. In the simulation, the magnetic field is only increased in the direction opposite to the initial condition and the reverse process is not considered in this paper. As seen, the magnetization reversal process for all 9 NWs occurs in 5 steps (instead of a nearly square loop in a single NW with an abrupt jump). Each staircase is caused by the magnetization reversal of one or more NWs. For example, in the first step, the magnetization reversal occurs along the whole NW 5, while in the second step, NWs 2 and 8 complete their magnetization reversal processes. In Figure 4(b), the numbers in each staircase correspond to the NWs whose magnetization reversal has already occurred. Similar to the single NW, the reversal processes nucleate at both ends of the NWs via a localized vortex mode and propagate toward the NW center. Similar magnetization reversal processes are observed in Refs. 8 and 11. For given NWs dimensions, it is also found that, if the number of NWs increases in an array, the local field experienced by each of the NWs increases. Moreover, the coercivity field decreases as a result of the magnetostatic interactions between the NWs. Note that in the empirical cases the smooth hysteresis curve without any steps is expected; that is because, for an infinite array of wires in the z-axis and y-axis, an infinite number of steps cause smooth magnetization reversal.

The Zeeman, demagnetization, and total energies in terms of applied fields are demonstrated in Figure 4(b). The total



FIG. 2. Plane view of the right half end NW magnetization at the middle of the unit cell. At (a) point a, (b) point b, (c) point c, (d) point d of the hysteresis curve shown in Figure 1. For all four cases, the applied field direction is from right to left. Public domain micromagnetic software OOMMF is used for the simulation.



FIG. 3. The cross section of the NW right end during the reversal process at point b (see Figure 1).

free energy is a sum of Zeeman and demagnetization energies; although the magnetocrystalline anisotropy and exchange energies play important roles in the magnetization reversal process, these energies are negligible in the equilibrium configuration. For large wires' diameters, the magnetostatic energy dominates the anisotropy and exchange energies. The minimum demagnetization energy corresponds to the maximum Zeeman and total energies where half of the NWs already completed their magnetization reversal process (i. e. half of the NWs are magnetized parallel to the external field while the rest of the NWs are magnetized antiparallel to the external fields.).

Since the middle NW (i.e. NW number 5) has four neighbors in the y direction, the interactions with farther NWs are neglected, and the magnetization reversal process of this NW is studied. Figure 5(a) demonstrates the NW schematic; the magnetization of three sections of the NW denoted as t_1 , t_2 , and t_3 are exhibited in Figures 5(b), 5(c), and 5(d), respec-

tively. First, the NW is already magnetized in the *x* direction. Then, by applying an external field in the -x direction, (in a similar trend of a single NW) the magnetic moments at both ends of the NW start to rotate and align with the external field. As seen in Figure 5(b) (which shows section t_1 of the NW), the magnetic moments of the left end of the NW rotate in a vortex trend and propagate to the NW center. At t_2 (see Figure 5(c)), the magnetic moments of the left end are already aligned along the applied field, while the vortex propagation moves toward the center of the NW. Finally, at t_3 (see Figure 5(d)), the magnetization distribution is shown for the center of the NW, while the magnetic moments of both ends aligned along the applied field. Here, the vortex core is not in the center of the NW as mentioned previously.

The reversal process in nanoscale wires to some extent is similar to that of microscale wires. Stoleriu *et al.*¹⁹ studied the domain structure and magnetization distribution of amorphous microwires (MWs). For Fe-based MW without a glass



FIG. 4. a) Top view schematic of 9 NWs (labeled with numbers) located along the *y*-axis with PBC in the *z*-axis. b) Normalized magnetization (red curve), Zeeman energy (black curve), demagnetization energy (blue curve), and total energy (green curve) in terms of external magnetic field. For the magnetization curve, the numbers in each staircase are related to the NW that the magnetization reversal has occurred and is completed. In the simulation, the diameter, lengths, and center-to-center distance between each NW are 124 nm, 3200 nm, and 160 nm, respectively.



FIG. 5. (a) Schematic of NW number 5 where part of the NW length is defined with t_1 , t_2 , and t_3 . The NW is already magnetized from left to right. Plane view magnetization at the middle of the NW unit cell number 5 for length (b) t_1 , (c) t_2 , (d) t_3 . For all three cases, the applied field direction is from right to left.

cover, the reversal process in the wire is divided into two switching regions: close to the center and close to the surface of the wire. Initially, the reversal process starts from both ends of the MW close to the center of the wire and moves toward the middle of the MW. At this stage, the magnetic moments close to the center of the wire are axially aligned in the direction of the external field, while the magnetic moments close to the surface are anti-parallel to the external field. Then, the reversal process radially extends to the entire wire for the magnetic moments close to the surface. The first step of the reversal process in the MW reported by Ref. 19 is similar to what is observed in this work for the reversal process of the



FIG. 6. Normalized hysteresis loss in terms of NW diameter for an array of NWs (circles). The curve shows the fitting curve $\frac{D_0}{D}$, where *D* is the wire diameter and $D_0 = 20 \text{ nm}$ is the simulated minimum diameter. In the simulations, the length and intrawire distance are 30*D* and 1.27*D*, respectively.

NW array (as well as a single NW). Therefore, the computationally affordable micromagnetic analysis of NWs provides a picture of the magnetization reversal process in wires with higher diameters.

IV. HYSTERESIS LOSS IN AN ARRAY OF NANOWIRES

Hysteresis loss is a major concern in magnetic materials, and depends on the dimensions and frequency. The hysteresis loss (the hysteresis loop area) in terms of the NW diameter is illustrated in Figure 6 for an array of long NWs (circles) using OOMMF. The values are normalized to the maximum calculated loss in the whole range of diameters. In the simulations, the length and center-to-center distance between each NW are 30D and 1.27D, respectively, where *D* is the diameter.

As seen, if the diameter increases, the hysteresis loss decreases as well. That is, the coercivity and remanence magnetization decrease as the NWs diameter increases, while the saturation magnetization increases. Shape anisotropy, demagnetizing field, and dipolar interaction between the NWs in the array contribute to such behavior²⁰. Similar results are presented in Refs. 21 and 20. When the diameter increases from 1 to 0.5. A fitting curve shows that the hysteresis loss reduces as $\frac{D_0}{D}$ where D_0 is the simulated minimum diameter (i.e. 20 *nm*).

The results shed light on the understanding of the hysteresis loss on a larger scale, as this behavior has been numerically and experimentally observed in microscale dimensions^{19,22–24}.

V. CONCLUSION

Using the minimization of free energy, the magnetization reversal processes of a single NW and an array of NWs are studied to qualitatively understand their magnetic properties. In an array of NWs with a diameter range of hundreds of nanometers, the Zeeman and demagnetization energies are dominant, while the anisotropy and exchange energies are negligible. The study shows that the hysteresis loss of an array of long NWs decreases when the diameter of the wires increases. The results presented in this work facilitate the design of composites made of highly packed ferromagnetic NWs where the coercivity and hysteresis loss play a key role.

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