Micromagnetic investigation of low-symmetry 3D particles

T Blachowicz\textsuperscript{1} and A Ehrmann\textsuperscript{2}

\textsuperscript{1}Institute of Physics – Center for Science and Education, Silesian University of Technology, 44-100 Gliwice, Poland
\textsuperscript{2}Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences, 33619 Bielefeld, Germany

E-mail: tomasz.blachowicz@polsl.pl

Abstract. Investigating the anisotropies of magnetic nanoparticles is crucial for further development of magnetic data storage media, MRAM, magnetic logical circuits, or magnetic quantum cellular automata. Former theoretical and experimental examinations have revealed the possibility to gain highly symmetric nanoparticles with increased numbers of magnetic states per storage element. In a recent project, we have investigated low-symmetry T-shaped 2D and 3D particles from iron using the micromagnetic simulation software MAGPAR which is based on solving the Landau-Lifshitz-Gilbert (LLG) equation of motion for a mesh built from tetrahedral finite elements. To examine the influence of the reduced symmetry, simulations were performed on the 3D double-T particle with the field applied in different directions in the x-y base plane, ranging from 0 to 180° in 5° steps. Additionally, the external magnetic field was rotated laterally under different angles with respect to the x-y plane, i.e. 5°, 22.5°, and 45°. Similar simulations were executed for the 2D single-T particle. Our results show the strong impact of the shape anisotropy and the respective possibility to tailor magnetic anisotropies according to the desired behaviour by modifying the nanoparticles’ form.

1. Introduction

Magnetic nanoparticles can be used for several applications, including magneto-electronic devices. In these low-dimensional structures, the shape anisotropy dominates over magneto-crystalline and magneto-elastic anisotropies, enabling tailoring the overall anisotropies by designing the geometry of the nanoparticle properly [1]. Magnetic nanostructures can also depict exotic magnetic states, such as flux-closed vortex states with significantly reduced stray fields in nano-rings [2,3]. Perpendicular rings can also exhibit stable onion states [4,5], while ellipses show onion, horseshoe, vortex, and domain wall states [6,7]. 3D-forms, such as half-spheres, tend to mixed in-plane and out-of-plane magnetization components [8-10].

Square magnetic nanoparticles show another special feature: Such systems can have stable intermediate states at remanence [11], as it is also known from exchange bias systems [12], allowing to use them as quaternary memory cells with 2 bits per storage position. This property depends on the geometrical dimensions of the nanoparticles, as shown in theory and experiment [13,14].

Since symmetric 2D nanoparticles with higher numbers of edges, such as sixfold or eightfold particles, only offer instable intermediate states which cannot be used for practical applications [15], it would be interesting to investigate asymmetric and three-dimensional magnetic nanoparticles. Our
article thus aims at simulating two-dimensional T-shaped as well as three-dimensional double-T-shaped particles under different angles to get an insight into the impact of such symmetry breaks.

2. Methods
Magnetic nanoparticles were modelled using the micromagnetic simulation program Magpar, based on the finite element method [16]. Dynamical integration of the Landau-Lifshitz-Gilbert equation of motion is used in this program to simulate hysteresis loops.

For the simulation of the nanoparticles depicted here, mesh dimensions of maximum 2 nm were used. The dimensions of the 2D T-shaped nanoparticle are 250 nm x 250 nm x 10 nm; for the 3D particle, two of these particles were combined under an angle of 90°. Both systems are depicted in Fig. 1. As material, we chose iron (Fe) with an exchange constant of $A_{Fe} = 2.0 \cdot 10^{-11}$ J/m, magnetic polarization at saturation $J_{Fe} = 2.1$ T and Gilbert damping constant $\alpha = 0.01$. The y-axis is directed along the upper part of the T, the x-axis is directed along the base part of the T, while the second T in the 3D case is directed along negative z-direction. The out-of-plane angle $\theta$ is measured with respect to the surface normal (z-axis), while the in-plane angle $\phi$ is measured with respect to the x-axis.

The simulation was performed sweeping from zero external field up to +600 kA/m (with the external field in the sample plane or along an out-of-plane direction specified in the respective graph) and back up to -600 kA/m and to +600 kA/m again, using a field sweeping speed of 10 kA/(m ns).

Figure 1. Geometries of simulated 2D T-shaped nanoparticle (left panel) and of 3D double-T-shaped nanoparticle (right panel).

3. Results
A necessary property of a hysteresis loop which shows four stable states at remanence is a step in the hysteresis loop, resulting from partly switched magnetization [11]. Fig. 2 depicts the results of in-plane measurements of the 2D nanoparticle for four different in-plane angles of the external magnetic field, measured with respect to the x-axis. Although a small step is visible in all cases at vanishing external magnetic field, there are only two stable states at remanence (those with smaller magnetization). Apparently in the 2D case the asymmetry of the T-shape does not support creation of additional stable states at vanishing external field.

In the 3D case, however, more degrees of freedom are available. Since optical as well as electrical detection methods allow measuring the magnetization in-plane or perpendicular to the plane with relatively simple means and intermediate angles necessitating more sophisticated methods, the most use-oriented measurement directions are out-of-plane (perpendicular to the sample plane) and in-plane along the magnetization direction, along the x- and the y-axis.

The results of these different evaluation methods is depicted in Fig. 3 for the double-T-shaped particle with the magnetization at an out-of-plane angle of 22.5° to the surface normal and an in-plane angle of 5°. Obviously, the highest magnetization is reached, approaching saturation, for the out-of-plane case, which fits to the external magnetic field being oriented strongly out-of-plane. However, in this hysteresis loop (blue line), no steps are visible which could indicate additional stable states at remanence. Such steps are only visible in the measurement along the y-direction. This shows that it may be helpful to examine different possible measurement directions to find special features.
For a “symmetric” out-of-plane angle of 45°, i.e. the magnetic field being oriented in the middle between both parts of the double-T, most in-plane angles do not reveal any indication for steps in the hysteresis loops. For an in-plane angle of 90° (Fig. 4), evaluations along the x- or y-direction as well as along the z-direction (not shown here) only show a small area where “ringing” occurs, a precession of the magnetization typical after switching processes. Evaluation along an intermediate angle (here $\phi = 45^\circ$), however, shows clear steps stemming from partial magnetization reversal processes. Thus, the system could be used in this orientation to create quaternary memory cells.

Figure 2. Hysteresis loops, simulated for the single-T-shaped particle, simulated for an external magnetic field along the x-y-plane ($\theta = 90^\circ$) and different in-plane-angles $\phi$ with respect to the x-axis.

Figure 3. Hysteresis loops, examined in different directions for a double-T-shaped particle, simulated for an external magnetic field with an out-of-plane angle of 22.5° and an in-plane-angle of 5°.
While systems with one step can be created as 2D forms [11,14], 3D forms should offer a significant advantage to compensate the increased effort to create them. In Fig. 3, a system with two steps, i.e. 6 possible states at remanence, was depicted. All other systems, tested at out-of-plane angles of 5°, 22.5° and 45° with respect to the z-axis and in-plane angles of 0°, 5°, 20°, 45°, and 90° with respect to the x-axis, did not reveal signs of more than these two steps.

Figure 4. Hysteresis loops, simulated for the double-T-shaped particle, simulated for an external magnetic field with an out-of-plane angle of 22.5° and an in-plane-angle of 5°.

4. Conclusion
To conclude, we have shown that using asymmetric nanoparticles with 3D shapes can result in hysteresis loops with one or two steps on each side of the loop, corresponding with additional states at remanence. The stability of these additional states against small changes of the external field and erroneous shape modifications has to be tested carefully in future micromagnetic simulations.

Future simulations can investigate more 3D shapes to gain an insight into the mechanisms leading to additional stable states at remanence, finally resulting in a possibility to maximize the number of such stable states and thus the data storage capacity of a single nanoparticle.

5. Acknowledgements
This work was partially supported by the internal project BK-243/RIF/2016 of the Institute of Physics – CSE, Silesian University of Technology.

6. References
[1] Nogués J, Sort J, Langlais V, Skumryev V, Surinach S, Munoz JS, and Baro MD 2005 Phys. Rep. 422 65
[2] Zhang W and Haas S 2010 Phys. Rev. B 81 064433
[3] Zhu FQ, Fan DL, Zhu XC, Zhu JG, Cammarata RC, and Chien CL 2004 Adv. Mater. 16 2155
[4] Subramani A, Geerpuram D, Domanowski A, Baskaran V, and Metlushko V 2004 Physica C 404 241
[5] Wang J, Adeyeye AO, and Singh N 2005 Appl. Phys. Lett. 87 262508
[6] Gao XS, Adeyeye AO, Goolaup S, Singh N, Jung W, Castaño FJ and Ross CA 2007 J. Appl. Phys. 101 09F505
[7] Vavassori P, Grimsditch M, Novosad V, Metlushko V, and Ilic B 2003 Phys. Rev. B 67 134429
[8] Soares MM, de Biasi E, Coelho LN, dos Santos MC, de Menezes FS, Knobel M, Sampaio LC, and Garcia F 2008 Phys. Rev. B 77 224405
[9] Leong TG, Zarafshar AM, and Gracias DH 2010 Small 6 792
[10] Amaladass E, Ludescher B, Schütz G, Tyliszczak T, Lee MS, and Eimüller T 2010 J. Appl. Phys. 107 053911
[11] Blachowicz T and Ehrmann A 2011 J. Appl. Phys. 110 073911
[12] Tillmanns A, Oertker S, Beschoten B, Güntherodt G, Leighton C, Schuller IK, and Noguès J 2006 Appl. Phys. Lett. 89 202512
[13] Blachowicz T, Ehrmann A, Steblinski P, and Palka J 2013 J. Appl. Phys. 113 013901
[14] Ehrmann A, Blachowicz T, Komraus S, Nees MK, Jakobs PJ, Leiste H, Mathes M, and Schaarschmidt M 2015 *J. Appl. Phys.* **117** 173903
[15] Blachowicz T, Ehrmann A 2013 *J. Magn. Magn. Mat.* **331** 21-23
[16] Scholz W, Fidler J, Schrefl T, Suess D, Dittrich R, Forster H and Tsiantos V 2003 *Comp. Mat. Sci.* **28** 366