

MICROMAGNETIC SIMULATIONS AND APPLICATIONS

T. Schrefl, H. Forster, R. Dittrich, W. Scholz, D. Suess, V. Tsiantos, J. Fidler
Vienna University of Technology, Wiedner Hauptstr. 8-10, A-1040 Vienna, Austria,
phone: +43 1 58801 13729, fax: +43 1 58801 13729, email: thomas.schrefl@tuwien.ac.at

<http://magnet.atp.tuwien.ac.at>

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 minimum energy path provides a tool to calculate the energy barriers in large scale micromagnetic systems.

2 Numerical Methods

The following numerical methods are used for the simulation of magnetic elements:

- MCS/Patran to create the finite element mesh
- software package VODPK to perform a time integration
- finite element program library DIFFPACK
- hybrid FE/BE method for the open boundary problem
- Treecode for the long range magnetostatic interaction
- hierarchic matrices for speeding up the FE/BE method
- AVS for visualization of the results

The simulations (especially large models) were carried out partly on the following servers of the computational center of TU-Vienna (*ZID*): *sc.zserv*, *fe.zserv*, *cfid.zserv* and *fpr.zserv*.

3 Applications

3.1 ENERGY BARRIERS IN MAGNETIC RANDOM ACCESS MEMORY ELEMENTS

Minimum energy paths and energy barriers are calculated for the free data layer in MRAM (magnetic random access memory) elements using a recently developed method [2] which combines the CINEB method [3] (climbing image nudged elastic band method) with finite element micromagnetics. The method calculates the magnetic states along the most probable reversal paths for applied fields below the zero temperature switching field.

[1] T. Shimatsu, H. Uwazumi, Y. Saki, A. Otsuki, I. Watanabe, H. Muraoka, Y. Nakamura, IEEE Trans. Mag. 37(2001) 1567

[2] R. Dittrich, T. Schrefl, D. Suess, W. Scholz, H. Forster and J. Fidler, J. Magn. Mater. 250, 12 (2002)

[3] G. Henkelman, B. P. Uberuaga, H. Jonsson, J. Chem. Phys. 113, 9901 (2000)

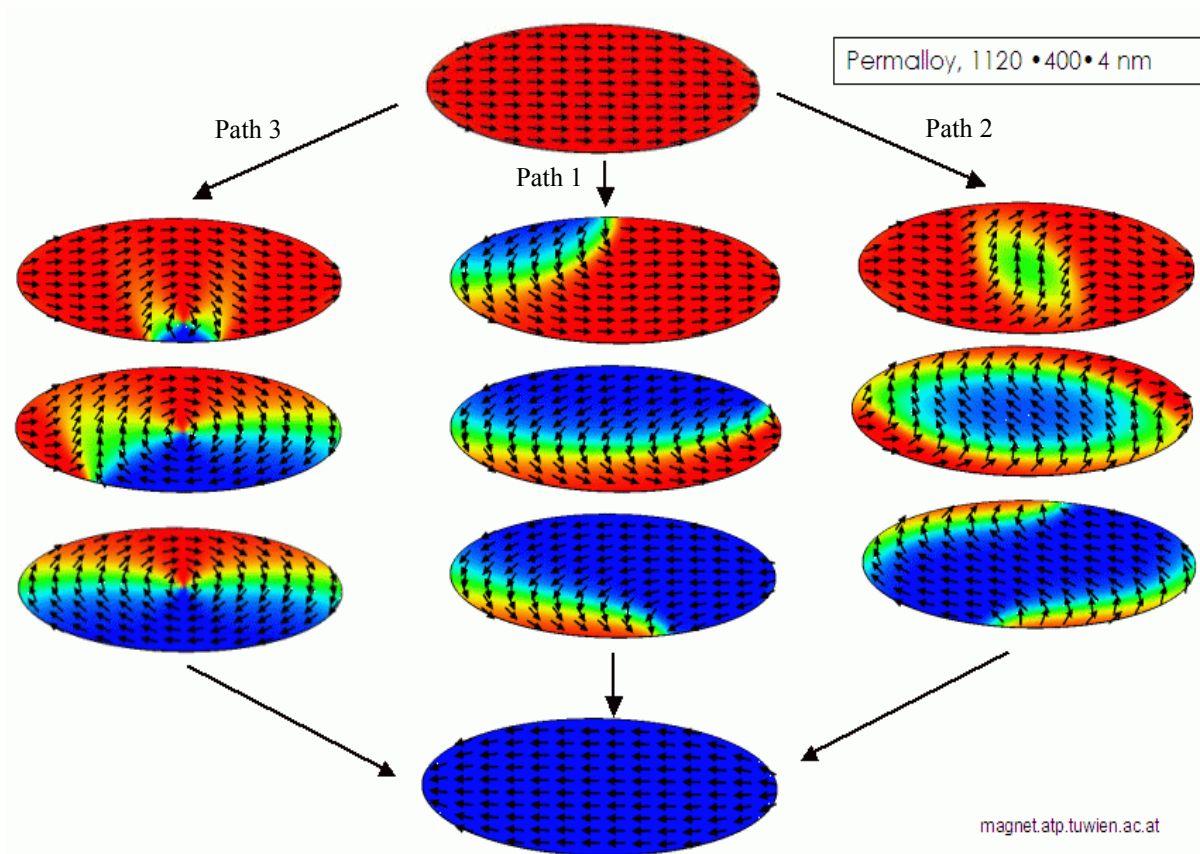


Figure 1. Three Minimum energy paths for the thermal reversal of a thin NiFeCo MRAM element are found between the two stable states. In Paths 1 and 2 the magnetization stays in plane crossing a single barrier. In path 3 a two step reversal mode is found passing a metastable state (vortex in the center).

The predicted transition rates are compared with an experimental work [4], which studies the thermal reversal of elliptical NiFeCo MRAM elements. Fig. 1 shows a top view of the 3D finite element model of the free layer. The long axis is 1120 nm, the diameter 400 nm and the thickness 4 nm. The material parameters of NiFeCo were used ($J_s=1.068$ T, $A=10$ pJ/m, $K=5.1 \cdot 10^2$ J/m³) with the easy axis along the long axis of the element. The minimum energy paths (MEP) were calculated as a function of an external field along the easy axis of an strength below the zero temperature switching field ($= 90$ Oe).

The results show three possible minimum energy paths. Two of them shows a single energy barrier where the magnetization reverses by an inhomogeneous rotation in the film plane (path1 and path2 in figure 1). The third mode is a two step reversal process which passes a metastable state where a vortex is in the center (path3 in figure1). At zero field this two step reversal by vortex motion has smaller energy barriers than the in plane process. With increasing field however, the in plane mode becomes energetically favorable. This is in agreement to the single energy barrier behavior of the observed relaxation times in the experiment.

[4] N. D. Rizzo, M. DeHerrera, J. Janesky, B. Engel, J. Slaughter and S. Tehrani, Appl. Phys. Lett. 80, 2335 (2002)

3.2 FAST BOUNDARY METHODS FOR MAGNETOSTATIC INTERACTIONS IN MICROMAGNETICS

Micromagnetic simulations of realistic magnetic devices require the calculation of the magnetostatic interactions between distinct magnetic parts. Hybrid finite element/boundary element (FE/BE) algorithms as originally proposed by Fredkin and Koehler are very efficient, since they require no mesh between the particles [5]. In addition the FE/BE discretization allows arbitrarily shaped structures. However the BE part of this algorithm leads to a fully populated matrix of size N^2 , where N is the number of boundary nodes. As a consequence storage and CPU-time scale with N^2 , which causes performance problems in structures with high aspect ratio where most nodes are on the boundary. To overcome this problem various techniques to accelerate the BE method have been proposed. In this work we compared (1) a treecode-method as used for particle simulations [6], (2) hierarchical matrices or so called supermatrices [7], and (3) the fully populated boundary element matrix.

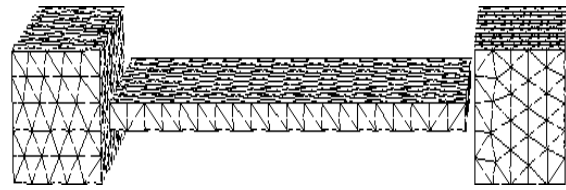


Figure 2. Surface mesh with 996 boundary nodes.

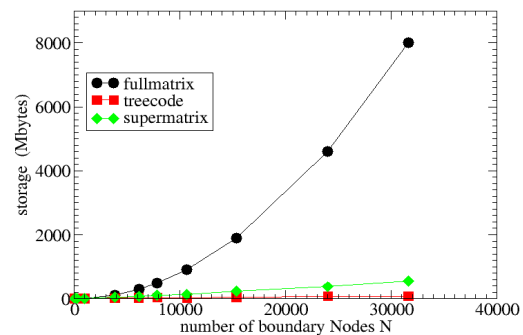


Figure 3. Storage requirements dependent on the number of boundary nodes.

The different methods are tested for a soft magnetic film stabilized by two permanent magnets. Fig. 2 gives an example of a surface mesh. The CPU-time for the setup-phase, the CPU-time for the matrix vector multiplication and the required storage are compared as a function of the number of boundary nodes. Therefore the same structure is remeshed with grids of different element size. Fig. 3 gives the memory requirement for the different methods. CPU-time tests with the full matrix method are only possible for $N < 10000$, because of the N^2 -dependence and the limited memory in our workstation. We found that both, the treecode and the supermatrix approach, drastically reduce the CPU-time of the setup-phase as compared to the N^2 -dependence of the full matrix method. Finally we evaluated the required CPU-time for 1000 matrix vector multiplications according to (3). Even for a small problem size, $N=10000$, the supermatrix method reduces the CPU-time by a factor of 10 as compared to the multiplication of the full matrix. With increasing problem size the speedup becomes more significant. The treecode scales with $N \times \log(N)$. The high amount of bookkeeping increases the CPU-time for matrix vector multiplications for small problems. Because of the N^2 -dependence the full matrix method is not suitable for large systems. Due to the very short setup-phase the treecode method is recommended for moving parts, for example recording simulations using a fully discretized head. The supermatrix is faster in the matrix vector multiplication. So it is the method of choice for the solution of the Landau-Lifshitz-equation on a fixed grid.

[5] D. R. Fredkin, T. R. Koehler, IEEE Trans. Magn. 26, 415, (1990)

[6] J. Barnes, P. Hut, Nature 324, 446, (1986)

[7] S. Börm, L. Grasedyck, W. Hackbusch, Mathematica Bohemica 127, 229, (2002)

4 List of publications (2002)

D. Suess, W. Scholz, T. Schrefl, and J. Fidler, "Fast switching of small magnetic particles", *J.M.M.M.* 242-245 (2002) 426-429.

V.D. Tsiantos, W. Scholz, D. Suess, T. Schrefl and J. Fidler, "The effect of the cell size in Langevin micromagnetic simulations", *J.M.M.M.* 242-245 (2002) 999-1001.

W. Scholz, J. Fidler, T. Schrefl, D. Suess and T. Matthias, "Micromagnetic simulation of domain wall pinning in Sm(Co,Fe,Cu,Zr)_z magnets", *J.M.M.M.* 242-245 (2002) 1356-1358. J. Fidler, T. Schrefl, V.D. Tsiantos, W. Scholz and D. Suess

W. Scholz, H. Forster, D. Suess, T. Schrefl and J. Fidler, "Micromagnetic simulation of domain wall pinning and domain wall motion", *Computational Materials Science* 25 (2002) 540-546.

J. Fidler, T. Schrefl, V.D. Tsiantos, W. Scholz and D. Suess, "Fast switching behaviour of nanoscopic NiFe- and Co-elements", *Computational Materials Science* 25 (2002) 554-561.

I. Panagiotopoulos, T. Matthias, D. Niarchos, J. Fidler, "Magnetic properties and microstructure of melt-spun Sm(Co,Fe,Cu,Zr)₈ magnets", *J.M.M.M.* 247 (2002) 355-362.

D. Suess, V. Tsiantos, T. Schrefl, J. Fidler, W. Scholz, H. Forster, R. Dittrich, J. Miles, "Time resolved micromagnetics using a preconditioned finite element method" *J.M.M.M.* 248 (2002) 298-311.

H. Forster, T. Schrefl, D. Suess, W. Scholz, V. Tsiantos, R. Dittrich, J. Fidler, "Domain wall motion in nano-wires using moving grids", *JAP* 91 (2002) 6914-6919.

W. Scholz, D. Suess, T. Schrefl and J. Fidler, "Domain structures and domain wall pinning in arrays of elliptical NiFe nanoelements", *JAP* 91 (2002) 7047-7049.

J. Fidler, T. Schrefl, V.D. Tsiantos, W. Scholz, D. Suess and H. Forster, "Ultrafast switching of magnetic nanoelements using a rotating field", *JAP* 91 (2002) 7974-7976.

D. Suess, V. Tsiantos, T. Schrefl, W. Scholz, J. Fidler, "Nucleation in polycrystalline thin films using a preconditioned finite element method" *JAP* 91 (2002) 7977-7979.

W. Scholz, J. Fidler, T. Schrefl, D. Suess, T. Matthias, "Micromagnetic 3D simulation of the pinning field in high temperature Sm(Co,Fe,Cu,Zr)_z magnets", *JAP* 91 (2002) 8492-8494.

J. Fidler, T. Schrefl, H. Forster, D. Suess and R. Dittrich, "FE-Simulation of fast switching behaviour of magnetic nanoelements", *Proceedings of 5th Int. Conference on Modeling and Simulation of Microsystems, Puerto Rico*, Eds: M. Laudon and B. Romanowicz, 2002, pp. 348-351.

Dittrich, R.; Schrefl, T.; Forster, H.; Suess, D.; Scholz, W.; Fidler, J.; Tsiantos, V.

"Finite element simulation of discrete media with granular structure" *IEEE Trans Magn.* 38 (2002) 1967-1969.

Suess, D.; Schrefl, T.; Scholz, W.; Kim, J.-V.; Stamps, R.L.; Fidler, J. ; "Micromagnetic simulation of antiferromagnetic/ferromagnetic structures" *IEEE Trans Magn.* 38 (2002) 2397-2399.

Fidler, J.; Schrefl, T.; Tsiantos, V.D.; Forster, H.; Dittrich, R.; Suess, D. "FE-simulation of fast switching behavior of granular nanoelements" *IEEE Trans Magn.* 38 (2002) 2520-2522.

Forster, H.; Schrefl, T.; Dittrich, R.; Suess, D.; Scholz, W.; Tsiantos, V.; Fidler, J.; Nielsch, K.; Hofmeister, H.; Kronmuller, H.; Fischer, S. "Magnetization reversal in granular nanowires" IEEE Trans Magn. 38 (2002) 2580–2582.

R. Dittrich, T. Schrefl, D. Suess, W. Scholz, H. Forster, J. Fidler, "A path method for finding energy barriers and minimum energy paths in complex micromagnetic systems", JMMM 250 (2002) L12-L19.

J. Fidler, T. Matthias, W. Scholz, T. Schrefl, T.S. Rong, I. Jones, I. R. Harris, "The role of the precipitation structure on the coercivity of Sm(Co,Fe,Cu,Zr)_z magnets for HT applications" Proc. of XVII Rare Earth Magnets Workshop, University of Delaware, ed: G. Hadjipanayis and M.J. Bonder, 2002, pp. 853-860.

T. Schrefl, H. Forster, J. Fidler, R. Dittrich, D. Suess and W. Scholz, "Magnetic hardening of exchange spring multilayers", Proc. of XVII Rare Earth Magnets Workshop, University of Delaware, ed: G. Hadjipanayis and M.J. Bonder, 2002 pp. 1006-1026.

R. Dittrich, T. Schrefl, V. Tsiantos, H. Forster, D. Suess, W. Scholz, J. Fidler, "Micromagnetic simulation of thermal effects in magnetic nanostructures", Materials Research Society Symposium Proceedings Vol. ????: xxx, 2002, in press.

H. Forster, T. Schrefl, W. Scholz, D. Suess, V.D. Tsiantos and J. Fidler, "Micromagnetic simulation of domain wall motion in magnetic nano-wires", Proc. of Int. Workshop on Wires (IWMW), San Sebastian, Spain, June 2001, (2002) in press.

T. Schrefl, J. Fidler, D. Suess W. Scholz and V. Tsiantos, "Micromagnetic simulation of dynamic and thermal effects", Advanced magnetic materials, Eds: Y. Liu, D.J. Sellmyer and D. Shindo, (2002), in press.

D. Payer, D. Suess, T. Schrefl and J. Fidler, "Reversal processes in circular nanomagnets", J.M.M.M. (2002) in press.

T. Schrefl, M. Schabes, B. Lengsfeld, "Fast reversal dynamics in perpendicular magnetic recording media with soft underlayer", JAP 91 (2002) 8662 -8665.

M. Schabes, B. Lengsfeld, T. Schrefl, "Micromagnetic modelling of soft underlayer magnetization processes and fields in perpendicular magnetic recording", IEEE Trans. Magn. 38 (2002) 1670 - 1675.

D. M. Newns, W. E. Donath, G. J. Martyna, M. E. Schabes, B. E. Lengsfeld, T. Schrefl "Performance of a Novel Algorithm for Perpendicular Magnetic Recording Simulation" Proceedings of The 3rd Workshop on Parallel and Distributed Scientific and Engineering Computing with Applications (PDSECA-02) (2002) pp. 232 -238.

D. Suess, "Micromagnetic simulations of antiferro- and ferromagnetic structures for magnetic recording" Doctor Thesis, Institute for Solid State Physics, TU Wien, 2002.

M. Stehno, "Intergranular exchange in perpendicular recording media", Diplom Thesis, Institute for Solid State Physics, TU Wien, 2002.