MICROMAGNETIC SIMULATIONS OF DOMAINSTRUCTURES IN SOFTMAGNETIC THIN FILMS

T. Schrefl, W. Scholz, R. Dittrich, H. Forster, D. Suess, M. Stehno, 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 development of advanced magnetic materials requires a precise understanding of the magnetic behavior. A prominent example are magnetic recording systems future high density information storage, where both recording medium and recording heads have to meet certain characteristics [1]. These structures are so small that quantum mechanical effects like exchange have to be taken into account. However, they are too large for a pure quantum mechanical description, which would exceed the capabilities of today's ab-initio computational models. On this intermediate level between the macroscopic world and a description with atomic resolution, micromagnetic models provide a useful tool for detailed predictions of the magnetic properties and magnetization processes. The theory of micromagnetism combines Maxwell's equations for the magnetic field with an equation of motion describing the time evolution of the magnetization. The local arrangement of the magnetic moments follows from the complex interaction between intrinsic magnetic properties such as the magnetocrystalline anisotropy and the physical/chemical microstructure of the material.

The finite element method is a highly flexible tool to describe magnetization processes, since it is possible to incorporate the physical grain structure and intergranular phases. Recent developments of advanced numerical methods allows for the first time the modelling and dynamic simulation of an entire media-head system including sub-grain dicretization of the media and a full 3D finite element mesh of the entire ring head. Moreover the development of high performance parallel finite element micromagnetics packages (see section 2.1) take full use of the computational power of novel multiprocessor machines and allows the use of large scaled complex models.

The computational models provide great freedom in the choice of experiment conditions and in the variation of material parameters. This provides useful hints for artificial structuring of future magnetic materials [2]. In addition to measurements of the remanent magnetization and the coercive field, it is possible to study the details of the magnetization distribution and the magnetization reversal processes, which are difficult to investigate experimentally.

[1] D.E. Speliotis, Magnetic recording beyond the first 100 years, J. Magn. Magn. Mat. 193, 29-35 (1999).
[2] E.D. Dahlberg, J.G. Zhu, Micromagnetic Microscopy and Modeling, Physics Today 48, 34-40 (1995).

2 Numerical Methods

2.1 magpar - Parallel Finite Element Micromagnetics Package

In the light of the importance of the microstructure of magnetic materials the finite element method has been chosen for the implementation of a micromagnetic model. There are several commercial and open source micromagnetics packages available, however all of them use the finite difference method. In addition, static energy minimization methods for the study of SmCo permanent magnets as well as dynamic time integration methods for the investigation of the magnetization dynamics in magnetic nanoparticles are desirable.

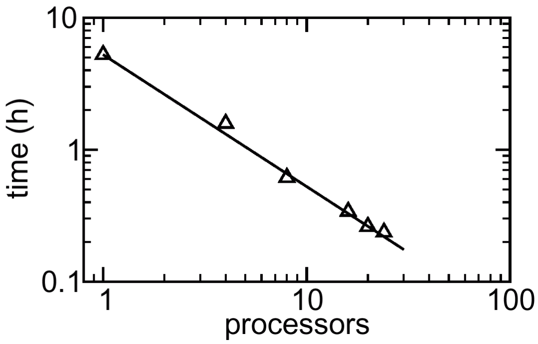


Fig. 1 *Execution time of a static energy minimization problem (nucleation in FePt nanoparticles) as a function of the number of processors. The solid line represents the ideal scaling behavior. On eight processors a "superlinear" scaling behavior due to caching effects is observed.*

Therefore, a new high performance scalable (Fig .1) parallel finite element micromagnetics package [3]-[4] has been implemented which combines several unique features: It is entirely based on portable, free, open source software packages (Fig. 2), highly portable to different hardware platforms, which range from simple PCs to massively parallel supercomputers, highly optimized, scalable and well integrated. It includes solvers for static energy minimization, time integration of the Landau-Lifshitz-Gilbert equation, and the nudged elastic band method.

Simulations (especially large models) were carried out partly on the following servers of the computational center of TU-Vienna (*ZID*): sc.zserv and fe.zserv. A first release of the freeware under GNU General Publick License [5] can be found on the web [6].

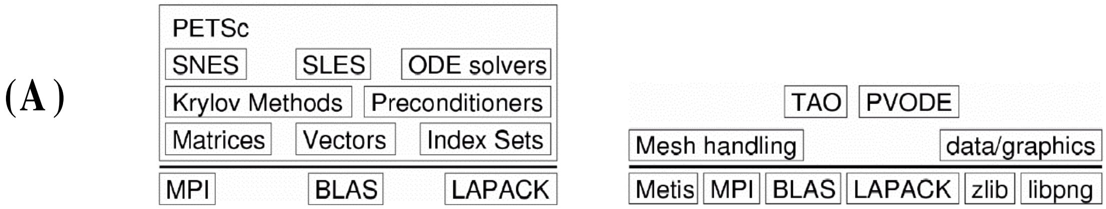
---

[3] W. Scholz, "Scalable Parallel Micromagnetic Solvers for Magnetic Nanostructures", dissertation, Vienna University of Technology, Vienna, Austria, 2003

[4] W. Scholz, J. Fidler, T. Schrefl, D. Suess, R. Dittrich, H. Forster, V. Tsiantos, "Scalable Parallel Micromagnetic Solvers for Magnetic Nanostructures", Comp. Mat. Sci (2003), submitted.

[5] http://www.gnu.org/licenses/gpl.html/

[6] http://magnet.atp.tuwien.ac.at/scholz/magpar/



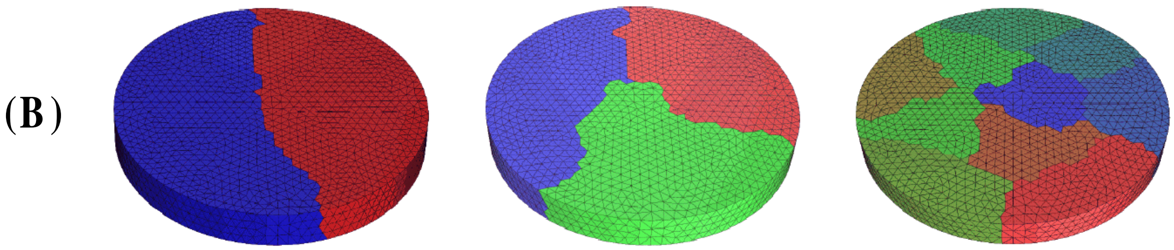


Fig. 2A *The micromagnetics package is based on PETSc, the "Portable, Extensible Toolkit for Scientific Computation". PETSc uses MPI for message passing, BLAS and LAPACK for low level linear algebra. The "Toolkit for Advanced Optimization" is used for energy minimization and PVODE for the time integration of the Landau-Lifshitz-Gilbert equation. METIS handles the mesh partitioning, zlib is used for the compression of output data and libpng for the generation of PNG graphics files.* **Fig. 2B** *Example of the mesh partitioning for 2 processors, 3 processors and 10 processors using the METIS library is shown at the bottoem sequence.*

3 Applications

3.1 Permalloy Nanodots

The static and dynamic properties of magnetic nanodots with curling in-plane magnetization distribution (vortex) are studied using 3D dynamic micromagnetic simulations. The magnetization state of such a vortex stae is shown in Fig. 3. The magnetization distribution, contributions to the total energy, hysteresis behavior, and surface charges are calculated and compared with an analytical vortex model. A phase diagram of the magnetic ground states of magnetic nanodots as a function of the radius and height is calculated and compared with analytical and experimental investigations.

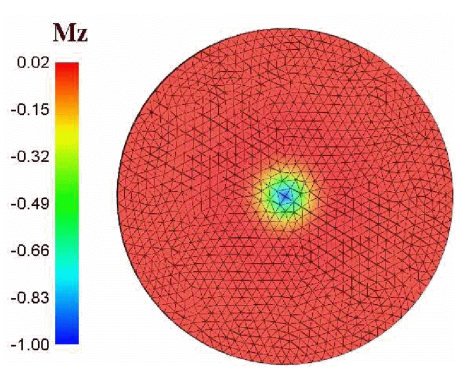


Fig. 3 *Magnetization distribution of the vortex state on a fine 3D finite element mesh.The vortex core is properly resolved.*

The dynamic properties, which are important for high frequency applications, are reported for in-plane and out-of-plane fields. The simulations [7] show that the shape of the vortex core and its exchange energy have been found to be very stable (“rigid”) even for large vortex shifts in an external field. The phase diagram of magnetic ground states shows sharp transitions from the “in-plane” state to the perpendicular magnetization distribution and the magnetic vortex state, whereas the transition from the perpendicular magnetization to the magnetic vortex state is not well defined.

3.2 Exchange bias in F/AF systems with perfectly compensated interfaces

The phenomena of exchange anisotropy and exchange bias, particularly, were discovered in the year 1956 by Meiklejohn and Bean when studying Co particles surrounded with antiferromagnetic oxide (CoO). They found that the field required to switch the ferromagnet from the field cooled state into the reversed state is larger than that to rotate the ferromagnet back to its original direction. Our present work concerning exchange bias focus on bilayer systems with perfectly compensated interfaces [8] (see Fig. 4).

The interacting grain model assumes perfectly compensated interfaces between the granular ferro- and antiferromagnet and gives bias fields and coercivities comparable to those observed experimentally. The behavior of the hysteresis shift (shown in Fig. 5 on the left) and the coercivity for varying material parameters is investigated. For certain material parameters our simulations resulted in substantially stable 360° domain wall [9] loops (shown in Fig 5 on the right) or lines within the softmagnetic ferromagnic layer, similar to those observed experimentally.

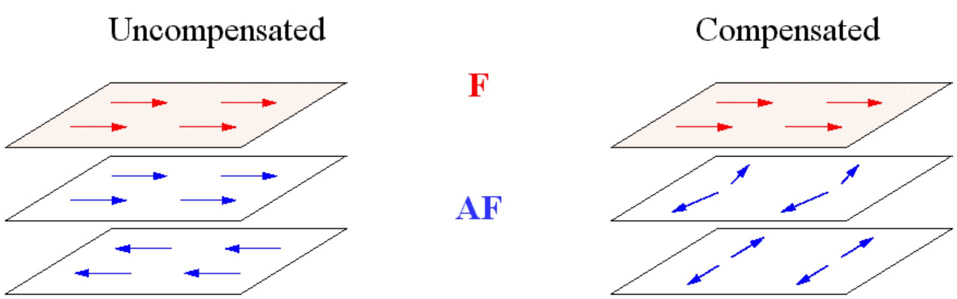


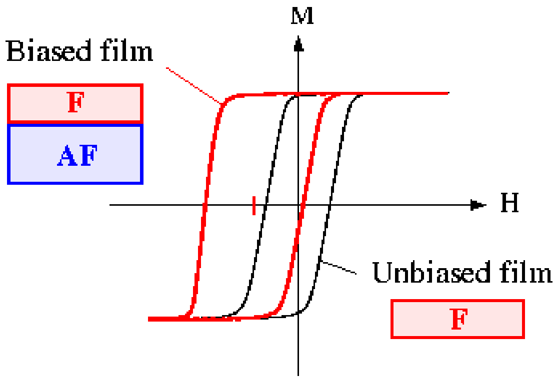
Fig. 4 (on the left) *For uncompensated interfaces the antiferromagnetic spins of one sublattice dominate at the AF/F contact surface.* **(on the right)** *At perfectly compensated interfaces the net spin of the antiferromagnet averaged over a microscopic length scale is zero. A fully compensated antiferromagnetic interface will lead to a 90° or spin flop coupling between the two layers. A weak canting of the AF spins close to the interface provide a small net moment parallel to the interface to which the ferromagnet is able to couple. Simple models predict that AF/F layers with compensated interfaces exhibit an enhanced coercivity but no exchange bias. However, our simulations resulted in exchange bias fields and coercivities comparable to experimentally found data.*

---

[7] W. Scholz, K. Y. Guslienko, V. Novosad, D. Suess, T. Schrefl, R. W. Chantrell, J. Fidler, "Transition from single-domain to vortex state in soft magnetic cylindrical nanodots", J. Magn. Magn. Mater. 266 (2003) 155-163. .

[8] D. Suess, M. Kirschner, T. Schrefl, J. Fidler, R.I. Stamps, J.V. Kim "Exchange bias of polycrystalline antiferromagnets with perfectly compensated interfaces", Phys. Rev.B 67 (2003) 54419-8.

[9] M. Kirschner, D. Suess, T. Schrefl, J. Fidler, J. N. Chapman, "Micromagnetic calculation of bias field and coercivity of exchange biased IrMn/NiFe bilayers, IEEE Trans. Magn. (2003), in press



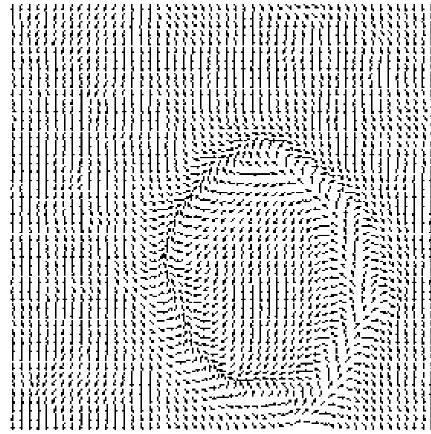


Fig. 5 (on the left) *The antiferromagnetical exchange bias leads to a shift of the hysteresis as compared to an unbiased single layer film.* **(on the right)** *For certain material parameters our simulations resulted in substantially stable 360° domain wall loops or lines within the ferromagnet, similar to those observed experimentally. The figure shows the stable magnetization state (360° domain wall) in the ferromagnetic layer F obtained in the simulation of the hysteresis loop.*

3.3 Vortex core reversal by Bloch points

Thin permalloy disks support a vortex configuration. We study how micromagnetic calculations can be applied to processes that involve a singularity of the magnetization field, namely the Bloch point [10]. The reversal of the core of the vortex under an field applied perpendicularly to the disk plane is investigated. We apply two different procedures to evaluate switching fields and processes: direct micromagnetic time-dependent calculation, and the evaluation of the energy barrier that separates the two orientations of the vortex core in the configuration space, using the nudged elastic band method [11]. Both methods show the occurrencse of Bloch points (see Fig. 6) during reversal.

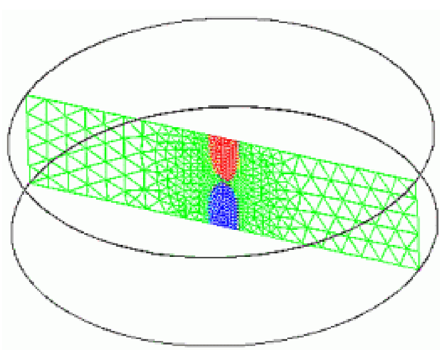


Fig. 6 *Minimum energy paths for the thermal reversal of the vortex core in a softmagnetic disk are calculated. The vortex core reverses by the nucleation and displacement of a Bloch point singularity. Shown is a cut across the thickness of the finite element mesh (Permalloy disk, 100 nm radius, 50 nm thickness). The colour code corresponds to the z-component of the magnetization. The magnetization state has a Bloch point in the center of the disk.*

---

[10]A. Thiaville, J.M. Garcia, R. Dittrich, J. Miltat, T. Schrefl, "Micromagnetic study of Bloch points nucleated vortex core reversal", Phys. Rev. B. 67, 94410-1-12 (2003)

[11]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", J. Magn. Magn. Mater. 250 (2002) L12-L19.

4 List of publications (2003)

[1] Scholz Werner, Schrefl Thomas, Suess Dieter, Dittrich Rok, Forster Hermann, Tsiantos Vassilios, Fidler Josef Implementation of a scalable parallel finite element package for micromagnetic simulations, submitted

[2] W. Scholz, J. Fidler, T. Schrefl, D. Suess, H. Forster, R. Dittrich, V. Tsiantos, Numerical Micromagnetic Simulation of Fe-Pt Nanoparticles with Multiple Easy Axes, J. Magn. Magn. Mater. (2003), submitted.

[3] W. Scholz, D. Suess, R. Dittrich, T. Schrefl, V. Tsiantos, H. Forster, J. Fidler, Implementation of a high performance parallel finite element micromagnetics package, J. Magn. Magn. Mater. (2003), submitted.

[4] Rok Dittrich, "Finite element computation of energy barriers in magnetic systems", Ph.D thesis, Vienna University of Technology, 2003

[5] W. Scholz, "Scalable Parallel Micromagnetic Solvers for Magnetic Nanostructures", dissertation, Vienna University of Technology, Vienna, Austria, 2003.

[6] H. Forster, "Reversal Modes in Mesoscopic Structures" Doctor Thesis, Institute for Solid State Physics, TU Wien, 2003.

[7] I. Rungger, Magnetische Wirbelstrukturen in quadratischen Nanoelementen, Diplom Thesis, Institute for Solid State Physics, TU Wien, 2003.

[8] M. Kirschner, Exchange Bias in Ferro-/Antiferromagnetic Bilayers, Diplom Thesis, Institute for Solid State Physics, TU Wien, 2003.

[9] V. Tsiantos, T. Schrefl, W. Scholz, H. Forster, D. Suess, R. Dittrich, J. Fidler, "Thermal Fluctuations in Magnetic Sensor Elements," Sensor and Accutors A 106, 134-136 (2003).

[10] D. Suess,T. Schrefl, J. Fidler, R. C. Woodward, T. G. St.Pierre, R. Street, S. Sun, C. Murray, L. Folks, B. Terris, "Reversal Processes in FePt Nanoparticle Arrays," IEEE Trans. Magn., submitted

[11] D. Suess, M Kirschner, T. Schrefl, J. Fidler, R.L. Stamps, T. Schrefl, J.V. Kim, "Exchange bias of polycrystalline antiferromagnets with perfectly compensated interface", Phys. Rev. B 67, 54419-1-8 (2003).

[12] W. Scholz, K. Yu Guslienko, V. Novosad, D. Suess, T. Schrefl, R.W. Chantrell, J. Fidler, "Transition from single-domain to vortex state in soft magnetic cylindrical nanodots", J. Magn. Magn. Mater. (2003) in press.

[13] T. Schrefl, H. Forster, R. Dittrich, D. Suess, "Reversible magnetization processes and energy density product in Sm-Co/Fe bilayers", J. Appl. Phys. 93, 6489-6491 (2003).

[14] D. Suess, T. Schrefl, W. Scholz, J. Fidler, "Micromagnetic calculation of coercivity and remanence of self assembled FePt nanoparticle arrays", J. Appl. Phys. 93, 7041-7043 (2003).

[15] R. Dittrich, T. Schrefl, D. Suess, W. Scholz, H. Forster, J. Fidler, "Thermally induced magnetization reversal in AFC media", J. Appl. Phys. 93, 7405-7407 (2003).

[16] V. Tsiantos, T. Schrefl, W. Scholz, J. Fidler, "Thermal magnetization noise in submicron spin valve sensors", J. Appl. Phys. 93, 8576-8678 (2003).

[17] D. Suess, M. Kirschner, T. Schrefl, W. Scholz, R. Dittrich, H. Forster, J. Fidler, "Micromagnetic calculations of bias field and coercivity of compensated ferromagnetic/antiferromagnetic bilayers", J. Appl. Phys. 93, 8618-86120 (2003).

[18] R. Dittrich, A. Thiaville, J. Miltat, T. Schrefl, "A rigorous micromagnetic computation of configurational anisotropy energies in nanoelements", J. Appl. Phys. 93, 7891-7893 (2003).

[19] A. Thiaville, J.M. Garcia, R. Dittrich, J. Miltat, T. Schrefl, "Micromagnetic study of Bloch points nucleated vortex core reversal", Phys. Rev. B. 67, 94410-1-12 (2003) .

[20] R. Dittrich, V. Tsiantos, T. Schrefl, D. Suess, W. Scholz, H. Forster, J. Fidler, "Micromagnetic simulations of thermal effects in magnetic nanostructures," in Magnetoelectronics and Magnetic Materials--Novel Phenomena and Advanced Characterization, S. Zhang, G. Guntherodt, A. Kent, I. Schuller, T. Shinjo (eds), MRS Proceedings Volume 746 (2003) 183-188.

[21] M. Kirschner, D. Suess, T. Schrefl, J. Fidler, R.L. Stamps, J.V. Kim, "Exchange bias and training effect in polycrystalline antiferromagnetic/ferromagnetic bilayers," in Magnetoelectronics and Magnetic Materials--Novel Phenomena and Advanced Characterization, S. Zhang, G. Guntherodt, A. Kent, I. Schuller, T. Shinjo (eds), MRS Proceedings Volume 746 (2003) 25-30.

[22] H. Forster, N. Bertram, X. Wang, R. Dittrich, T. Schrefl, "Energy barrier and effective thermal reversal volume in columnar grains," J. Magn. Magn. Mater, in press.

[23] H. Forster, T. Schrefl, R. Dittrich, W. Scholz, J. Fidler, "Fast boundary methods for magnetostatic interactions in micromagnetics", IEEE Trans. Magn. (2003), in press.

[24] M. Stehno, T. Schrefl, R. Dittrich, H. Forster, J. Fidler, Y. Uesaka, "Numerical switching experiments for perpendicular media," IEEE Trans. Magn. (2003), in press.

[25] V. Tsiantos, T. Schrefl, W. Scholz, H. Forster, D. Suess, R. Dittrich, J. Fidler, "Thermal magnetization rotation of small nanoparticles," IEEE Trans. Magn. (2003), in press.

[26] W. Scholz, T. Schrefl, J. Fidler, T. Matthias, D. Suess, "Micromagnetic simulation of pinning and depinning processes in permanent magnets," IEEE Trans. Magn. (2003), in press.

[27] R. Dittrich, T. Schrefl, H. Forster, D. Suess, W. Scholz, "Energy barriers in magnetic random access memories," IEEE Trans. Magn. (2003), in press.

[28] M. Kirschner, D. Suess, T. Schrefl, J. Fidler, J. N. Chapman, "Micromagnetic calculation of bias field and coercivity of exchange biased IrMn/NiFe bilayers, IEEE Trans. Magn. (2003), in press.

[29] H. Forster, T. Schrefl, R. Dittrich, W. Scholz, J. Fidler, "Anisotropic magnetorisistivity effect in a Co nanowire," Physica B, in press.

[30] J. Fidler, T. Schrefl, W. Scholz, D. Suess, V. Tsiantos, H. Forster, R. Dittrich, "Magnetostatic spinwaves in nanoelements", Physica B, in press.

[31] T. Schrefl, H. Forster, M. E. Schabes, B. Lengsfield, "Finite Element Simulation of Head / Media Interactions in Perpendicular Recording," Proceedings of the 14th Compumag Conference on the Computation of Electromagnetic Fields, Saratoga Springs, NY, July 2003, volume I, pp. 4-5.

[32] R. Dittrich, T. Schrefl, A. Thiaville, J. Miltat, V. Tsiantos, J. Fidler, "Comparison of Langevin dynamics and direct energy barrier computation", J. Magn. Magn. Mater. (2003), in press.

[33] W. Scholz, J. Fidler, T. Schrefl, D. Suess, H. Forster, R. Dittrich, V. Tsiantos, "Numerical Micromagnetic Simulation of Fe-Pt Nanoparticles with Multiple Easy Axes", J. Magn. Magn. Mater. (2003), in press.

[34] W. Scholz, D. Suess, R. Dittrich, T. Schrefl, V. Tsiantos, H. Forster, J. Fidler, "Implementation of a high performance parallel finite element micromagnetics package", J. Magn. Magn. Mater. (2003), in press.

[35] W. Scholz, J. Fidler, T. Schrefl, D. Suess, R. Dittrich, H. Forster, V. Tsiantos, "Scalable Parallel Micromagnetic Solvers for Magnetic Nanostructures", Comp. Mat. Sci (2003), in press.

[36] T. Schrefl, R. Dittrich, V. Tsiantos, W. Scholz, H. Forster, D. Suess and J. Fidler "Simulation of thermally induced magnetization processes for sensor and storage applications", Computer Methods in Applied Mechanics and Engineering, in press

[37] T. Schrefl, R. Dittrich, V. Tsiantos, D. Suess, H. Forster, W. Scholz, J. Fidler, "Switching fields and energy barriers of soft magnetic nano-elements," JMMM in press

[38] J. Fidler, T. Schrefl, W. Scholz, D. Suess, H. Forster, R. Dittrich, Micromagnetic modeling and magnetization processes, International Conference on Magnetism, JMMM in press

[39] R. Dittrich, T. Schrefl, H. Forster, V. Tsiantos, D. Suess, J. Fidler, Comparison of Langevin dynamics and direct energy barrier computation, JMMM in press