MA 32: Micromagnetism and computational magnetics

Time: Wednesday 15:00–16:45 Location: H 0112

MA 32.1 Wed 15:00 H 0112

Micromagnetic studies of exchange-biased spherical half shells — •Rico Huhnstock, Meike Reginka, Andreea Tomiţa, Dennis Holzinger, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Magnetic Janus particles show a highly promising dynamical behavior in microfluidic experiments especially if the particles consist of a spherical metallic half shell that exhibits a spatially fixed and directed magnetization due to the exchange bias effect. Understanding the magnetic properties of these half shells becomes a difficult task since the underlying curved geometry heavily influences the configuration of the magnetization distribution in the considered system. Thus, in this work the Python based micromagnetic simulation package Nmag [1] was used in order to compute magnetic equilibrium states of the modeled half shells. The results of parameter studies concerning the influence of different energy and size related contributions will be presented and discussed.

[1] Fischbacher, T., Franchin, M., Bordignon, G., Fangohr, H. (2007), A Systematic Approach to Multiphysics Extensions of Finite-Element-Based Micromagnetic Simulations: Nmag. IEEE Transactions on Magnetics, 43: 2896-2898.

MA 32.2 Wed 15:15 H 0112

The role of longitudinal spin dynamics during magnetisation switching in FePt thin films — •Matthew Ellis, Mario Galante, and Stefano Sanvito — School of Physics and CRANN, Trinity College, Dublin 2, Ireland

$L1_0$ ordered FePt is a magnetic material of great interest for magnetic recording applications due to its large uniaxial anisotropy. Previous ab-initio studies observed that the magnetic moments localised on the Pt atoms arise due to the local exchange field provided by the neighbouring Fe atoms. As such an effective spin Hamiltonian can be derived without the Pt degrees of freedom. However, the applicability of this model in out-of-equilibrium cases where the longitudinal dynamics are important is not clear.

Here, we employ an atomistic spin model that incorporates the longitudinal fluctuations of the spin magnetic moment following the Landau Hamiltonian given by Ma and Dudarev [1]. Using this, we construct a model for $L1_0$ FePt, where the Pt magnetic moment depends linearly on its local exchange field. At temperatures close to the Curie point, we observe that despite a low net magnetisation the local ordering of Fe atoms preserves to magnetic moment of the Pt atoms. Finally, we apply this model to switching in FePt thin films using atom-resolved ab-initio computed spin-transfer torque. Whilst the torque on the Fe atoms is dominant and promotes switching the Pt torque opposes this but the exchange interaction sustains the collinearity in the film.

[1] P.-W. Ma and S. L. Dudarev, Phys. Rev. B 86, 54416 (2012).

MA 32.3 Wed 15:30 H 0112

Spirit: a modern framework for spin dynamics — •Gideon P Müller[1,2], Nikolai Kiselev[1], Stefan Blügel[1], and Hannes Jónsson[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Science Institute of the University of Iceland, VR-III, 107 Reykjavík, Iceland

Spin simulations using atomistic models have great importance in theoretical work on solid state magnetism, as they provide valuable predictions and help interpret experimental data. We present our framework of modern cross-platform computational tools for atomistic spin dynamics providing direct user interaction and powerful real-time visualisations. It is designed to increase scientific productivity by simplifying workflows and to minimize time spent on problem-specific programming. Through live visual feedback and parameter control, the time needed to study and understand properties and dynamics of a system is significantly reduced. Thanks to simplified programming interfaces (C/C++ or Python), time- consuming or repetitive tasks can be executed e.g. on a cluster, as all steps taken in the graphical user interface can be easily reproduced.

The framework is the ideal tool for the simulation of localized magnetic objects, such as magnetic skyrmions, chiral bobbers and complex domain walls. Its capabilities include Landau-Lifshitz-Gilbert dynamics simulations and direct energy minimization, as well as the calculation of minimum energy paths and energy barriers for transitions between states, using the geodesic nudged elastic band method.

MA 32.4 Wed 15:45 H 0112

Experiment, mean field theory and Monte Carlo simulations of the magnetocaloric effect in Pr0.65Sr0.35MnO3 perovskite — •rachid masrour — Cady Ayyed University, National School of Applied Sciences, Safi, Morocco.

Magnetic properties and magnetocaloric effect of the Pr0.65Sr0.35MnO3 perovskite are studied by means experiment, mean field theory and Monte Carlo simulations. The temperature dependence of the magnetic entropy change and of the adiabatic temperature is also obtained. We have used the experiment results, mean field theory and MCSs. The Curie temperature of Pr0.65Sr0.35MnO3 perovskite has been deduced The field dependence of relative cooling power of Pr0.65Sr0.35MnO3 perovskite has been given.

MA 32.5 Wed 16:00 H 0112

ab-initio phase stabilities of Ce-based hard magnetic materials — •halil ibrahim sözen, fritz körmann, tilmann hickle, and jörg neugebauer — Max-Planck-Institut für Eisenforschung, D-40237 Düsseldorf, Germany

Due to the developments in electrical transportation and renewable energies, hard magnetic materials composed of rare earths (RE) and transition metals (TM) have gained increasing importance in the last decades. Recently, there are attempts to develop alternative hard magnetic materials, RE-TM-X (X=Ti, W, Mo, Si, Al), that lift the dependence on a small number of RE elements. In order to support the efforts to find alternative materials concepts for hard magnetic applications, we performed ab initio calculations of finite temperature phase stabilities of Ce-based alloys. The Helmholtz free energy F(T,V) is calculated for all relevant competing phases using a sophisticated set of methods capturing vibrational, electronic, magnetic and configurational entropy contributions. The study includes unary Ce, binaries of Ce-Fe and Fe-Ti phases, and ternary Ce-Fe-Ti phases, for which the performance of our approach for rare-earth metals is tested. Theoretical results are compared with experimental findings. We observe that the presence of the CeFe2 phase retards any formation of promising hard magnetic Ce-Fe-Ti alloys. The study has therefore been extended to the impact of quaternary alloying elements such as Cu, La and Ga, in order to provide strategies to solve this challenge.

MA 32.6 Wed 16:15 H 0112

Macrospin rotation mechanism in discrete and continuum systems. Analytic approach. — •Grzegorz Kwiatkowski — Immanuel Kant Baltic Federal University, Kaliningrad, Russia

Macrospin rotation escape rate is calculated analyticaly for both discrete N-spin and continuous systems with arbitrary potential in harmonic approximation. Method for continuous systems is based on path integral approach to semiclassical quantisation. Influence of material and geometric parameters is discussed and well known limits for macrospin rotation mechanism are explicitly derived.

MA 32.7 Wed 16:30 H 0112

Demagnetazing tensor for two arbitrary oriented uniformly magnetized blocks — •Mikhail Vereshchagin[1], Pavel Bessarab[2], Valerian Yurov[1], and Grzegorz Kwiatkowski[1] — [1]Center for Functionalized Magnetic Materials (FunMagMa), Immanuel Kant Baltic Federal University, 236041 Kaliningrad, Russian Federation. — [2]Department Faculty of Physical Sciences, University of Iceland, Sæmundargötu 2, 101 Reykjavik, Iceland

A classical analytical formula for demagnetization tensor of two uniformly magnetized parallel to each other blocks (Newell et al.(1993)Newell, Williams, and Dunlop) has been generalized for the case when the bodies are oriented arbitrary with respect to each other. Account of arbitrary orientation of the blocks makes computations much more complex and tedious, nevertheless the final formula can be expressed as a sum of several repeated expressions with small differences the similar manner as it is done for parallel blocks' case. The result can be applied for spin ice systems.