MA 4 Mikromagnetismus / Computational Magnetism

Zeit: Freitag 12:00–12:45 Raum: TU H1028

MA 4.1 Fr 12:00 TU H1028

Exact parametrization of the adiabatic magnetic energy hypersurface — •Ralf Drautz[1,2] and Manfred Fähnle[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Department of Materials, University of Oxford, OX1 3PH, UK

The complexity of magnetic interactions in nanostructured magnetic systems makes it necessary to establish a parameter-free multi-scale framework for modelling. First-principles-based dynamics and statistical mechanics for magnetic systems thereby require an accurate and sufficiently general but at the same time computationally efficient representation of the adiabatic magnetic energy of many interacting atoms. We exactly parameterize the adiabatic magnetic energy of generalized interacting spins for the important special case of zero spin-orbit coupling and no applied external field. The expansion classifies the classical Heisenberg model as a first order approximation to the energy, extensions of the Heisenberg model in literature are shown to be of second order. We relate the symmetry-based energy expansion presented in this talk to the more general spin-cluster expansion that we published recently [1].
[1] R. Drautz and M. Fähnle, Phys. Rev. B **69**, 104404 (2004)

MA 4.2 Fr 12:15 TU H1028

Ferromagnetic hollow nanoparticles — •D. Goll[1], A.E. Berkowitz[2], and H.N. Bertram[2] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Center for Magnetic Recording Research, La Jolla, USA

Single-domain nanoparticles are an important prerequisite for ultra-high density magnetic recording. Recently, ferromagnetic nanoparticles with a nonmagnetic core have been successfully produced by spark erosion and colloid chemistry methods. We have analytically calculated and compared the total magnetic energies of zero-field magnetization states of such particles to find out the conditions for single-domain behavior. Therefore, the size of the particles and the thickness of the spheroidal shell have been systematically varied for different hard and soft magnetic materials. From the micromagnetic calculations the corresponding phase diagrams of the lowest-energy configurations have been derived. The phase diagrams identify two phases which are for hard magnetic materials as $Nd_2Fe_{14}B$ or FePt the single-domain state and the two-domain state. For soft and middle-hard magnetic materials as permalloy, Fe or Co the single-domain state and the curling-vortex state occurr. It turns out, that in the case of hard magnetic materials the critical diameter for which the single-domain state becomes energetically unfavorable can become more than doubled for ultrathin spheroidal shells compared to the corresponding bulk sphere. The magnetization reversal process takes place inhomogeneously starting at the magnetic poles of the inner surface. *This project was sponsored by DAAD, Bonn.*

MA 4.3 Fr 12:30 TU H1028

Micromagnetism and the microstructure of cell boundaries in nanostructured Sm_2Co_{17} based magnets — •H. Kronmüller and D. Goll — Max-Planck-Institut für Metallforschung, Stuttgart, Germany

High-quality permanent magnets on the basis of rare earth intermetallic compounds achieve large coercive fields either by large nucleation fields or by strong pinning forces of domain walls (dws). Sm_2Co_{17} based magnets are characterized by pinning of dws at the cell walls of 1:5 structure within the pyramidal nanostructure. For a micromagnetic calculation of the interaction force between a dw and an extended phase boundary we consider a space dependent magnetocrystalline anisotropy constant, $K_1(r)$, and an exchange constant, $A(r)$, which vary over a distance, d, from the values $K_1^{2:17}$, $A^{2:17}$ of the 2:17 matrix phase to a value $K_1^{1:5}$, $A^{1:5}$ of the 1:5 cell wall phase. Using the $K_1(r)$ profiles as determined by EDX measurements the coercive field due to dw pinning is determined self consistently by numerical methods as a function of the profile parameters taking into account the modification of the spin structure of the dw by the space dependent material parameters.