Theoretical study of the magnetic ordering of thin films and nanostructures

Nagyfalusi Balázs

The investigation of magnetic thin films and nanostructures has been a focus of interest in solid-state physics for a long time. To understand numerous phenomena, it is essential to know the electronic and magnetic structure of the system, and today's computing capacity already permits to determine these theoretically, even starting from first principles. In my doctoral work, I investigated the properties of various magnetic systems: thin films and spin chains, whose behavior plays an important role in the development of magnetic data storage devices.

In one part of my work, I investigated the temperature dependence of the magnetic anisotropy energy (MAE) of thin films using Monte Carlo simulations. MAE is the result of several effects that often favour opposite magnetic ordering. These contributions respond in different ways to changes in the thickness and temperature of the system, which can ultimately lead to a change in the sign of the MAE and thus to a spin reorientation transformation (SRT). To map the free energy, I used a procedure based on the well-tempered metadynamics method. During the work, first I validated the operation of the method on model systems, and then examined real, experimentally motivated physical systems. The couplings and magnetic anisotropy parameters necessary for the simulation of the latter have been calculated from first-principles. In the model mono- and bilayers, I successfully reproduced the temperature dependence expected from the literature and examined the SRT in details as a function of anisotropy. My research confirmed the SRT between the double and triple Fe layers placed on the Au(001) surface. My investigations on the Fe double layer on the W(110) surface revealed that the finite temperature effective anisotropy contribution caused by the Dzyaloshinsky-Moriya interaction plays an important role in the SRT that takes place during the temperature increase.

The important task of the doctoral work was to further develop the metadynamics code, so that I could investigate topological structures, i.e. skyrmions and antiskyrmions, based on the topological charge as a collective variable. The simulations were performed in $(Pt_{0.95}Ir_{0.05})$/Fe/Pd(111) and Pd/Fe/Ir(111) bilayers. The topological charge that characterizes the magnetic configuration itself not enough to identify different skyrmions. However, by carefully examining the configuration, the various objects can be identified. This allowed me to identify, depending on the temperature and the external magnetic field, a range where the skyrmions behave as particles on the lattice, and thus I was able to calculate their chemical potential. Finite temperature chemical potential curves showed that for the investigated $(Pt_{0.95}Ir_{0.05})$/Fe/Pd(111) bilayer both skyrmion and antiskyrmion creation is energetically unfavourable, but for Pd/Fe/Ir(111) in a given magnetic field range, where the ground state is field polarized I found negative chemical potential for skyrmions, showing that their formation is a favourable process, i.ė. with the given $B - T$ parameters their creation from the field polarized background is a favourable process.

Another main direction of the research was the investigation of magnetic atomic Fe chains placed on non-magnetic supports by means of *ab initio* optimization. The significance of the investigation of the chains placed on the Re(0001), Rh(111) and Nb(110) surfaces was that the ground state magnetic ordering can be determined directly from the electronic structure without the assumption of an underlying spin model. I successfully reproduced the spin spiral structure in the Fe chains placed on the Re(0001) and Nb(110) surfaces, in good agreement with the experimentally measured wavelength. My investigations extended to the investigation of the effect of the $\ell_{\max}$ cutoff in the angular momentum space used in the electronic structure calculation, and to the comparison of the resulting magnetic configurations with the results based on classical quadratic spin model calculations.