Magnetic properties of Fe-based ultrathin films – first principles calculations

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Abstract

One of the key aspects of technological development is the increasing miniaturization of electronic circuits and their components. In the case of data storage devices, the main challenge in this miniaturization is the magnetic recording trilemma. It describes the competition between the density of stored information, the thermal stability of the memory cell and the possibility of recording. Several different approaches to this problem are proposed. One way to reduce the magnetic field required for recording may be to use the tilt of the magnetic easy axis of the material relative to the magnetic field used for recording. This approach – applied to $L1_0$ FePt and $L1_0$ FeNi layers – is one of the main issues discussed in the presented doctoral dissertation.

In this dissertation, I investigated the properties of the above-mentioned ultrathin magnetic films with $L1_0$ structure, as well as another Fe-based material: $Fe_{0.7}Co_{0.3}$. The research focused on determining the effect of film's modification on their basic magnetic properties: the direction of the easy magnetization axis, the magnetocrystalline anisotropy energy, and the spin and orbital magnetic moments. The considered modifications were the film's thickness change in the $L1_0$ structures and octahedral interstitial doping with B, C, and N atoms in the $Fe_{0.7}Co_{0.3}$ alloy. I performed the electronic structure calculations. I used density functional theory – mainly in the implementation of the full-potential local-orbital (FPLO) computational code and using the exchange-correlation potential in the form proposed by Perdew, Burke, and Ernzerhof.

The basic differences between layers of different thickness and dopant type were observed in the values of magnetocrystalline anisotropy energy and orbital magnetic moments. The orientation of the film's surface also affects the direction of the easy magnetization axis. In the (010) $L1_0$ FePt and $L1_0$ FeNi systems, I observed a preference for the tetragonal [001] direction of the $L1_0$ phase, located in the plane of the ultrathin layer. The use of the (111) surface allowed obtaining a tilted magnetization direction, and changing the thickness of the (111) surface layer allowed for setting a specific tilt value. The observed properties may prove useful in designing computer memories using the tilt of the magnetization axis with respect to the magnetic switching field.

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