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Temperature dependent magneto-crystalline anisotropy of thin films: A relativistic disordered local moment approach

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Abstract

In order to study the temperature dependence of the magnetic anisotropy energy of thin ferromagnetic films from first principles we combined the relativistic extension of the disordered local moment approach with the screened Korringa–Kohn–Rostoker technique for layered systems. We first apply the new method for a Fe monolayer on a Cu(1 1 1) surface and a Co monolayer on a Cu(1 0 0) surface referring to an out-of-plane and an in-plane magnetization, respectively. Interestingly, the magnetic anisotropy energy follows a remarkably different temperature dependence for these two cases. This different behavior is also demonstrated in terms of the relationship between the magnetic anisotropy energy and the average magnetization.

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Keywords: Magneto-crystalline anisotropy; Ultrathin films; Finite temperature magnetism

1. Introduction

The recent development of advanced fabricating techniques of atomic sized nanostructures [1] promises the design of ultrahigh density magnetic data storage media built up from nanoparticles with a diameter less than 20 nm [2]. The stability of the magnetic information is clearly governed by the magneto-crystalline anisotropy (MCA) energy, K, of the particles stemming from relativistic effects, namely from spin–orbit coupling. While a considerable amount of ab initio theoretical work has been published over the past two decades to calculate the MCA energy and to explain its trends in different bulk ferromagnets, thin magnetic films and finite nanostructures at zero temperature, there appeared only very recently the first attempts o describe its temperature dependence from first principles [3–5]. These studies successfully explained, e.g., the $K(T) \propto M(T)^{\gamma}$ ($\gamma \approx 2.1$) dependence of the MCA observed experimentally for the ordered bulk FePt system [6].

In the present work we develop the relativistic version of the disordered local moment (RDLM) approach used in Refs. [3,4] to layered systems such as surfaces and thin films by combining this method with the screened Korringa–Kohn–Rostoker method (SKKR) [7]. The proposed method is first applied to the temperature dependence of the MCA energy of $Fe_1/Cu(1\,1\,1)$ and the $Co_1/Cu(1\,0\,0)$, the obtained results are compared to the prediction of a single-ion model by Callen and Callen [8].

2. Theory

The theory of disordered local moments in conjunction with the coherent potential approximation and the Korringa–Kohn–Rostoker method has been laid more than 20 years ago by Györffy et al. [9] and has recently been generalized to a relativistic level by Staunton et al. [3,4]. Here we briefly outline the formalism as applied to systems with two-dimensional translational invariance. By using a mean field approach, below the Curie temperature,

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T_C, of a layered ferromagnet with a direction of the magnetization, $\hat{n}$, the Weiss field in a given layer p, $h_p^{(\hat{n})}$, can be expressed as

$$h_p^{(\hat{n})} = \frac{3}{4\pi} \int (\hat{e}_{pi} \cdot \hat{n}) \langle \Omega^{(\hat{n})} \rangle_{\hat{e}_{pi}} \, \mathrm{d}\hat{e}_{pi}, \tag{1}$$

where the site i within a given layer can be chosen arbitrarily, the $\hat{e}_{pi}$ denote orientations of the local magnetic moments, and $\langle \Omega^{(\hat{n})} \rangle_{\hat{e}_{pi}}$ stands for a restricted average of the grand-canonical potential of the electron system described in terms of the local spin-density approximation (LSDA). Alternatively, by assuming an uniaxial anisotropy term for $\langle \Omega^{(\hat{n})} \rangle_{\hat{e}_{pi}}$, $K_p \cos^2 \vartheta_{pi}$, the Weiss field can safely be approximated by

$$\frac{\partial \langle \Omega^{(\hat{n})} \rangle_{\hat{e}_{pi}}}{\partial \varphi_{pi}} \approx h_p^{(\hat{n})} \hat{n} \cdot \frac{\partial \hat{e}_{pi}}{\partial \varphi_{pi}}, \tag{2}$$

where ϑ_{pi} and φ_{pi} are the spherical coordinates of $\hat{e}_{pi}$. The probability distributions,

$$P_p^{(\hat{n})}(\hat{e}_{pi}) = \frac{\beta h_p^{(\hat{n})} \exp(-\beta h_p^{(\hat{n})} \hat{n} \cdot \hat{e}_{pi})}{4\pi \sinh \beta h_p^{(\hat{n})}}, \tag{3}$$

($\beta = 1/k_B T$) are then used in a multi-component CPA to determine the effective scattering medium that replaces the fluctuating moments when evaluating thermal averages. In particular, the average magnetizations, $M_p(T)$, are given by

$$M_p(T) = \int (\hat{e}_{pi} \cdot \hat{n}) P_p^{(\hat{n})}(\hat{e}_{pi}) \, \mathrm{d}\hat{e}_{pi}. \tag{4}$$

The free energy of the system

$$F^{(\hat{n})}(T) = N \sum_p F_p^{(\hat{n})}(T), \tag{5}$$

with N being the number of sites in a plane and

$$F_p^{(\hat{n})}(T) = \int P_p^{(\hat{n})}(\hat{e}_{pi}) \langle \Omega^{(\hat{n})} \rangle_{\hat{e}_{pi}} \, \mathrm{d}\hat{e}_{pi} + \frac{1}{\beta} \int P_p^{(\hat{n})}(\hat{e}_{pi}) \ln P_p^{(\hat{n})}(\hat{e}_{pi}) \, \mathrm{d}\hat{e}_{pi} \tag{6}$$

is then used to calculate the temperature-dependent uniaxial MCA energy, $K(T)$, most conveniently in terms of the torque method [10],

$$K(T) = -\frac{\partial F^{(\hat{n})}(T)}{\partial \vartheta}\bigg|_{\vartheta = \pi/4}. \tag{7}$$

Note that by neglecting the dependence of the magnitudes of the Weiss fields, $h_p^{(\hat{n})}$, on the orientation, $\hat{n}$, only the first term in Eq. (6) contributes to the MCA energy, Eq. (7). We implemented the RDLM scheme described in this section in the relativistic SKKR program package for layered systems [7]. Further details of this implementation and the computations will be communicated elsewhere.

3. Results and discussion

We applied the above method to the monolayer systems $Fe_1/Cu(1\,1\,1)$ and $Co_1/Cu(1\,0\,0)$. First, we performed non-relativistic self-consistent calculations in the paramagnetic state where the multi-component CPA procedure can be mapped onto a 50–50% mixing of spin-up and spin-down components [9]. Corresponding calculations for the ferromagnetic state at $T = 0$ revealed that the obtained local moments, $1.66\,\mu_B$ for Co and $2.47\,\mu_B$ for Fe, change only within 15% in magnitude over the whole temperature range in the ferromagnetic phase. Therefore we neglected self-consistency effects for the RDLM calculations, i.e., we kept the effective potentials and fields fixed to those obtained for the paramagnetic state.

By changing the temperature we determined the Weiss fields, average magnetizations and the MCA energies by using Eqs. (2), (4) and (7), respectively. As can be read off from Fig. 1 the Curie temperature (at which the Weiss field drops to zero) was determined to be about 750 and 1300 K for the Fe and the Co monolayer, respectively. Note that experimentally much lower Curie temperatures were found [11,12] most likely due to the large thermal fluctuations clearly missing in a mean-field description of order–disorder phase transitions.

In Fig. 2 the calculated MCA energy is shown for both systems as a function of the temperature. In agreement with the experiments, $Co_1Cu(1\,0\,0)$ is magnetized in-plane ($K > 0$) while $Fe_1Cu(1\,1\,1)$ is magnetized out-of-plane ($K < 0$) for the whole range of the ferromagnetic phase. Interestingly, for low temperatures $K(T)$ even increases in magnitude in the case of the Fe monolayer and drops rapidly to zero above 100 K. Quite differently, $K(T)$ of the

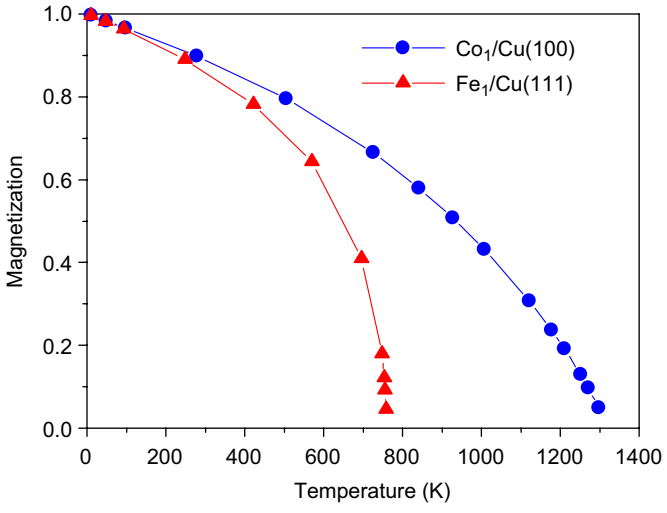

Fig. 1. Calculated temperature dependence of the magnetization for $Co_1/Cu(1\,0\,0)$ and $Fe_1/Cu(1\,1\,1)$ monolayers.

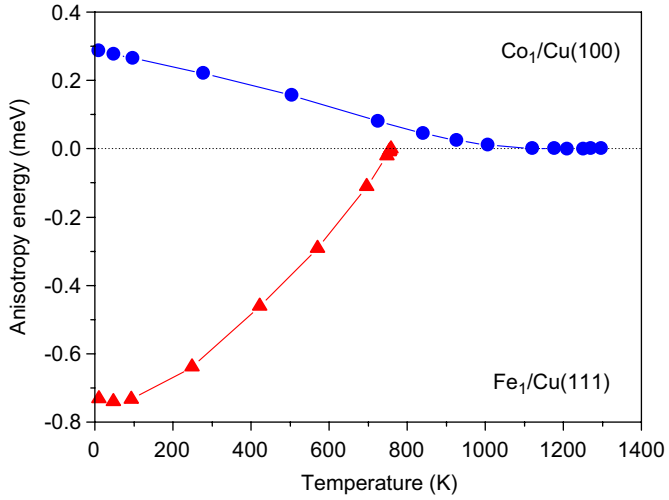

Fig. 2. Calculated temperature dependence of the uniaxial MCA energy for $Co_1/Cu(1\,0\,0)$ and $Fe_1/Cu(1\,1\,1)$ monolayers.

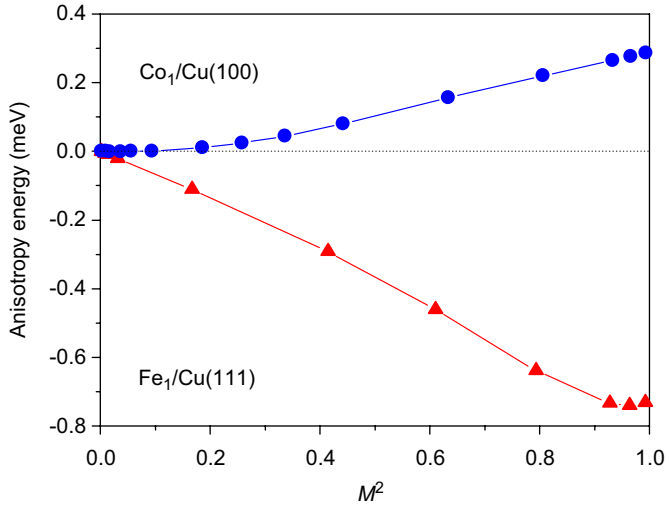

Fig. 3. Calculated uniaxial MCA energies as a function of the squared average magnetization.

Co monolayer decreases monotonously, vanishing in fact much below the Curie temperature.

In a previous study of ordered FePt we found a nearly $K(T) \propto M(T)^2$ dependence [3,4] over a large temperature range in contradiction to the single-ion model that predicts a $K(T) \propto M(T)^3$ dependence for low temperatures [8] but in agreement with experiment [6]. As seen from Fig. 3, apart for large magnetizations, i.e., near $T = 0$ the MCA energy of the Fe monolayer also behaves like $M(T)^2$. For the Co monolayer we can conclude a $K(T) \propto (M(T) - 0.2)^2$ dependence for $M(T) > 0.2$, while $K(T)$ is in fact zero for $M(T) < 0.2$. Most probably this dependence is due to the strongly itinerant character of the Co moments. In order to obtain a deeper insight into the mechanism leading to this unexpected behavior of $K(T)$ we plan to perform model calculations based on an extended Heisenberg Hamiltonian [13]. Our future studies will be related to multi-layers and to ab initio descriptions of temperature dependent reorientation transitions.

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