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First principles and metadynamics study of the spin-reorientation transition in Fe/Au(001) films

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Abstract. Based on first principles calculations, we investigate the magnetic anisotropy and spin reorientation transition (SRT) for Feₙ/Au(001) (n=2,3) films. The SRT occurs at three atomic layer of Fe in agreement with experiments due to competing on-site and two-site anisotropy. We also study the temperature dependence of the magnetic anisotropy energy (MAE) by means of metadynamics Monte Carlo simulations.

1. Introduction
Magnetic anisotropy in multilayers and nanoparticles is of high technological importance in magnetic data storage [1, 2]. In general, thickness dependent SRT is explained as the result of competing volume and surface anisotropies. The most important contribution to the volume part is the shape anisotropy related to the magnetic dipole-dipole interaction and prefers the in-plane orientation of the magnetization, whereas the surface anisotropy due to the spin-orbit coupling favours in most case a normal-to-plane configuration. In the present paper we study the magnetic anisotropy of thin Fe films on Au(001) surface from first principles. The Fe/Au(001) system has been a subject of numerous investigations concerning its structural and magnetic properties, see eg. Ref. [3] and the references therein. Fe monolayers grown on Au(001) have also been referred as a model two-dimensional ferromagnet [4]. The SRT for Fe layers on Au(001) occurs between two and three atomic layers [3]. Based on our computational results we will argue that, in this particular case, the SRT is the consequence of the competition between the on-site uniaxial anisotropy and the anisotropy of the exchange couplings.

2. Methods of calculations
The electronic structure of the overlayer was calculated in terms of the fully relativistic screened Korringea-Kohn-Rostoker (KKR) method applying the surface Green’s function technique to treat the semi-infinite Au system [5]. Since the lattice mismatch between the bcc Fe(001) and the fcc Au(001) is 0.6 % we supposed a perfect 2D translational symmetry for the whole system using the lattice constant of Au (2.87 Å). The Fe-Fe interlayer distance has been chosen to be the same as the bulk value (1.44 Å). Due to the fact that the magnetic anisotropy energy is sensitive to the lattice relaxation the electronic structure has been determined for different values of the...
Fe-Au interlayer distance changing from 1.6 Å to 1.7 Å. The range of the interlayer distance is in agreement with measurements [3] and previous ab-initio calculations [6].

We describe the magnetic system in terms of an extended Heisenberg model:

\[
H = -\frac{1}{2} \sum_{pi,qj} s_{pi}^{T} J_{pi,qj} \cdot s_{qj} + \sum_{pi} K_{p}(s_{pi} \cdot \hat{z})^{2},
\]

where \(s_{pi}\) is a unit vector parallel to the atomic magnetization at site \(i\) in layer \(p\), T denotes the transpose of the vector, \(J_{pi,qj}\) is a \(3 \times 3\) exchange tensor, \(K_{p}\) is the uniaxial anisotropy constant at layer \(p\) and \(\hat{z}\) denotes a unit vector normal to the surface of the magnetic layer. The exchange tensor and the uniaxial anisotropy constant have been determined by using the relativistic torque method [7]. The thermodynamic quantities of the system such as the magnetization, the magnetic susceptibility and the specific heat, have been calculated by means of Monte Carlo (MC) simulations. The temperature dependence of the magnetic anisotropy has been calculated by applying metadynamics [8] implemented in the Metropolis MC simulations. The free energy has been sampled along a collective variable (CV) defined as the \(z\) component of the normalized magnetization: \(\eta = M_{z}/M\), where \(M_{z} = \hat{z}M\), and \(M = |M|\) with the total magnetization \(M = \sum_{p,i} s_{pi}\).

3. Results and discussion

The calculated magnetic moments for \(\text{Fe}_{2}\text{Au}(001)\) and \(\text{Fe}_{3}\text{Au}(001)\) and the corresponding Curie temperatures are summarized in Table 1. The values changed within a few percent in the whole relaxation range. The Curie temperatures are in relatively good agreement with the experiments in Ref. [9].

Table 1. Calculated magnetic moments of the Fe layers and simulated Curie temperatures for \(\text{Fe}_{2}/\text{Au}(001)\) and \(\text{Fe}_{3}/\text{Au}(001)\). The first layer is on the top of the Au(001) surface.

|        | 1  | 2  | 3  | \(T_{C}^{\text{calc}}\) | \(T_{C}^{\text{exp}}[9]\) |
|--------|----|----|----|--------------------------|--------------------------|
| \(\text{Fe}_{2}/\text{Au}(001)\) | 2.7 \(\mu_{B}\) | 3.0 \(\mu_{B}\) | 440 K | 430 K |
| \(\text{Fe}_{3}/\text{Au}(001)\) | 3.0 \(\mu_{B}\) | 2.3 \(\mu_{B}\) | 3.0 \(\mu_{B}\) | 500 K | 550 K |

In our model the exchange interaction between two spins is described by a \(3 \times 3\) matrix. One third of the trace of this matrix is associated with the usual exchange coupling appearing in a conventional Heisenberg model, the anti-symmetric part can be identified as the Dzyaloshinsky-Moriya interaction and the symmetric part is the pseudo-dipolar interaction. Beyond the on-site anisotropy, this two-site term contributes to the MAE. Both terms are the consequence of the spin orbit coupling. The calculated total MAE and the on-site anisotropy contributions of the Fe layers are given in Table 2. For \(\text{Fe}_{2}/\text{Au}(001)\) both the on-site and two-site terms prefer normal-to-plane magnetization in the relaxation range considered. In the case of \(\text{Fe}_{3}/\text{Au}(001)\) the on-site anisotropy still prefers normal to plane configuration, but it is counterbalanced by the two-site anisotropy resulting in to an in-plane magnetization in the whole relaxation range.

Crespo et al. [10] have shown that the magnetization as a collectice variable can be used to explore the free energy of the Ising model. In the left panel of Fig. 1 the parabolic behavior of the biasing potential is depicted as a function of the CV. Obviously, \(\eta = \pm 1\) belongs to the normal-to-plane, while \(\eta = 0\) to the in-plane magnetic configuration. The curvature of the parabolas is decreasing as the temperature is increasing and the biasing potential will be flat when the system reaches the paramagnetic phase. In the right panel of Fig. 1 the MAE extracted from the curvature of the biasing potential is shown as a function of the magnetization. According to the Callen-Callen’s law [11], at low temperature the MAE curve behaves as \((M/M_{0})^{3}\). At
Table 2. Calculated total MAE and sum of the layer-dependent on-site anisotropy constants for Fe$_2$/Au(001) and Fe$_3$/Au(001). All energies are given in meV.

|                | Fe$_2$/Au(001) | Fe$_3$/Au(001) |
|----------------|----------------|----------------|
| $d_{\text{Fe-Au}}$ | $E_z - E_x$   | $K_1 + K_2$  |
| 1.58 Å         | -0.669        | -0.263        |
| 1.61 Å         | -0.649        | -0.223        |
| 1.64 Å         | -0.605        | -0.184        |
| 1.67 Å         | -0.565        | -0.150        |

higher temperature it is close to ($M/M_0$)$^2$ due to the two-site anisotropy present in the model, similar to the case of bulk FePt [12].

Figure 1. Biasing potential at different temperatures in the metadynamics simulations of Fe$_2$/Au(001) with the interlayer distance, $d_{\text{Fe-Au}} = 1.58$ Å (left panel). The normalized MAE as a function of the normalized magnetization is shown in the right panel on a log-log scale. Different symbols refer to different sizes of the 2D lattice used in the simulations.

4. Conclusions
In the present paper we used metadynamics to study the temperature dependence of the magnetic anisotropy for Fe$_2$/Au(001) system. From ab-initio calculation we concluded that the thickness driven SRT is the consequence of the competing on-site anisotropy and the anisotropy of the exchange interactions due to the spin-orbit coupling.

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