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Magnetic Properties of Fe/Ni Thin Films: First Principles Study

Dongyoo Kim and Jisang Hong*

Department of Physics, Pukyong National University, Busan 608-737, Korea

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This study examined the magnetic properties of ultrathin Fe/Ni films on a Cu(001) surface using the full potential linearized augmented plane wave (FLAPW) method. The magnetic moment of Fe/Ni films was found to be insensitive to strain. Nevertheless, strain had a significant influence on the magnetization direction. For example, Fe/Ni films showed a thickness-dependent spin reorientation transition in the presence of strain, while the Fe/Ni films grown pseudomorphically on Cu(001) always showed perpendicular magnetization. In addition, the theoretically calculated X-ray magnetic circular dichroism (XMCD) was examined.

Keywords : spin reorientation transition, FLAPW, Fe/Ni, XMCD

1. Introduction

The magnetic properties of thin film magnetism have attracted considerable research effort because this peculiar physical phenomenon is not found in bulk or macroscopic materials and has potential device applications. One of the most fundamental and important issues in a study of thin film magnetism is magnetic anisotropy, which determines the magnetization direction of a material. In this respect, the spin reorientation transition (SRT) [1] and perpendicular magnetic anisotropy are of particular interest. The perpendicular magnetic anisotropy is indeed closely associated with high density spin information storage. To this end, two conditions should be satisfied a large perpendicular magnetic anisotropy to overcome spin fluctuations arising from thermal energy and high saturation magnetization for a writing field.

Recently the thickness dependent SRT in Fe/Ni films were reported [2, 3]. However, these experimental studies showed different thickness-dependent spin reorientation transitions. For example, R. Thamankar *et al.* reported that Fe/Ni films display SRT from perpendicular to the film surface to in-plane magnetization at 9 monolayers (ML) of Ni when the Fe coverage is approximately 1.5 ML [2]. On the other hand, Abe et al. reported that the Fe/Ni film still has a perpendicular magnetization up to 3 ML Fe coverage [3]. Such disparities can be observed in other film thicknesses. Since the magnetic anisotropy of nano scale materials is strongly dependent on changes in the underlying electronic structure, the disagreement between the two experimental studies may be due to the different interface structure, sample conditions or strain. The thickness dependent magnetic anisotropy of Fe/Ni films has not studied extensively. Therefore, this study examined the thickness dependent magnetic properties of ultra thin Fe/Ni films.

2. Numerical Method

The thin film version of the full potential linearized augmented plane (FLAPW) method was employed in these calculations. Therefore, there was no shape approximation assumed in the charge, potential, and wavefunction expansions [4-6]. The core electrons were treated fully relativistically, and the spin orbit interaction between the valence electrons was examined with second variations [7]. The generalized gradient approximation was used to describe the exchange correlation [8]. Spherical harmonics with $\lambda_{max} = 8$ were used to expand the charge, potential, and wavefunctions in the muffin tin region. Energy cutoffs of 225 Ry and 13.7 Ry were implemented for the plane wave star function and basis expansions in the interstitial region, respectively. Four hundred k-mesh points were used during the course of the entire calculations discussed in this report. In order to explore the main issue, the Fe coverage was changed from 0.5 ML to 2.5 ML on a Ni underlayer, which has a 5 ML and 7 ML

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*Corresponding author: Tel: +82-51-629-5573
Fax: +82-51-629-5549, e-mail: hongj@pknu.ac.kr

thickness. Two types of Fe/Ni films were considered; (i) pseudomorphically grown films on Cu(001), and (ii) Fe/Ni with a Ni(001) lattice parameter to consider strain.

3. Results and Discussions

The optimized atomic structures of Fe/Ni films were first examined because the magnetic properties of materials are sensitive to changes in the underlying electronic structure. $d_{i,j}$ means the interlayer distance between two adjacent layers. The interface Ni neighboring a Fe adlayer is represented by Ni_S, and the subsurface layer is denoted as Ni_{S-1}. Tables 1 and 2 show the calculated vertical distances with 7 and 5 ML of the Ni underlayer thickness, respectively.

As shown in Table 1 and 2, the optimized atomic structure was dependent on strain. Outward relaxation was observed in the presence of 2-3% strain. Nevertheless, it was realized that strain has almost negligible influence on the magnetic moment. Intensive discussion of the magnetic moments is reported elsewhere [9].

Table 1. The vertical distances (in Å) of Fe/Ni with a 7 ML Ni underlayer.

Fe coverage	0.5 ML	1 ML	1.5 ML	2 ML	2.5 ML
pseudomorphic growth on Cu(001): 7 ML Ni					
$d_{3,2}$					1.59
$d_{2,1}$			1.6	1.85	1.79
$d_{1,S}$	1.47	1.74	1.70	1.75	1.68
$d_{S,S-1}$	1.77	1.76	1.74	1.71	1.70
with Ni(001) lattice parameter					
$d_{3,2}$					1.71
$d_{2,1}$			1.71	1.98	1.88
$d_{1,S}$	1.54	1.85	1.78	1.89	1.77
$d_{S,S-1}$	1.85	1.83	1.83	1.82	1.76

Table 2. The vertical distances (in Å) of Fe/Ni with a 5 ML Ni underlayer.

Fe coverage	0.5 ML	1 ML	1.5 ML	2 ML	2.5 ML
pseudomorphic growth on Cu(001): 7 ML Ni					
$d_{3,2}$					1.59
$d_{2,1}$			1.63	1.85	1.79
$d_{1,S}$	1.48	13.76	1.66	1.74	1.70
$d_{S,S-1}$	1.74	1.72	1.75	1.69	1.71
with Ni(001) lattice parameter					
$d_{3,2}$					1.75
$d_{2,1}$			1.72	1.92	1.89
$d_{1,S}$	1.54	1.84	1.79	1.83	1.77
$d_{S,S-1}$	1.85	1.78	1.78	1.78	1.78

The density of states(DOS) features were examined. Fig. 1 shows the DOS of a 2.5 ML Fe coverage. Fe_i denotes the i^{th} layer measured from the interface Ni layer. The dotted lines represent the DOS of Fe/Ni film grown with a Cu(001) lattice constant, and the solid lines indicate the films affected by strain. Fig. 1(a), (b), and (c) show the DOS of Fe/Ni with a 5 ML Ni underlayer thickness. Fig. 1(d), (e), and (f) show the DOS with 7 ML Ni underlayers. Broadening at the interface layer can be clearly observed compared with the DOS in the other layers, while band narrowing was found in the surface layer resulting in surface enhancement of the magnetic moment. The different band width according to the layer position is definitely due to the different hybridization effect. The majority spin DOS at the interface is almost filled below the Fermi level indicating an almost half metallic state, while the half metallic features disappear in the other layer. In addition, strain has minimal effect on the DOS character regardless of the underlayer thickness. This can account for the stable magnetic moment even in the presence of strain. Here, only the DOS results of 2.5 ML Fe coverage are presented. However, a similar conclusion has been reported in other systems.

The main aim of this study was to understand the thickness dependent magnetic anisotropy of ultrathin Fe/Ni films. To this end, the torque method was used [10]. Fig. 2 shows the calculated magnetocrystalline anisotropy energy (MCA) of Fe/Ni films for the two different systems. The open and solid symbols are the MCA of a Fe/Ni film grown with Cu(001) and Ni(001) lattice parameters, respectively. The figure presents the results from two different Ni underlayer thicknesses. The positive magnetic anisotropy energy means perpendicular magnetization, whereas the negative one denotes in-plane magnetization. Pseudomorphically grown Fe/Ni thin films always have perpendicular magnetization, even though the magnitude of magnetic anisotropy energy depends on the film thickness. However, interestingly, the Fe/Ni manifests a thickness dependent SRT due to strain. It is known that the orbital anisotropy and magnetocrystalline anisotropy cannot be correlated if the magnitude of spin orbit coupling through the spin flip interaction is comparable to that through the minority spin channel. A more generalized approach was proposed by Van der Laan [11]. However, the relationship between orbital anisotropy and magnetocrystalline anisotropy is unclear. Indeed, it was found that the spin flip interaction is sizable compared with that of spin orbit coupling through minority spin channel for all systems, as reported in other studies. Overall, the simple interpretation of thickness dependent magnetic anisotropy is not possible. Figs. 3 presents the distribution of mag-

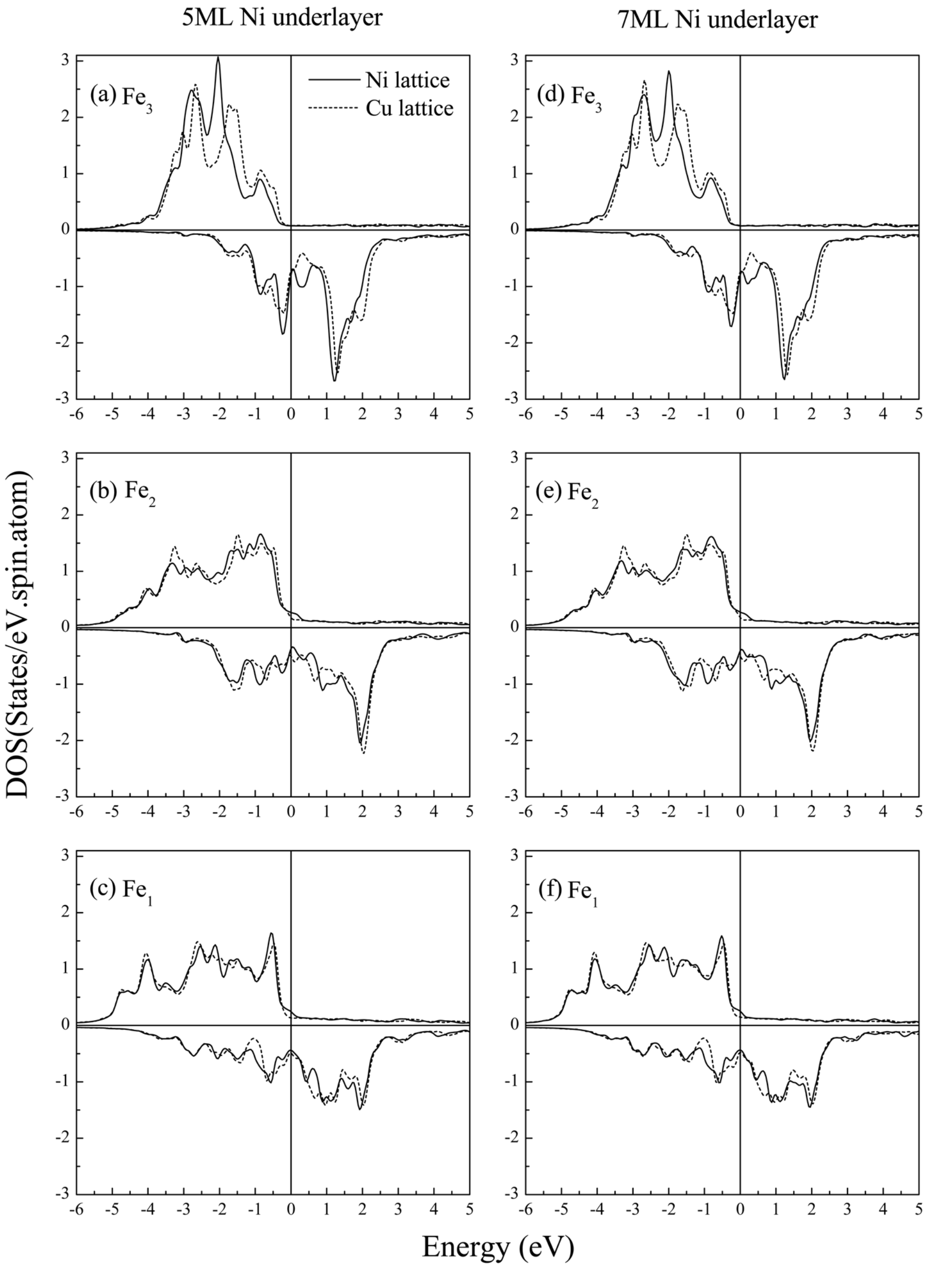

Fig. 1. DOS of Fe/Ni film for 2.5 ML Fe coverage. The solid lines denotes the DOS of Fe atoms grown with the Ni(001) lattice parameter and the dotted lines indicate the DOS with the Cu(001) lattice constant.

netic anisotropy over a two dimensional Brillouin zone (BZ) showing the distribution of the 2.5 ML Fe coverage system. The contribution to perpendicular magnetization at a given k-point is represented by the red circle, while the blue circle denotes the contribution to in-plane magnetization. The magnitude of magnetic anisotropy is proportional to the size of the circle. Fig. 3(a) and (b) show the distributions of magnetic anisotropy energy with Cu(001) lattice constants, and Fig. 3(c) and (d) show the distributions influenced by strain. It can be seen that a large portion of BZ contains perpendicular magnetization contributions, even though the distribution is different. In contrast, a rather different behavior was observed in the presence of strain. The area that previously made a contribution to perpendicular magnetization now maintains in-plane magnetization for both 5 and 7 ML Ni underlayer thicknesses. Overall, the Fe/Ni film has in-plane magnetization in the presence of strain. This is mostly observed around the corner of BZ. In addition, enhanced in-plane contributions from the BZ center can be seen. It should be

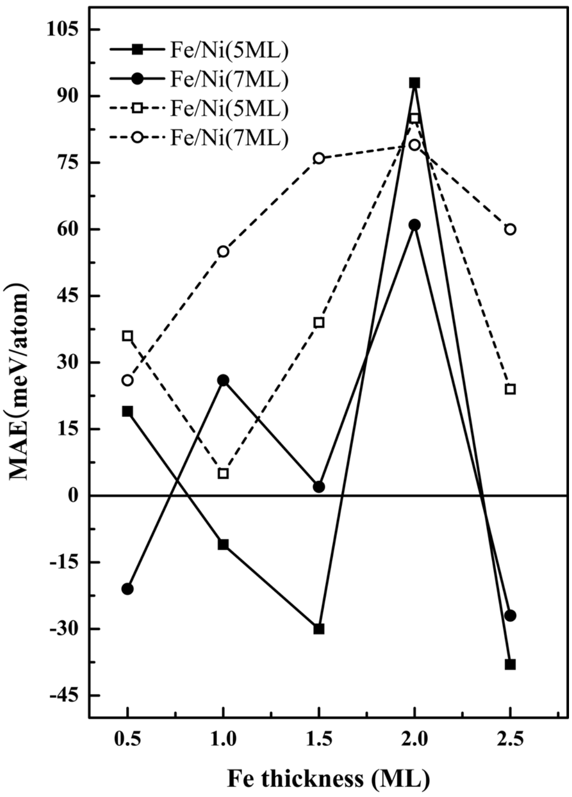

Fig. 2. Calculated magnetic anisotropy energy per atom. The positive MAE means perpendicular magnetization, whereas the negative one denotes in-plane magnetization.

noted that the magnetic moment is simply the difference in the number of electrons occupied below the Fermi level and the wavefunction character has no influence on the magnitude of the moment if the electron state is occupied. In contrast, magnetic anisotropy is substantially dependent on the wavefunction character, and the distribution shown in Fig. 3 suggests that the wavefunction feature is modified substantially according to the film thickness and strain. Here, there is no single dominant k-point contribution to magnetic anisotropy. Rather, many k-points have a similar magnitude of perpendicular magnetic anisotropy energy, which are cumulative.

X-ray magnetic circular dichroism (XMCD) was examined. Only the dipole transition was considered assuming rigid core-hole relaxation. Therefore, the precise peak position should be shifted when comparing with experimental data. The Doniach-Sunjic shape was employed [12] with a life time broadening of 0.12 eV. Fig. 4 only shows the calculated L edge XMCD of Fe atoms for 2.5 ML Fe coverage. The dotted and solid lines denote the XMCD with the Cu(001) and Ni(001) lattice parameters, respectively. As expected from the DOS results, the XMCD with the two different lattice constants show a

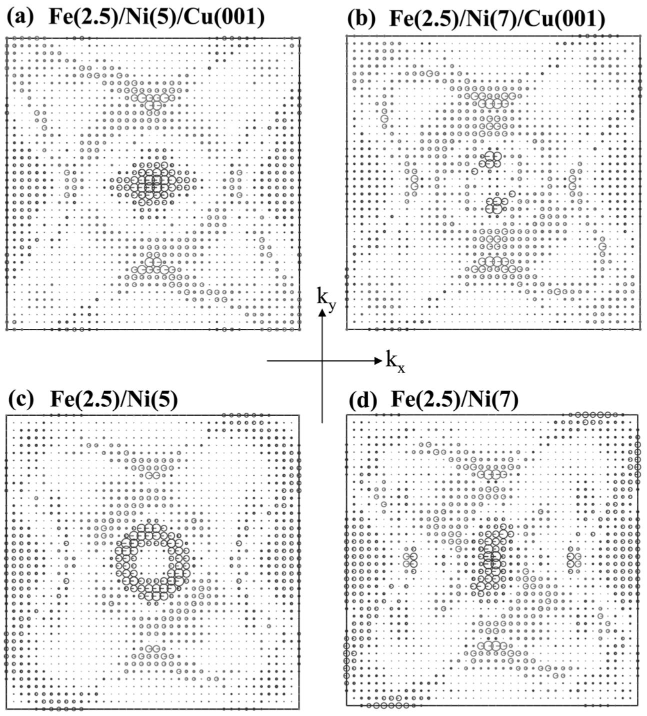
(a) Fe(2.5)/Ni(5)/Cu(001) **(b) Fe(2.5)/Ni(7)/Cu(001)** **(c) Fe(2.5)/Ni(5)** **(d) Fe(2.5)/Ni(7)**

Fig. 3. Distribution of magnetic anisotropy over the two dimensional Brillouin Zone. The contributions to perpendicular magnetization at given k-point are represented by red circles, while the blue circles show the in-plane contributions.

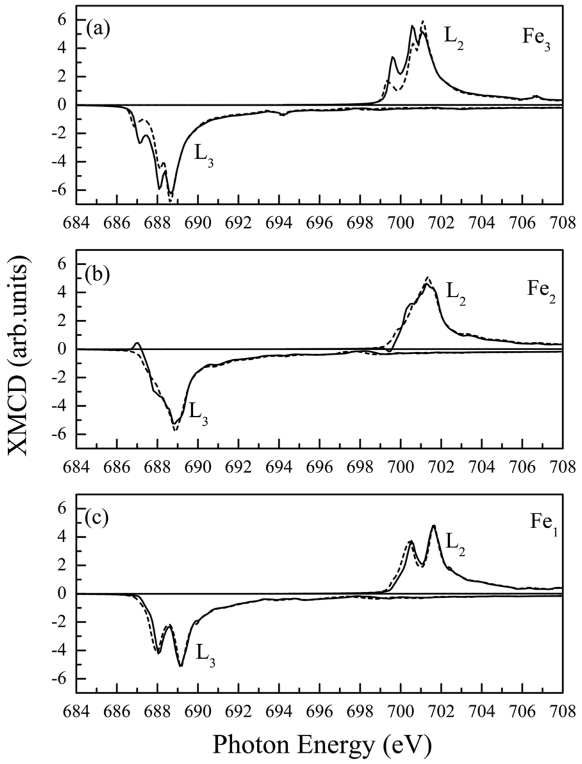

Fig. 4. Calculated L edge XMCD spectra. The dotted and solid lines are for XMCD with Cu(001) and Ni(001) lattice parameters, respectively.

similar trend. It was reported that both L_3 and L_2 edges have clear double peak structures in Fe_3 and Fe_1. The L edges of Fe_2 are rather weak but a shoulder state 1 eV below the main peak state was observed. The unoccupied DOS of Fe shown in Fig. 1 can account for the observed XMCD spectral shapes because the splitting of two peaks in DOS agrees with the energy between the two peaks in the calculated XMCD spectra. The L_3 edge extends over to the L_2 edge, which may cause an overestimation of the orbital moment. The insensitivity of the XMCD spectral shapes to strain has been reported for all systems (data not shown).

4. Summary

In conclusion, this study examined the thickness dependent magnetic anisotropy of ultrathin Fe/Ni films. It was found that strain does not influence the magnetic moments but the magnetic anisotropy is affected substantially by strain with a thickness dependent SRT being observed. The XMCD spectra showed that Fe atoms have double peak structures. In addition, the XMCD is not sensitive to strain, which is similar to that observed with the magnetic moments.

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