10-2011

Magnetoelectric Effect in L10-CoPd Thin Films

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Manchanda, Priyanka; Skomski, Ralph; Solanki, A.; Kumar, P. S. A.; and Kashyap, Arti, "Magnetoelectric Effect in L10-CoPd Thin Films" (2011). *Ralph Skomski Publications*. 72.
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Magnetoelectric Effect in $L1_0$-CoPd Thin Films

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The effect of an applied electric field on the magnetic properties of $L1_0$-ordered CoPd thin films is investigated by first-principle calculations. Both the magnetic moment and the magnetocrystalline anisotropy of the surface atoms are changed by the electric field, but the net effect depends on the surface termination. The magnetocrystalline anisotropy switches from in-plane to perpendicular in the presence of external electric field. Typical magnetic-moment changes are 0.1 μ_B per eV/Å. The main mechanism is the shift of the Fermi level, but the anisotropy change also reflects a crystal-field change due to incomplete screening.

***Index Terms*—Anisotropy, magnetoelectric material, magnetic moment, thin films.**

I. INTRODUCTION

IN the last few years, the magnetoelectric effect has sparked intense research, partially motivated by potential applications in spintronics and high-density magnetic recording [1]. The effect consists in the creation of a magnetization change due to an electric field [2] and is related to electrically controlled exchange bias [3] and magnetocrystalline anisotropy [4]. There are two main magnetoelectric (ME) mechanisms [5], [6]. The first mechanism involves mechanical strain, that is, the external electric field changes the magnetization of the multiferroic by displacing ions from their original positions. In the second mechanism, the ferroelectric and ferromagnetic degrees of freedom couple through electronic effects [5], [11]. The electron screens the electric field over the screening length of the metal and the electron does not penetrate into the bulk of metals and the induced electric charge is confined to a depth of the order of atomic dimensions from the surface. The effect is therefore also known as the surface magnetoelectric effect.

Very recently, it has been found that an electric field modifies the coercivity of $L1_0$-ordered FePd and FePt thin films in an electrochemical environment [4]. Furthermore, the magnetization direction of the magnetic semiconductors (Ga, Mn)As in a metal–insulator–semiconductor structure can be tuned by the application of an electric field [12]. Using first-principle calculations it has been demonstrated that ferromagnetism is created at Pd thin-film surfaces through the application of an external electric field [14]. It has also been reported that an external electric field modifies the magnetization of $L1_0$-CoPd thin films [7] and changes the magnetization state of a Fe/Cu(111) thin film [8]. The effect of electric field on the magnetocrystalline anisotropy of transition-metal monolayers has also been predicted using first-principle calculations [13].

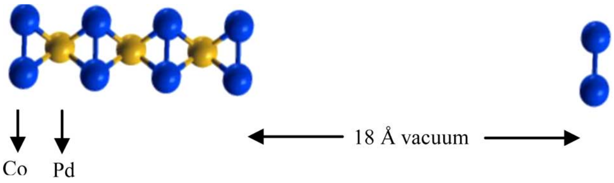

Fig. 1. Atomic structure of the considered Pd–Co thin film. Both the top and the bottom of the film are Co-terminated, which is important for the physical understanding of the ME effect.

Motivated by these experimental and theoretical findings, we use first-principle calculations to study the influence of external electric effect on the magnetic properties of $L1_0$-ordered CoPd films. Our calculations show that an electric field yield substantial change in surface magnetization and anisotropy, due to change in the surface electric density at the Fermi level.

II. NUMERICAL DETAILS

The calculations have been performed using the density-functional calculations for $L1_0$-CoPd thin-films ($a = 3.70$ Å, $c = 3.67$ Å) having a thickness of seven monolayers (MLs) with vacuum of 18 Å. The $L1_0$-CoPd films were modeled by tetragonal supercell, as shown in Fig. 1. The calculations are based on projector augmented wave (PAW) implemented in the Vienna *ab-initio* simulation package (VASP) [9]. Exchange and correlations are treated within the generalized gradient approximation (GGA), and the electronic wave functions are represented by plane waves with a cutoff energy of 500 eV. We have used a $13 \times 13 \times 1$ Monkhorst–Pack grid for k-point sampling for the self-consistent calculations. All structure relaxations are performed until the Hellmann–Feynman forces on the relaxed atoms become less than 0.01 eV/Å. The external electric field is introduced by the planar dipole layer method [10]. The spin-orbit coupling was included to determine the magnetocrystalline anisotropy (MCA) and calculated using the difference between the total energy for the magnetization perpendicular (001) and parallel (100) to the surface.

Manuscript received February 21, 2011; accepted April 13, 2011. Date of current version September 23, 2011. Corresponding author: A. Kashyap (e-mail: arti.kashyap@lnmiit.com).

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Digital Object Identifier 10.1109/TMAG.2011.2147293

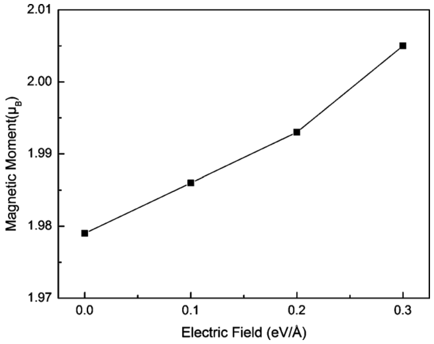

Fig. 2. Magnetic moment per Co surface atom as a function of applied electric field.

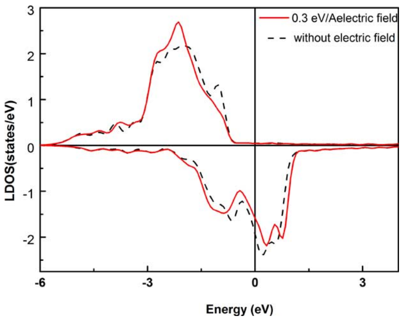

Fig. 3. Effect of the electric field on the local density of states (LDOS).

III. Results

Fig. 2 shows the calculated magnetic moment of the surface Co atoms of $L1_0$ -CoPd thin film as a function of the applied electric field. The magnetic moment of the surface atoms increases with the electric field. The electric field shifts the Fermi level E_F, thereby changing the densities of states (DOSs) of spin-up and spin-down electrons at E_F, and this change in E_F may increase or decrease the magnetization. The magnetization changes at both sides of film, decreasing and increasing at the positive and negative electrodes, respectively. The magnitude of the change is about 0.1 μ_B per Co atom and per eV/Å.

Table I shows the spin and orbital moment of surface Co atom in the presence of electric field, a calculation that requires the inclusion of spin-orbit coupling. Our results show that only surface Co atoms are affected by the field. Zhernenkov *et al.* reported the modification of the magnetization depth profile of an 18.5-nm-thick $Co_{50}Pd_{50}$ film immersed in an electrolyte using an electric field [7]. Inside the film, the external electric field is nearly completely screened. Typical local densities of states of surface Co atom in the absence of electric field and in the presence of 0.3 eV/Å electric field are shown in Fig. 3. Basically, the applied field is screened by Co $4s$ electrons and $3d$ electrons at the surface and the electric field does not penetrate into the bulk. Correspondingly, the change in magnetic moment reflects a change in the number of d electrons at the surface. We also find that at the electric field greater than 0.3 eV/Å the deformation of the atomic structure occurs.

The external electric field changes not only the magnetization but also the anisotropy. Fig. 4 shows the electric-field dependence of the effect. At zero electric field, the anisotropy -0.047 meV/atom, indicating that the magnetization energetically favors pointing in the in-plane (100) direction. When the electric field 0.3 eV/Å is introduced, we find that the spin moment is strongly enhanced as shown in Table I. As shown in Table I, the orbital moment of surface Co atom increases as the magnitude of external electric field increases.

TABLE I
CHANGES OF THE LOCAL MAGNETIC MOMENT IN SOME APPLIED ELECTRIC FIELDS

Electric field (eV/Å)	In-plane		Perpendicular	
	μ_s	μ_l	μ_s	μ_l
0.0	1.970	0.160	1.969	0.133
0.1	1.979	0.161	1.981	0.133
0.2	1.985	0.163	1.990	0.134
0.3	1.995	0.162	2.123	0.131

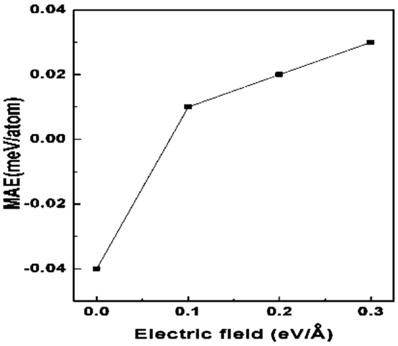

Fig. 4. Magnetic anisotropy energy as a function of applied electric field.

Fig. 4 shows the magnetic anisotropy energy as a function of external electric field. It is clear that magnetic anisotropy increases with respect to external electric field. This is due to recently proposed new type of transient magnetic anisotropy induced by external electric field [15]. At 0.3 eV/Å, the magnetic anisotropy is strongly enhanced to 0.03 meV/atom, which favors perpendicular magnetization alignment. This means that an external magnetic field can be used to control the magnetic anisotropy and that it may be possible to design thin films with the anisotropy switchable between in-plane and out-of-plane orientation.

IV. Discussion and Conclusion

The above findings indicate that the magnetization change is basically a band-filling effect, related to the strong ferromagnetism of the Co atoms in the $L1_0$ alloys such as CoPd. The electric field is effectively screened in the middle of the film, but at the surface, this screening is incomplete, leading to a redistribution of electrons. The magnetocrystalline anisotropy also exhibits a strong and generally oscillating dependence of the band filling [16], but this is not the only consideration. Magnetocrystalline anisotropy is also a crystal-field effect [6], and the shifting of electrons near the surface has a pronounced effect on the crystal field, irrespective of the whether the number of d-electrons changes. For example, an electric field may change a nearly isotropic environment (roughly the same electron density in all directions) into a uniaxial environment (charge density predominantly in one direction).

In the present system, magnetization and anisotropy change at both sides of the films. The effects have the same magnitudes at the top and bottom surfaces of the film but opposite signs. This is a consequence of the CoPd-…-PdCo structure of the film (Fig. 1). If the top and bottom surfaces were differently terminated, then the magnetization and anisotropy changes at the two surfaces would be different and yield a net magnetization and anisotropy change.

In conclusion, we have investigated how an external electric field affects the magnetism of $L1_0$-ordered CoPd thin films. Due to screening by conduction electrons, the magnetization and anisotropy changes are limited to surfaces of the film. The net effect depends on the surface terminations, because top and bottom Co layers exhibit effects of equal magnitudes but opposite signs. While the electric field affects both the magnetization and the anisotropy by changing the number of d electrons at the surface, there is also an independent crystal-field change with implications for the anisotropy.

ACKNOWLEDGMENT

The authors would like to thank Ch. Binek and D. Le Roy for stimulating discussions on some experimental aspects of the magnetoelectric effect. This work was supported by DST (India-EU collaborative project "DYNAMAG" INT/EC/ /CMS, 24/233552, and Nano Mission, SR/NM/NS-20/2008) and NRI.

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