

## First-Principles Study of Magnetic Properties of Co/Pt(111) Film in Electric Field

Sho YASUDA and Shugo SUZUKI

*Division of Materials Science, Faculty of Pure and Applied Sciences, University of Tsukuba,  
Tsukuba, Ibaraki 305-8573, Japan*

KEYWORDS: Co/Pt(111), magnetic properties, electric field, first-principles calculations

Technology of electric field (EF) control of magnetic properties is attractive for spintronic devices. In particular, it has been shown that the EF can change the magnetization and the magnetic anisotropy.<sup>1-3)</sup> According to an experimental study,<sup>2)</sup> an EF less than 0.1 V/nm causes a large change of 40% in the magnetic anisotropy energy (MAE) of the Fe/Au(001) film. Also, another experimental study<sup>3)</sup> using the Co/Pt(111) film in the EF has shown that the Curie temperature of the film is changed up to 6 K by applying an EF of about +0.2 V/nm while down to -6 K by applying an EF of about -0.2 V/nm.

A first-principles study of the MAE in the EF for the Fe/Pt(001) film was carried out;<sup>4)</sup> it has been found that the change in the MAE is in proportion to the EF with the slope rate of 0.03 meV/Fe per V/nm for Fe/Pt(001). Another first-principles study of the MAE in the EF for the Fe monolayer was carried out;<sup>5)</sup> it has been found that the MAE is affected considerably by applying the EF. On the other hand, to our knowledge, there are no first-principles studies of the Co/Pt(111) film in the EF although the Co films are as important as the Fe films.

In this study, we investigate the magnetic properties of the Co/Pt(111) film in the EF carrying out the first-principles calculations. We take account of the EF by introducing electrode far above Co/Pt(111) and changing the total number of electrons in the film. We calculate the spin moments and the numbers of electrons of the constituent atoms as well as the MAE of the film self consistently.

We employ the fully relativistic full-potential linear-combination-of-atomic-orbitals method based on the density-functional theory within the local spin density approximation.<sup>6)</sup> The exchange-correlation energy functional used in this study is the Perdew-Wang parameterization of the Ceperley-Alder results.<sup>7,8)</sup>

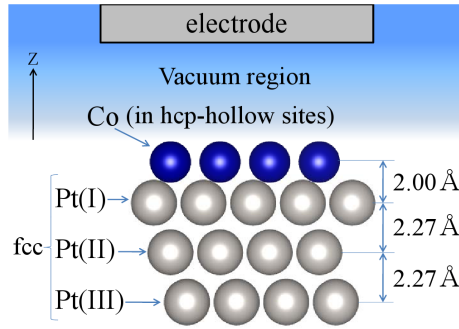
As shown in Fig.1, the Pt(111) surface is modeled by a 3-layer slab. We denote the Pt atoms in the top, middle, and bottom Pt layers by Pt(I), Pt(II), and Pt(III), respectively. We

assume hcp stacking of the Co adlayer on the Pt(111) surface because the Co adatom prefers to occupy an hcp-hollow site on the Pt(111) surface.<sup>9)</sup> We use the lattice constant of the triangular lattice, 2.78 Å, which is calculated from the lattice constant of fcc Pt, 3.92 Å. All the interlayer distances between adjacent atomic layers of Co/Pt(111) are optimized calculating the forces acting on the Co and Pt atoms in the absence of the EF. The optimized interlayer distances are shown in Fig.1.

The EF is applied as follows. We change the total number of electrons in the film; we denote this change per Co atom by  $\Delta N$ . We introduce the following external potential originated in the electrode shown in Fig.1:

$$V_{\text{EF}}(z) = -\frac{2\pi e^2 \Delta N}{A_{\text{cell}}} z. \quad (1)$$

Here,  $A_{\text{cell}}$  is the area of the unit cell of the triangular lattice. We also use the two-dimensional Ewald method.<sup>10,11)</sup> All the atomic positions are fixed at those optimized in the absence of the EF.

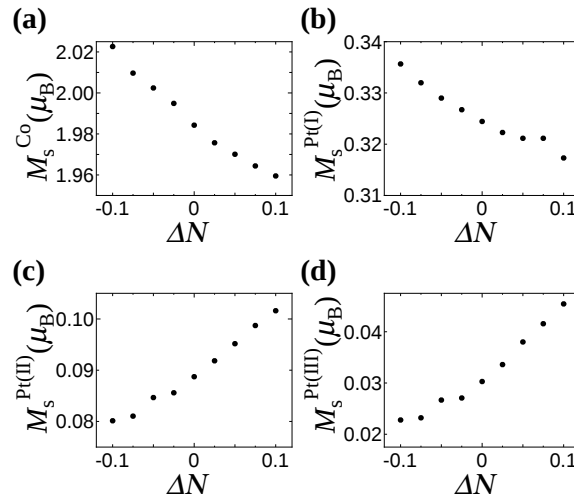


**Fig. 1.** (Color online) Schematic diagram of the computational model. The model constitutes of the Co/Pt(111) film and the electrode. The Co monolayer is on the Pt(111) substrate. The Co atoms are in the hcp-hollow sites and the Pt(111) substrate is composed of three Pt layers.

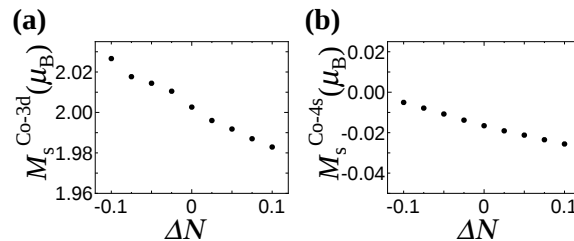
We evaluate the MAE from the difference between the total energies for the easy and hard axis magnetization directions:  $\text{MAE} = E_{\text{tot}}^{[1\bar{1}0]} - E_{\text{tot}}^{[111]}$ , where the easy and hard axes are the [111] and  $[1\bar{1}0]$  directions, respectively. The dipolar contribution to the MAE is not considered. The basis functions adopted in this study consist of the following atomic orbitals: 1s, 2s, 2p, 3s, 3p, 3d, and 4s orbitals of the neutral Co atom, 3d, 4s, and 4p orbitals of the  $\text{Co}^{2+}$  atom, 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, 5s, 5p, 5d, and 6s orbitals of the neutral Pt atom, and 5d, 6s, and 6p orbitals of the  $\text{Pt}^{2+}$  atom. The Brillouin-zone integration is carried out using the good-lattice-point method with 610  $k$  points. The convergence of the MAE with

respect to the number of  $k$  points is about 0.04 meV/Co, which occurs almost systematically with the same set of  $k$  points, irrespective of the magnitude of the EF; hence, this error does not affect the dependence of the MAE on the EF very much. To speed up the convergence, we use a modest Fermi distribution smearing of eigenstates with a small width of 30 meV.

The calculated spin moments of the Co, Pt(I), Pt(II), and Pt(III) atoms are shown in Fig.2(a), (b), (c), and (d), respectively. Also, the calculated spin moments of the Co 3d and Co 4s electrons are shown in Fig.3(a) and (b), respectively. The spin moments of the Co and Pt(I) atoms decrease with increasing  $\Delta N$ . On the contrary, the spin moments of the Pt(II) and Pt(III) atoms increase with increasing  $\Delta N$ . Also, the spin moments of the Co 3d and Co 4s electrons decrease with increasing  $\Delta N$ . The sum of the spin moments of the Co 3d and Co 4s electrons is almost equal to the spin moment of the Co atom for each  $\Delta N$ .



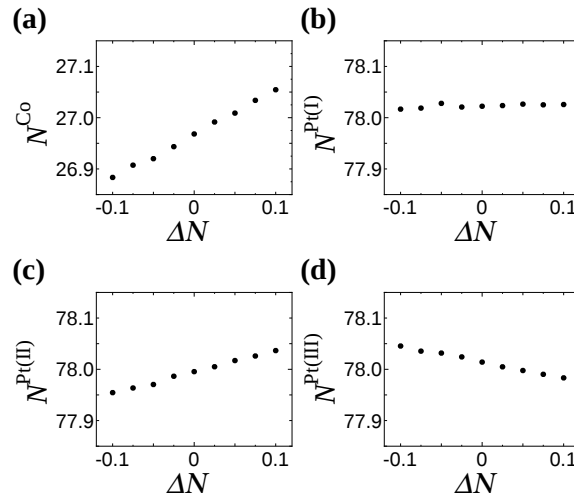
**Fig. 2.** Spin moments of (a) Co, (b) Pt(I), (c) Pt(II), and (d) Pt(III) atoms as a function of external electric field.



**Fig. 3.** Spin moments of (a) Co 3d and (b) Co 4s electrons as a function of external electric field.

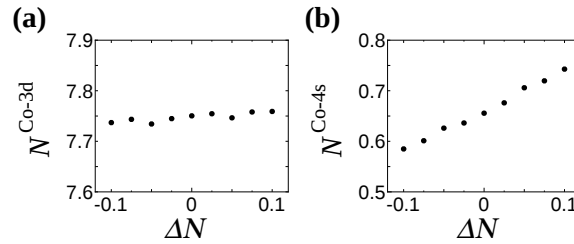
The calculated numbers of electrons of the Co, Pt(I), Pt(II), and Pt(III) atoms are shown

Fig.4(a), (b), (c), and (d), respectively. Also, the calculated numbers of electrons of the Co 3d and Co 4s electrons are shown in Fig.5(a) and (b), respectively. The number of electrons of the Co atom increases with increasing  $\Delta N$ . The number of electrons of the Pt(I) atom depends very little on  $\Delta N$ . On the other hand, the number of electrons of the Pt(II) atom increase with increasing  $\Delta N$  while the number of electrons of the Pt(III) atom decrease with increasing  $\Delta N$ . Also, the number of the Co 3d electrons is almost unchanged; this does not contradict the decrease in their spin moment,  $-0.04 \mu_B$ , which is the difference between  $\Delta N = -0.1$  and  $0.1$  shown in Fig.3(a), because one half of this decrease is due to a slight increase in the number of the Co 3d electrons shown in Fig.5(a),  $+0.02$ , and the other half is due to their redistribution. On the other hand, the number of the Co 4s electrons is changed noticeably; this change explains the change in the number of electrons of the Co atom shown in Fig.4.(a). The reason for this behavior might be that, compared with the Co 3d electrons, the Co 4s electrons play a major role in the screening of the EF.



**Fig. 4.** Numbers of electrons of (a) Co, (b) Pt(I), (c) Pt(II), and (d) Pt(III) atoms as a function of external electric field.

We now discuss the dependence of the MAE on the EF. The calculated MAE depend very little on the EF within the range of  $\Delta N$  considered in this study; the calculated MAE is  $0.76 \pm 0.03$  meV/Co. Fitting a straight line to the calculated MAE as a function of the EF, the slope rate is found to be  $-0.0004 \pm 0.0008$  meV/Co per V/nm. The experimental study of Fe/Au(001) indicates that the slope rate is about  $0.02$  meV/Fe per V/nm.<sup>2)</sup> The large change in the Curie temperature due to the EF observed in the experimental study of Co/Pt(111) also indicates a large change in the MAE.<sup>3)</sup> The theoretical study of Fe/Pt(001) has shown that



**Fig. 5.** Numbers of (a) Co 3d and (b) Co 4s electrons as a function of external electric field.

the slope rate is 0.03 meV/Fe per V/nm.<sup>4)</sup> Compared with these results, our calculated MAE show almost no dependence on the EF.

This might be originated in the difference between Fe and Co. Another possibility is that we did not take account of the structure change of Co/Pt(111) due to the application of the EF or the insulator layer on Co/Pt(111). In particular, the structure change due to the EF can alter the dependence of the MAE on the EF. We need to study the effects of the EF on the MAE, taking these points into account in the future.

**References**

- 1) M. Weisheit, S. Fähler, A. Marty, Y. Souche, C. Poinignon, and D. Givord: *Science* **315** (2007) 349.
- 2) T. Maruyama, Y. Shiota, T. Nozaki, K. Ohta, N. Toda, M. Mizuguchi, A. A. Tulapurkar, T. Shinjo, M. Shiraishi, S. Mizukami, Y. Ando, and Y. Suzuki: *Nature Nanotech.* **4** (2009) 158.
- 3) D. Chiba, S. Fukami, K. Shimamura, N. Ishiwata, K. Kobayashi, and T. Ono: *Nature Mater.* **10** (2011) 853.
- 4) M. Tsujikawa and T. Oda: *Phys. Rev. Lett.* **102** (2009) 247203.
- 5) K. Nakamura, R. Shimabukuro, Y. Fujiwara, T. Akiyama, T. Ito, and A. J. Freeman: *Phys. Rev. Lett.* **102** (2009) 187201.
- 6) S. Suzuki and K. Nakao: *J. Phys. Soc. Jpn.* **68** (1999) 1982.
- 7) J. P. Perdew and Y. Wang: *Phys. Rev. B* **45** (1992) 13244.
- 8) D. M. Ceperley and B. J. Alder: *Phys. Rev. Lett.* **45** (1980) 566.
- 9) P. Błoński and J. Hafner: *J. Phys.: Condens. Matter* **21** (2009) 426001.
- 10) D. E. Parry: *Surf. Sci.* **49** (1975) 433.
- 11) F. E. Harris: *Int. J. Quantum Chem.* **68** (1998) 385.