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Magnetoelectric effect in Fe linear chains on Pt(001)

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The effect of an electric field on the magnetic properties of Fe chains on Pt(001) is investigated by first-principle calculations. The calculated magnetic anisotropy of the chains yields a preferential magnetization perpendicular to the surface. We predict a linear change in the Fe magnetic moment as a function of the external electric field, which is due to spin-dependent screening of electrons. In the presence of electric field, we also obtain an enhancement in magnetic anisotropy as well as an orbital-moment anisotropy. The enhancement in magnetic anisotropy is due to a change in the *d*-electron occupancy of the surface atoms. © *2014 AIP Publishing LLC*.
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I. INTRODUCTION

Nanostructured magnetic materials play an important role in technology due to their fascinating physical properties.[1] Magnetic anisotropy is one of the most important properties of magnetic nanostructures, because it determines, for example, the stability of the magnetization direction against thermal fluctuations. It is well known that the anisotropy is strongly enhanced in nanomaterials as compared to the bulk due to reduced symmetry. Many magnetic nanostructures consisting of 3*d* and 5*d* elements show significantly enhanced magnetic moments and anisotropies, in analogy to $L1_0$-FePt and CoPt alloys, and therefore play an important role in ultra-high density magnetic recording.[2,3]

Advanced fabrication techniques make it possible to produce low-dimensional structures such as ultrathin films, nanowires, and clusters on various substrates.[4] Co nanowires on Pt(997) substrate have been fabricated by Gambardella *et al*. where they found an increased orbital moment and enhanced anisotropy as compared to bulk alloys and thin films.[5,6] Furthermore, giant magnetic anisotropy of about 9 meV per atom has been reported for Co atoms on Pt(111).[2] The influence of Pt substrate on the magnetic properties of monoatomic Fe and Co nanowires has been studied using first-principle calculations. It is found that Pt substrate has strong influence on magnetic moment and magnetic anisotropy of nanowires.[7] Cheng *et al*. investigated the magnetic properties of Fe nanostripes on Pt experimentally[3] and observed that the in-plane and out-of-plane orientations of magnetic properties depend on the thickness of nanostripe. It has been observed that FePt surface alloys supported by a Pt substrate show huge magnetic anisotropy energies, comparable to those in the bulk $L1_0$-FePt alloys.[8] Experimental and theoretical study of the magnetic properties of Fe double chains on Ir(001) has been investigated[9,10] It has been found that antiferromagnetic configuration is more stable for double Fe chains on Ir(001).[10]

Recently, the control of magnetic properties of magnetic nanomaterials by external electric field has attracted much attention.[11–13] For example, it has been observed that an electric field modifies the coercivity of $L1_0$-ordered FePd and FePt thin films in an electrochemical environment,[11] and a strong influence of electric field on the magnetic anisotropy of Fe on MgO has been predicted.[14] Tsujikawa and Oda reported the linear variation of the anisotropy with respect to electric field in Fe/Pt(001) and Pt/Fe/Pt(001).[15] Ferromagnetism has been induced in the presence of applied electric field in nonmagnetic nanoparticles[16] and thin films.[17] An enhanced magnetic anisotropy has been predicted for Co-Pt nanowires on Pt(111) in the presence of electric field.[18] Furthermore, the effect of electric field on magnetic anisotropy energy (MAE) has been studied for Fe monolayers on Pd(001) and Pt(001) surfaces, and it has been found that the magnetic anisotropy energy depends linearly on the electric field.[19] The enhancement of magnetic anisotropy in Pt/Fe/Pt(001) is found to be more pronounced than in Pd/Fe/Pd(001) surface.[19]

Now, the question arises, for which nanostructures the above-mentioned effects are more pronounced. In the present paper, we use first-principle calculations to investigate the magneto-electric effect of Fe chains on Pt(001) as shown in Fig. 1.

II. COMPUTATIONAL DETAILS

The calculations are performed within the framework of density-functional theory using the projector augmented wave (PAW) method[20,21] as implemented in the VASP code.[22,23] The exchange-correlations are described by a spin-polarized generalized-gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) functional. The supercell slab consists of four layers of Pt atoms stacked in (001) direction using the optimized lattice parameter of Pt ($a = 3.98$ Å) calculated using GGA-PBE. The system is fully relaxed until

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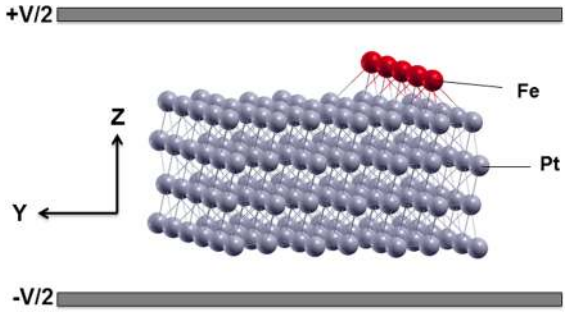

FIG. 1. Schematic of Fe chains on Pt(001) surface used in the present calculations.

the Hellmann-Feynman forces acting on each atom become less than 5 meV/Å. The energy cut-off is used to be 450 eV and the ground-state energies are converged to the 10^{-6} eV. We used $17 \times 17 \times 1$ Monkhorst-Pack grid in the full Brillouin zone for *k*-point sampling.

The external electric field is applied in the direction perpendicular to the surface, using the dipole-layer method.[24] The direction of positively charged plate is towards the side of the slab where chain is located and vice-versa for negative electric field. The magnetic anisotropy is calculated by taking the energy difference between in-plane and out-of-plane orientations of the magnetization direction in the presence of spin-orbit interaction.

III. RESULTS AND DISCUSSION

First, we discuss the influence of electric field on the magnetic moment of Fe chain on Pt(001) substrate. Figure 2 shows the calculated magnetic moment as a function of external electric field. We find that the magnetic moment of Fe chain varies linearly as a function of electric field. This variation is much more pronounced than the previously calculated magneto-electric effect in $L1_0$-CoPd thin-films[25] and Fe monolayers.[26] The magnetic moment increases when the negatively charged plate is towards the side of the slab where chain is located, i.e., in the -Z direction. In the absence of an electric field, the calculated magnetic moment per Fe atom in the chains is 3.272 μ_B, which is comparable to previous

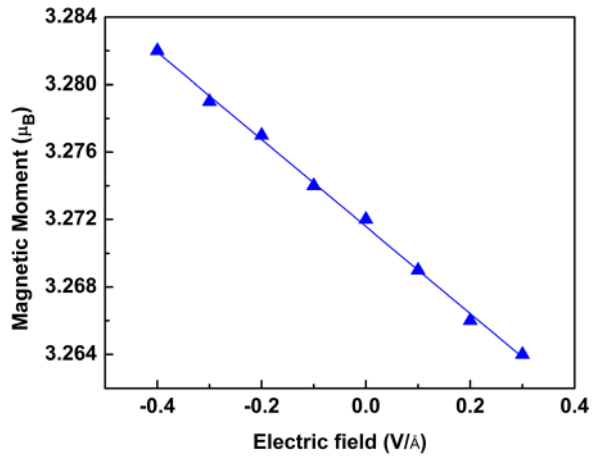

FIG. 2. The effect of an electric field on the magnetic moment of the Fe chain on Pt(001).

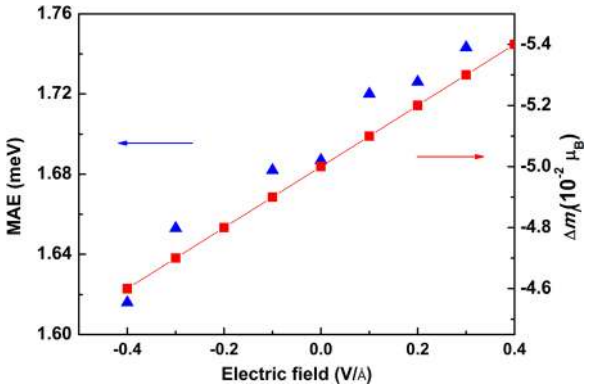

FIG. 3. Magnetic anisotropy energy (MAE, triangles) and orbital-moment anisotropy (Δm_l, squares) as a function of the electric field.

findings.[8,27] The change in magnetic moment mainly arises from the shift of minority *d*-states, as majority states are completely filled in the Fe atom.

The induced magnetic moment ΔM at the surface is $\mu_0 \Delta M = \alpha_S E$, where α_S is the surface magnetoelectric coefficient.[26] The value of $\alpha_S \approx 6.7 \times 10^{-14}$ G cm^2/V for the Fe chains on Pt(001). This value is 2.3 times larger than that of Fe(001) monolayers but smaller than that of Fe/MgO (1.11×10^{-13} G cm^2/V).[14]

Second, we consider the effect of an electric field on orbital moment and magnetic anisotropy. The calculated MAE in the absence of an electric field is 1.687 meV per Fe atom, with the easy magnetization axis perpendicular to the (001) plane.

Figure 3 shows the magnetic anisotropy and the orbital-moment anisotropy ($\Delta m_l = m_l[001] - m_l[100]$) as a function of the electric field. We found the increase in orbital moment anisotropy as well as magnetic anisotropy as a function of the electric field. According to Bruno's theory, the magnetic anisotropy is proportional to the orbital moment anisotropy. The variation of orbital moment anisotropy as a function of electric field is large as compared to Fe monolayers on Pt(001).[15] Therefore, the change in MAE is more pronounced than in Fe monolayers on Pt(001). These two anisotropies are linearly related to each other when the majority *d* bands are fully occupied and spin-flip terms between up and down states are ignored.[28]

In zero electric field, our Fe chains have values of $m_l[100] = 0.115\,\mu_B$ and $m_l[001] = 0.065\,\mu_B$. We found that $m_l[001]$ decreases with increasing electric field whereas $m_l[100]$ remains constant. Since the direction of orbital moment is perpendicular to the plane of the orbitals containing the electrons, so the orbitals contributing to the [001] direction will be d_{yz}, d_{xz}, and d_z^2, whereas the ones contributing to orbital moment along the [100] direction are d_{xy} and $d_{x^2-y^2}$. Therefore, the main contribution to change in MAE is due to the change of d_{xy} and $d_{x^2-y^2}$ occupation.

IV. CONCLUSIONS

In summary, we have used first-principle calculations to calculate the magnetic moment and the magnetic anisotropy of Fe chains on Pt(001) as a function of electric field. The

magnetic moment varies linearly with electric field. This variation is more pronounced for Fe wires on Pt(001) than for Fe monolayers. The easy magnetization axis is perpendicular to the (001) plane. We found that the electric field yields a significant change in the magnetic anisotropy as well as in the orbital-moment anisotropy.

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