Journal of Magnetics 16(3), 197-200 (2011) http://dx.doi.org/10.4283/JMAG.2011.16.3.197

Magnetic Properties of Ordered $L1_2$ $FePt_3$: A First Principles Study

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(Received 11 July 2011, Received in final form 7 September 2011, Accepted 16 September 2011)

Using the full potential linearized augmented plane wave (FLAPW) method, the influences of uniform and tetragonal strains on the magnetic state have been explored for chemically ordered bulk $L1_2$ $FePt_3$. The ordered state displays antiferromagnetic Q_1 (AFM-Q_1) state but it transitions into antiferromagnetic Q_2 (AFM-Q_2) state at about 10% uniform strain. The ferromagnetic (FM) state is observed at 11% uniform strain. For tetragonal strain, it is also seen that the transition from AFM-Q_1 to AFM-Q_2 depends on the strength and direction of the applied strain. The FM state does not appear in this case. Magnetocrystalline anisotropy (MCA) calculations for tetragonal distortion reveal that the spin reorientation transition occurs. In addition, we find that the direction of magnetization and the magnitude of magnetic anisotropy energy strongly depend on the *c*/*a* ratio.

Keywords : L1 $FePt_3$, strain, magnetic anisotropy

1. Introduction

Exchange bias systems which are composed of ferromagnetic (FM) and antiferromagnetic (AFM) materials are currently generating many research interests because antiferromagnetic materials play essential roles in innovative magnetic devices, even though the exact mechanism of the exchange interaction that arises at the interface between FM and AFM materials is still unsolved. From this point of view, ordered $L1_2$ $FePt_3$ has been extensively studied since it is typically employed as the antiferromagnetic counterpart [1]. $L1_2$ $FePt_3$ is an APt_3 binary alloy compound, where A stands for a 3d transition metal element. One can find various magnetic states in this alloy formation according to the type of 3d element. For instance, $CrPt_3$ becomes a ferromagnetic material. On the other hand, CoPt3 and MnPt3 display ferromagnetic states [2-4].

Indeed, $L1_2$ $FePt_3$ is a particularly interesting material in which one can find very rich physics. For instance, it is reported that the antiferromagnetic ground state is observed in the chemically ordered state, while the ferromagnetic state is seen in the chemically disordered state. Besides, it is known that the chemically ordered $L1_2$ $FePt_3$ displays one of two different magnetic states, called AFM-Q_1 and AFM-Q_2, depending on the temperature [5]. In the iron rich state phase, a temperature dependent magnetic state is reported [5]. It is claimed that the AFM-Q_1 state is changed to the AFM-Q_2 state below 100 K. Extensive research efforts have been focused on this material due to the variety of physics that it displays and its importance for technological purposes. As is briefly mentioned above, $L1_2$ $FePt_3$ is mostly considered as the antiferromagnetic counter part in an exchange bias material. Interestingly, it is also reported that a slight change of chemical composition can induce ferromagnetism in this material. This may give rise to an intriguing issue in the field of permanent magnet study.

The development of rare earth free permanent magnets has become one of the most essential issues in permanent magnet research. The exchange spring magnet [6] composed of hard and soft magnets has been proposed as a potential rare earth free permanent magnet. In this respect, it will be of particular interest if $L1_2$ $FePt_3$ can be utilized for this exchange spring magnet. Note that the influence of surface relaxation on the magnetic state in a thin film structure has been explored [6]. In our report, we will focus on the fundamental magnetic properties of bulk $L1_2$ $FePt_3$. The central issue is to find the influence of strain on the magnetic state. To this aim, we consider two different cases: (1) uniform strain along *a*, *b*, and *c* directions (2) tetragonal distortion in which the volume of the unit cell is fixed. One of the most essential issues in mag-

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netism is to understand magnetic anisotropy, because of its device applications. For example, the magnetic exchange coupling at the interface between AFM and FM materials should be clarified to improve current understanding of the exchange bias system. Besides, the direction of magnetization also plays an essential role in applications utilizing an exchange spring magnet system. Therefore, we will also calculate the MCA.

2. Numerical Method

The full potential linearized augmented plane wave (FLAPW) method is used to find the magnetic ground state in our calculation. Therefore, no shape approximation is assumed in charge, potential, and wave-function expansions [8-10]. We treat the core electrons fully relativistically, and the spin orbit interactions between valence electrons are dealt with using a second-variation method [11]. The generalized gradient approximation is used to describe exchange and correlation potentials [12]. Spherical harmonics with l_{max} = 8 are used to expand the charge, potential, and wave-functions in the muffin tin region. Energy cut offs at 225 Ry and 13.7 Ry are implemented for the plane wave star function and basis expansions in the interstitial regions, respectively. We use 210 k-points for all calculations in the irreducible three dimensional Brillouin zone to evaluate integrals in the reciprocal space and a muffin-tin (MT) radius of 2.2 atomic units (a.u.) to model 3d transition elements. For 5d elements, we use an MT radius of 2.5 a.u.

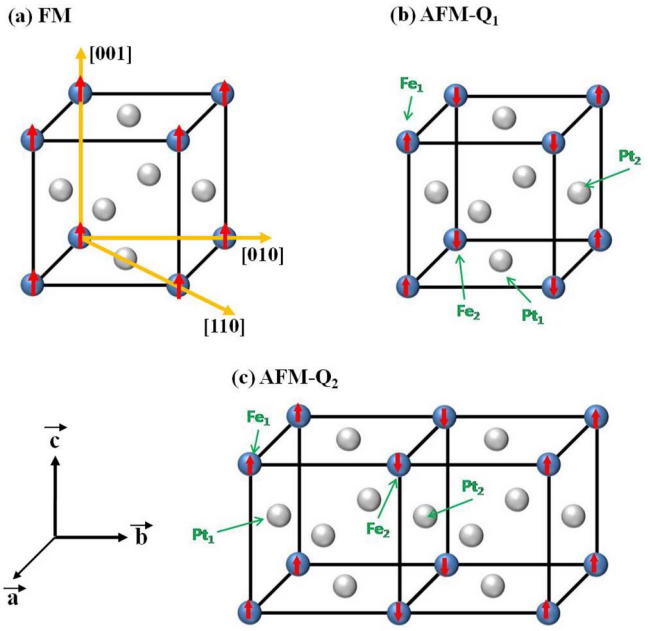

Fig. 1. (Color online) Schematic illustrations of spin structures (a) FM (b) AFM-Q_1 (c) AFM-Q_2.

3. Numerical Results and Discussion

In Fig. 1, we present the schematic illustration of magnetic structures for FM, AFM-Q_1 and AFM-Q_2, respectively. Note that $Q_1 = 2\pi/a$ (1/2, 1/2, 0) and $Q_2 = 2\pi/a$ (1/2, 0, 0). The ideal bulk $L1_2$ $FePt_3$ has a cubic structure with a lattice constant of 3.86 Å. In Fig. 2(a), we first show the calculated total energies in each magnetic state under uniform strain in three different directions. The total energy of the ferromagnetic state is set to zero as a reference. In the chemically ordered state without any strain, the ground state is found in the AFM-Q_1 state, which agrees with previous results [5]. As strain increases, the spin configuration changes from AFM-Q_1 to AFM-Q_2 and finally converges to the FM state. The transition from AFM-Q_2 to the FM state occurs at 11% strain. Next, we focus on the effect of tetragonal strain and these results are presented in Fig. 2(b). In this case, the volume is fixed and the *c*/*a* ratio is changed accordingly. It is found that

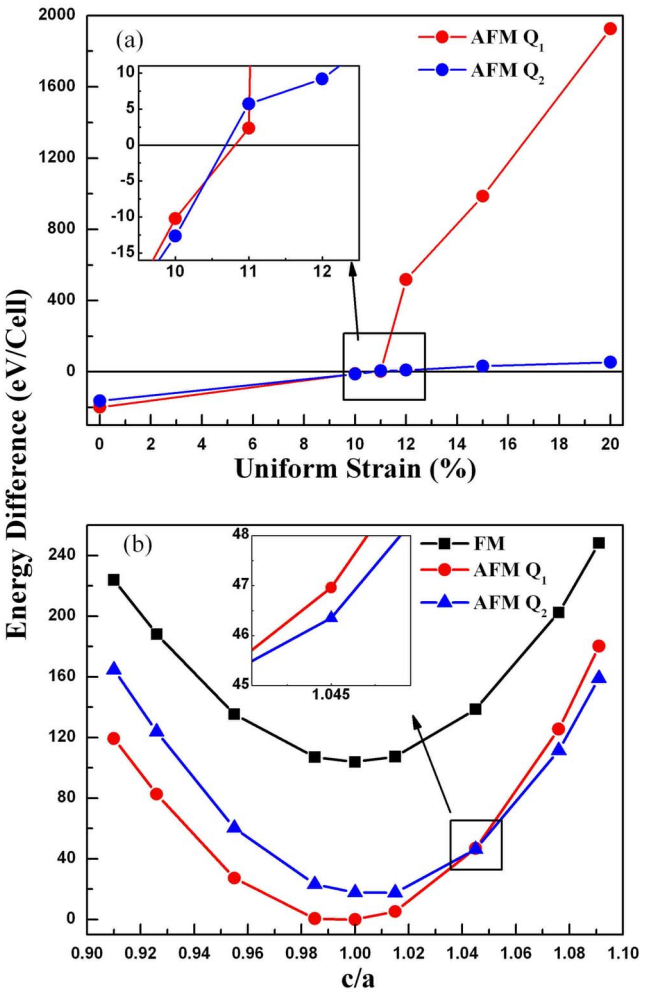

Fig. 2. (Color online) Total energy differences according to magnetic state for (a) uniform strain (b) tetragonal strain.

Table 1. Calculated spin magnetic moments (in μ_B) of Fe and Pt atoms for uniform strain

Strain (%)	0	10	11	12	15	20
Fe_1	3.21	3.51	3.49	3.50	3.53	3.54
Fe_2	-3.21	-3.51	3.49	3.50	3.53	3.54
Pt_1	0	0.15	0.43	0.43	0.42	0.42
Pt_2	0	-0.15	0.43	0.43	0.42	0.42

Table 2. Calculated spin magnetic moments (in μ_B) of Fe and Pt atoms for tetragonal strain

c/*a* ratio	1.092	1.045	1.0	0.955	0.926	0.912
Fe_1	3.24	3.24	3.21	3.21	3.21	3.21
Fe_2	-3.24	-3.24	-3.21	-3.21	-3.21	-3.21
Pt_1	0.14	0.15	0	0	0	0
Pt_2	-0.14	-0.15	0	0	0	0

the antiferromagnetic ground state is still observed even under the influence of tetragonal distortion. However, we observe different behavior. For a wide range of distortion as shown in Fig. 2(b), the ground state is observed in AFM-Q_1. However, the spin structure changes from AFM-Q_1 to AFM-Q_2 state when the *c*/*a* ratio is larger than approximately 1.045. Note that there is no FM state for tetragonal strain. From these results, we conclude that the FM ground state is hardly achievable in the bulk system because a uniform strain of about 11% seems unrealistic in nature. In Tables 1 and 2, we present the calculated magnetic moments of Fe and Pt atoms in the ground state. It is observed that the magnetic moments of Fe and Pt atoms are strongly sensitive to the type of strain. In particular, we observe a strain induced spin magnetic moment in Pt under tetragonal distortion. We found that no magnetic moment was induced by expansion in the *ab* plane, whereas expansion in the *c*-axis resulted in a spin polarized state in the Pt atom.

We have calculated the MCA energy using a torque method [13, 14]. Since the tetragonal strain is more realistic, we only consider this system. In Fig. 3, the calculated results are shown. Through MCA calculations, we find the dependence of the spin reorientation transition phenomenon on the strength of distortion. Firstly, we found that the direction of magnetization points along the [110] direction at the *c*/*a* ratio of 1.075 and it is changed to [010] at *c*/*a* ratio of 1.045 . With decreasing the *c*/*a* ratio, the [001] axis magnetization is found. At the *c*/*a* ratio of 0.98, we find the [010] axis magnetization with a very small magnetic anisotropy energy. Below this ratio of 0.98, the magnetization along the [110] direction is obtained. Besides the changes in magnetization, the magnitude of the magnetic anisotropy energy is also strongly

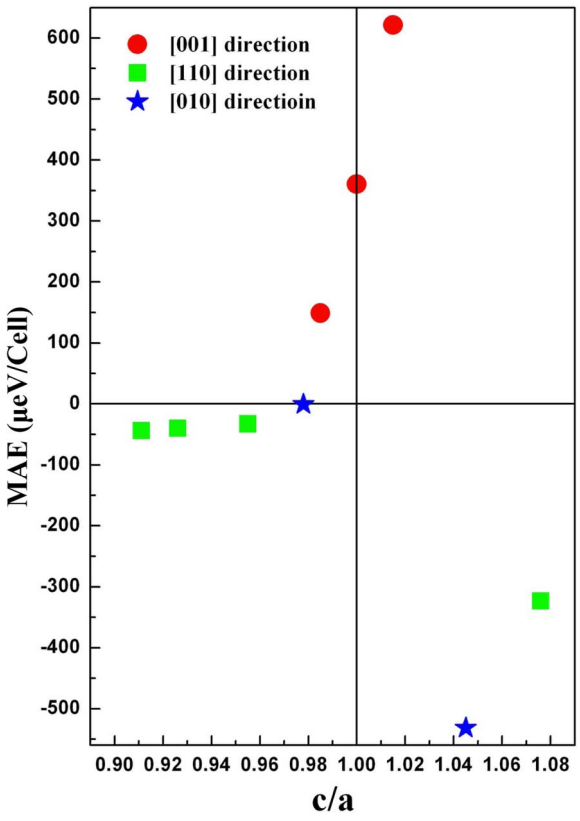

Fig. 3. (Color online) Calculated magnetocrystalline anisotropy energy.

fluctuating. It is clearly shown that the magnetic anisotropy is strongly dependent on the distortion strength. The results obtained for tetragonal strain may indicate that thin film structures or materials grown on suitable substrates can manifest different magnetic behavior.

4. Summary

In conclusion, we have explored the magnetic properties of bulk $L1_2$ $FePt_3$. We find that the magnetic state is strongly dependent on the strain. For instance, the AFM-Q_1 state is achieved under uniform strain and the transition from AFM-Q_1 to AFM-Q_2 is observed as the strain increases. The FM state is realized upon further increasing the strain beyond 11%. For tetragonal distortion, the magnetic ground state changes from AFM-Q_1 to AFM-Q_2. We find no FM state for the given tetragonal distortion range. Through MCA calculations, we find that the direction of magnetization and magnetic anisotropy energy are strongly sensitive to the distortion strength. This indicates that one can manipulate the magnetic properties of this material in thin film geometry or hetrostructured multilayer systems.

Acknowledgments

This work was supported by the Korea Science and Engineering Foundation (KOSEF) grant funded by the Korean government (MEST) (No. R01-2008-000-20014-0) and by the National Research Foundation (NRF) of Korean grant funded by the Korean government (MEST) (No. 2010-0028604).

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