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Metamagnetism in Fe_3Al Alloy

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Abstract

In this study we report the results of *ab initio* first-principles calculations to investigate the possibility of metamagnetic behavior in Fe3Al alloy. We used the WIEN2k package of full-potential linearized-augmented- plane-wave method within the local-spin-density approximation to the density-functional theory. The exchange-correlation functional is the generalized-gradient approximation of Perdew-Burke-Ernzerhof. The theoretical lattice constant, which is about 0.5% smaller than the experimental one, is obtained by minimizing the total energy. If the volume decreases about 9 % from the equilibrium, the total magnetic moment decreases abruptly from 4.6 μ_B/f.u. to 4.0 μ_B/f.u. Since this change is considerably large (~14%), it is possible to measure by a simple high-pressure experiment at about 180 kbar.

Keywords : Metamagnetism, Fe_3Al alloy, Electronic-structure calculations

1. Introduction

Metallic iron (Fe) is in its ferromagnetic ground state with body-centered-cubic (*bcc*) structure. However, the *ab-initio* total-energy calculations within the local-spin-density approximation (LSDA) to the density-functional theory predict that the fictitious nonmagnetic Fe with a face-centered-cubic (*fcc*) structure is energetically more stable [1,2], and the expansion of *fcc*-Fe could exhibit metamagnetic behavior, high-spin and low-spin states.

Fe_3Al alloy forms a cubic DO_3 structure in which two types of Fe positions are possible; one similar to that of *bcc*-Fe (2 Fe atoms: Fe_I) and the other similar to *fcc*-Fe (one Fe atom: Fe_{II}). Therefore, it is quite possible that Fe_3Al alloy may exhibit a metamagnetism. This possibility was investigated by Christensen *et al.* [3] for the first time, however, they never published the results.

In this study we report the results of our first-principles calculations of electronic structures to investigate the possibility of metamagnetic behavior in Fe_3Al alloy. We used a feature named fixed-spin-moment (FSM) calculation, which will be explained later, of the WIEN2k package [4].

2. Calculational Details

We used the WIEN2k package [4] of full- potential linearized-augmented-plane-wave method within LSDA to the density-functional theory. The exchange-correlation functional is the generalized-gradient approximation of Perdew-Burke-Ernzerhof [5], which is known to be most accurate one for the magnetic system.

The Bravais lattice of DO_3 structure is *fcc* and a chain of Fe_I-Al-Fe_I-Fe_{II} is formed along the [111] direction. If Fe_{II} is exchanged with different atom, it becomes Heusler alloy.

We used the FSM calculation of the WIEN2k package to investigate the possibility of meta-magnetism in Fe_3Al alloy more clearly. In the FSM calculation it is possible to constrain the total spin magnetic moment per unit cell to a fixed value and thus force a particular

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ferromagnetic solution, which may not correspond to the equilibrium. This is particularly useful for systems with several metastable magnetic solutions, where the conventional spin-polarized calculation would not converge or the solution may depend on the starting density. In each fixed magnetic moment the equilibrium lattice constant was found by minimizing the total energy. In the minimization process, the equation of states of Murnaghan [6] was used.

3. Results and Discussion

Fig. 1 displays the total energy (E_{TOT}) curves as a function of the unit-cell volume (V_{cell}) in the paramagnetic and ferromagnetic phases. It is clear that the ferromagnetic $D0_3$ phase is the ground state. The equilibrium lattice constant is about 0.5% smaller than the experimental one.

The magnetic moments change abruptly at $V_{cell} \approx$ 278 (a.u.)^3, which is about 9 % smaller than the equilibrium volume. This is a clear indication of metamagnetic behavior of Fe_3Al alloy. As the unit-cell volume decreases, Fe_3Al alloy undergoes a phase transition from the high-spin to low-spin states. The total magnetic moment changes from 4.6 μ_B/f.u. to 4.0 μ_B/f.u, when the unit-cell volume decreases across $V_{cell} \approx 278$ (a.u.)^3. Since this change is considerably large (~14%), it is possible to measure by a simple high-pressure

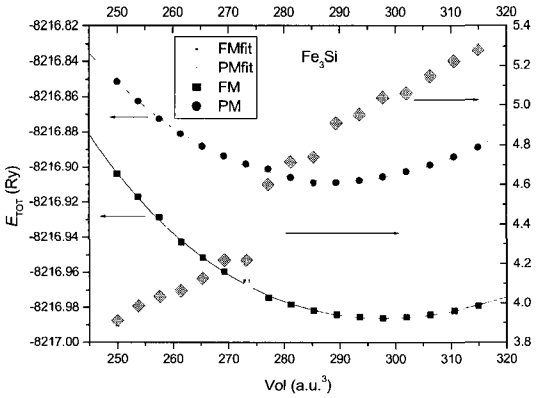

Fig. 1. E_{TOT}-vs.- V_{cell}. Large symbols are for the magnetic moments in the units of μB.

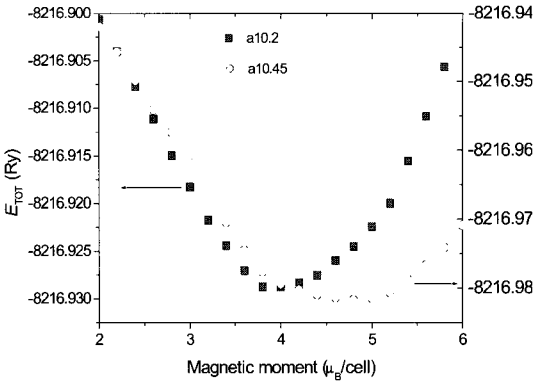

Fig. 2. E_{TOT}-vs.- M, where M is the magnetic moment, at two different lattice constants.

experiment. The corresponding pressure for the volume decrease is about 180 kbar, which is easily attained by the current technology.

In order to understand the metamagnetism, we demonstrate E_{TOT}-vs.-M graphs at two different lattice constants. For the case of a=10.2 a.u. the minimum occurs at M=3.80 μ_B/f.u. and there is a peculiarity at ~5.0 μ_B/f.u. Meanwhile, the case of a=10.45 a.u. the minimum occurs at M=4.80 μ_B/f.u. and there is a peculiarity at ~3.80 μ_B/f.u. Therefore, there might be a double-minimum structure in E_{TOT}-vs.-M curve for a certain lattice constant. Detailed analysis of the density of states reveals that the Fe atoms similar to *bcc*-Fe (Fe_I) exhibit metamagnetis (see Table 1).

Table 1. Site-decomposed magnetic moments for the high-spin and low-spin states.

	High spin(μ_B)	Low spin(μ_B)
Al	-0.08119	-0.06878
Fe_I(*bcc*)	1.31561	1.07338
Fe_{II}(*fcc*)	2.19834	2.25305
Total	4.600	4.200

4. Conclusions

Ab-initio first-principles electronic-structure calculations with the fixed-spin moment predict that Fe_3Al may have metamagnetism depending on the pressure (about

180kbar). The Fe atoms similar to *bcc*-Fe (Fe_I) exhibit metamagnetism. To confirm this calculational results the high-pressure measurement will be done in a near future to check our theoretical prediction.

Acknowledgments

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