Volume and Magnetization Dependence of Local Magnetic Moments of Mn in bcc Fe: First-principles Study

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1. Introduction

According to the phase diagram of Hansen and Ardenko[1], the body-cantered cubic (bcc) phase of Fe-Mn alloys is stable only up to 5 % Mn, and there is a large amount of experimental and theoretical work on the magnetic properties of bcc Fe-Mn. However, the ferromagnetic bcc Fe-Mn alloys have been studied insufficiently; there is a controversy between the existing data on the magnitude of local magnetic moments at Mn atoms both in absolute value ($0.0\pm0.2\mu_B$, $1.0\pm0.2\mu_B$) and in the direction ($0.77\mu_B$ and $-0.82\mu_B$). From theoretical point of view, the bcc Fe-Mn is showing different local magnetic moments of Mn depending on the theoretical approaches, Mn concentrations, and valence electron concentrations. To address the origin of this controversy, we studied the effect of lattice contraction and expansion on the local magnetic moment of Mn in bcc Fe.

2. Computational Method

First-principles calculations were carried out for a $3\times3\times3$ supercell of bcc Fe and the body centre Fe atom was replaced by Mn. The Kohn-Sham equation was solved self-consistently in terms of the full-potential linearized augmented plane wave (FLAPW) method [2] based on both the generalized gradient approximation (GGA) and the local spin density approximation (LSDA). The LAPW basis set was expanded by a plane wave cutoff of 19 Ry. Lattice harmonics with $l\leq8$ were employed to expand the charge density, potential, and wave functions inside each muffin-tin (MT) sphere. The star-function cutoff of 280 Ry was employed for depicting the charge density and potential in the interstitial region. Integrations inside the 3 dimensional (3D) Billouin zone (BZ) were performed by improved tetrahedron method on a $13\times13\times13$ mesh, which corresponds to 84 k-points inside the irreducible wedge of the 3D BZ. Self-consistency was assumed when the difference between input and output charge (spin) density was less than 1.0×10^{-5} electrons/a.u^3 All the atoms were fully relaxed at each lattice volume.

3. Results and Discussions

A series of calculations were carried out at different lattice volumes, and the calculated local magnetic moments at Mn site as a function of volume are shown in Fig. 1. One can see that the local magnetic moment of Mn (*m*) in bcc Fe strongly depends on the lattice volume, and *m* can couple ferromagnetically as well as antiferromagneticaly with the host bcc Fe. As we decrease the volume of the unit cell, *m* changes it sign around $1.026V_0$. In 1.020-$1.026V_0$ region around the equilibrium volume, *m* is very sensitive to the volume change and a spin reversal occurs in this region. Note that such anomalous behavior of Mn in bcc Fe was not observed for

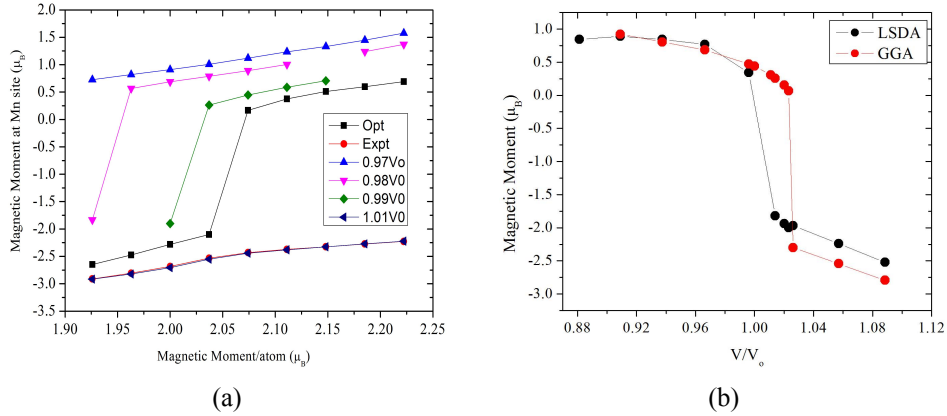the other *3d* transition-metal impurities in bcc Fe[3].

Fig. 1 (a) Magnetic moment at Mn site vs lattice volume lattice volume of Mn_1Fe_{26} and (b) Fixed magnetic moment /atom vs GGA calculated local magnetic moments of Mn at different lattice volumes. V_0 represents the GGA equilibrium lattice volume of Mn_1Fe_{26}

We further carried out fixed moment calculations, which are the counterpart of calculations in the applied magnetic field and have been successfully used to study magnetic systems, at different lattice volumes. It is concluded that the local magnetic moments at Mn site also depend on the magnetization of the unit cell, and m can couple ferromagnetically and antiferromagnetically with the host (Fig 1(b)). It is considered that the atomic character of Mn atom is dominant at volume larger than the critical volume.

4. Conclusions

The behavior of the local magnetic moments of 3.7 at.% Mn in bcc Fe was investigated in terms of the first-principles calculations. It is shown that the local magnetic moments at Mn site couple to the host bcc Fe depending on the lattice volume and magnetization. The dominant atomic character for the large volumes is considered to be responsible for the abrupt magnetic moment of Mn atom.

6. References

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