First-principles Investigation on Fundamental Magnetism and Electronic Structures of α-Mn

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1. Introduction

Manganese is known to be the most complex metallic element and have four allotropic modifications exhibiting a complex phase diagram [1]. From the various experimental results, α-Mn, which is the stable phase below 1000 K, orders in non-collinear antiferromagnetic (AFM) structure [2, 3]. The 29 atoms per primitive unit cell (58 atoms per cubic cell) are distributed over four crystallographically inequivalent sites (denoted as Mn_I, Mn_{II}, Mn_{III}, and Mn_{IV}) with complex simple cubic structure. α-Mn undergoes a paramagnetic to AFM phase transition at the Nëel temperature of T_N = 95 K.

In density functional study, Hobbs *et al.* [4] exhausted extensively structural and magnetic properties of α-Mn using first-principles calculations with reviews. The α-Mn formed by strongly magnetic (Mn_I, Mn_{II}) and weakly magnetic (Mn_{III}) or even nearly nonmagnetic (NM) (Mn_{IV}) atoms in its AFM state. Note that a pseudopotential method very occasionally predicts erroneous higher magnetic moment than a real value due to disregarding the spin polarization of core electrons. For this reason, the studies for more reliable information to the electronic and magnetic properties of α-Mn have been required. Therefore, we used the all-electron full-potential linearized augmented plane wave (FLAPW) method [5], well known for its most suitable in magnetic system calculation.

2. Computational Method

The Perdew-Burke-Ernzerhof form of the generalized gradient approximation (GGA) [6] for the exchange correlation potential was used. An energy cutoff of 4.58 ($2\pi/a$), where a is the lattice parameter, was employed for expanding the linearized augmented plane wave basis set. An 18.44 ($2\pi/a$) star function cutoff was used for depicting the charge density and potential in the interstitial regions. Lattice harmonics with $l \leq 8$ were employed to expand the charge density, potential, and wave functions inside each muffin-tin sphere, with radii of 2.0 a.u. for Mn atom. Integrations inside the Brillouin zone (BZ) were performed using the improved tetrahedron method over a 15×15×15 mesh within the three-dimensional (3D) BZ.

3. Results and Discussions

From previously reported literatures [2-4], the bulk α-Mn for AFM phase crystallized in a tetragonal structure with the I-42m space group. However, the resultant c/a ratio estimated too small values which have 0.99955 and 0.9999 for experimental observation [3] and first-principles calculation [4], respectively. Therefore, our calculation was performed that the atomic structure of α-Mn assumed as cubic symmetry (I-43m space group) for two magnetic states (NM and AFM).

As a result, the equilibrium lattice constant calculated to be 8.572 and 8.667 Å for NM and AFM states, respectively. In ferromagnetic (FM) state case, we could not determine equilibrium lattice constant since the calculated data did not fit well. As compared to experiment [3], these values are reduced to 3.31 and 2.37 % for NM and AFM states, respectively. Furthermore, the AFM state of α-Mn is energetically favored by 33.55 meV/Mn over the NM state. Above mentioned, there are four inequivalent sites in a simple cubic system, of which the calculated magnetic moments per Mn atoms are listed in Table I. For comparison, the results for neutron diffraction experiment and another first-principles calculation also given. As shown in Table I, our results are in well agreement with theoretical results, but calculated the magnetic moments of Mn_{III} and Mn_{IV} are not in perfect agreement with experimental results.

Table I. The calculated spin magnetic moments (in units of μB/Mn) at the crystallographically four inequivalent sites of α-Mn.

Site	Present work	Lawson *et al.*[a]	Hobbs *et al.*[b]
MnI	2.82	2.83	2.79
MnII	2.28	1.83	2.22
MnIII	1.34	0.55	1.00
MnIV	0.02	0.47	0.0

[a]Ref. [3] (neutron diffraction measurement)

[b]Ref. [4] (pseudopotential calculation)

4. Summary

In this study, the magnetic and electronic properties of α-Mn have been investigated using the all-electron FLAPW method based on the GGA. The local magnetic moment of Mn atoms are consistent with previously calculated results. Detailed discussion on the structural, magnetic, and electronic properties of α-Mn will be given.

5. References

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