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Fundamental Magnetism of Fe_3P Intermetallic Compound

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1. Introduction

The effect of phosphorous (P) inclusion in steels is quite detrimental on the mechanical properties. For instance, the decrease of the strength and plastic properties of steel G13L (high-manganese steel) is half when it contains 0.065 wt% P compared to the case of 0.028 wt% P steel[1]. It has been demonstrated that one form of intergranular embrittlement in steel is related to high concentrations of the impurities antimony and P in the grain boundaries[2,3].

Besides the iron based alloys, Cu based alloys have utilized P to enhance wear and water corrosion resistant Phosphor Bronze[4]. One of the increasing yield strength properties in Phosphor Bronze is considered by the precipitation of Cu_3Sn-type ε'-phase precipitation in the Cu matrix. The crystal structure of Cu_3Sn phase is similar to that of Fe_3P intermetallic compound. Thus, we raise a fundamental question whether is it possible to precipitate Fe_3P intermetallic compound from the austenite matrix.

However, there is no systematic first-principles study done for understanding the FexP compounds. In this work, we carried out fundamental electronic structures and magnetism of Fe_3P intermetallic compounds using a first-principles calculation.

2. Computational Method

The crystal structure of Fe_3P intermetallic compound is tetragonal cell with space group $I\bar{4}$. There are three nonequivalent Fe atoms in 8(g) sites with eight formula units (f.u.) per cell. In this calculation, we used experimental lattice parameters a = 9.107 Å and c = 4.460 Å[5]. The Kohn-Sham equations were solved by using the full potential linearized augmented plane wave (FLAPW) method[6] within the generalized gradient approximation (GGA)[7]. An energy cutoff of 5.0 ($2\pi/a$) was employed for expanding the linearized augmented plane wave basis set. A 18 ($2\pi/a$) cutoff was used for the star functions depicting the charge density and potential in the interstitial regions. Lattice harmonics with $l \leq 12$ were employed to expand the charge density, potential, and wave functions inside each muffin-tin (MT) sphere, with a radii of 2.2 and 1.9 a.u. for Fe and P atoms, respectively. A 13×13×13 mesh within the three-dimensional (3D) Brillouin zone (BZ), corresponding to 199 k-points inside the irreducible wedge of the 3D BZ.

3. Results and Discussions

The ground magnetic state was investigated by calculating the total energy of Fe_3P intermetallic compound with the nonmagnetic (NM) and ferromagnetic (FM) states. As a result, the FM state is more stable than the NM one by big energy difference of about 809 meV/f.u.

Table I. calculated magnetic moments (in unit of μB) inside each MT sphere for Fe_3P in FM state.

	Present Result	Experiment[1)]
Fe_I	2.367	2.12
Fe_{II}	1.665	1.25
Fe_{III}	2.104	1.83
P	-0.078	-

[1)] Neutron diffraction study in Ref.[9]

Table I list the calculated spin magnetic moments (in unit of μB) and also include the experimental data[9] due to compare. As mentioned before, there exist three nonequivalent Fe site in Fe_3P intermetallic compound as denoted FeI, FeII, and FeIII. Overall the magnitudes of magnetic moments are rather overestimated compared to the experimental study by neutron diffractions. The magnetic moment of P atom is coupled negatively to Fe atoms, even though its magnitude is small.

4. Summary

The fundamental properties of Fe_3P intermetallic compound was investigated in terms of the FLAPW method within GGA. The FM state of Fe_3P was found to be energetically more stable compared to the NM one. It is consistent with the experiment. In addition, the calculated magnetic moments of Fe atoms were calculated to be 2.367, 1.665, and 2.104 μB for FeI, FeII, and FeIII atoms, respectively.

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