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Effects of Al Impurity on Magnetism in bcc Fe by a First-principles Calculation

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1. Introduction

Recent progress on search for new lightweight high strength steels attracts much attention for achieving the energy saving automobile structure design. Al is considered as the most attracting alloying element, because it reduces the density of the final products [1]. It is well known that Al is ferrite former by destabilize of austenite domain [2]. However, the high Al contents create many side effects on steels, e.g., complicated Fe-Al compounds, Fe-Al-C compounds, or κ-carbide, which affects much on the creep properties or deformation mechanics. Contrary to the 3*d* alloying elements in bcc Fe, the Group III-VI elements shows a strong spin-orbit coupling (SOC) effects, especially on magnetism, e.g. Si in bcc Fe [3]. In this work, we investigate the effects of Al impurities on bcc Fe magnetism in terms of first-principles calculations.

2. Computational Methodology

The Al impurity in bcc Fe was model as a substitution of an atom in the 3×3×3 supercell of the primitive cell of the bcc unit cell. This corresponds to ~3.7 at.% Al impurities in bcc Fe and we designate it as $Fe_2$6Al. Fe atoms are distinguished by the distance from Al atoms; we note them as Fe1, Fe2, and Fe3, respectively. First-principles calculations were performed by using the full-potential linearized augmented plane wave (FLAPW) [4] method based on the generalized gradient approximation (GGA). Lattice harmonics with $l \leq 8$ were employed to expand the charge density, potential, and wave functions inside the muffin-tin (MT) sphere. The core electrons are treated fully relativistically, whereas the valence electrons are treated scalar relativistically. In order to see the effects of SOC, the Hamiltonian were solved second variation method [5] and spin-diagonal densities were subjected to the self-consistent loop. All the atoms were fully relaxed until the atomic forces on each atom were negligible and 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}

3. Results and Discussions

It is found, from the calculated total energy, that the SOC corrected system is about 4.5 mHartree lower than the SOC uncorrected system. Bulk modulus was calculated to be 175.9 (175.4) GPa with (without) SOC: the solid solution hardening is not so significant at this Al contents compared to that (175.8) GPa of the pure bcc Fe with the comparable convergence parameters [6]. The calculated spin magnetic moments at each atom were -0.125, 2.111, 2.226, and 2.226 μ_B without SOC and -0.124, 2.109, 2.223, and 2.222 μ_B with SOC, respectively for Al, Fe1, Fe2, and Fe3 atoms. The orbital magnetic moments were calculated to be 0.002 μ_B in <$\underline{1}$00>-direction for Al, 0.017 μ_B in <$\underline{1}$10> direction for Fe1, 0.026 μ_B in <111> direction for Fe2, and 0.016 μ_B in <00$\underline{1}$> direction for Fe3, approximately. Compared with the results of the Si impurity case [3], the orbital magnetic moments of Fe3 atom is large. This feature

imply that the screening of impurities is weaker than that of Si impurity, in bcc Fe.

4. Summary

First-principles calculations were carried out to investigate the effects of Al impurities on bcc Fe magnetism by considering SOC. No significant solid solution hardening effect was found. Albeit the effects of the SOC by Al on spin magnetic moments were minor, there are sizeable orbital magnetic effects. It is concluded that the orbital magnetism due to the Al impurity is strongly related with the impurity screening of the system as seen in Si impurity case [3], but the effects of Al impurity is stronger than those of Si impurity in terms of orbital magnetism.

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