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Phase Stability of $Fe_{16}C_2$ and $Fe_{16}C_4$ from First-principles Calculations

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1. Introduction

Experimental analysis of Fe-Ni-C martensite showed that carbon atoms in as-quenched marteniste were distributed uniformly in the virgin martensite, but when the samples were aged for various times, images of carbon-enriched region were found. Aging studies by Mössbauer spectroscopy have been interpreted to indicate the formation of a metastable Fe4C configuration within the martensite [1]. However, the exact crystal structure of high carbon phase in martensite is unknown. There is controversy about the phase stability between $Fe_{16}C_4$ (Fe_4C) and $Fe_{16}C_2$ (Fe_8C). To address this issue, we carried out first-principles calculations.

2. Computational Methodology

First-principles calculations were performed by using the full-potential linearized augmented plane wave (FLAPW) [2] 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. 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}

To investigate the structure of high carbon phase, we considered two different models, known as J and T model in the literature, to describe the atomic positions of Fe_4C ($Fe_{16}C_4$) and Fe_8C ($Fe_{16}C_2$). Initially, for $Fe_{16}C_4$ and $Fe_{16}C_2$ structures, we considered the lattice parameters of $Fe_{16}N_2$ [3] and then the optimized lattice parameters were determined by total energy minimization.

3. Results and Discussions

It is found that the ferromagnetic (FM) states are stable for both systems. The formation energy was calculated in the FM state and our preliminary results show that $Fe_{16}C_2$ (Fe_8C) is more stable than $Fe_{16}C_4$ (Fe_4C). The spin density contours in the (110) plane of $Fe_{16}C_2$ are shown in Fig. 1. The magnetic properties arecalculated and it is observed that C atoms are negatively polarized. Our analysis showed that those Fe atoms which were nearest to C atoms have smaller magnetic moment due to strong bonding with the C atoms.

4. Summary

First-principles calculations were carried out to investigate the crystal stability and magnetism of $Fe_{16}C_2$ and $Fe_{16}C_2$. Our precise calculations show that the structure of high carbon phase is $Fe_{16}C_2$ and this structure is more stable in the ferromagnetic state than the nonmagnetic state. The Fe atoms induced negative magnetic moment at the C

atoms, which interact with the nearest Fe atoms.

References

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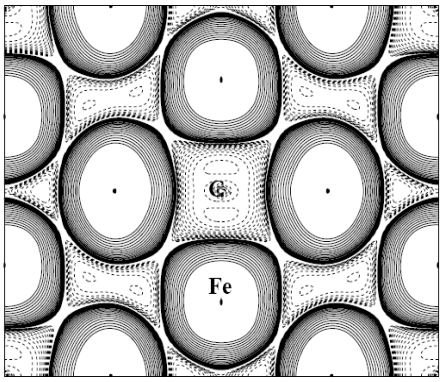

Fig. 1 Spin contours of $Fe_{16}C_2$ plotted in (110) plane. The lowest contours start from than 2.0×10^{-4} electron/a.u. and subsequest lines differ by a factor of $\sqrt{2}$. Solid (dottedl) lines represent majority (minority) spins.