Electronic structure and magnetism of FeGe with B20-type structure

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Abstract

The electronic structure of FeGe with B20-type crystal structure is calculated by a self-consistent LMTO method. A ferromagnetic state is obtained with the magnetic moment of about 1 μ_B per Fe at the observed lattice constant, being consistent with the observed induced moment. It is shown at smaller lattice constants that a non-magnetic semiconducting state with a very narrow band-gap becomes stable, where a magnetic field-induced metamagnetic transition takes place from a non-magnetic state (semiconductor) to a ferromagnetic one (metal), similar to that in FeSi with the same crystal structure. It is concluded that the difference between the magnetic states of Fe in FeGe and FeSi comes from the band-gap width in the nonmagnetic state.

Key words: FeGe; Field-induced metamagnetic transition; Narrow-gap semiconductor

The magnetic ordering of the cubic FeGe with B20-type crystal structure has a long-wavelength spiral structure with a period of 683∼700 Å below the Néel temperature 278.7 K [1]. The field-induced ferromagnetic state with about 1 μ_B/Fe is stabilized at the magnetic field of 0.2 T. On the other hand, FeSi with the same crystal structure is known as a narrow-gap semiconductor and behaves similarly to the strongly correlated electron system [2]. Kudasov et al. [3] have observed the semiconductor-metal transition for FeSi under extremely strong magnetic fields. The present authors [4] have shown by the band calculations that FeSi shows such a phase transition from the non-magnetic semiconductor to the metallic ferromagnet. The anomalous temperature dependence of the magnetic susceptibility has been shown to be reproduced by the spin-fluctuation theory [5].

The aim of the present paper is to study why the Fe states in FeGe and FeSi are so different from each other, by calculating the electronic structures by a self-consistent LMTO method. The details of the band calculations are given in [4]. Figure 1 denotes the local density-of-states (DOS) curves Fe and Ge calculated at the non-magnetic state for some lattice constants. (The observed lattice constant for FeGe is 4.7 Å [1].) The Fermi level lies in the narrow band-gap for each case. The calculated band-gap decreases with increas-

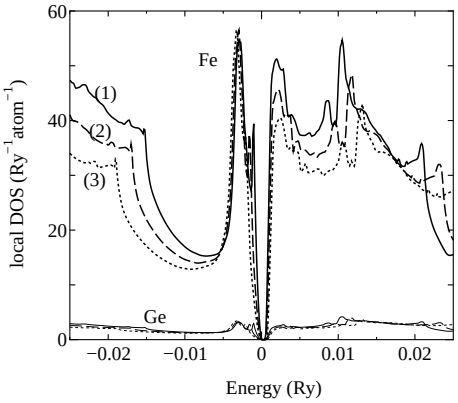

Fig. 1. Local DOS curves of Fe and Ge. The solid, broken and dotted curves (1), (2) and (3) are those calculated at the lattice constants 4.7, 4.6 and 4.5 Å, respectively.

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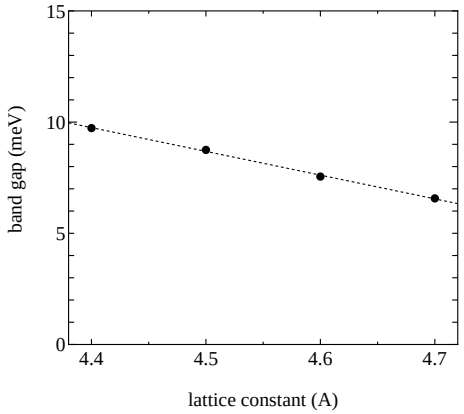

Fig. 2. Calculated value of the band-gap for the non-magnetic FeGe as a function of lattice constant.

ing the lattice constant, as shown in Fig. 2. It is noted that the band-gap for FeGe is less than 10 meV for these lattice constants, while that for FeSi with the observed lattice constant 4.49 Å is about 60 meV [6]. The difference of the band-gap widths for FeGe and FeSi will be attributed to the p-states of Ge and Si.

By the fixed-spin-moment method, the magnetic energy $\Delta E(M)$ is calculated as a function of the magnetic moment M, as shown in Fig. 3 for some lattice constants. The calculated values of the local moments on Fe and Ge at the observed lattice constant 4.7 Å are 1.16 and -0.086 $\mu_{\rm B}$/atom. By the lack of the inversion symmetry of the present crystal structure, the Dzyaloshinskii-Moriya type magnetic structure is stabilized without magnetic field. However, the ferromagnetic moment of 1 $\mu_{\rm B}$/Fe is induced at the magnetic field of 0.2 T [1]. As shown in Fig. 3, the ferromagnetic state becomes unstable at the smaller lattice constants. But the two minima of $\Delta E(M)$ appear at the small and large values of M, as shown by the curve (3). In this case, a first-order magnetic transition from

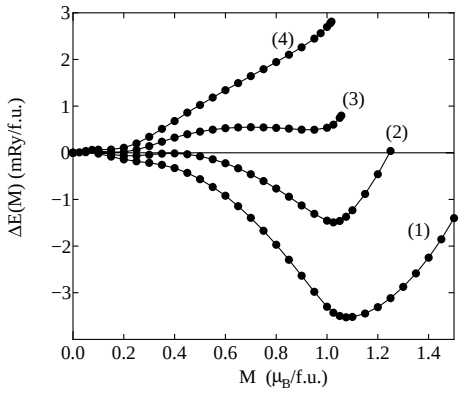

Fig. 3. Calculated results of $\Delta E(M)$ as a function of M. The curves (1)-(4) are those at lattice constants 4.7, 4.6, 4.5 and 4.4 Å, respectively.

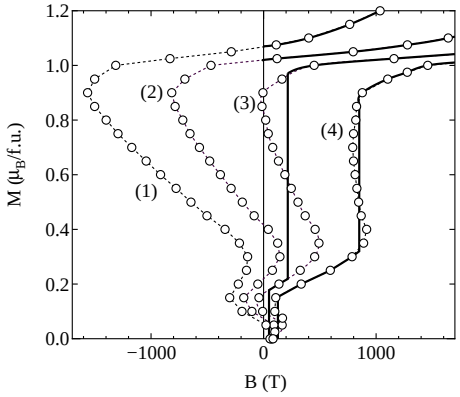

Fig. 4. Calculated results of the magnetization curve. The curves (1)-(4) are those at lattice constants 4.7, 4.6, 4.5 and 4.4 Å, respectively.

the small moment state to the large moment one takes place at a certain magnetic field, as discussed for FeSi. The magnetization curve $M(B)$ is obtained in the same method used in [4]. The calculated results are shown in Fig. 4. There is no physical meaning in the negative region of B. A clear metamagnetic transition is seen from the small moment state to the large moment one for the curves (3) and (4). Then, it is expected that the metamagnetic transition will take place for FeGe under extremely strong pressures.

In conclusion, the difference between the magnetic states of Fe in FeGe and FeSi comes from the band-gap width in the non-magnetic state. The measurements of the metamagnetic transition at the strong pressures are desired to confirm the present calculations.

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