On the Correlation and Magnetism of B2-FeAl

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It is a long quest for finding a reliable exchange-correlation potential for the many-body theory for describing the electronic structures within reasonable computational resources. The local density approximation (LDA) by Kohn-Sham [1] is a triumph of the density functional theory (DFT) [2] in many-body physics, but it is a certain class of mean-field approximation, which cannot capture correlation effects correctly. The LDA+U method [3], which is a combination of two extreme theoretical approaches in solid states physics, has been successfully described many important physical properties of various classes of correlated materials [4]. The success of the LSDA+U method is due to the rather *ad hoc* engineered inclusion of a parameter, the Hubbard U, for controlling the localization of electrons instead of the Stoner parameter I responsible to control localization in the local spin density approximation as well as in the generalized gradient approximation. Since the LSDA+U method is based on the static Hartree-Fock approximation to the Hubbard model, a further progress for considering the dynamical effects has been made in terms of the dynamical mean field approximation (DMFT) [5].

The LSDA+U method [6] was applied to investigate the origin of the observed paramagnetism [7] or spin glass behavior [8] of B2-FeAl intermetallic compound at low temperature. The investigation of Ref. [6] claimed that the correlation correction within the LSDA+U scheme yields a nonmagnetic ground state for U being greater than 3.7 eV and attributed that the disappearance of the magnetic ground state occurs since Fe-t_{2g} and Fe-e_g manifolds are affected differently by a common U. However, there have been many doubts on the conclusion of Ref. [6] by considering the effects of thermal disorder [7,9,10] including the effects of antisites [11]. Moreover, the authors of Ref. [6] made a conceptual mistake in distinguishing nonmagnetism and paramagnetism, although they are conventionally treated equivalent. It is therefore necessary to investigate again the effects of correlation on the magnetism of B2-FeAl with more precise calculations.

The crystal structure of the target is simply B2-FeAl whose experimental lattice constant is 5.496 a.u. (see Ref. [6]) and we vary the lattice constant from 95 % to 115 % of the experimental one for find the equilibrium lattice constant. The Kohn-Sham equation was solved in terms of the total energy all-electron full-potential linearized augmented plane wave method [12] implemented in the QMD-FLAPW software package [13]. The convergence parameters were carefully selected for checking the accuracy of the calculations such that a $21 \times 21 \times 21$ mesh for the integration inside the Brillouin zone, lattice harmonics with the maximum l=10 for both potential and wave function expansion inside the muffin-tin spheres of radii 2.2 a.u. with 481 radial exponential meshes. The important parameters for the plane wave cutoff and the star function cutoff were chosen to be respectively 4.5 ($2\pi/a$) and 18.0 ($2\pi/a$), where a is the lattice constant.

We used the various correlation effects to the Kohn-Sham potential such as the local density approximation (LDA) by Hedin-Lundqvist [14], the local spin density approximation (LSDA) by von Barth-Hedin [15], the generalized gradient approximation by Perdew-Burke-Ernzerhof [16], and the screened exchange LDA (sx-LDA)

[17] implemented in the FLAPW method by Asahi-Mannstadt-Freeman [18] as well as the LDA+U method [3] combined with the LDA, LSDA, and GGA implemented in the FLAPW method [13]. The required U and J parameters were chosen to be the same with those of Ref. [6].

With all the possible cases of the correlation potentials including the variations of U and lattice constants, we always obtain the ferromagnetic ground states, which is contradict to that of Ref. [6]. We attribute the discrepance is originate from the implementation error of Ref. [6] and warn that the consequent study based on the Wien 97 and Wien 2k packages with the LDA+U should be investigated again.

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