Origin of the magnetic moment enhancements of the ordered $Fe_{50}Co_{50}$ alloys

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We investigated the physical origin of the magnetic moment enhancements of the ordered $Fe_{50}Co_{50}$ alloys, by using the all-electron total-energy full-potential linearized augmented plane wave (FLAPW) method [1] within the generalized gradient approximation (GGA) [2] to exchange correlation potential. Two ordered cubic structures were assumed for the $Fe_{50}Co_{50}$ alloys, i.e., the bcc related CsCl-type (B2) and the fcc related CuAu-type ($L1_0$). The Wigner-Seitz radii (R_{WS}) were determined from the total energy minimization, and they are 2.642 a.u. and 2.636 a.u. for the B2 and $L1_0$ alloys, respectively. These values are smaller than that (2.668 a.u.) of bcc Fe and larger than that (2.619 a.u.) of fcc Co. It is also found that the B2 alloy is more stable (~0.23 eV) than the $L1_0$ alloy.

The calculated magnetic moments of the B2 alloy are 2.80 μ_B for Fe and 1.81 μ_B for Co, while those of the $L1_0$ alloy are 2.57 μ_B for Fe and 1.61 μ_B for Co. For comparison, we also calculated pure Fe and Co systems with the same R_{WS} for bcc (B2) and fcc ($L1_0$) structures. The calculated magnetic moments of the pure Fe are 2.24 μ_B for bcc and 1.37 μ_B for fcc, and those of the pure Co are ~1.7 μ_B for both structures. Our results, thus, show that the magnetic moments of Fe in the alloys are enhanced significantly.

Compared to the pure Fe and Co structures, the charge transfer from the muffin-tin (MT) sphere of the Fe atom to that of the Co atom in the alloy is only ~0.06 and ~0.04 electrons, which are negligible to affect the magnetic moment of each atom. Instead, the spin-down charge of the Fe atoms flips to the spin-up by about 0.24 and 0.58 electrons for the B2 and $L1_0$ alloys, respectively. Twice the number of those is comparable to the enhancement of Fe magnetic moments in each alloy. The calculated local density of states show that the enhancements of the Fe magnetic moments are due to the filling the unoccupied majority d-bands of the pure Fe atoms. The calculated orbital-decomposed number of electrons reveals a quantitative understanding on the origin of the spin-flip. Most of the spin-flip in the Fe atoms occurs in the t_{2g} electrons, and total Fe majority spins shift toward higher binding energy, i.e., increasing the exchange splitting, to fill the majority d electrons completely, for both the B2 and $L1_0$ alloys. On the other hand, the change of the magnetic moments of Co in the alloys can be explained in terms of crystalline electric field (CEF) splitting: Compared to the pure Co, the Co atom of the B2 alloy "feels" larger CEF splitting, while that of the $L1_0$ alloy "does" smaller CEF splitting.

References

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