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Electronic and magnetic properties of $Co_2Fe(Ga_{1-x}Si_x)$ and $Co_2Fe(Al_{1-y}Si_y)$ Heusler alloys with high Curie temperature

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ABSTRACT

We investigate the electronic and magnetic properties of $Co_2Fe(Ga_{1-x}Si_x)$ and $Co_2Fe(Al_{1-y}Si_y)$ alloys using first-principles density functional theory based method. With increasing concentration of Si, lattice constant decreases linearly whereas bulk modulus and total magnetic moment increase. Electronic structure calculations show that the minority DOS exhibits a gap around Fermi level confirming the half-metallic character of the material for all the concentrations studied and the Fermi level can be shifted within the energy gap by changing the Si concentration. The Heisenberg exchange coupling parameters obtained from our calculations predict strong ferromagnetic coupling and high Curie temperatures, which is in accord with the experimental results.

1. Introduction

Co-based Heusler alloys have attracted considerable attention for their potential use as applicable materials in the field of spin-electronics and magnetoresistive devices. They are particularly of interest because of their predicted full spin polarization at the Fermi edge, making them the so-called half-metallic ferromagnets (HMFs) [1]. Several kinds of Co-based Heusler alloys have been investigated and reported to HMFs based on theoretical calculations [2–7]. Co-based Heusler compounds have the formula Co_2YZ, where Y may be Ti, V, Cr, Mn or Fe and Z may be Al, Ga, Si, or other main group metal. Co-based Heusler alloys with high spin polarization are good candidates for applications since they have large magnetic moments, high Curie temperatures (T_C) and easily grow on substrates in fabrication of multi-layered thin films. From the viewpoint of applicability, not only high T_C and high spin polarization but also high $L2_1$ phase stability are required in the ferromagnetic materials used as an electrode of magnetic tunnel junctions (MTJs). Actually, it has been reported that the MTJs using Co-based Heusler alloys such as Co_2MnAl, Co_2MnSi, $Co_2(Cr_{1-x}Fe_x)Al$, and $Co_2Fe(Al_{1-x}Si_x)$ display large TMR ratios even at room temperature [8–12]. Therefore, Co-based Heulser alloys ordering easily to the $L2_1$ structure have an advantage as applicable materials.

Moreover, Co_2FeZ compounds have recently attracted much theoretical and experimental attention for applications since it has unique half-metallic band structure with high Curie temperature and exhibits the high magnetic moment. Also the phase stability and the position of Fermi level in the band gap play an important role in industrial applications. Many theoretical calculations show magnetic moment and spin polarization variation and shifting the position of Fermi level in the band gap can be achieved through substitution of main group element in place of constituent Z atoms [13–15]. The concentration dependence of the order–disorder phase transformation temperature, spin polarization and magnetic properties of $Co_2Fe(Ga_{1-x}Si_x)$ and $Co_2Fe(Al_{1-y}Si_y)$ Heusler alloys have been reported [16,17]. In the experimental investigations, where the order–disorder phase transformation temperature increases with increasing Si content, in accord with a tendency that the degree of order of the $L2_1$ phase becomes higher with increasing Si content and the spin polarization increases at first then decreases by substituting Si for Al. The spontaneous magnetization in both alloys almost follows the generalized Slater–Pauling rule. Therefore, keeping in view these findings and important applications of Co_2FeZ compounds, our main purpose is to study the effect of substitution of main group element on electronic and magnetic properties of Co_2FeGa and Co_2FeAl in this paper.

2. Computational details

First-principles calculations of $Co_2Fe(Ga_{1-x}Si_x)$ and $Co_2Fe(Al_{1-y}Si_y)$ are performed in a plane-wave basis set using the

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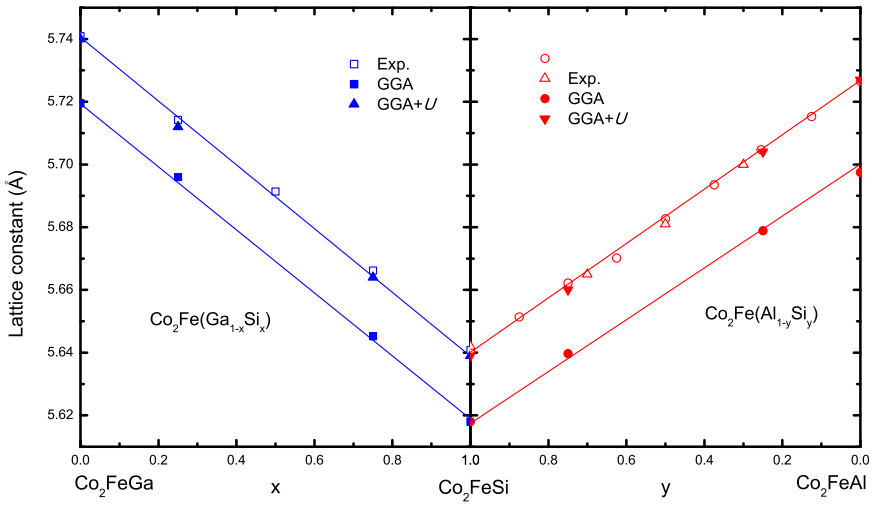

Fig. 1. Concentration dependence of the lattice constant for $Co_2Fe(Ga_{1-x}Si_x)$ and $Co_2Fe(Al_{1-y}Si_y)$ alloys, together with the reported experiment data (Refs. [16,17]).

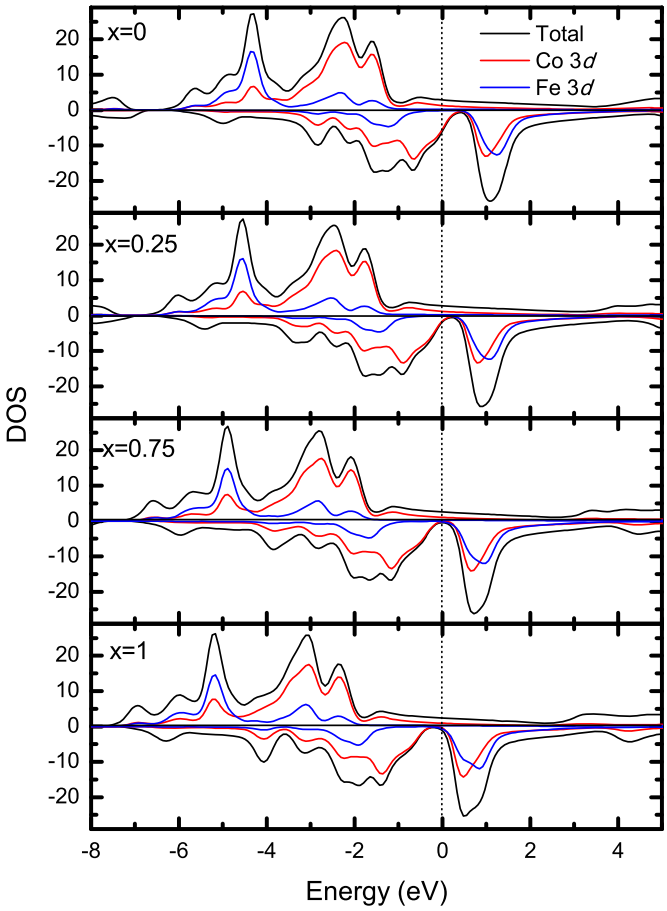

Fig. 2. Concentration dependence of the total densities of states (DOS) and partial densities of states (PDOS) of Co 3*d* and Fe 3*d* for $Co_2Fe(Ga_{1-x}Si_x)$ alloy. The energy zero is taken at the Fermi level and the majority spin and minority spin DOS are shown above and below the abscissa axis, respectively.

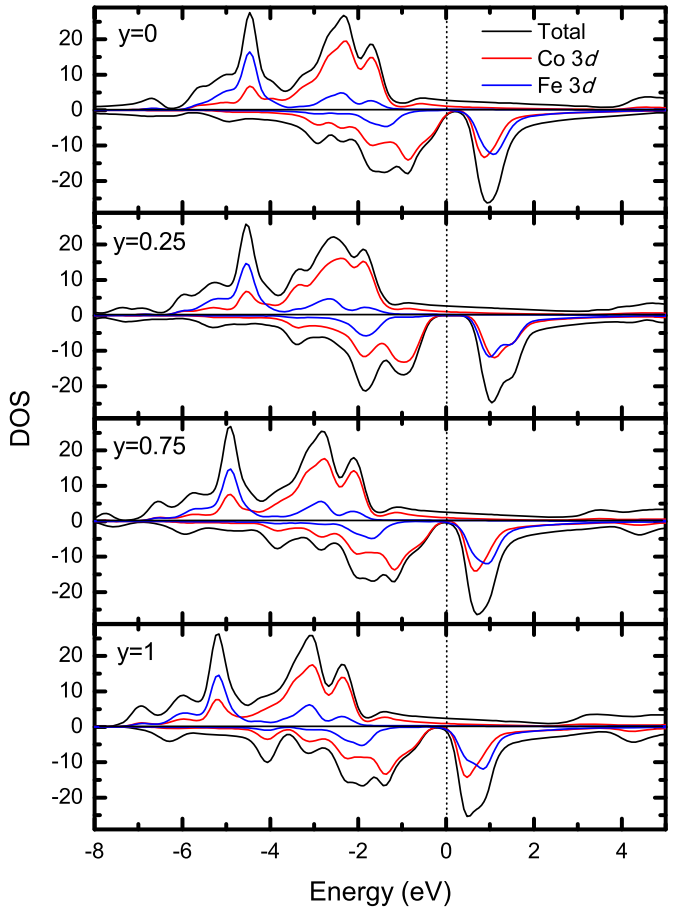

Fig. 3. Concentration dependence of the total densities of states (DOS) and partial densities of states (PDOS) of Co 3*d* and Fe 3*d* for $Co_2Fe(Al_{1-y}Si_y)$ alloy. The energy zero is taken at the Fermi level and the spin-up and spin-down DOS are shown above and below the abscissa axis, respectively.

projector augmented wave (PAW) [18,19] method in the generalized gradient approximation (GGA) as it is implemented in the Vienna *ab initio* simulation program (VASP) [20,21]. To treat exchange and correlation effects, we use both GGA and the semi-empirical GGA+*U* [22–25] methods within a rotationally invariant formalism for a better description of the localized transition metal *d* electrons. Here, we choose U=3.5 eV, J=0.9 eV for the 3*d* orbitals of Co atoms and U=3.4 eV, J=0.9 eV for the 3*d* orbitals of Fe atoms which are consistent with the first-principles Hartree–Fock-calculated values of effective U parameter for transition-metal elements. The 16 atoms in the $L2_1$ unit cell composed of eight Co, four Fe, and four Ga/Al atoms were taken for the self-consistency calculations. The Si addition was carried out by a gradual replacement of those four Ga/Al atoms by Si atoms. In such a way, one of the four Ga/Al atoms replaced by an Si atom results in x=0.25/y=0.25, etc. in the $Co_2Fe(Ga_{1-x}Si_x)$ and $Co_2Fe(Al_{1-y}Si_y)$