Effect of local atomic disorder on the half-metallicity of full-Heusler Co_2FeSi alloy: a first-principles study*

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(Received 18 December 2009; revised manuscript received 23 March 2010)

This paper investigates the effect of atomic disorder on the electronic structure, magnetism, and half-metallicity of full-Heusler Co_2FeSi alloy by using the full-potential linearized augmented plane wave method within the generalized gradient approximation (GGA) and GGA+U schemes. It considers three types of atomic disorders in Co_2FeSi alloy: the Co–Fe, Co–Si, and Fe–Si disorders. Total energy calculations show that of the three types of disorders, the Fe–Si disorder is more likely to occur. It finds that for the Co–Si disorder, additional states appear in the minority band-gap at the E_F and the half-metallcity is substantially destroyed, regardless of the disorder level. On the other hand, the Co–Fe and Fe–Si disorders have little effect on the half-metallicity at a low disorder level. When increasing the disorder levels, the half-metallcity is destroyed at about 9 % of the Co–Fe disorder level, while that stays at 25 % of the Fe–Si disorder level.

Keywords: half-metallicity, full-Heusler alloy, electronic structure, full-potential linearized augmented plane wave method

PACC: 7115A, 7120H

1. Introduction

Half-metallicity was first predicted by de Groot and collaborators[1] for the half-Heusler NiMnSb alloy in 1983. Half-metallic ferromagnets have a unique property in their band structure: the minority spin band is semiconducting, while the majority spin band is metallic, which brings 100 % spin polarisation at the Fermi energy (E_F). A significant number of full-Heusler alloys have been predicted to be half-metallic ferromagnets.[2] The full-Heusler alloys have a chemical formula of X_2YZ (X and Y are usually transition metals and Z is a main group element) and they crystallize in the $L2_1$ structure, where the X atoms are sitting on the 8c (1/4, 1/4, 1/4 and 3/4, 3/4, 3/4) sites and the Y and Z atoms are placed on the 4a (0, 0, 0) and 4b (1/2, 1/2, 1/2) sites in Wyckoff coordinates. The total spin magnetic moment of full-Heusler alloys scales with the number of valence electrons and can be described with the Slater–Pauling rule.[3]

The full Heusler Co_2FeSi alloy attracts particular interest because it has a Curie temperature of 1100 K, a saturation magnetic moment of 6 μ_B per formula unit (f.u.), and a high spin polarisation at the Fermi level. These properties fulfill the essential requirements for magnetic sensors or spin valve structures.[4] Recent band structure calculations for Co_2FeSi have demonstrated that the local spin density approximation (LSDA)[5,6] and the generalized gradient approximation (GGA)[7] schemes for the exchange–correlation potential are not sufficient for correctly describing the electronic structure and magnetism. A good agreement with the experimental results can be achieved by using the LDA+U scheme.[4,8] Here U is on-site electron–electron Coulomb interaction. The LDA+U, as described by Anisimov *et al.*,[9] adds an orbital-dependent on-site electron–electron Coulomb interaction, which is not included in the LSDA and GGA schemes. By investigating the dependence of the electronic structure on the lattice parameter of Co_2FeSi, Kandpal *et al.*[8] found that an effective Coulomb exchange interaction $U_{\rm eff} = U - J$ in the range of approximately $2 \sim 5$ eV leads to half-metallic ferromagnetism and a measured integer magnetic moment at the experimental lattice parameter.

It is well known that the disorder, defect, and surface have a significant influence on the electronic structure and magnetism of the materials.[10−15] Picozzi *et al.*[15] have investigated the effects of several kinds of defects, such as atomic swaps and antisites

*Project supported by the National Natural Science Foundation of China (Grant No 10664005).
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on Co_2MnSi and Co_2MnGe alloys by using the full-potential linearized augmented plane wave (FLAPW) method. The results show that the Mn antisites have the lowest formation energy and they retain half-metallicity, in contrast with the Co antisites. The effect of doping and disorder on the magnetic properties of Co_2MnSi, Co_2MnGe, and Co_2MnSn full-Heusler alloys has been studied by Galanakis *et al.*,[16] using the first-principles density functional theory. They found that both disorder and doping have little effect on the half-metallic character of the alloys, and keep a high degree of spin polarisation. A high degree of disorders in Co_2FeSi was investigated by Gercsi *et al.* using an *ab initio* calculation with the U values of the magnitude of ~ 2 eV.[17] They reported that the 25 % B2-type disordered (swapping the position of an Fe atom for an Si atom) and the 12.5 % DO_3-type disordered (a Co atom was swapped with an Fe atom) systems retain the half-metallic character, while the 12.5 % A2-type disordered (a Co atom and an Si atom swap their sites) system lost the half-metallicity. By means of x-ray diffraction (XRD) and Mössbauer spectroscopies, Wurmehl *et al.*[4] detected a small disorder (< 10 %) between the Fe and Si atoms (B2-type disorder) in the Co_2FeSi alloy.

In this paper, we have studied effects of atomic disorder with different disorder levels on the electronic structure, magnetism, and half-metallicity of Co_2FeSi by using the all-electron FLAPW[18] method with GGA and GGA+U. We considered three types of atomic disorders: (a) the Co–Fe disorder; (b) the Co–Si disorder; (c) the Fe–Si disorder. In Section 2, we briefly describe the calculational model and method. The results and discussions are presented in Section 3, and a brief summary is given in Section 4.

2. Model and method

We have considered four types of structures: (a) the ordered $L2_1$; (b) the Co–Fe disorder (DO_3-type disorder, where a Co–Fe nearest-neighbouring pair shows exchanging the positions in comparison with the ideal bulk); (c) the Co–Si disorder (A2-type disorder, where a Co–Si nearest-neighbouring pair shows swapping the positions in comparison with the ideal bulk); and (d) the Fe–Si disorder (B2-type disorder, where an Fe–Si next-nearest-neighbouring pair shows exchanging the positions in comparison to the ideal bulk). To describe a low and high level of disorder, we have adopted two unit cells: one is a 16 atom $L2_1$ unit cell and the other is a 32 atom unit cell obtained by doubling the $L2_1$ bulk unit cell (with four atoms) Bravais vectors, i.e., $2 \times 2 \times 2$ times the $L2_1$ unit cell. For the 32 (16) atom unit cell, the levels of disorder are 6.25 (12.5) %, 6.25 (12.5) %, and 12.5 (25.0) % for the Co–Fe, Co–Si, and Fe–Si disorders, respectively. The lattice parameter was chosen to be the experimental value ($a = 10.658$ a.u.).[4] No geometrical optimisation was taken into account for the disordered systems.

The Kohn–Sham equation[6] was solved self-consistently in terms of the FLAPW method as implemented in the FLEUR (a new Flapw-code the development of which is partly funded by the European research network)[19] within the GGA and GGA+U schemes. We denote the effective Coulomb-exchange interaction $U_{\text{eff}} = U - J$ (the U and J are the Coulomb and exchange parameters) by U_x, where the subscript x stands for the values (in %) relative to the neutral atomic values. The U_{eff} values were chosen to be 1.92 (1.80) eV, 2.52 (2.38) eV, 3.78 (3.56) eV, and 5.04 (4.76) eV at the Co (Fe) atom, which corresponds to $U_{7.5}$, U_{10}, U_{15}, and U_{20}. These values ensure that the ordered Co_2FeSi is a half-metallic ferromagnet. Lattice harmonics with $l \leq 8$ were employed to expand the charge density, potential, and wave functions inside the muffin-tin (MT) radius of 2.20 and 2.00 a.u. for the Co (and Fe) and Si atoms, respectively. Integrations inside the Brillouin zone (BZ) were performed by summations over $10 \times 10 \times 10$ and $6 \times 6 \times 6$ meshes inside the BZs, for the 16 and 32 atoms unit cells, respectively. All core electrons were treated fully relativistically, while valence states were treated as scalar relativistically, i.e., not taking account of the spin–orbit coupling.[20] Self-consistency was assumed when the difference between the input and the output charge (spin) density was less than 1.0×10^{-5} electrons/(a.u.)^3.

3. Results and discussion

In Table 1, we present the calculated relative total energies per f.u. with respect to the ordered system for the disordered systems with different U_{eff} in the 16 and 32 atoms unit cells. A larger relative total energy indicates a lower possibility of the disorder. As shown in Table 1, the relative total energy of the Co–Si disorder is larger than that of the others; thus, the disorder is a highly unfavourable metastable state. On the other hand, although the relative total energies of the Fe–Si and Co–Fe disorders are similar at

the low disorder level, the relative total energy of the Co–Fe disorder rapidly increases when increasing the disorder level in comparison with the Fe–Si disorder. Thus, it is expected that the Fe–Si disorder is more likely to occur in comparison with the Co–Fe disorder. The results agree with the experimental results obtained by Wurmehl *et al.*[4] They have fabricated polycrystalline Co_2FeSi samples by arc melting and found a small (< 10%) Fe–Si disorder, while a Co–Fe disorder can be excluded from the XRD Rietveld refinement as well as from neutron scattering data. A detailed neatron magnetic resonance (NMR), x-ray, and neutron-diffraction study on $Fe_{3-x}Co_xSi$ samples showed that the Co–Fe, Fe–Si, and Co–Si disorders have values ranging from 10% to 16% for the $x = 2.00$ composition.[21] Niculescu *et al.*[22] suggested that the degree of disorder in the Huesler alloys is very sensitive to the way they are heat treated.

Table 1. Relative total energies per f.u. (in eV) with respect to the ordered structure and total magnetic moments (in μ_B/f.u.) for the three types disorder with different $U_{\rm eff}$ values. The subscript of 16 and 32 denote the 16 and 32 atoms unit cells, respectively.

disorders	Co–Fe disorder		Co–Si disorder		Fe–Si disorder	
$U_{\rm eff}$	$\triangle E_{16}$	$\triangle E_{32}$	$\triangle E_{16}$	$\triangle E_{32}$	$\triangle E_{16}$	$\triangle E_{32}$
$U_{7.5}$	0.25	0.10	0.81	0.43	0.21	0.15
U_{10}	0.33	0.14	0.81	0.44	0.21	0.16
U_{15}	0.47	0.22	0.76	0.40	0.21	0.20
U_{20}	0.51	0.26	0.66	0.33	0.20	0.24

The calculated total (/f.u.) and atom-resolved local magnetic moments (in μ_B) are given in Table 2 for the three types of disorder, along with the ordered systems with different U_{10} and U_{15} in a 32 atoms unit cell. For the ordered system, the total magnetic moment (6.0 μ_B) is in good agreement with the experimentally measured saturation magnetic moment (6.0 μ_B/f.u. interpolated to 0 K) and satisfies the Slater–Pauling rule. The integer magnetic moment indicates that the ordered Co_2FeSi is half-metallic ferromagnet. The magnetic moments of Co and Fe are calculated to be 1.54 and 3.20 μ_B, respectively, which agree well with previous band structure calculations.[4,23] The magnetic moments of Co and Fe were previously reported to be 1.70 and 2.37±0.12 μ_B by neutron-diffraction at room-temperature, but with a rather high degree of disorder (about 10% for Co–Fe, 12% for Fe–Si, and 16% for Co–Si disorders),[21] while the magnetic moments of 2.6±0.1 μ_B and 1.2±0.1 μ_B for Fe and Co were obtained from the recent x-ray magnetic circular dichroism (XMCD) experiment at $T = 300$ K and $\mu_0 H = 0.4$ T with a sum rule analysis.[4] We suggest some possible reasons for such disagreement between the theoretical and the experimental values of the magnetic moments. (i) The first-principles calculations are performed at zero temperature, which do not take into account spin fluctuations occurred at room temperature as in the case of the actual measurements. (ii) A local atomic disorder may play an important role. The neutron-diffraction measurement was performed at room temperature and the sample of Co_2FeSi has a high degree of disorder (about 10% Co–Fe, 12% Fe–Si, and 16% Co–Si disorders). The measured magnetic moment of Fe actually represents an average value in the neutron-diffraction and the total magnetic moment ($\sim$ 5.6 μ_B/f.u. interpolated to 0 K) is significantly smaller than that (6.0 μ_B/f.u.) of the recent experiment (with a small (< 10%) disorder between Fe and Si atoms) by magnetometry. Our calculation indicates that the Fe–Si disorder does not affect the total magnetic moment of the system, which is consistent with the experiment.[4] (iii) The magnetic moments obtained from XMCD with a sum

Table 2. The total and atom-resolved local magnetic moments (in μ_B) for the three types disorder as well as the ordered systems with different $U_{\rm eff}$ values for the 32 atoms unit cell.

system	$U_{\rm eff}$	$M_{\rm Co}$	$M_{\rm Fe}$	$M_{\rm Si}$	$M_{\rm total/f.u.}$
Co–Fe disorder	U_{10}	1.34 $\sim$ 1.64	1.95 – 3.12	–0.03 – –0.04	5.50
	U_{15}	1.36 $\sim$ 1.78	1.94 – 3.20	–0.07 – –0.08	5.50
Co–Si disorder	U_{10}	1.49 $\sim$ 1.89	3.01 – 3.15	–0.01 – –0.03	6.05
	U_{15}	1.58 $\sim$ 2.06	3.13 – 3.24	–0.01 – –0.04	6.26
Fe–Si disorder	U_{10}	1.38 $\sim$ 1.67	3.12 – 3.21	–0.01 – –0.02	6.00
	U_{15}	1.41 $\sim$ 1.68	3.16 – 3.26	–0.03 – –0.04	6.00
$L2_1$ order	U_{10}	1.53	3.17	–0.02	6.00
	U_{15}	1.55	3.24	–0.05	6.00

rule could be corrected due to the adequacy of the sum rules which varies from very good (within 5% agreement) to very poor (up to 50% discrepancy).[24] The summarized magnetic moments, $\sim 5.0\ \mu_B$/f.u. resulting from XMCD, are smaller than the experimental value of $6\mu_B$. It was reported that the sum rule evaluations may underestimate the spin magnetic moments of Ni, Co and Fe by about 10%.[25] Therefore, we have multiplied the value by 1.1 to obtain the Co and Fe 3d magnetic moment. As a result, we can obtain magnetic moments of 2.86 μ_B for Fe and 1.32 μ_B for Co, respectively. In addition, the XMCD experiment was carried out at $T = 300$ K and $\mu_0 H = 0.4$ T, thus the magnetic moments interpolated to 0 K may further increase the magnetic moments of Co and Fe and thus may be finally close to our calculated values. The ratio of M_{Fe}/M_{Co} is 2.1 from our LDA+U calculations, which agrees very well with the measured value, 2.2, at 300 K and $\mu_0 H = 0.4$ T. (iv) Other possibilities, such as nonstoichiometry at surface may also be important.

We found that the total magnetic moments for the Co–Fe disorder decreased from 6.00 to 5.50 μ_B due to the decrease of the local magnetic moment of the disordered Fe atom from 3.10 to 1.95 μ_B. On the other hand, for the Co–Si disorder, the total magnetic moment increased to about 6.10 μ_B due to the increase of the local magnetic moment of the disordered Co atom from about 1.50 to 1.90 μ_B. The increased magnetic moment of disordered Co can be attributed to the reconstruction of the energy band due to the change of local symmetry. In the ordered system, the symmetry of the Fe and Si atoms is O_h with eight Co atoms as the first coordination shell (1nn), whereas the Co atom has T_d symmetry with four Fe and four Si as the 1 nn. For the Fe–Si disorder, when an Fe was exchanged by a next-nearest-neighbouring Si, the disordered Fe also has eight Co as the 1nn, while although the swapped Co has four Fe and four Si as the 1nn but the T_d symmetry was destroyed by the disorder. In the Co–Si disordered system, when a Co was swapped by a nearest-neighbouring Si, the disordered Co has seven Co and one Si as the 1nn, which is similar to that of the bcc Co where the Co has eight Co atoms as the 1nn. Indeed, the magnetic moment of disordered Co atom is close to that (1.81 μ_B) of the bcc Co.[26] The study of effect of disorder on the half-metallic character of Co_2MnSi is also suggested that the 1nn mainly dictates the behaviour of the magnetic moments of transition metals.[15] For the Fe–Si disorder, the local magnetic moments of the Co and Fe atoms are affected very little, and the total magnetic moment remains at an integer value of 6.00 μ_B, as in the ordered system, thus, we can expect that the Co_2FeSi keeps its half-metallicity against this kind of disorder. A similar behaviour was found in Co_2MnSi by first-principles calculations,[27] i.e., the total magnetic moments/f.u. are decreased to 4.5 μ_B for Co-Mn disorder, increased to 5.25 μ_B for Co–Si disorder, and unchanged for Mn-Si disorder, respectively, with respect to that (5.0 μ_B) of the ideal case. In the Co–Si disordered system the magnetic moment (about 1.6 μ_B) of disordered Co atom increases than that (1.07 μ_B) of the ordered Co, while the disordered Mn in Co–Mn disorder has a magnetic moment of around –1 μ_B. For the three types of disorders, the 16 atoms unit cell has similar results to the 32 atoms unit cell. The above results are also consistent with the previous first-principles calculation performed by Gercsi *et al.* in a 16 atoms unit cell.[17]

In order to discuss the novel properties of half-metallicity, the spin-polarised total density of states (TDOS) for the three types of disordered systems within a wide range of $U_{eff} \approx U_{7.5}$–U_{20} are presented in Fig. 1. The thick and thin solid lines denote disorders in the 32 and 16 atoms unit cells, respectively. The TDOS of the ordered system (thin broken line) is also given for comparison. The values of the TDOS of the minority spin states were multiplied by -1 and the E_F was set to zero. It is found that in the ordered Co_2FeSi, the E_F shifts gradually from the upper band edge of the minority spin gap to the lower band edge of the minority spin gap when the magnitude of U_{eff} increases from $U_{7.5}$ to U_{20}. It should be noted that not only the Co e_u and Co t_{1u} orbitals, but also the Fe e_g orbitals, will contribute to the conduction bands around the half-metallic gap due to the partially occupied Fe e_g orbitals in the minority band of Co_2FeSi.[28]

For the Co–Fe disorder, we found that at a low level of disorder (6.25%), two new sharp peaks appear within the minority spin-gap of the ordered material below the E_F, which leads to a reduced minority-spin band-gap, while the half-metallic character was still retained in the system. Those peaks mainly originate from the disordered Co and Fe 3d orbitals due to the breaking of the crystal field symmetry. At a high level of disorder (12.5 %), those peaks become strongly dispersed and cross the E_F, thus the half-metallic character was destroyed. We estimated the critical level of disorder, 9.7 % and 8.6 % for U_{10} and

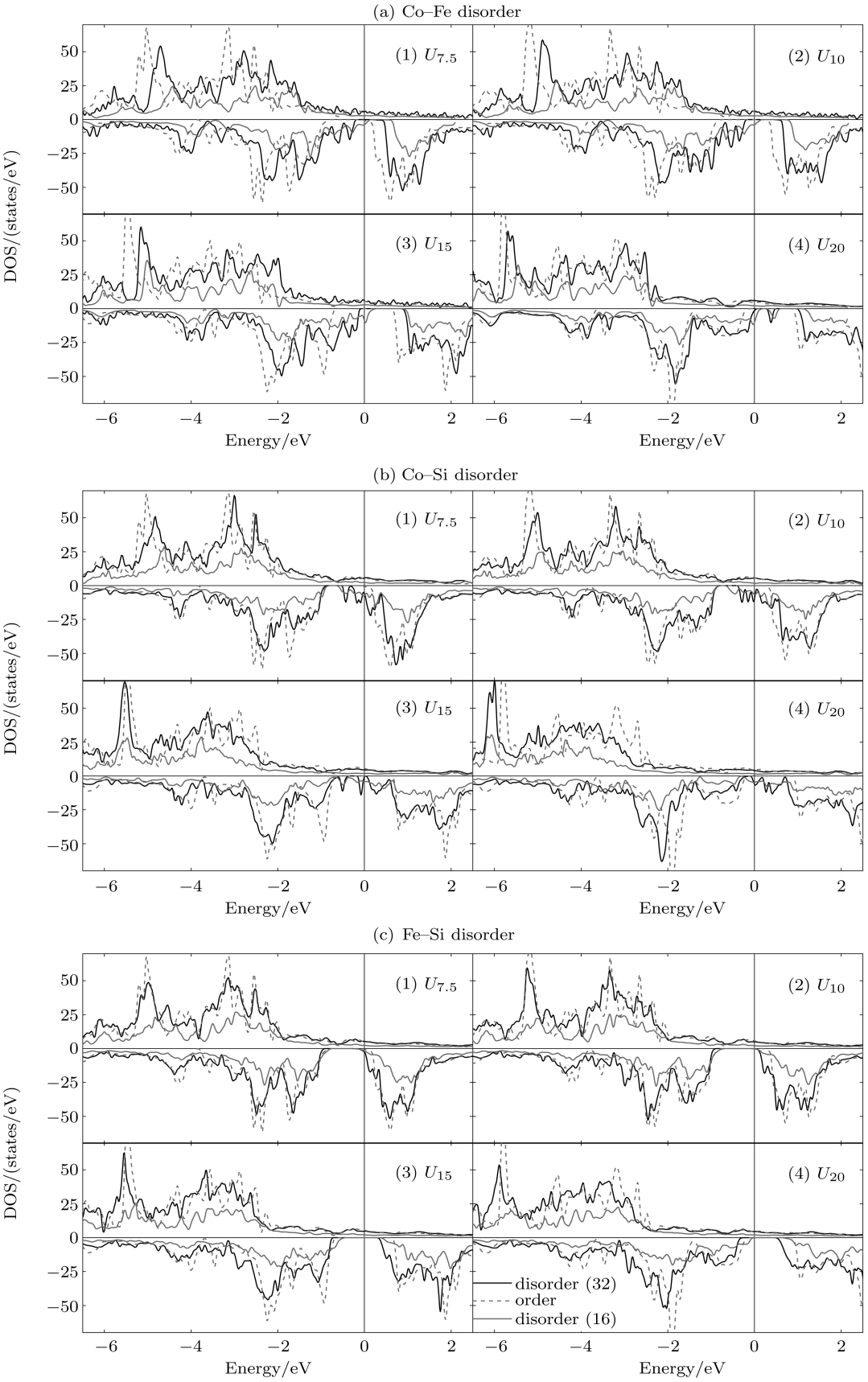


Fig. 1. The TDOS for three types of disordered cells (solid line) and ordered cell (dashed line) with variation of the U_{eff} values. Positive and negative values correspond to majority and minority spin states. The Fermi level is set to zero.

U_{15}, respectively, from the relative positions of the E_F with respect to the right edges of the dispersed states, where we assumed that the distance between the E_F and the right edges of the dispersed states decreased monotonically when increasing the levels of disorder. Other first-principles calculations performed by the OpenMX software package pointed out a 100 % spin polarisation at the E_F for 12.5 % of the disorder.[17] We think that this quantitative disagreement with our FLAPW results are probably to be ascribed to the use of the pseudopotential approach in the OpenMX. Our results are overall consistent with those reported by Orgassa *et al.*[29] for NiMnSb: in the case of a Ni–Mn disorder similar to the Co–Fe disorder studied here, a peak arises just below the E_F in the minority spin band. The peak broadens in energy when increasing the disorder levels, finally reaching the E_F and resulting in the loss of half-metallicity.

A dramatic change of the TDOS in the minority band-gap at the E_F is found for the Co–Si disorder, regardless of the disorder levels. One can see additional states in the minority band-gap at the E_F; thus, the half-metallcity was destroyed by the disorder. The atom resolved DOSs (not presented here) show that the disordered Co 3d orbitals are main contributors to the additional states.

The most interesting finding is that the half-metallicity was preserved for the Fe–Si disorder, regardless of the disorder levels, as was indicated from the integer total magnetic moment. At a low level (12.5%) of the disorder, the TDOS of minority valence bands is very similar for both ordered and disordered systems, while that of the minority conduction bands were shifted toward low energy regions by $\sim$ 0.27 eV, resulting in the reduced band-gap; nevertheless, the half-metallic character still remained as for the ordered alloy. The atom resolved DOSs (not shown here) show that the antibonding minority spin e_g states of disordered Fe mainly contribute to the shifting of the minority conduction bands. When increasing the level of disorder up to 25.0 %, the Fe 3d derived state appears just below the E_F in the minority spin band due to the increased next-nearest Fe–Fe interactions, which reduce their band-gap.

The above results indicate that at a low level of the disorder, the 1nn is the most relevant to the half-metallicity, while at a high level of the disorder, the next-nearest neighbouring interaction between the transition metal atoms also plays an important role, which would reduce (or destroy) the band-gap.

4. Summary

In this work, we have investigated the electronic structure, magnetism, and half-metallicity of three types of disorder in Co_2FeSi by using the FLAPW method within the GGA and GGA+U schemes. We have considered three types of atomic disorders: the Co–Fe, Co–Si, and Fe–Si disorders in the full-Heusler Co_2FeSi alloy. From the total energy calculations, we found that among the three types of disorders, the Fe–Si disorder was most likely to occur. The total magnetic moment for the Co–Fe (Co–Si) disorder is decreased (increased), while that remains at an integer value of 6.00 μ_B for the Fe–Si disorder. It is found that for the Co–Si disorder, additional states appear in the minority band-gap at the E_F, and the half-metallcity was substantially destroyed, regardless of the disorder level. On the other hand, the Co–Fe and Fe–Si disorder have a litter effect on the half-metallicity at a low disorder level. When increasing the disorder levels, the half-metallcity was destroyed at about 9 % of the Co–Fe disorder level, while that stays at 25.0% of the Fe–Si disorder level. We found that at a low level of the disorder, the first coordination shell is the most relevant to the half-metallicity, while at a high level of the disorder, the next-nearest neighbouring interaction between the transition metal atoms also plays an important role, which would reduce (or destroy) the band-gap.

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