Search for half-metallic ferrimagnetism in V-based Heusler alloys Mn_2VZ (Z = Al, Ga, In, Si, Ge, Sn)

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Abstract
Using a state-of-the-art full-potential electronic structure method within the local spin density approximation, we study the electronic and magnetic structure of Mn_2V-based full Heusler alloys: Mn_2VZ (Z = Al, Ga, In, Si, Ge and Sn). We show that small expansion of the calculated theoretical equilibrium lattice constants restores the half-metallic ferrimagnetism in these compounds. Moreover, a small degree of disorder between the V and Z atoms, although it induces some states within the gap, preserves the Slater–Pauling behaviour of the spin magnetic moments and the alloys keep a high degree of spin polarization at the Fermi level, opening the way for a half-metallic compensated ferrimagnet.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Recently rapid development of magneto-electronics intensified the research on ferromagnetic materials that are suitable for spin injection into a semiconductor [1]. One of the promising classes of materials is the half-metallic ferrimagnets, i.e., compounds for which only one spin channel presents a gap at the Fermi level, while the other has a metallic character, leading to 100% carrier spin polarization at E_F [2, 3]. Half-metallic ferromagnetism (HMF) was discovered by de Groot *et al* in 1983 when studying the band structure of semi-Heusler compound NiMnSb [4]. Ishida *et al* have also proposed that the full-Heusler alloy compounds of the type Co_2MnZ, where Z stands for Si and Ge, are half-metals [5]. Since then many others have been predicted on the basis of ground state calculations, such as magnetic oxides (CrO_2 and Fe_3O_4) and colossal magnetoresistance materials (Sr_2FeMoO_6 and $La_{0.7}Sr_{0.3}MnO_3$) [6]. Finally, the diluted magnetic semiconductors ($Ga_{1-x}Mn_xAs$) and MnAs and CrAs in the zinc-blende crystal structure have attracted a lot of attention [7–9].

Heusler alloys have been particularly interesting systems because they exhibit much higher ferromagnetic Curie temperature than other half-metallic materials [10]. Among the other properties useful for the applications are the crystal structure and lattice matching compatible with zinc-blende semiconductors used industrially [11, 12].

Mn_2VAl received much experimental and theoretical attention. The neutron diffraction experiment by Itoh *et al* [13] revealed the ferrimagnetic ordering in this compound with a Mn magnetic moment of 1.5 ± 0.3 μ_B and a V moment of -0.9 μ_B. Yoshida *et al* studied the magnetic and structural properties of $Mn_2V_{1+x}Al_{1-x}$ as a function of x [14]. The authors found that the structure preserved the $L2_1$-type phase for $-0.3 < x < 0.2$ with linearly varying saturation moment. For $x \geqslant 0.2$ a structural transformation from $L2_1$-phase to a disordered B2-type phase has been detected. Recently, Jiang *et al* examined the magnetic structure of Mn_2VAl by x-ray diffraction and magnetization measurements [15]. They found that Mn_2VAl was nearly half-metallic with the total magnetic moment of 1.94 μ_B at 5 K. The loss of half-metallic character was attributed to the small amount of disorder in V and Al sublattices.

The electronic structure of Mn_2VAl has been studied for the first time by Ishida *et al* [16]. The authors used the local-density approximation (LDA) to the density functional theory and showed that the ground state of Mn_2VAl was close to half-metallicity. Recently, a detailed theoretical study of the magnetism of Mn_2VAl was reported by Weht and Pickett [17], who used the generalized gradient approximation (GGA) for the exchange–correlation potential and have shown that Mn_2VAl is a half-metallic ferrimagnet with the atomic moments of 1.5 and -0.9 μ_B for Mn and V atoms respectively, in very good agreement with experiment. The Fermi level was found to lie in the minority spin band. In 2005 Şaşıoğlu *et al* studied the exchange interaction and Curie temperature in the Mn_2VZ (Z = Al, Ge) half-metallic compounds and showed that the antiferrimagnetic coupling between the V and Mn atoms stabilizes the ferromagnetic alignment of the Mn spin moments [18].

2. Motivation

Half-metallic ferrimagnetic materials, like FeMnSb or the Mn_2VZ compounds, are much more desirable than their ferromagnetic counterparts in magneto-electronic applications. This is mostly due to the fact that the small value of the total magnetic moment in these systems provides additional advantages. For example, they do not give rise to strong stray fields in devices and are less affected by external magnetic fields.

The ideal case for applications would be a half-metallic antiferromagnet like CrMnSb. It is a special antiferromagnet in the sense that the majority spin and minority spin densities of states are not identical, as for common antiferromagnets, and the material is better described as a fully compensated ferrimagnet, having a magnetic moment that is, due to the half-metallic character, precisely equal to zero. Such a half-metallic antiferromagnet would be a very interesting magneto-electronic material since it would be a perfectly stable spin-polarized electrode in a junction device. Moreover, if used as a tip in a spin-polarized STM, it would not give rise to stray flux, and hence would not distort the domain structure of the soft-magnetic systems to be studied. Unfortunately, CrMnSb does not crystallize in the ordered $C1_b$ crystal structure adopted by the half-Heusler alloys. However, these results show that such an important magneto-electronic material could exist. Van Leuken and de Groot have recently suggested a possible route towards a half-metallic antiferromagnet starting from the semiconducting $C1_b$-type compound FeVSb [19]. It is isoelectronic with the non-existing half-metallic antiferromagnet CrMnSb. A 12.5% substitution of Mn for V, and (in order to keep the system isoelectronic) In for Sb, was predicted to already yield half-metallic ferrimagnetism, with local Mn moments of about 2.3 μ_B and a bandgap of about 0.35 eV.
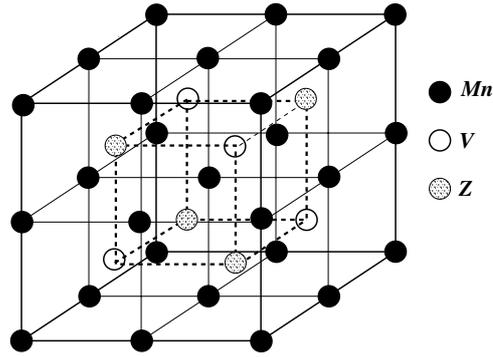
Figure 1. Schematic representation of the L2$_1$ structure adapted by the full Heusler compounds. The lattice consists of four interpenetrating fcc sublattices with the positions $(0, 0, 0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ for the Mn and $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ and $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ for the V and sp (Z) atoms, respectively.

In the present paper, we systematically study the electronic and magnetic structure of V-based full Heusler alloys Mn$_2$VZ (Z = Al, Ga, In, Si, Ge and Sn) to search for new half-metallic ferrimagnetic candidates and search for a way to decrease their spin-moment in order to reach the ideal case of the half-metallic compensated ferrimagnet. Among the systems studied Mn$_2$VZ (Z = Al, Ga, In and Sn) are predicted to be nearly half-metallic at theoretical equilibrium lattice constants. We demonstrate that half-metallicity can be achieved in Mn$_2$VZ (Z = Al, Se, Ge and Sn) by expanding the lattice parameter by a few per cent and can be maintained for a small range of lattice constants. Finally, the effect of disorder, and more specifically the intermixing of V and sp atoms, on the half-metallicity and spin polarization of Mn$_2$VAl is discussed.

The paper is organized as follows. In section 3 we present the calculational approach. Section 4 contains the results and the discussion on the total energy calculations and section 5 is devoted to the effect of disorder. Finally, in section 6 we summarize and conclude.

3. Calculational method

Full Heusler compounds crystallize in the L2$_1$-type structure (see figure 1). The lattice consists of four interpenetrating fcc sublattices and is characterized by the formula X$_2$YZ. In the compounds under study, Mn atoms occupy the X sites in contrast to the majority of the Heusler alloys, for which the Mn atom usually enters as the Y element. Vanadium atoms occupy the Y sites while the Z site corresponds to the sp element (in our case Al, Ga, In, Si, Ge, or Sn).

The electronic structure calculations are performed using the full-potential nonorthogonal local-orbital minimum-basis band structure scheme (FPLO) [20]. We use the scalar relativistic formulation and thus the spin–orbit coupling is not taken into account. The exchange–correlation potential is chosen in the local spin density approximation (LSDA) [21]. The self-consistent potentials were calculated on a $20 \times 20 \times 20$ **k**-mesh in the Brillouin zone, which corresponds to 256 k points in the irreducible Brillouin zone. The sets of valence orbitals in the FPLO calculations were selected as 3s, 3p, 4s, 4p, 3d for Mn, Ga, Ge and V, 4s, 4p, 5s, 5p, 4d for In and Sn and 2s, 2p, 3s, 3p, 3d for Al and Si. All lower states were treated as core states.

Disorder in Mn$_2$V$_{1-x}$Al$_{1+x}$ was introduced within the coherent potential approximation (CPA) implemented in FPLO code [20].
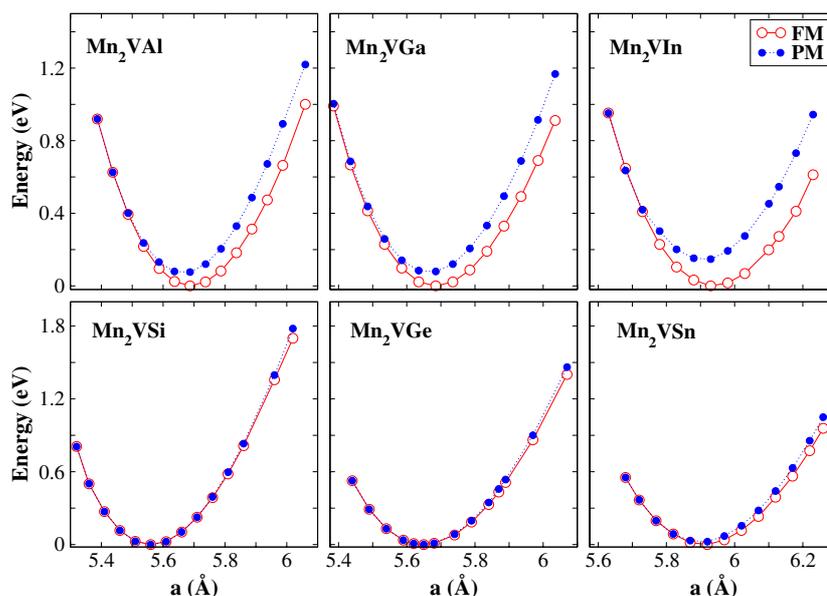
Figure 2. Calculated total energy for all studied compounds as a function of lattice constant for both the non-magnetic (PM) and ferrimagnetic (FM) cases. The total energies have been rescaled so that the zero energy corresponds to the calculated equilibrium lattice constant. Spheres represent calculated values.

4. Half-metallic ferrimagnetism in Mn$_2$VZ (Z = Al, Ga, In, Si, Ge, Sn)

4.1. Total energy and lattice parameter

The first task which we undertook was to calculate how the total energy changes with the lattice constant and thus to find the theoretical equilibrium lattice parameter. We performed calculations both for the non-magnetic and the ferrimagnetic cases and we summarize our results in figure 2. There is a clear difference when the sp atom belongs to the IIIB column of the periodic table (Al, Ga or In) having three valence electrons with respect to the case of a IVB column sp element (Si, Ge or Sn) with four valence electrons. For Mn$_2$VAl (Ga or In) it is clear that the ferrimagnetic state is the most stable one and the stability (relative energy difference between the FM and PM curves) increases when the sp element is heavier, reaching a value of around 0.15 eV for Mn$_2$VIn at the equilibrium lattice constant. In table 1 we have gathered the equilibrium lattice constants, the difference in energy between the FM and PM states and the atom-resolved and total spin moments. Interestingly, Mn$_2$VAl has a similar lattice constant to Mn$_2$VGa and one has to go to Mn$_2$VIn to see an important difference in the calculated equilibrium lattice constant. Note also that the total spin moments are not integers and thus the system is not half-metallic at the equilibrium lattice constants.

The case of Mn$_2$VSi (Ge or Sn) compounds is more interesting. Here the non-magnetic and ferrimagnetic configurations are almost degenerated. As we can see in figure 2, around the equilibrium lattice constants it is impossible to distinguish the black spheres representing the non-magnetic state from the empty ones representing the ferrimagnetic state. Exactly at the equilibrium lattice constant we were not able to converge the ferrimagnetic solution for Mn$_2$VSi and Mn$_2$VGe compounds and thus in table 1 we give only the equilibrium lattice constant. On the other hand in the case of the Mn$_2$VSn compound the ferrimagnetic state is

Table 1. The calculated equilibrium lattice parameters (in ferrimagnetic state), the energy difference ΔE between the ferrimagnetic and non-magnetic state at the equilibrium lattice constant and the atom-resolved spin magnetic moments in μ_B for the Mn_2VZ (Z = Al, Ga, In, Si, Ge and Sn) compounds. The last column is the total spin magnetic moment in the primitive cell. Note that for Si and Ge compounds we could not converge a ferrimagnetic calculation at the equilibrium lattice constant (see the text).

Compound	a (Å)	ΔE (eV)	m_{Mn}	m_V	m_Z	m_{Cell}
Mn_2VAl	5.687	0.076	−1.264	0.581	0.017	−1.93
Mn_2VGa	5.685	0.079	−1.254	0.603	0.040	−1.865
Mn_2VIn	5.930	0.140	−1.404	0.853	0.038	−1.917
Mn_2VSi	5.560	0.000	0.000	0.000	0.000	0.000
Mn_2VGe	5.650	0.000	0.000	0.000	0.000	0.000
Mn_2VSn	5.920	0.025	−0.696	0.447	0.024	−0.921

energetically preferable with respect to the non-magnetic one but the energy difference at the equilibrium lattice constant is only 0.025 eV, much smaller than the Al-, Ga- and In-based compounds. Unfortunately, only the Mn_2VAl compound has been grown experimentally. But we expect the magnetic properties of the Mn_2VSi (Ge or Sn) compounds to strongly depend on the substrate and the growth conditions and the latter compounds will very easily oscillate between the magnetic and non-magnetic configurations.

Finally, we should also note for the Mn_2VSi and Mn_2VGe compounds that a very small expansion of the lattice parameter with respect to the theoretical equilibrium lattice constant of the order of 1% now stabilizes the ferrimagnetic state, leading to a jump in the spin magnetic moments, being the sign of a metamagnetic transition. The intermediate region requires a systematic study with the fixed spin moment approach, which is out of the scope of the present work. For the Mn_2VSi compound the Mn spin moment reaches a value of -0.87 μ_B and V a moment of 0.35 μ_B, with the total spin moment being -0.62 μ_B. For Mn_2VGe the corresponding moments are $-0.82, 0.32$ and -0.57 μ_B. Similar behaviour to Mn_2VSi and Mn_2VGe has also been found in the Fe_2FeSi and Fe_2FeAl Heusler compounds [22] and in Ni_2MnSn [23].

4.2. Effect of the lattice parameter: appearance of half-metallicity

All compounds under study are not half-metallic at their theoretical equilibrium lattice constants. This is obvious from table 1, where the total spin moments in a cell are not integer numbers. Galanakis and collaborators have shown that in the case of half-metallic full-Heusler alloys the total spin moment in μ_B follows the relation $Z_t - 24$, where Z_t is the total number of valence electrons, even for compounds with less than 24 electrons such as the ones under study [24]. Mn_2VAl (Ga or In) have 22 valence electrons per cell and thus they should have a total spin moment of -2 μ_B while the other three compounds Mn_2VSi (Ge or Sn) have in total 23 valence electrons and a total spin moment per cell of -1 μ_B in the case of half-metallicity. This is obviously not the case in table 1.

But even if these compounds are not half-metallic in their equilibrium lattice constants, small expansion of the lattice parameter restores the half-metallicity. In figure 3 we have drawn the spin-resolved density of states (DOS) projected on each atom for Mn_2VAl and Mn_2VSi compounds. The rest of the compounds present DOSs similar to their isoelectronic counterparts. If we follow the nomenclature introduced in [24] to denote the spin-up and spin-down bands in Heusler alloys, for the Mn_2VZ compounds the situation is reversed to all other full-Heusler alloys. Now the minority spin-band is the spin-up one and the majority is the
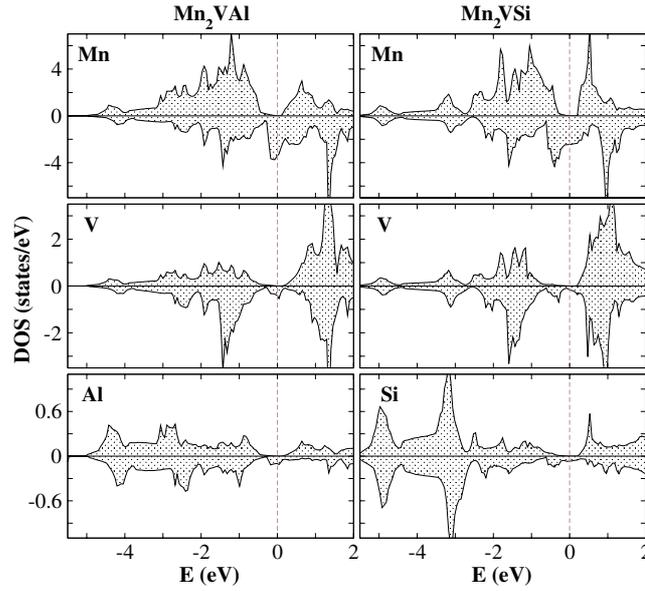
Figure 3. Calculated atom and spin-resolved density of states (DOS) for the Mn$_2$VAl and Mn$_2$VSi compounds when they are half-metallic.

Table 2. Half-metallic lattice parameters and spin magnetic moments (in μ_B) of Mn$_2$VZ (Z = Al, Si, Ge and Sn).

Compound	a (Å)	m_{Mn}	m_V	m_Z	m_{Cell}
Mn$_2$VAl	5.987	−1.510	0.967	0.053	−2.00
	6.117	−1.655	1.233	0.076	−2.00
Mn$_2$VSi	6.06	−0.863	0.675	0.052	−1.00
	6.29	−1.092	1.105	0.078	−1.00
Mn$_2$VGe	6.18	−0.976	0.905	0.048	−1.00
	6.27	−1.082	1.111	0.054	−1.00
Mn$_2$VSn	6.25	−0.980	0.922	0.038	−1.00
	6.31	−1.050	1.059	0.041	−1.00

spin-down. Thus the gap is situated in the spin-up band and not the spin-down one [24]. This also explains why in table 1 the total spin moment is negative. When we pass from Mn$_2$VAl to Mn$_2$VSi which has one electron more we populate one more spin-down state and the total spin moment changes from −2 to −1 μ_B. The charge of this electron is attributed one-third to V and two-thirds to Mn. We also remark in figure 3 that the gap is larger for V and Al or Si atoms with respect to the Mn ones. The states responsible for this difference are the t$_{1u}$ states of Mn just below the Fermi level (see discussion in [24]).

In table 2 we have gathered the half-metallic parameters and the spin moments for four of the compounds under study. We provide for each compound the smallest and largest lattice constant for which half-metallicity is present. Of course, the heavier the system the larger the lattice parameters. We also note that the range of parameters for which half-metallicity appears is doubled in the case of Mn$_2$VAl (Si) with respect to Mn$_2$VGe and even tripled with respect to Mn$_2$VSn. The lighter the elements, the smaller the Coulomb repulsion, and this leads to larger
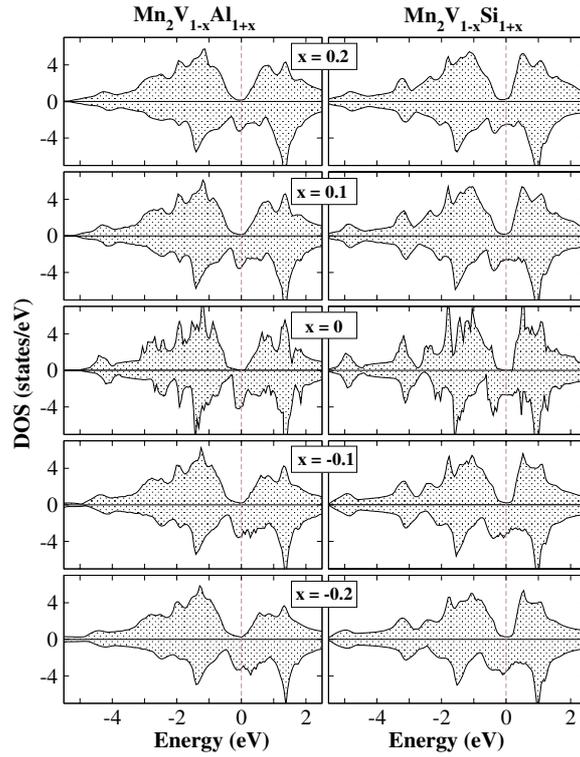
Figure 4. Spin-resolved DOS for the $Mn_2V_{1-x}Al_{1+x}$ (left panel) and $Mn_2V_{1-x}Si_{1+x}$ (right panel) compounds.

gaps covering a larger area of lattice constants. Expansion of the lattice leads in all cases to a small rearrangement of the charge and the absolute values of the spin moments of all atoms increase. In particular, in the case where the sp belongs to the IVB column the spin moment of V is comparable to the spin moment of each Mn atom. Concluding, we should note that half-metallicity is feasible in these compounds depending on the lattice parameter adopted, and thus the choice of the proper substrate in experiments is of primordial importance to get the highest possible spin polarization in experiments.

5. Effect of disorder on the half-metallicity: $Mn_2V_{1-x}Al_{1+x}$ and $Mn_2V_{1-x}Si_{1+x}$ alloys

The effect of mixing the sp atom has already been extensively studied for the full Heusler alloys, and in particular in [25] it was shown that mixing the Al and Ge atoms does not destroy the gap. On the contrary, the $Mn_2V[Al_xGe_{1-x}]$ remains half-metallic for any concentration of Al and Ge atoms. This implies that it also shows the Slater–Pauling behaviour and the total spin moment scales following the rule $Z_t - 24$. In our study we will seek the influence of now mixing the lower valent transition metal atom (V) and the sp atom. We took as prototypes Mn_2VAl and Mn_2VSi at such a lattice constant that the Fermi level lies in the middle of the gap, and then studied the families $Mn_2V_{1-x}Al_{1+x}$ and $Mn_2V_{1-x}Si_{1+x}$ for $x \in [-0.2, 0.2]$ with a step of 0.05.

In figure 4 we have gathered the spin-resolved DOS for all cases under study. The left panel contains the results for the Al-based compounds. We note that for $x = 0$ we have a half-
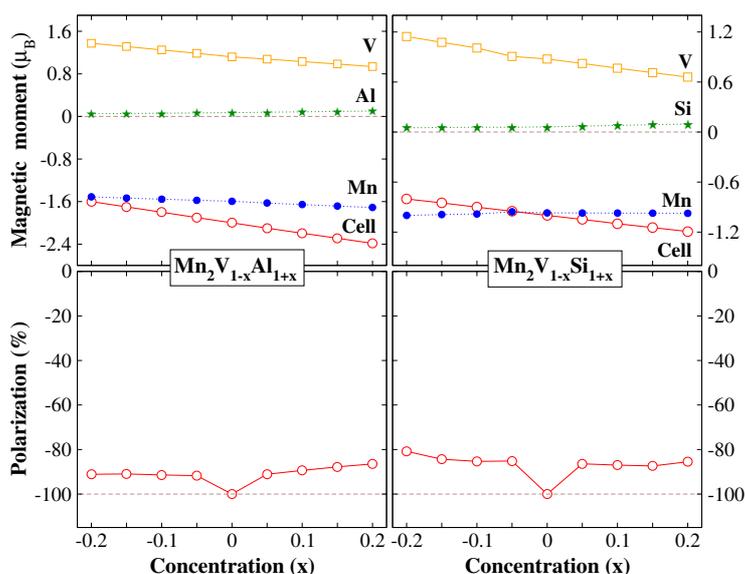
Figure 5. Variation of the spin magnetic moments and the spin polarization at the Fermi level with the concentration x for the $Mn_2V_{1-x}Al_{1+x}$ and $Mn_2V_{1-x}Si_{1+x}$ compounds.

metallic compound as already stated. When we have a surplus of Al atoms ($x = 0.1$ and 0.2) then the gap shrinks to almost zero but the Fermi level continues to fall within it. An excess of V atoms ($x = -0.1$ and -0.2) has a similar effect. The physics is even clearer when we look at figure 5, where we represent the variation of the spin moments and spin polarization with the concentration. When we are away from $x = 0$ the system keeps a high degree of spin polarization of about -90%, which means that almost all electrons ($\sim 95\%$) are of spin-down character. The spin-magnetic moment of the Mn atom is not influenced by the disorder and remains almost constant for all values of x. The spin moment of Al is almost negligible and has no real effect on the total spin moment. It is the spin moment of V which changes, but as we can see from the total spin moment in the cell it follows the Slater–Pauling behaviour. For $x = -0.2$ we have the $Mn_2V_{1.2}Al_{0.8}$ compound, which has on average 22.4 electrons per unit cell and thus the total spin moment should be $-1.6\ \mu_B$ for the half-metallic case. For $x = 0.2$, the compound $Mn_2V_{0.8}Al_{1.2}$ has on average 21.6 valence electrons and thus half-metallicity corresponds to $-2.4\ \mu_B$. These values coincide with the calculated one presented in figure 5.

In the case of the $Mn_2V_{1-x}Si_{1+x}$ compounds the effect of disorder is much larger and as we can see from figure 5 away from half-metallicity the spin polarization is as low as -80% and thus $\sim 90\%$ of electrons at the Fermi level are of spin-down character. But the system remains almost half-metallic as we can conclude by studying the variation of the total spin moment. The values $x = -0.2$ and $x = 0.2$ correspond to 23.2 and 22.8 total valence electrons in the cell on average, respectively. The calculated total spin moments are about 0.8 and 1.2 μ_B as expected from the Slater–Pauling curve for the half-metallic systems. Thus although disorder leads to a decrease of the spin polarization, a small amount of disorder keeps an almost half-metallic character in the system.

The case of $Mn_2V_{1-x}Si_{1+x}$ compounds is a very interesting one. Decreasing slightly the concentration in Si keeps a really high spin polarization and in the meantime the total spin moment in the cell decreases, reaching a value of less than 1 μ_B while the individual spin moments of V and Mn atoms stay really high. In this respect the case of $Mn_2V_{1.2}Si_{0.8}$ is very

near to what we can call an ideal half-metallic compensated ferrimagnet. Moreover, even in the ideal case, half-metallicity would be lost in the case of surfaces or interfaces [26], making such a system even more attractive and a possible candidate for spintronic devices.

6. Conclusions

We have studied the possibility of appearance of half-metallicity in the case of the full Heusler compounds Mn_2VZ, where Z is an sp atom belonging to the IIIB or IVB column of the periodic table. These compounds show ferrimagnetism with the V and Z spin moments being antiparallel to the Mn ones. Firstly we performed total-energy calculations for both the non-magnetic and ferrimagnetic configurations to find the stable magnetic configuration and the equilibrium lattice constant. We found that when Z is Al, Ga, In and Sn the ferrimagnetic is stable with respect to the non-magnetic state, while for the Si and Ge compounds at the equilibrium lattice constant we could converge only the non-magnetic solution. A small expansion of the lattice leads to the emergence of ferrimagnetism also in these compounds.

Although all compounds are not half-metallic at their equilibrium lattice constant, small expansion of the lattice pushes the Fermi level within the gap, which is now situated in the spin-up band, in contrast to all other full Heusler alloys. The total spin moment is $-2\ \mu_B$ for the Mn_2VAl (Ga or In) compounds, which have 22 valence electrons per unit cell, and $-1\ \mu_B$ for the Mn_2VSi (Ge or Sn) compounds, with 23 valence electrons. Thus these compounds follow the Slater–Pauling behaviour and the 'rule of 24' [24]. The lighter the element and the smaller the number of valence electrons, the wider is the gap and the more stable is the half-metallicity with respect to the variation of the lattice constant.

Finally, we examined in the case of the half-metallic Mn_2VAl and Mn_2VSi compounds the effect of intermixing V with the Al or Si atoms. We found that a small degree of disorder decreases the spin polarization at the Fermi level from its ideal -100% value, but since this effect is only local the resulting alloys still show an almost half-metallic behaviour.

A small degree of substitution of V atoms for Si ones in Mn_2VSi keeps a high degree of spin polarization, and as shown by the total spin moment in the cell the compound stays almost half-metallic. In the meantime the total spin moment considerably decreases and the alloy is very near to what we can call an ideal half-metallic compensated ferrimagnet, which has several advantages for realistic spintronic applications. Our work urges experimentalists to grow new half-metallic alloys on suitable substrates to get new candidates for spintronic applications.

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