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Half-metallic ferrimagnetism in the $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys adopting the zincblende and wurtzite structures from first-principles

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ABSTRACT

Employing first-principles calculations we study the structural, electronic and magnetic properties of the $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys assuming that they crystallize in the zincblende and wurtzite structures. Both structures are degenerated with respect to the total energy. For all concentrations the alloys in these lattice structures are half-metallic with the gap located in the spin-down band. The total spin moment follows the Slater–Pauling behavior varying linearly between the $-1\,\mu_B$ of the perfect ScC and ScSi alloys and the $+1\,\mu_B$ of the perfect VC and VSi alloys. For the intermediate concentrations V and Sc atoms have antiparallel spin magnetic moments and the compounds are half-metallic ferrimagnets. At the critical concentration, both $[Sc_{0.5}V_{0.5}]C$ and $[Sc_{0.5}V_{0.5}]Si$ alloys present zero total spin-magnetic moment but the C-based alloy shows a semiconducting behavior contrary to the Si-based alloys which is a half-metallic antiferromagnet.

1. Introduction

Half-metallic ferromagnets have attracted considerable attention during the last decade due to their potential applications in magnetoelectronic devices [1]. The term "half-metal" was initially introduced by de Groot et al. to denote the peculiar behavior exhibited by a Heusler compound: NiMnSb [2]. The have found using first-principles calculations that the majority-spin band was metallic while the minority-spin band was semiconducting leading to 100% spin-polarization of the electrons at the Fermi level. This behavior was later on confirmed both by infrared absorption [3] and by spin-polarized positron annihilation [4] experiments.

Although Heusler alloys have attracted a lot of interest as potential half-metallic systems, the discovery of Akinaga et al. has shown the possibility to grow new half-metallic systems in metastable structures usually adopted by thin films [5]. They have shown that the CrAs/GaAs multilayers are ferromagnets and surprisingly the X-ray diffraction measurements suggested that CrAs adopts the lattice structure of GaAs and grows in the metastable zincblende structure. Moreover SQUID measurements have shown that CrAs exhibits an integer total spin magnetic moment of $3\,\mu_B$ per unit cell [5]. These findings have intensified the interest on transition-metal pnictides and chalcogenides like CrAs and CrSe which crystallize either in the zincblende or wurtzite structures of binary semiconductors and an extended review can be found in Ref. [6]. Galanakis and Mavropoulos have studied using first-principles calculations several such compounds and have determined the lattice constants for which half-metallicity is present [7]. Moreover they have explained the gap in terms of the $p-d$ repulsion; the p orbitals of the sp atom hybridize with the t_{2g} orbitals of the transition metal atoms creating three bonding and three antibonding states. The gap is created between these states. The e_g orbitals of the transition metal atom are very localized in energy since they do not hybridize with other orbitals and they are placed above the Fermi level in the spin-down band. Their relative position with respect to the antibonding $p-t_{2g}$ orbitals depends on each system. It has been also shown in the same reference that except the three bonding $p-t_{2g}$ bands below the Fermi level exists also a deep s band. Thus, since there are exactly four spin-down occupied bands, the total spin moment, M_t, follows a Slater–Pauling behavior and it equals in μ_B units: $M_t = Z_t - 8$ where Z_t the total number of valence electrons in the unit cell.

As we mentioned above most of the studies concern cases where the sp atom belongs to the Vth (pncitides) or the VIth (chalcogenides) column of the periodical table. The case where the sp atom comes from the IVth column of the periodical table

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has attracted much less attention in literature and to the best of our knowledge only the cases of MnC [8–10], MnSn [9] and MnSi [11–13] in the zincblende lattice have been studied. In this manuscript we study using the full-potential nonorthogonal local-orbital minimum-basis band structure scheme (FPLO) [14] within the local density approximation (LDA) [15] the case of $[Sc_{1-x}V_x]C$ and $[Sc_{1-x}V_x]Si$ alloys for x taking the values $0, 0.1, 0.2, \ldots, 0.9, 1$. The disorder is simulated using the coherent potential approximation [16]. ScC and ScSi compounds have seven electrons per unit cell and, if they are half metals, they should show a total spin moment of $-1\,\mu_B$. On the other hand VC and VSi have nine electrons and, if they are half-metals, should exhibit a total spin moment of $+1\,\mu_B$. Thus within these families of alloys we can study the transition at the $x = 0.5$ concentration where the total spin moment changes sign. In Section 2 we study the perfect compounds to determine the equilibrium lattice constants. In Section 3 we continue our study with the case of the magnetic zincblende and wurtzite structures which are degenerated with respect to their total energy and we study both the electronic and magnetic properties. We show that for the intermediate concentrations the total spin moment scales linearly with the concentration and the Sc and V atoms have antiparallel spin magnetic moments. We also try to explain why for $x = 0.5$ the C-based alloy is a semiconductor while the Si-based alloys is a half-metallic antiferromagnet [17]. The latter property is highly desirable for applications since such materials create vanishing stray fields and thus minimize energy losses in devices. Finally in Section 4 we summarize and present our conclusions.

2. Total energy calculations

We will start the presentation of our results discussing the equilibrium lattices and lattice constants. We have taken into account two different lattices: (i) the zincblende and (ii) the wurtzite (WZ) structures, and we present in Fig. 1 the calculated total energy as a function of the volume of the unit cell. Before proceeding with the discussion and presentation of our results we should focus on the characteristics of the two structures under study. Both ZB and WZ structures are open structures. In the ZB structure the lattice is an fcc with four sites as basis set along the diagonal, but now two out of the four sites are empty. The WZ is the hexagonal analogue of the ZB structure. In our WZ calculations we have varied only the in-plane lattice parameter a and we have considered that the c/a ratio is for all calculations the ideal $(\frac{8}{3})^{1/2}$ for which the nearest environment in the WZ structure is the same with its cubic ZB analogue. Finally we should mention that in the ZB there is one transition-metal atom and one sp atom per unit cell while in the WZ structure there are two atoms of each chemical kind. We have divided in the WZ case by two all the properties, which are calculated per unit cell (total density of states, total spin magnetic moment and total energy), in order to compare them directly to the ZB case.

For all four perfect compounds presented in Fig. 1 the total energy calculations suggest that the ZB and WZ structure are almost degenerated and thus, when grown as thin films on top of semiconductors, the unit cell can easily deform itself. In the same figure we have also denoted the equilibrium lattice constants both

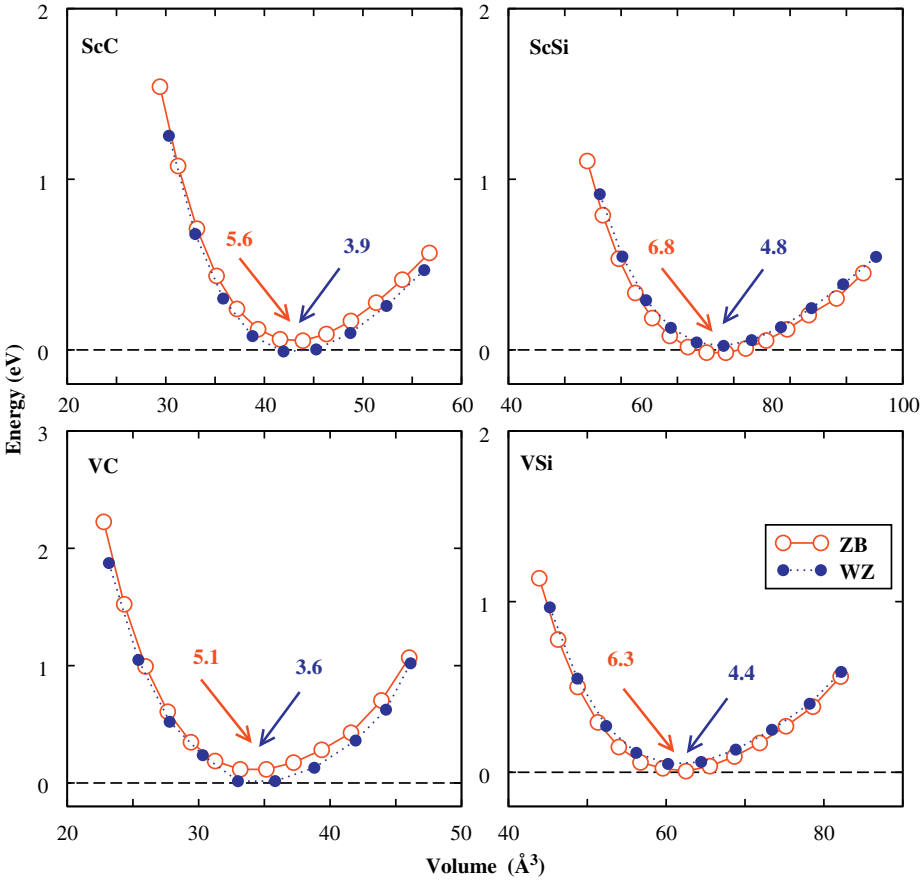

Fig. 1. (Color online) Calculated total energy as a function of the volume of the unit cell for ScC, ScSi, VC and VSi in the zincblende (ZB) and wurtzite (WZ) structures. The zero of the total energy is defined as the energy of the global equilibrium volume and with arrows we represent the corresponding equilibrium lattice constant; for the WZ structure which is not cubic we give the in-plane lattice parameter a and the c/a ratio is for all calculations the ideal $(\frac{8}{3})^{1/2}$ for which the nearest environment in the WZ structure is the same with its cubic ZB analogue. In the ZB there is one transition-metal atom and one sp atom per unit cell. In the WZ structure there are two atoms of each chemical kind but we have divided the energy by two to compare it directly to the other two cases.