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Design of half-metallic Heusler-based superlattices with vanishing net magnetization

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Employing first-principles electronic structure calculations, we show that it is possible to achieve half-metallic antiferromagnetism in artificial superlattices based on Heusler compounds. Suitable alternation of full-Heusler compounds with more and less than 24 valence electrons in the unit cell results in superlattices with zero total spin magnetic moment keeping the half-metallic character of the initial compounds. We demonstrate it considering superlattices made up from Mn_2TiGe (Mn_2VGa) and Co_2TiGe (Co_2VGa) compounds, which have 22 and 26 valence electrons, respectively. Moreover, these compounds posses similar lattice constants and have been already grown as thin films making them promising for spintronics devices. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4789361]

I. INTRODUCTION

Half-metallic compounds play a central role in contemporary materials science due to their potential applications in spintronics/magnetoelectronics.[1–3] With the term "half-metal," we describe solids for which the one of the two spin-electronic band structures is metallic while the other is semiconducting resulting in 100% spin polarization of the conduction electrons at the Fermi level.[2,3] Several full-Heusler compounds have been shown to be half-metalllic magnets.[4] They have the chemical formula X_2YZ, where X and Y are transition metal atoms and Z is an *sp*-element. When the valence of X is larger than the valence of Y, they crystallize in a dense cubic structure called $L2_1$, which is similar to the zincblende structure of binary semiconductors.[5] Moreover, they are suitable for applications since most of them present very high Curie temperatures.[5] Galanakis and collaborators have elucidated the origin of the gap in these alloys and have shown that the total spin-magnetic moment exhibits a Slater-Pauling (SP) behavior being per unit cell in μ_B the total number of valence electrons minus 24.[6]

For applications, it would be more desirable if half-metallicity could be combined with a zero net magnetization, since this would mean that no external magnetic fields are created minimizing the energy losses. These compounds are known in literature as half-metallic antiferromagnets or half-metallic fully compensated ferrimagnets.[7–16] Full-Heusler alloys with exactly 24 valence electrons in the unit cell are expected to combine half-metallicity with a zero total spin magnetic moment as predicted by the SP rule while they are made up of magnetic elements.[8] Contrary to the conventional antiferromagnets, here the zero magnetization stems from different magnetic sublattices with opposite and equal magnitude of spin magnetic moments. However, in contrast to the zero-temperature limit in which the total spin magnetic moment vanishes, at finite temperatures, spin fluctuations induce a net magnetization in half-metallic antiferromagnets leading to a ferrimagnetic state.[17] Several Heusler compounds with 24 valence electrons have been predicted to be half-metallic antiferromagnets: Mn_3Ga,[8] Cr_2MnZ (Z = P, As, Sb, Bi) alloys,[18] Co-doped Mn_2VZ (Z = Al, Si) half-metallic ferrimagnetic alloys,[19] Cr-doped Co_2CrAl,[20] Cr_2CoGa,[21,22] and $Cr_{2+x}Se$ alloys.[23]

II. MOTIVATION AND CALCULATIONAL DETAILS

Experimentally, half-metallic antiferromagnetism has been identified in the case of Cr_2CoGa polycrystalline ingots,[21] while Meinert *et al*. have tried unsuccessfully due to disorder to achieve half-metallic antiferromagnetism by growing $(Mn_{0.5}Co_{0.5})_2VAl$ films.[24] Thus, it seems that the growth of films combining half-metallicity and antiferromagnetism is still an open issue. An alternative route towards such structures would be the growth of artificial multilayer superlattices made up of two different half-metallic compounds with opposite spin magnetic moments. Superlattices made up of half-metallic transition metal pnictides and chalcogenides in the zincblende structure have been extensively studied theoretically,[25–28] and Nakao has proposed in 2008 that some combinations should result in half-metallic antiferromagnetism.[29] But such structures do not seem feasible experimentally; only CrAs and CrSb have been grown as ultrathin films since the zincblende structure is not the ground state of transition-metal pnictides and chalcogenides (see Ref. 30, and references therein). Alternatively, to achieve half-metallic antiferromagnetism in multilayer superlattices, one could combine half-metallic full-Heusler compounds with less and more than 24 valence electrons since, due to the SP rule,[6] they should have total spin magnetic moments of opposite signs and this is the aim of the

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TABLE I. Lattice constants (taken from Refs. 31–34), spin polarization at the Fermi level (see text for the definition), and the atom-resolved spin magnetic moments (in μ_B) as well as the total spin moment in the unit cell for the bulk parent compounds. "Int" corresponds to the interstitial region.

Compound	a(Å)	P(%)	$m_{[X]}$	$m_{[Y]}$	$m_{[Z]}$	$m_{[Int]}$	$m_{[Cell]}$
Mn_2TiGe	5.87	96	−1.22	0.40	0.04	0.03	−1.97
Mn_2VGa	5.91	98	−1.53	0.96	0.03	0.08	−1.99
Co_2TiGe	5.83	100	1.04	−0.03	0.03	−0.08	2.00
Co_2VGa	5.79	100	0.95	0.18	−0.02	−0.06	2.00

present study. We study using *ab-initio* calculations superlattices made up of Mn_2TiGe (Mn_2VGa) and Co_2TiGe (Co_2VGa) compounds. The two Mn-based compounds have 22 valence electrons per unit cell and thus a total spin magnetic moment of $-2\,\mu_B$, while the Co-based compounds have 26 valence electrons per unit cell and a total spin magnetic moment of $+2\,\mu_B$. Moreover, with the exception of Mn_2TiGe,[31] the other three compounds have been already grown in the form of thin films and their half-metallicity has been confirmed.[32–34] Thus, the growth of such heterostructures seems plausible with modern growth techniques.

To perform the calculations, we have used the full-potential linearized augmented-plane-wave (FLAPW) method[35] in conjunction to the Perdew-Burke-Ernzerhof formulation of the generalized gradient approximation (GGA) to the exchange-correlation potential.[36] We have used for the bulk compounds the lattice constants from Refs. 31–34 (see Table I) while for the superlatices we have used the mean values of the bulk lattice constants of constituents (see Table II). For the superlattices, the lattice mismatch between the constituent compounds is quite small; the maximum value is about 2% in the case of the Mn_2VGa/Co_2VGa. Thus, we expect relaxation effects at the interface to be minimal. Moreover, in the case of the half-metallic GaAs/CrAs thin superlattices, experiments have shown that the multilayers adopt the lattice constant of the substrate crystallizing in a perfect zinc-blende lattice which is similar to the $L2_1$ structure of the full-Heusler alloys.[37] We have taken into account all four possible combination of the Mn_2TiGe (Mn_2VGa) and Co_2TiGe (Co_2VGa) compounds as constituents of the superlattice and three different values of the constituent thickness for the $[Mn_2YZ]_n/[Co_2Y'Z']_n$ superlattice along the (001) direction as shown in Fig. 1(a). When $n=0.5$, we have alternating layers of Mn_2-YZ-Co_2-Y′Z′ type, and when $n=1$ or $n=2$, we increase the

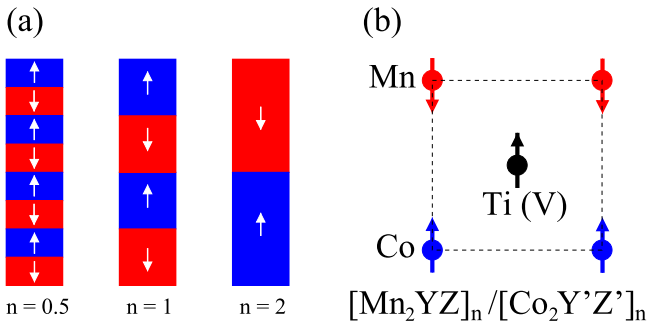

FIG. 1. (a) Schematic representation of the $[Mn_2YZ]_n/[Co_2Y'Z']_n$ periodic superlattices along the (001) direction for three different constituent thicknesses n. $n=0.5$, 1, and 2 corresponds to 2, 4, and 8 layers in each constituent, respectively. With red (blue), we show the Mn_2YZ ($Co_2Y'Z'$) constituents, where YZ and Y′Z′ can be either TiGe or VGa. Arrows show the orientation of the Co (Mn) spin magnetic moments in each constituent. Note that when $n=0.5$ the sequence of the layers in periodic superlattice is …-Co_2-Y′Z′-Mn_2-YZ-Co_2-… (b) Structure of the interface projected on the [100] plane. The Co and Mn atoms form a cube and at the center of the cube, we have either a Ti (V) or a Ge (Ga) atom. Arrows represent the orientation of the atomic spin magnetic moments.

thickness of each constituent of the superlattice by 2 or 4 times, respectively. At the interface as shown in Fig. 1(b), we have a Ti (V) atom having as nearest neighbors Mn atoms from one side and Co atoms at the other side. As shown in Refs. 31–34 and confirmed by our bulk calculations presented in Table I, the Mn and Ti (V) atoms are antiferromagnetically coupled in the Mn-based Heusler compounds while the Co and Ti (V) atoms are ferromagnetically coupled in the Co-based Heusler compounds. Thus, the presence of the Ti (V) atom at the interface ensures and stabilizes the antiferromagnetic coupling between the two constituents of the superlattice presented in Fig. 1(a). Finally, we should notice that in the case of $[Mn_2TiGe]_n/[Co_2TiGe]_n$ and $[Mn_2VGa]_n/[Co_2VGa]_n$ superlattices, we have two equivalent interfaces while in the two other cases we have two inequivalent interfaces.

III. RESULTS AND DISCUSSION

Before discussing our results on the superlattices, we should shortly present our results on the bulk compounds. In Fig. 2, we present the total and atom-resolved density of states (DOS). In all cases, there is an energy gap at the Fermi level in the spin-down electronic band structure and the four compounds are half metals. In Table I, we present the spin-polarization at the Fermi level, P, defined as $P=\frac{N^{\uparrow}-N^{\downarrow}}{N^{\uparrow}+N^{\downarrow}}$, where $N^{\uparrow}$ ($N^{\downarrow}$) is the number of spin-up (spin-down) states at

TABLE II. For the four superlattices under study and for all three values of the constituent thickness n, we present the lattice constant used in the calculation (the mean value of the bulk ones of the parent compounds presented in Table I), the spin-polarization at the Fermi level and the spin magnetic moments of the V (Ti) atoms at the interface. The total spin magnetic moments in the unit cell are multiplied by 4 in the $n=0.5$ case and by 2 in the $n=1$ case to be comparable to the $n=2$ case.

		$n=0.5$				$n=1$				$n=2$			
Superlattice	a (Å)	P (%)	$m_{[Ti]}$	$m_{[V]}$	$m_{[Cell]}$	P (%)	$m_{[Ti]}$	$m_{[V]}$	$m_{[Cell]}$	P (%)	$m_{[Ti]}$	$m_{[V]}$	$m_{[Cell]}$
$[Mn_2TiGe]_n/[Co_2TiGe]_n$	5.85	75	0.08		0.52	93	0.18		0.12	94	0.17		0.12
$[Mn_2VGa]_n/[Co_2VGa]_n$	5.85	78		0.52	0.20	95		0.67	0.08	98		0.66	0.07
$[Mn_2TiGe]_n/[Co_2VGa]_n$	5.89	81	0.14	0.41	0.24	92	0.16	0.58	0.16	96	0.16	0.56	0.16
$[Mn_2VGa]_n/[Co_2TiGe]_n$	5.87	79	0.14	0.40	0.24	96	0.21	0.70	0.06	98	0.21	0.69	0.05

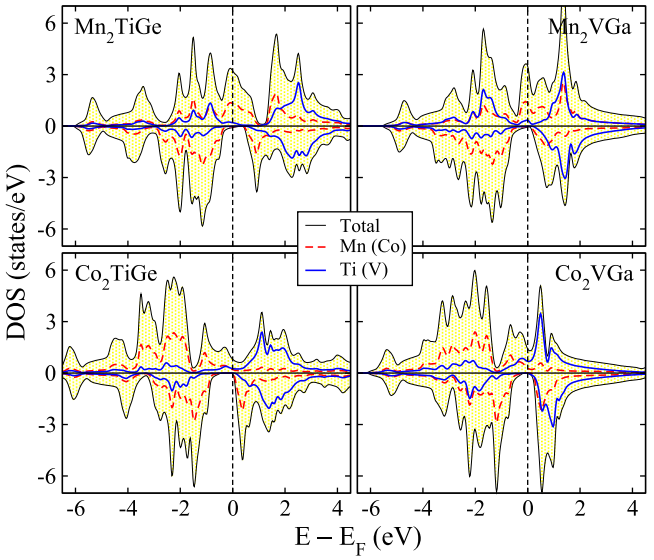

FIG. 2. Total and atom resolved DOS for the four parent bulk compounds. Positive (negative) DOS values correspond to the spin-up (spin-down) states. For the Mn-based compounds, the majority-spin states are the spin-down states while for the Co-based compounds they are the spin-up states. All four compounds exhibit an energy gap at the Fermi level in the spin-down electronic band structure. Note that the Fermi level has been set as the zero of the energy axis.

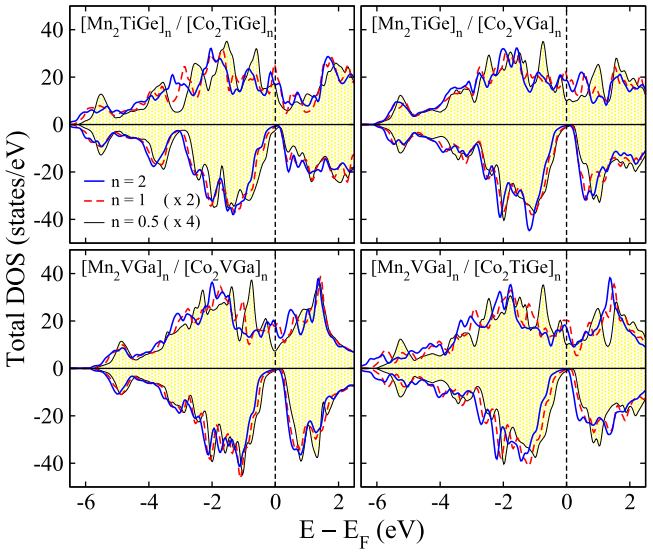

FIG. 3. Total DOS for the four superlattices under study and for all three values of the constituent thickness n. The DOS for $n=0.5$ ($n=1$) has been multiplied by 4 (2) in order to be comparable to the $n=2$ case (see Fig. 1 for the number of layers in each case). In all cases, a region of very low spin-down DOS around the Fermi level is preserved. Details as in Fig. 2.

the Fermi level. The two Co-compounds show 100% spin-polarization while the two Mn-compounds slightly deviate from the perfect half-metallicity (instead of a real gap, there is a region of vanishing DOS) but more than 99% of the electrons at the Fermi level are of spin-up character. In the case of the Mn-based compounds, the Mn and V atoms are antiferromagnetically coupled. The Mn atoms have negative spin magnetic moments and this is also illustrated in their DOS since their weight below the Fermi level is mainly in the spin-down bands. Co atoms show an opposite behavior with respect to the Mn atoms and they have their weight below the Fermi level in the spin-up bands being ferromagnetically coupled to the Ti (V) atoms. In the case of the Mn-compounds, the Ti (V) atoms carry significant spin magnetic moments contrary to the situation in the Co-compounds. Due to the use of muffin-tin spheres in FLAPW method, we have also very small spin magnetic moments in the interstitial region. Finally, the total spin magnetic moment in the unit cell follows the SP rule[6] being $+2\,\mu_B$ for Co_2TiGe (Co_2VGa) and almost $-2\,\mu_B$ for Mn_2TiGe (Mn_2VGa).

For the superlattices considered, the lattice constants are chosen as the mean value of the corresponding lattice constants of constituent bulk compounds. As we discussed above, the Ti (V) atoms at the interface stabilize the antiferromagnetic coupling between the two constituents since they are antiferromagnetically (ferromagnetically) coupled to the Mn (Co) atoms. We have also performed calculations assuming ferromagnetic coupling of the constituents and found that this configuration has a total energy of about 0.2 eV higher than the antiferromagntic one and thus the latter is the ground state. First, we have to examine if the multilayer superlattices are half-metallic. In Fig. 3, we present the DOS for all four cases and for the three values of the constituent thickness n which we took into account. As noted in the caption of Fig. 3, we have multiplied the DOS for $n=0.5$ ($n=1$) by 4 (2) to make them comparable to the $n=2$ case. In all cases, the Fermi level seems to fall within a narrow energy-gap in the spin-down band. To make it even clearer in Table II, we present the calculated spin-polarization at the Fermi level, P. For the $n=0.5$ case, P is about 80% meaning that 90% of the electrons at the Fermi level are of spin-up character. As the thickness of the constituent Heusler compounds increases, the behavior of P becomes more bulk like and when $n=2$, P assumes values more than 94% meaning that more than 97% of the electrons at the Fermi level are of spin-up character. Thus, although superlattices show no perfect half-metallicity, the ones with thicker constituents present a very high-degree of spin polarization and thus are suitable for spintronic devices.

To reveal whether the superlattices are antiferromagnets presenting zero net magnetization, we should examine the spin magnetic moments presented in Table II. Note that the Ti and V atoms at the interfaces present spin magnetic moments, which are close to their values for the Mn- and the Co-based parent compounds giving a first hint towards a zero net magnetization. As mentioned above in the first two cases presented in the Table II, we have two equivalent interfaces while in the latter two case there are two inequivalent interfaces. The Mn and Co atoms in the superlattices present spin magnetic moments (not shown here) similar to their values in the bulk compounds shown in Table I and the same stands also for their atom-resolved DOS. To draw safe conclusions, we present also the total spin magnetic moment in the cell shown in Fig. 1(a) where for $n=0.5$ ($n=1$), we multiply the total moment by 4 (2) to compare with the $n=2$ case. For $n=0.5$, the total spin magnetic moments are small but not zero. As we increase the thickness of the each constituent in the superlattice ($n=1$ and $n=2$), the total spin magnetic moment in the cell almost vanishes especially when Mn_2VGa is one of the two constituents. Interestingly,

both $n=1$ and $n=2$ cases show almost identical magnetic properties. Thus, the superlattices with thicker constituents can be considered as half-metallic antiferromagnets. Finally, we should also comment on the dependence of our calculated spin magnetic moments on the exchange-correlation functional used for the calculations. GGA, which is used for the present calculations, has the tendency to underestimate hybridization effects with respect to the local-spin-density approximation (LSDA)[38] leading to slightly larger values of the atom-resolved spin magnetic moments by less than $0.1\,\mu_B$.[39] Other properties like the magnetic anisotropy energy have been found to be much more sensitive to the choice of the exchange-correlation functional used in the calculations.[39] Moreover, at the same time for the same lattice constant, both GGA and LSDA yield similar electronic properties and identical total spin magnetic moments for the half-metallic Heusler alloys.[40] Thus, we expect that the use of LSDA instead of GGA will only marginally affect the calculated spin magnetic moments.

Although in the present work, we have considered half-metallic Heusler compounds with $\pm 2\mu_B$ spin magnetic moments, in general, we can envisage that superlattices made up of half-metallic Heusler compounds, which have in their bulk form total spin magnetic moments of the same magnitude but opposite sign, would exhibit zero net magnetization. Moreover, we have considered in our calculations the (001) direction, which is the usual growth direction in experiments but we expect that these superlattices would be also half-metallic antiferromagnets if the stacking is along the (110) or (111) directions.

IV. SUMMARY AND CONCLUSIONS

Employing first-principles electronic structure calculations, we have proposed a route towards half-metallic antiferromagnetism in artificial superlattices based on full-Heusler compounds. The superlattices as bulk materials follow the Slater-Pauling rule with their total spin magnetic moment in μ_B being the total number of valence electrons minus 24.[6] We have suggested that Mn_2TiGe (Mn_2VGa) with 22 and Co_2TiGe (Co_2VGa) with 26 valence electrons, and thus, total spin magnetic moments of -2 and $+2\,\mu_B$, respectively, are suitable for such half-metallic antiferromagnetic heterostructures. Our calculations have shown that superlattices with thick constituents and the (001) as growth direction keep the half-metallic character of the parent compounds while they exhibit a vanishing net magnetization. Such artificial structures should be easily grown since the constituents have similar lattice constants and they have already been grown independently in the form of thin films. Moreover, the bulk half-metallic Heusler compounds have in general very high Curie temperatures[31,41,42] and thus the superlattices are expected to show a similar behavior. These features combined with the dependence of the magnetic properties on the thickness of the constituents would allow the design of half-metallic superlattices of zero-net magnetization with predefined magnetic properties promising to be incorporated in future spintronics/magnetoelectronics devices.

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