Journal of Magnetism and Magnetic Materials 322 (2010) 2922–2928

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Electronic, magnetic and transport properties of Co_2TiZ (Z=Si, Ge and Sn): A first-principle study

Vinit Sharma [a], A.K. Solanki [b], Arti Kashyap [a,*]

[a] Condensed Matter Theory Group, The LNM Institute of Information Technology, Jaipur 302031, India
[b] Central Computer Center, Malaviya National Institute of Technology, Jaipur 302017, India

ARTICLE INFO

Article history:
Received 18 January 2010
Received in revised form
19 April 2010
Available online 6 May 2010

Keywords:
Heusler alloy
Band structure
Magnetic property
Transport property

ABSTRACT

We have studied the electronic structure, magnetic and transport properties of some Co based full Heusler alloys, namely Co_2TiZ (Z=Si, Ge and Sn), in the frame work of first-principle calculations. The calculations show that Co_2TiZ (X=Si, Ge and Sn) are to be half-metallic compounds with a magnetic moment of 2 μ_B, well consistent with the Slater–Pauling rule. The electronic structure results reveal that Co_2TiZ has the high density of states at the Fermi energy in the majority-spin state and show 100% spin polarization. Our results also suggest that both the electronic and magnetic properties in these compounds are intrinsically related to the appearance of the minority-spin gap. The origin of energy gap in the minority-spin states is discussed in terms of the electron splitting of Z (Z=Si, Ge and Sn) and 3*d* Co atoms and also the *d*–*d* hybridization between the Co and Ti atoms. The transport properties of these materials are discussed on the basis of Seebeck coefficients, electrical conductivity coefficients and thermal conductivity coefficients.

1. Introduction

The rapid advancement of spintronics [1–5] in recent years has intensified the research in the Heusler alloys [6]. The magnetoelectronic (spintronic) devices are mostly dependent on an imbalance in spin carriers, namely majority and minority spins, with 100% spin polarization at Fermi level for the ideal materials. One important class of materials suitable for such applications is some of the Heusler compounds also known to be Half-metallic ferromagnets (HMFs) [7]. In general, HMFs are exotic systems and can be treated as hybrids between metals and semiconductors as for one spin-direction these are normal metals and semiconductor for the other spin and thus the electrons near the Fermi level are of unique spin character. The HMF compounds are basically ternary intermetallic alloys with the stoichiometric composition of 2:1:1. In general they are of X_2YZ type Heusler alloys, where X and Y are different 3*d* transition metals and Z is a nonmagnetic *s*–*p* element. The full Heusler alloys crystallize in $L2_1$ structure (space group no. 225) where the lattice consists of four interpenetrating *fcc* sublattices. The unit cell is a *fcc* lattice with four atoms as X at (0 0 0) and (½ ½ ½), Y at (¼ ¼ ¼) and Z at ($^3/_4$ $^3/_4$ $^3/_4$). In this arrangement, each X atom has four Y and four Z atoms as nearest neighbors while each Y and Z atom is surrounded by eight X atoms.

The electronic structure calculations from *ab initio* first-principles methods play an important role in determining the magnetic properties of Heusler compounds and, in particular, for predicting half-metallic ferromagnetism. The first attempt to calculate the band structure of some Co based compounds was performed by Ishida et al. [8], however, their results did not show any half-metallic ferromagnetism. They found a minimum of the minority density of states (DOS) at Fermi energy but without any gap. In 1984, Kübler et al. [9] have reported the formation of local moments in various Mn-based Heusler alloys using first-principles calculations; they concluded that at the Fermi energy minority spin density vanishes in these compounds. Barman et al. [10] have studied the Ni_2MnGa and found that the total magnetic moment has the maximum contribution from Mn atom that is located at Y position. The nature of the ferromagnetism of various Mn-based semi- and full-Heusler alloys, has also been explained by Şaşıoğlu et al. [11]. Electronic structures of similar type Heusler alloys, Co_2MnZ (Z=sp elements), were calculated by Ishida et al. [12]. Galanakis et al. [13] have reported full-potential screened Korringa Kohn Rostoker calculations for various Co, Fe, Rh and Ru based Heusler compounds, with Mn at Y position. They have found that the top edge of the lowest unoccupied spin-down band and the bottom edge of the lowest unoccupied spin down band touch the Fermi level, practically destroying the indirect gap. Their results were compatible with those found for the Mn compounds as calculated by Picozzi et al. [14] using the generalized gradient approximation (GGA) instead of the pure LSDA. Sargolzaei et al. [15] have studied the spin and orbital magnetism

* Corresponding author.
E-mail address: arti.kashyap@lnmiit.com (A. Kashyap).

0304-8853/$ - see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2010.05.006

of Co_2YZ (Y=Mn, Fe; Z=Al, Si, Ga, Ge) full Heusler compounds. The review on various Co_2 and Mn based Heusler compounds clearly indicates that the Mn atom has strongly localized magnetic moment, which is absent if Y is not Mn [9–15].

The half metallic properties of some Co and Ti based compounds have been reported by Lee et al. [16], while Mohn et al. [17] studied the magnetic ground state of Co_2TiZ (Z=Al and Sn) without observing a half-metallic state. Review on Ti based compounds indicates that band structure of Co_2TiSn has always been at the center, Hickey et al. [18] used CASTEP code to investigate the Fermi surface topology for this compound and Kandpal et al. [19] have performed both experimental and theoretical studies to obtain magnetic properties of Co_2TiSn. Very recently, experimental as well as theoretical study of, the electronic structure and transport properties of Co_2TiZ (Z=Si, Ge and Sn) Heusler alloys have been reported by Barth et al. [20]. Experimental study of Seeback coefficient of the of Co_2TiZ (Z=Si, Ge and Sn) compounds have been performed by Balke et al. [21]. Using circular dichroism in X-ray absorption spectroscopy (XMCD) and first principle calculations, Klaer et al. [22] have obtained that in Co_2TiZ (Z=Si, Ge and Sn) compounds, Co minority DOS reveals a maximum at above Fermi energy (E_F) and very low values at E_F in agreement with the expectation for half-metallic ferromagnetism. In past few years, attempts have been made by different groups to investigate the electronic and magnetic properties of Co_2TiSn using different experimental techniques [23–26].

The main difference in magnetic properties of Mn based and Ti based compounds is due to the localized magnetic moment of Mn. Therefore, in Mn based Heusler compounds the most of the magnetic moment contribution comes from Y site where Mn is located. While, in case of Ti based Heusler compounds the maximum contribution is produced to be from X sites. In this paper, a systematic study of electronic, magnetic and transport properties of Co_2TiZ (Z=Si, Ge and Sn) Heusler compounds has been carried out.

From the literature on theoretical exploration of the electronic structure of these HFMs, it has been observed that one principally needs both the full symmetry potentials and the GGA to find the correct electronic structure and ground state for the Heusler compounds. Therefore, the GGA introduced by Wu and Cohen [27] which accounts for gradients of the density that are absent in the pure LSDA parameterization of the exchange-correlation functional used in earlier calculations has been used for the calculations reported here.

2. Computational details

To perform the present calculation, we have used the density functional theory in connection with the full potential linear augmented plane wave (FP-LAPW) method as embodied in WIEN2k code [28]. The exchange and correlation effects were treated using the generalized gradient approximation (GGA) [27]. In the present study, we expand the basis function up to $R_{MT}K_{max}=8$, where R_{MT} is the plane wave radius and K_{max} the maximum modulus for the reciprocal lattice vector. The maximum value for partial waves inside the atomic sphere (l_{max}) is kept 10. Moreover, the potential cut-off extends up to 14, so no shape approximation to the potential is necessary.

The lattice constants used in the present work, were obtained by minimizing the total energy (E_{tot}) with respect to the experimental lattice parameters. In the total energy calculation spin–orbit coupling is excluded. The energy convergence criterion was set to 10^{-5}. For k-space integration, a $10\times10\times10$ mesh was used resulting into 47 k points of the irreducible part of the Brillouin zone. While to calculate different transport coefficients, a $50\times50\times50$ mesh was used.

Using the energy eigenvalues and eigenvectors at these points, the DOS was determined by the tetrahedral integration method [29]. The muffin tin radius was set to 2.30 a.u. for Co and Ti. While in case of Z (Z=Si, Ge and Sn) the values of muffin tin radii were 2.16, 2.18 and 2.23 a.u., respectively.

3. Results and discussion

3.1. Electronic properties

In order to compute the ground state properties, we performed a systematic volume optimization as shown in Fig. 1. To start the optimization, initially experimental lattice constants were taken from Ref. [16]. Calculated lattice constants (in a.u.) are 10.740, 10.936 and 11.366 for Co_2TiZ (Z=Si, Ge and Sn), respectively.

The calculated spin-polarized band structures of Co_2TiZ (Z=Si, Ge and Sn) along with the total DOS are displayed in Fig. 2(i–iii). The overall band shapes in all three compounds are quite similar, as Fig. 2(i–iii) shows that these Heusler compounds present a prominent energy gap at the Fermi level in one spin direction (minority) while the majority spin bands show the metallic character.

In the minority spin state, the Fermi level is near the edge of conduction bands for all these compounds. This spin gap in minority spin channel leads to 100% spin polarization at Fermi level and thereby, bringing in the half-metallic magnetism at an equilibrium state. It is worth mentioning here that in present calculations spin–orbit coupling is not incorporated, which may have strong influence on spin polarization, mainly when the Z atom is a heavy element such as Sn [19].

To further illustrate the nature of electronic structure, we have also plotted the partial DOS as shown in Fig. 3(a–c). The partial DOS of Co (d), in all cases, shows the same trend as majority spin

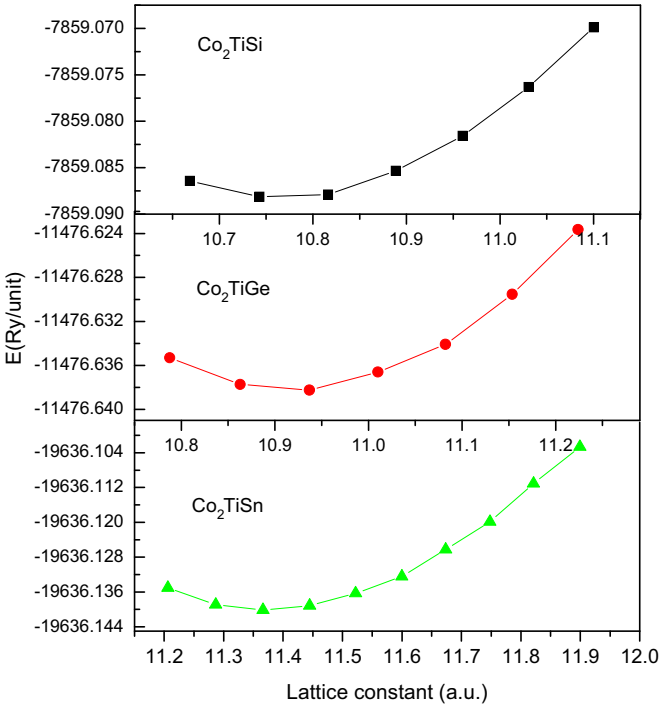

Fig. 1. Optimization of the lattice parameter. Shown is the dependence of the total energy on the lattice constant of Co_2TiZ (Z=Si, Ge and Sn). The solid line is the result of the equation of states fit.