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Electronic structure, Mechanical and Thermodynamic properties of CoYSb (Y= Cr, Mo, W) half-Heusler compounds as potential spintronic materials

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Abstract

The CoYSb (Y = Cr, Mo and W) compounds which are XYZ type half-Heusler alloys and also exist in the face centred cubic MgAgAs-type structure conform to $F\bar{4}3m$ space group. In the present work, these compounds are investigated in different atomic arrangements called, Type-I, Type-II and Type-III phases, using Generalized Gradient Approximation (GGA) in the Density Functional Theory (DFT) implemented in QE (Quantum Espresso *Ab-Initio* Simulation Package). The ferromagnetic state of these alloys is studied after investigating their stable structural phase. The calculated electronic band structure and the total electronic density of state indicated nearly half-metallic behaviour in CoMoSb with a possibility of being used in spintronic application, metallic in CoWSb and half-metallic in CoCrSb, with the minority-spin band gap of 0.81 eV. Furthermore, the calculated mechanical properties predicted an anisotropic behaviour of these alloys in the stable phase. Finally, due to its high Debye temperature value, CoCrSb possesses a stronger covalent bond than CoMoSb and CoWSb, respectively.

Keywords: nearly half-metal, Spin-polarization, Poisson's ratio, thermodynamic properties, Electronic band Structure

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1. Introduction

Ternary half-Heusler (HH) compounds involving Co atom have recently attracted attention due to their high curie temperature, and structural similarity with binary semiconductors with zinc-blende (ZB) structure that makes them potential candidates in optoelectronic and spintronic applications such as quantum sensors, resistors and computers devices, respectively in the near future [1]-[4], topological insulator [5]-[6], and thermoelectric devices [7], [14]. The wide range of usage of HH in applications is due to its excellent electrical, mechanical and electronic properties and thermal stability. The crystal structure, $C1_b$, of any HH alloy is similar to the structure, $L2_1$, of a full-Heusler alloy (X_2YZ) but missing one X atom. The absence of inversion symmetry due to an empty X site and the low coordination number of the d-band metals in the HH alloys are believed to be essential for these materials novel electronic and magnetic properties. Some research groups have reported three possible distinct atomic arrangements, called Type-I, Type-II, and Type-III phases, due to this missing X atom in the HH alloy [1], [8]-[18]. In Table 1, the positions occupied by the atoms and the vacancy are given according to the notations defined by Wyckoff [19]. Researchers such as [12]-[18], [7] have theoretically predicted and reported some Co-based HH compounds using Density Functional Theory in which they reported it to be semiconductor, metallic and half-metallic depending on the valence electron count (VEC) of the alloys. In the interest to study the structural, mechanical and thermodynamics properties of such predicted compounds, CoYSb (Y=Cr, Mo, W) compound has been chosen. To the best of our knowledge, we report here, for the first time, its band structure, mechanical and thermodynamics properties to explore their electronic transport behaviour and chemical bonding between their atoms. In Section 2, we explain a brief description of the computational details used. Then, in Section 3, the structural and magnetic properties for each phase of ferromagnetic HH CoYSb (Y=Cr, Mo, W) at its optimized lattice constant and the influence of the lattice parameter will be presented on the magnetic properties for each phase discussed. Next, in Section 4, the electronic properties of the stable phase showing both spin band and spin DOS will be presented and discussed. Also, the mechanical properties of the stable phase ferromagnetic HH CoYSb (Y=Cr, Mo, W) will be reported in Section 5. Finally, in Section 6, thermodynamic properties with summarising of our results in conclusion. To the extent we know, these detailed calculations have not been done before for all series of CoYSb alloys

considered in this work.

2. computational details

All computations have been performed using the Quantum Espresso *Ab-Initio* simulation package, which is a first-principles plane-wave pseudopotential [21]-[23] to study the electronic and magnetic properties of CoYSb (Y=Cr, Mo, W) in the three phases mentioned above. The generalized gradient approximation (GGA) was used in treating the effects of exchange-correlation potential with Perdew-Burke-Ernzerhof parameterization (PBE) [24]. The cutoff wave function was set at 680 eV, and the k-point of $14 \times 14 \times 14$ Monkhorst-Pack meshes [27] grid was used in the irreducible Brillouin zone to calculate the total charge density. The Plane-waves pseudopotential (PWPP) basis functions set consists of the $3d^7\ 4s^2$, $3d^5\ 4s^1$, $4d^5\ 5s^1$, and $5d^7\ 6s^2$ for Co, Cr, Mo and W respectively, as well as $5s^2\ 5p^3$ for Sb elements with a self-consistent convergence total energy of less than 10^{-4} Ry. Thermo_pw code [25], [26] was used to obtain the mechanical and thermodynamic properties based on our optimized lattice constant and cutoffs wave functions with denser k-points to get an accurate result.

3. Structural and Magnetic Properties

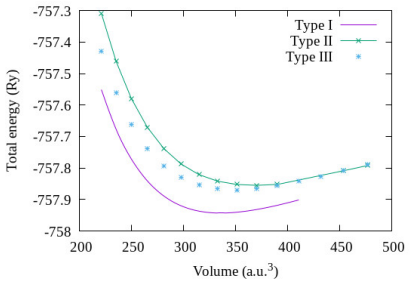
Firstly, we investigated the equilibrium lattice constant of the HH compound CoYSb (Cr, Mo, W) based on the three possible arrangement that was reported by researchers on the site preference of X and Y atoms which affects the properties of HH due to the high influence of the d elements and the position of the sp-valent element as shown on the Wyckoff positions of the atoms in Table 1.

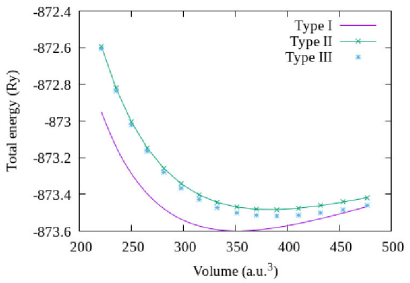
Table 1: The Wyckoff positions of the three atoms, X, Y, and Z: 4a = (0, 0, 0) a, 4b = (0.5, 0.5, 0.5) a and 4c = (0.25, 0.25, 0.25) a, with the 4d site vacant

Structural phase	**X**	**Y**	**Z**
Type I	4c	4b	4a
Type II	4b	4a	4c
Type III	4a	4c	4b

The optimized structural parameters of these alloys in each phase, energy–volume graphics of these systems were plotted by fitting to Murnaghan

equation of states [20] to obtain the equilibrium lattice constant (a_o), bulk modulus (B), the minimum energy (E_{min})and pressure derivative (B') of our alloys been studied in Type-I, Type-II and Type-III phases which conforms to $F\bar{4}3m$ space group as reported in Table 2. The minimum energy obtained from the fitted energy–volume curves of CoYSb (Y = Cr, Mo, W) alloys shows that the most stable and suitable phase is the Type-I phase, as shown in Fig.1. The lattice parameters are the smallest in the Type-I phase; Bulk moduli are more significant in the Type-I phase than the other structural phases. Also, they have large pressure derivatives of bulk moduli, which indicates that these alloys display strong sensitivity against pressure change in all structural phases. Type-I CoYSb alloys are the more stable phase, and hence, we shall focus our attention more on the study of this phase. Firstly, we investigated the equilibrium lattice constant of the HH compound CoYSb (Cr, Mo, W) based on the three possible arrangement that was reported by researchers on the site preference of X and Y atoms which affects the properties of HH due to the strong influence of the d elements and the position of the sp-valent element as shown on the Wyckoff positions of the atoms in Table 1.





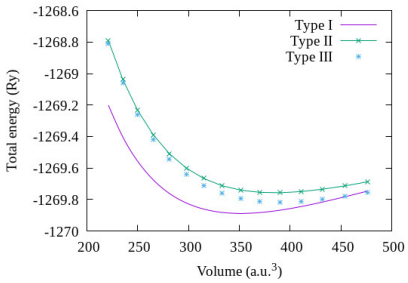


Figure 1: Calculated total energy as a function of volume in ferromagnetic state for the three possible structural phase for CoCrSb, CoMoSb and CoWSb respectively.

Table 2: The optimized lattice constants, a_o (Å), equilibrium energies, E_{min} (Ry), bulk modulus, B (GPa) and pressure derivative for the bulk modulus, B' for CoYSb (Y= Cr, Mo, W) for the three possible structural phases by Murnaghan equation of state.

Alloys	**Calculations**	**Structural phase**	a_o **(Å)**	**B (GPa)**	**B'**	E_{min} **(Ry)**
CoCrSb	This work	Type I	5.848	121.4	4.66	-757.944
	other calculations		5.79[a]			
			5.820[b]	135.4[b]		
			5.800[c]			
		Type II	6.031	97.6	4.33	-757.856
		Type III	5.935	98.6	4.71	-757.869
			5.935[d]			
CoMoSb		Type I	5.937	152.2	4.62	-873.598
	other calculations		5.935[d]			
		Type II	6.134	124.1	4.13	-873.484
		Type III	6.140	131.6	3.94	-873.520
CoWSb		Type I	5.939	164.9	4.32	-1269.888
		Type II	6.133	138.7	4.01	-1269.758
		Type III	6.145	148.2	3.81	-1269.819

a Ref.[14]
b Ref.[15]
c Ref.[16]
d Ref.[13]

The calculated total and partial magnetic moments for all phases are listed in Table 3., It is seen from the table that the main contribution to the

total magnetic moment for these alloys comes from the Y atom for CoCrSb and Co-atom for the Type-II and Type-III of CoYSb (Y= Mo, W). Since the total magnetic moment in CoYSb (Y = Cr, Mo and W) for the phases are greater than 1, it can be said that these materials show ferromagnetic properties. Hence, Type-I CoCrSb alloy exhibit a half-metallic behaviour, and its probably due to its small Y radius, which correlates with a decrease in its lattice parameter compared to CoMoSb and CoWSb, which have a larger lattice constant because Mo 4d and W 5d states have a smaller width relative to that of the Cr 3d state. So the oversized Co atom is effectively due to the enormously widened lattice because of the large Mo and W atoms. This possibly is the reason for the large change in the total magnetic moment compared with that of an integer number of Cr atom. Many half-Heusler alloys follow the Slater-Pauling (SP) rule M_t=Z_t –18 [28], [29] where Z_t is the total number of the valence electron and 18 means that there are 9 occupied spin-down states per unit cell. Thus CoMoSb and CoWSb, just like CoCrSb alloy has a total 20 valence electron count and should have a total magnetic moment of 2 μ_B that does not agree with the result obtained.

Table 3: The calculated spin magnetic moments in μ_B for CoYSb (Y=Cr, Mo, W) compounds for the three possible structural phases comparing with available data.

$m^{spin}(\mu_B)$	**Calculations**	**Structural phase**	**Co**	**Y**	**Sb**	**Void**	**Tota**
CoCrSb	This work	Type I	-0.4473	2.3766	-0.0573	0.138	2.01
	other calculations		-0.36^a	2.37^a	-0.06^a		2.00^a
		Type II	-0.4917	3.0659	-0.0625	0.328	2.84
		Type III	1.1219	1.8089	-0.0177	0.01169	3.03
CoMoSb		Type I	0.6685	0.9017	-0.0148	0.2346	1.79
		Type II	1.0329	0.4100	0.0136	0.0435	1.20
		Type III	0.9274	0.0711	0.0297	0.0082	1.02
	other calculations		0.650^b	1.111^b	-0.037^b		1.82^b
CoWSb		Type I	1.0274	1.2957	-0.0285	0.1955	2.49
		Type II	0.8804	0.1896	-0.0178	0.0078	1.06
		Type III	1.6376	0.4698	0.0133	0.0293	2.15

a Ref.[16]
b Ref.[13]

Our calculated values show slight deviation from other theoretical values available obtained by us for Type-I CoCrSb and CoMoSb [16], [13] with a

minimal discrepancy of only less than 1 % and suggesting that our computational method is reasonable and agreed with the available data.

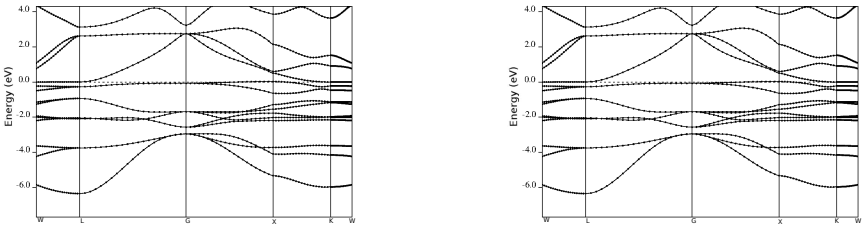
4. Electronic band structure

The band structures calculation of the minority-spin states, which lies within the semiconductor region and the majority states been metallic, was performed to analyze the half-metallic nature of these materials. These spin-polarized band calculations for Type-I CoYSb (Y= Cr, Mo, W) was carried out at equilibrium lattice constant in the ferromagnetic state along the high symmetry directions in the first Brillouin zone are shown in Fig. 2, in which the majority-spin band channels energy bands exhibit a metallic overlap with the E_F with their minority-spin band channel semiconductors the maximum of valence band occurs at the Γ-point and conduction band minimum is at the X-point, resulting in a band gap of 0.81 eV for CoCrSb half-Heusler alloy is slightly higher than the previous calculated value 0.77 eV, but the half-metallic gap is in good comparison with the previous calculation [16]. The minority-spin states gap of CoCrSb is also predicted for CoMoSb and CoWSb, respectively. But these gaps apparently becomes broader, and the Fermi level is pushed further away from the gap but closer to the conduction bands of the minority-spin electrons with the maximum valence band occurs at the L-point and conduction band minimum is at the X-point, which leads to a band gap of 0.32 eV for CoMoSb has seen in Fig. 3, which apparently distort the half-metallic property of these alloys. These distortions in the band gap width are found to be dependent on the lattice parameters and the atomic radius of the substitute Y element.

Table 4: The calculated minority-spin band gap, half-metallic (HM) gap and % spin polarization (SP) of Type I CoYSb (Y= Cr, Mo, W).

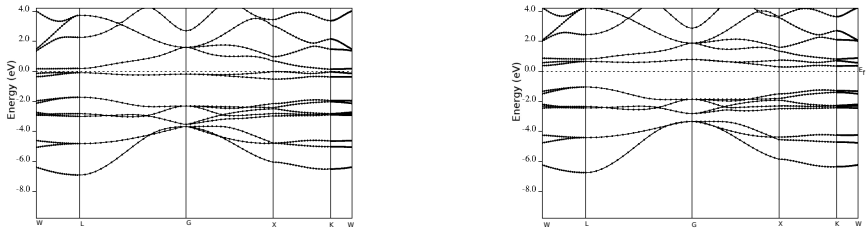
Compound	**Calculations**	**Band gap (eV)**	**HM gap (ev)**	**SP %**
CoCrSb	This work	0.81	0.21	100
	others	0.77[a]	0.22[a]	
CoMoSb		0.32		72
	others			23[b]
CoWSb				33

a Ref.[16]
b Ref.[13]



[a] [b]

Figure 2: Band structures for CoCrSb (a) majority-spin and (b) minority-spin. The Fermi level is indicated by the dashed horizontal line.



[a] [b]

Figure 3: Band structures for CoMoSb (a) majority-spin and (b) minority-spin. The Fermi level is indicated by the dashed horizontal line.

To further confirm the possible half-metallicity of CoYSb (Y = Cr, Mo, W), we show in Fig.4 the calculated total spin density of state (TDOS) for CoCrSb, CoMoSb and CoWSb, respectively in the Type-I arrangement. It can be seen that all these mentioned alloys show various degrees of half-metallic behaviours: in the majority-spin (up spin) channel, whose energy bands exhibit a metallic overlap with the E_F, whereas in the minority-spin (down spin) direction, an energy gap is opened and the E_F locates within the gap for CoCrSb and slightly close to the conduction band for CoMoSb and into the conduction band for CoWSb. This is seen from the spin polarization calculation in which it decreases from 100 % for CoCrSb to 33 % for CoWSb as shown in table 4., which is estimated by using the spin polarization (P) at the Fermi energy (E_F) following the expression:

$$P = \frac{n\uparrow(E_F) - n\downarrow(E_F)}{n\uparrow(E_F) + n\downarrow(E_F)} \times 100\% \quad (1)$$

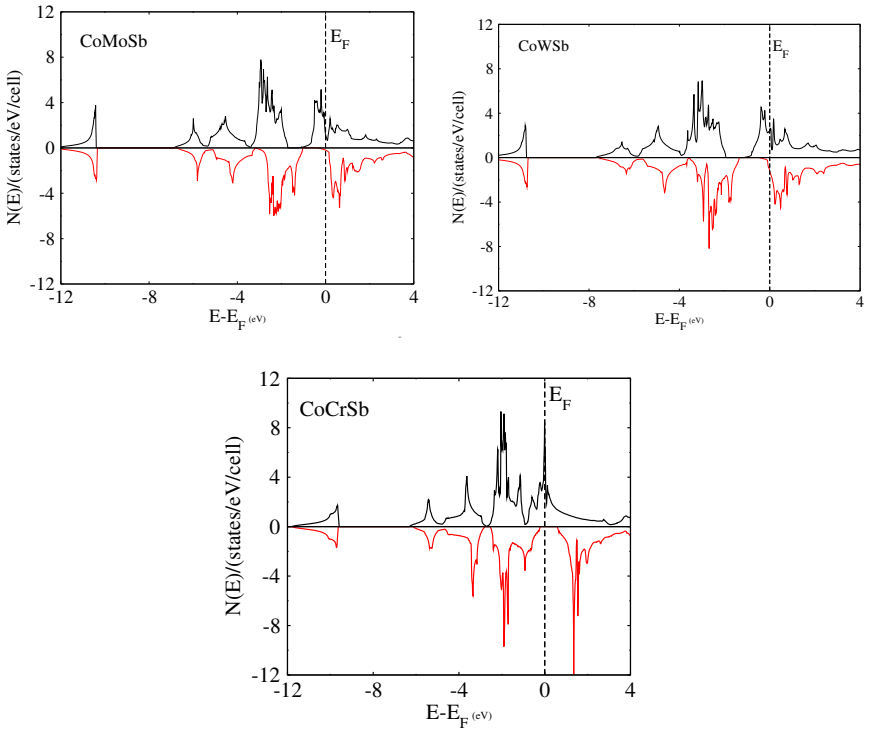


Figure 4: Calculated total spin density of states (DOS) of Type-I CoYSb alloy.

5. Mechanical Properties

In this section, we discuss the mechanical properties and phase stability. The stable structure (Type-I) mechanical properties, such as the elastic constants for a cubic structure which are reduced into Three independent elastic constants C_{11}, C_{12}, and C_{44}, respectively. The link between mechanical and dynamic behaviour of a material such as shear modulus (G), bulk modulus (B), and young modulus (E) is usually obtained through the stress-strain method [30]. First, we test the mechanical stability of these compounds based on the durability of the crystal against external forces, which is a desirable property to ensure its sustainability in any application. The mechanical stability according to the Born and Huang stability criteria for cubic structure [32]

$$C_{11}>0, C_{44}>0, C_{11}-C_{12}>0, and C_{11}+2C_{12}>0. \quad (2)$$

The calculated elastic values for the stable structures CoYSb (Y=Cr,

MO, and W) satisfy the above stability criteria. Hence, these compounds are mechanically stable, as shown by our results in Table 5. Furthermore, using the Voigt-Reuss-Hill approximation [33]-[34] which estimate the shear modulus (G), bulk modulus (B), Poisson's ratio (ν), and Young modulus (E) were calculated by using the following equations:

$$G = \frac{C_{11} + 2C_{12}}{3} \tag{3}$$

$$B = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{4}$$

$$\nu = \frac{3B - 2G}{2(3B + G)} \tag{5}$$

$$E = \frac{9BG}{3B + G} \tag{6}$$

The shear anisotropy (A), The Pugh's [31] ratio and the inverse which is Frantsevich's ratio given by the expression

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{7}$$

The bulk (B) and shear (G) are important in alloy applications due to the empirical rule, in which materials with high B and G tend to have a high melting point and high Debye temperature. Generally, B and G show how resistive these alloys are when subjected to fracture and plastic deformation, respectively. The higher the value B, the more its resistance to deformation due to pressure. CoWSb resistance to pressure is stronger compared to CoMoSb and CoCrSb, as shown in Table 5. The value of shear modulus G shows the resistance of a material to deformation by shear stress. The higher the value G, the higher its resistance to shear stress. Hence, CoCrSb>CoMoSb>CoWsb. The Young's modulus E characterizes the material's stiffness, and the higher the value E, the stiffer is the material. Therefore, as shown in Table 5, the relative order of stiffness, CoCrSb, is stiffer than CoMoSb, and CoWSb is the least stiffer. Also, the unidirectional elastic constant C_{11} is much higher than that of C_{44} indicating that these compounds present weaker resistance to pure shear deformation compared to resistance to unidirectional compression.

Table 5: Various mechanical properties of CoYSb (Y= Cr, Mo, W) stable phase obtained from the calculated lattice.

Calculated properties	**CoCrSb**	**CoMoSb**	**CoWSb**
C_{11} (GPa)	202.83	250.02	264.14
C_{12} (GPa)	79.61	117.98	131.46
C_{44} (GPa)	55.11	42.30	30.16
C_{11}–C_{12} (GPa)	123.22	132.04	123.68
$C_{11} + 2C_{12}$ (GPa)	362.04	485.97	527.05
B (GPa)	120.66	161.99	175.68
G (GPa)	57.63	50.59	41.61
E (GPa)	149.19	137.45	115.64
A	0.49	0.64	0.45
ν	0.29	0.36	0.39
Pugh's ratio	2.09	3.20	4.22

We also deduced the cubic Shear anisotropy factor [37] for these compounds based on equation 7. The calculated result shows anisotropy factors as 0.49, 0.64 and 0.45 for CoCrSb, CoMoSb and CoWSb, respectively. From these values, one can deduce that these compounds are substantially anisotropic in nature. The degree of ductility of a material is explained by the Pugh ratio, which is the ratio of the bulk and shear modulus of the material. The material is said to be more ductile if the Pugh's ratio increase more and it is greater than 1.75 (G/B<0.57) [38], otherwise it is brittle. As shown in Table 5, we can see that the compounds are ductile in nature because their values are greater than 1.75. The Poisson's ratio (ν) characterises the bonding forces in material and its compression against external forces [39]-[40]. The alloys reported in this work are central-force solid (ν is generally between 0.25 to 0.5) and incompressible because ν is due to their values that lie within this range. Hence, indicating that the metallic bonding contribution to the atomic bond is dominant.

6. Thermodynamic Properties

The effects of temperature at constant pressure on the thermodynamic properties of the CoYSb (Y= Cr, Mo, W) material from the state equation, under the considerations of the quasi-harmonic approximation of the Debye model, were analyzed as presented below. Fig. 5 shows the results of specific

heat at constant volume, C_V, as functions of temperature. As can be seen in the figure, the temperature was varied between 0 K and 800 K at constant pressure.

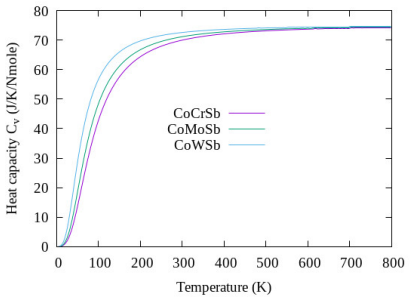


Figure 5: Heat capacity C_v against temperature for Type-I CoYSb alloy

Fig. 5 shows more clearly the trend of specific heat towards the Dulong-Petit limit, which is the specific heat value independent of temperature. From this limit value of Dulong-Petit, as the temperature increases, each of the atoms in the material absorbs the same amount of energy proportional to this temperature increase. This value corresponds to 72.63 J/Nmol.K for CoCrSb and CoMoSb respectively while 73.47 J/Nmol.K for CoWSb. The Debye temperature is a fundamental parameter of thermodynamic, which is linked with many physical properties of the material such as the melting temperature, lattice vibrations and specific heat at low temperature[41]. These properties listed in table 6 were obtained from the calculated elastic constants using the following equations.

$$v_l = \sqrt{\frac{3B + 4G}{3\rho}} \tag{8}$$

$$v_s = \sqrt{\frac{G}{\rho}} \tag{9}$$

Where, (v_l) is the compressional velocity and shear sound velocity (v_s). The average sound velocity (v_m) is expressed in terms of compressional and shear sound velocities as stated below.

$$v_m = \left(\frac{1}{3}\right)^{1/3} \left[\frac{2}{{v_s}^3} + \frac{1}{{v_l}^3}\right] \tag{10}$$

The Debye temperature θ_D is thus expressed as

$$\theta_D = \frac{\hbar}{\kappa}\left(\frac{3n}{4\pi}\left(\frac{\rho N_A}{M}\right)\right)^{1/3} v_m \tag{11}$$

Where, $\hbar$ is the reduced Planck's constant, κ is Boltzmann's constant, N_A is Avogadro's number, M is atomic mass of unit cell, n is the number of atomic per formula unit, and ρ is the density.

Table 6: Average sound velocity (v_m), compressional velocity (v_l), shear sound velocity (v_s), Debye temperature (θ_D) and predicted melting temperature (T_m) for the stable phase CoYSb (Y= Cr, Mo, W).

Compound	v_l **(m/s)**	v_s **(m/s)**	v_m **(m/s)**	θ_D **(K)**	T_m **(K)**
CoCrSb	5027.79	2723.03	3037.67	354.68	1751.73±300
CoMoSb	5105.36	2397.30	2688.55	308.93	2030.62±300
CoWSb	4459.49	1891.93	2113.76	243.05	2114.07±300

The Covalence bonds strength in solids is characterized by Debye temperature, which is listed in the table above along with the predicted melting temperature estimated from our elastic constant C_{11} calculated using the following expression [42].

$$T_(melting) = [555K + \left(\frac{5.91K}{GPa}\right) C_{11} \pm 300K] \tag{12}$$

Hence, CoCrSb has a stronger bond than CoMoSb and CoWSb due to its high Debye temperature.

6.1. Conclusions

The structural, mechanical, electronic and thermodynamic properties of Co-based half-Heusler CoYSb (Y= Cr, Mo, W) alloys which conform to $F\bar{4}3m$ space group in the three possible structural (Type-I, Type-II and Type-III) phases atomic arrangements, which are given by Wyckoff notation have been investigated in detail. We determined that our alloys are stable in the Type-I structural phase, which is half-metallic for CoCrSb, nearly half-metallic for CoMoSb due to its percentage spin polarization with the possibility of being used in a spintronic application and metallic character for CoWSb due to the absence of band gaps in their spin-polarized electronic

band structures. The calculated electronic band structures and total magnetic moments show that these alloys are ferromagnetic in all the phases. Finally, some mechanical properties of these materials have been examined in the most stable phase (Type-I), and it is clearly seen that these alloys are stable mechanically and anisotropic in nature.

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