

# Review on Thermoelectric properties of Co-based Full-Heusler compounds

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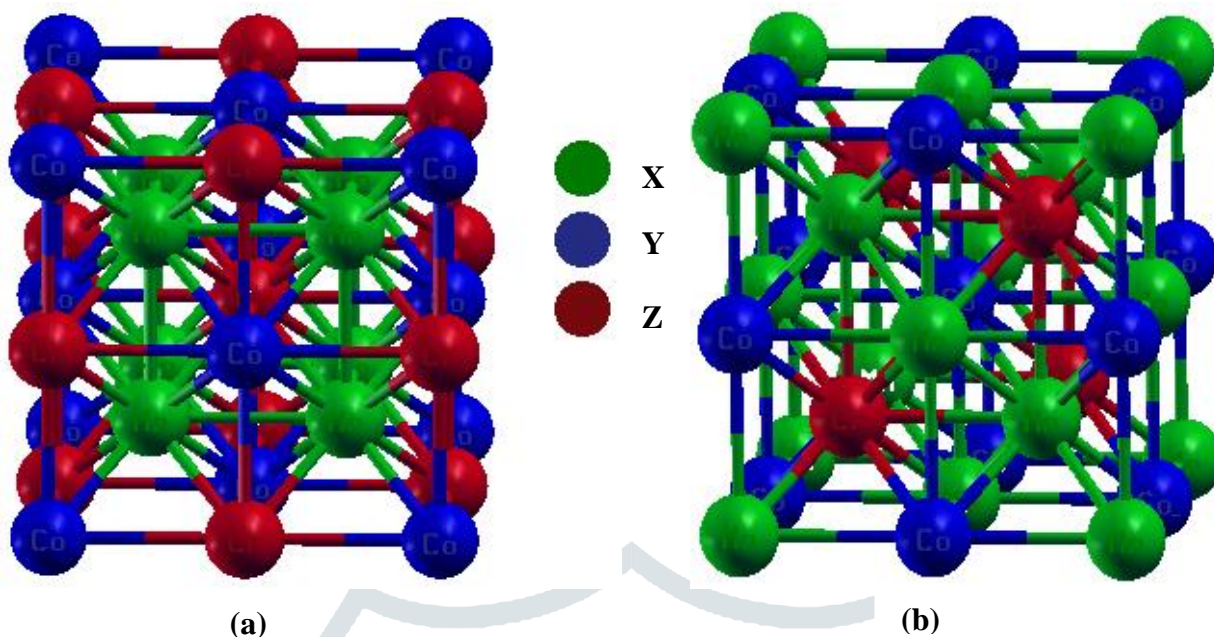
## Abstract

The applications of Heusler compounds in thermoelectric made them valuable for the theoreticians and experimentalists. In this paper thermoelectric properties of  $\text{Co}_2\text{MnAl}$ ,  $\text{Co}_2\text{MnSi}$  and  $\text{Co}_2\text{MnGe}$  full-Heusler compounds have been reviewed. The calculations were done by using BoltzTrap code which depends upon the Boltzmann semi-classical transport equation. Seebeck coefficient, electrical conductivity, and thermal conductivity for  $\text{Co}_2\text{MnSi}$  and  $\text{Co}_2\text{MnAl}$  were calculated by considering both magnetic phases.  $\text{Co}_2\text{MnSi}$  was found to be half-metallic in ferromagnetic phase and had the highest value for the power factor ( $2.9 \times 10^{-3} \text{Wm}^{-1}\text{k}^{-2}$ ).  $\text{Co}_2\text{MnGe}$  was found to be half-metallic and had the smallest value for figure of merit at room temperature. The calculated values for Seebeck coefficient for  $\text{Co}_2\text{MnSi}$  and  $\text{Co}_2\text{MnGe}$  were  $40 \times 10^{-6} \text{VK}^{-1}$  and  $16.7 \times 10^{-6} \text{VK}^{-1}$  respectively.

**Keywords:** Heusler compounds, Thermoelectric properties, Co-based Heusler, BoltzTrap code

## Introduction

The properties like high polarization at fermi level [1], thermoelectric performance [2], ferromagnetism and large Curie temperature [3] made Heusler compounds proficient candidates for spintronics, spin-value generators, magnetoresistive materials, memory devices and thermoelectric materials [4-7]. These eventful compounds were first introduced by Friedrich Heusler in 1903 and their shocking magnetic property of having ferromagnetic behavior without the presence of any magnetic element involve many researchers to investigate them.  $\text{Cu}_2\text{MnAl}$  was the first such full-Heusler compound [8, 9] and  $\text{NiMnSb}$  was the first half-Heusler compound investigated as the half-metallic [10]. There are always three elements in Heusler compounds generally named as X, Y, and Z in which transition elements are taken as X and Y whereas s, p elements are set at the place of Z. The composition of these three elements gives birth to two kinds of Heusler compounds named as half-Heusler (XYZ) and full-Heusler ( $\text{X}_2\text{YZ}$ ) compounds [11, 12]. The former crystallizes in  $\text{C1}_b$  structure and latter in  $\text{L2}_1$  or XA structure [13], therefore full-Heusler compounds can be investigate by considering two structures. One is  $\text{L2}_1$  also known as  $\text{Cu}_2\text{MnAl}$  lie under  $\text{Fm-3m}$  (225 SG no.) space group and another is XA also known as  $\text{Hg}_2\text{CuTi}$  or inverse Heusler compounds lie under  $\text{F-43m}$  (216 SG no.) space group. In  $\text{L2}_1$  structure (0.25, 0.25, 0.25), (0, 0, 0) and (0.5, 0.5, 0.5) are the atomic positions fixed to X, Y, and Z respectively whilst in XA structure atomic positions (0, 0, 0), (0.25, 0.25, 0.25), (0.5, 0.5, 0.5) and (0.75, 0.75, 0.75) are appointed to  $\text{X}_1$ ,  $\text{X}_2$ , Y and Z in the order [14].



**Figure 1:** (a) representing L<sub>21</sub> Phase and (b) representing XA Phase.

In this review paper thermoelectric properties of Co<sub>2</sub>MnZ (Z=Si, Al, Ge) has been calculated by using BoltzTrap code [15] which is based on Boltzmann semi-classical transport equation. The BoltzTrap code relies upon the data given by wien2k code.

### Thermoelectric properties

The semiconductors with a narrower gap or semimetals having high carrier mobility and low thermal conductivity are considered as the great aspirant for the thermoelectric materials [16-18]. A dimensionless physical quantity of a material known as figure of merit should be unity or larger for being a good candidate for thermoelectric materials and is defined as:

$$ZT = \frac{S^2 \sigma}{\kappa} T \quad [19]$$

where S is a Seebeck coefficient,  $\sigma$  is an electrical conductivity and  $\kappa$  is a thermal conductivity which is a sum of electronic ( $\kappa_e$ ) and lattice ( $\kappa_l$ ) thermal conductivity and the product of  $S^2$  and  $\sigma$  is known as the power factor whose value can be maximized by doping [16]. The thermoelectric properties of Co<sub>2</sub>MnAl and Co<sub>2</sub>MnSi were calculated by Hayashi et al. in a ferromagnetic state by considering electronic states and crystal structures. They found the high value of Seebeck coefficient and electrical conductivity for Co<sub>2</sub>MnSi as compare to Co<sub>2</sub>MnAl and as a result high value of power factor for Co<sub>2</sub>MnSi at 550K was obtained. The experimental lattice constant 5.758Å for Co<sub>2</sub>MnAl and 5.654Å for Co<sub>2</sub>MnSi was used for the further calculations. The L<sub>21</sub> structure was used for both the full-Heusler compounds whereas experimentally they found L<sub>21</sub> phase with small contribution B2 and A2 Phase for Co<sub>2</sub>MnSi and B2 phase for Co<sub>2</sub>MnAl from XRD patterns. Electronic band structure was calculated in both ferromagnetic and non-magnetic states as compounds showed variation in magnetic states within the different ranges of T<sub>C</sub>, which further help to assess the dependence of Seebeck coefficient S(T) and

division of electrical conductivity with time  $\sigma(T)/\tau$  on temperature. They considered the relaxation time to be the same for both the spins. The absolute value of Seebeck coefficient for  $\text{Co}_2\text{MnZ}$  ( $Z=\text{Al}, \text{Si}$ ) increased with increasing temperature and start decreasing beyond a particular temperature which indicated that the electronic states are related to the magnetic phases and lead to the lower value of Seebeck coefficient. They also explained the variation of absolute value of Seebeck coefficient ( $S$ ) with respect to the valence electrons, according to which  $\text{Co}_2\text{MnAl}$  should have large value of  $S$  as compare to  $\text{Co}_2\text{MnSi}$  because former has 28 valence electrons while latter has 29. But result showed the large value of  $S$  for  $\text{Co}_2\text{MnSi}$  and this contrast was due to the contribution of carriers in the electrical transport properties. DOS helped to conclude that dominant carriers for the  $S$  were roamed sp-electrons but not restricted d-electrons. They also found contrast in the absolute and calculated value of  $S$ , which might be because of the crystal structure or calculation method. The value of power factor for  $\text{Co}_2\text{MnSi}$  was  $2.9 \times 10^{-3} \text{Wm}^{-1}\text{K}^{-2}$  at 550K whilst absolute value of Seebeck coefficient was  $40 \times 10^{-6} \text{VK}^{-1}$  [20]. The electronic and thermoelectric properties of  $\text{Co}_2\text{MnGe}$  have been investigated by Joshi et al. by using density functional theory (DFT). By using experimental lattice constant they obtained  $5.6748 \text{\AA}$  lattice constant for further calculations. The calculated values of Seebeck coefficient ( $S$ ) and electrical conductivity ( $\sigma/\tau$ ) at room temperature were  $16.7 \times 10^{-6} \text{VK}^{-1}$  and  $2.92 \times 10^{22} \Omega^{-1}\text{m}^{-1}\text{s}^{-1}$  respectively. Electrical conductivity decreases below 25 K with increase in temperature and start increasing after that while became constant above 500 K. On the other hand for lower temperature thermal conductivity behaved same as the electrical conductivity and raised with rise in temperature above 40 K. The calculated value of figure of merit at room temperature was 0.008 which concluded that under ambient conditions half-metal  $\text{Co}_2\text{MnGe}$  is poor conductor for thermoelectric materials [21].

## Conclusion

The thermoelectric properties of full-Heusler compounds  $\text{Co}_2\text{MnZ}$  ( $Z=\text{Al}, \text{Si}, \text{Ge}$ ) has been reviewed.  $\text{Co}_2\text{MnZ}$  ( $Z=\text{Al}, \text{Si}$ ) also prepared experimentally and it was concluded that  $\text{Co}_2\text{MnAl}$  had B2 phase and  $\text{Co}_2\text{MnSi}$  had a mixture of B2, A2 and  $\text{L2}_1$  phase. From the review of three full-Heusler compounds it has been concluded that half-metallic  $\text{Co}_2\text{MnSi}$  is a good candidate for the thermoelectric materials whereas  $\text{Co}_2\text{MnGe}$  is also half-metallic compound but showed poor behavior for thermoelectric materials at room temperature. The obtained values for Seebeck coefficients for  $\text{Co}_2\text{MnSi}$  and  $\text{Co}_2\text{MnGe}$  were  $40 \times 10^{-6} \text{VK}^{-1}$  and  $16.7 \times 10^{-6} \text{VK}^{-1}$  respectively. The estimated value of figure of merit for  $\text{Co}_2\text{MnGe}$  was 0.008 which is far away from the efficient value.

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