The computational Investigation of Co based quaternary Heusler alloys compatible for spin flip device and thermoelectric applications

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ABSTRACT

In this work, we have employed Density Functional Theory (DFT) to study structural and mechanical stability, electronic, magnetic and thermoelectric properties of cubic Co-based new quaternary half- Heusler alloys CoZrCrZ (Z = Al, Ga, In) using WIEN2k. The volume optimization of all these three alloys suggest that they are stable in the Y1 structure and show ferromagnetic nature. The Generalised Gradient Approximation calculations confirm the half- metallic nature of the reported alloys, which show metallic nature in spin up channel and semiconducting band gaps exist in spin down channel. From the calculated cubic elastic constants, the reported Heusler alloys show ductile behaviour. The calculated spin-magneticmoments of CoZrCrZ (Z = Al, Ga, In) are consistent with the Slater-Pauling rule with total magnetic moments of 4μ B . Moreover, veryfine narrow band gap in the spin-down channel enhances the thermoelectric properties. The reported ferromagnetic half-metals with goodthermoelectric parameters suggest that these alloys have possible applications in spin-basedelectronics and green energy technology.

INTRODUCTION

- In recent years, with various structural symmetries, a large number of materials possessing half metallic (HM) character was identified, which includes perovskites, double perovskites, transition metal oxides, Heusler alloys (HAs) etc.
- Among these materials, HAs are well known for more than a century. German chemist Fredrich Heusler first discovered full HA Cu_2MnAl in 1903
- Based on the structural composition, they can be classified as full HAs with structural formula X_2YZ, half-HAs with structural formula XYZ and quaternary HAs having structural formula XX'YZ, where X, X' and Y are transition metals and Z is a main group (sp) element.
- These materials can easily be altered through chemical substitutions and structural variants. This tunability makes them fascinating candidates for the study of spintronics and thermoelectric applications
- First, experimental realization of HM in the Heusler compound NiMnSb was made by Groot *et al*.
- Though numerous HAs have been reported, these materials are still in demand because of their various properties including excellent controllability, simple fabrication and tunable physical properties.

FORMULAE AND THEORY

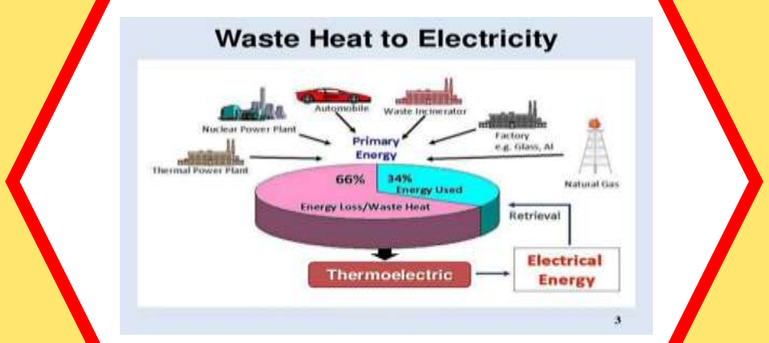
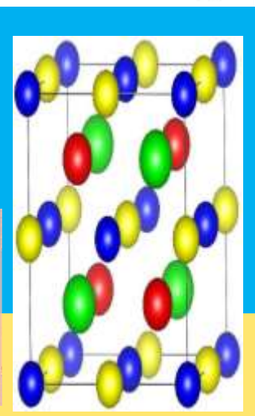


Fig.2. Applications of thermoelectricity

$$\eta = \frac{T_H - T_C}{T_H}\,\frac{\sqrt{1+ZT}-1}{\sqrt{1+ZT}+\frac{T_C}{T_H}}$$

$$ZT = \frac{\alpha^2 \sigma}{\kappa_l + \kappa_e} T$$

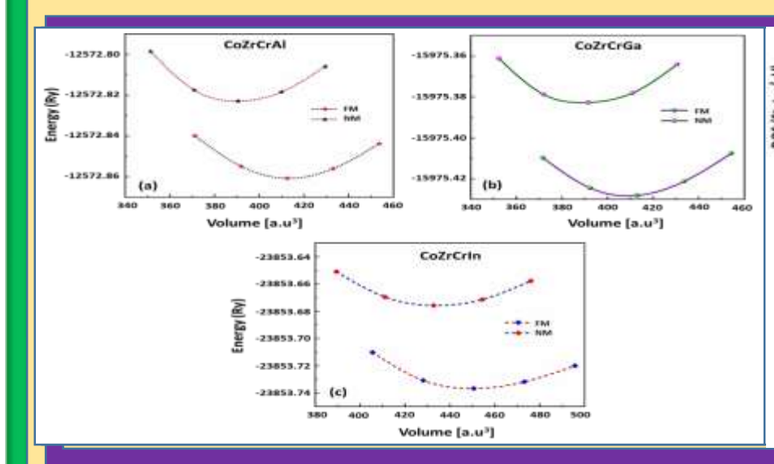
$$K = \frac{1}{3} C v l$$

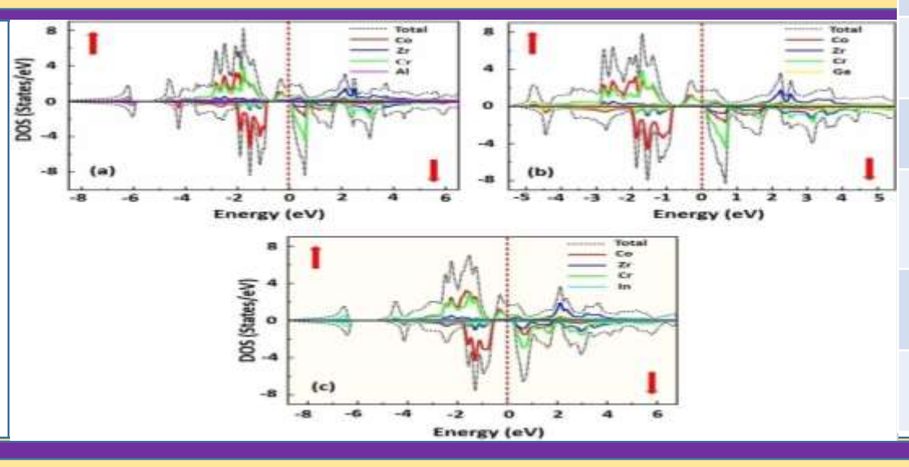


Alloys	Energy(Ry) FM	Energy(Ry) NM	a_0 (Å) FM	Volume FM
CoZrCrAl	-12572.86	-12572.82	6.2586	413.58
CoZrCrGa	-15975.43	-15975.38	6.2348	408.89
CoZrCrIn	-23853.74	-23853.68	6.4388	450.35

RESULT & DISCUSSION

- From the stability curve as shown in Figure 1 we can understand that all the three reported Heusler alloys are more stable in ferromagnetic phase compared to nonmagnetic phase.
- The calculated minimum energy and lattice constants for CoZrCrZ are listed in Table 1 in nonmagnetic and ferromagnetic phase.
- Among two phases ferromagnetic phase has least energy for all these three alloys which confirm that all the studied cubic quaternary Heusler alloys CoZrCrZ (Z=Al, Ga, In) are stable in ferromagnetic phase under equilibrium condition The possible atomic arrangements in the quaternary Heusler alloy XX'YZ: X (0, 0, 0), X' (0.25, 0.25, 0.25), Y (0.5, 0.5, 0.5) and Z (0.75, 0.75, 0.75) where X, X' and Y are transition metals and Z being a main group (sp) element and it belongs to F-43m space group.
- Pugh's ratio (B/G ratio) indicates the relationship between ductile and brittle nature of the materials. Direct
- If B/G > 1.75 then the material exhibits ductile behavior whereas for brittle nature B/G < 1.75
- The value of Poisson ratio is of the order of 0.1 for covalent materials whereas in case of ionic materials it is to be 0.25.
- In general crystals have anisotropic character i.e they exhibit directional property. For isotropic material A should be unity whereas in case of anisotropic materials A > 1.
- The chemical and thermodynamical stability of the materials is determined by its formation energy. The negative sign for studied alloys implies that these alloys are thermally stable and can be synthesized easily.
- The spin polarized band structures of CoZrCrZ (Z=Al, Ga, In) at equilibrium lattice constant is presented in Figure 3.
- From the investigated band structure we can see that the majority spin channel shows metallic nature whereas in spin down state the Fermi level is found to be presented in the gap between valence band and conduction band therefore the minority spin channel exhibits semiconducting band gap.
- In CoZrCrZ, the maxima of the valence band and minima of the conduction band are at the same symmetry point L in all the studied Heusler alloys.
- Thus these alloys exhibit direct band gap of 0.93eV, 0.9eV and 0.85eV for CoZrCrAl, CoZrCrGa and CoZrCrIn, respectively.





Alloy	Temperature (K)				ZT
CoZrCrAl	700	109	1.27	2	0.54
CoZrCrGa	700	103	1.2	1.9	0.48
CoZrCrIn	500	73	1.25	1.5	0.23
CoZrMnGe	600	-106			0.1
LaCoCrAl	600	-60.8			0.94

CONCLUSION

- Volume optimization of CoZrCrZ (Al, Ga, In) predicts that reported cubic quaternary Heusler alloys stable in ferromagnetic phase.
- As we go down in the periodic table from Al to In the band gap of CoZrCrZ get decreases from 0.93 eV to 0.85 eV in spin down state with simultaneous decrease of half metallic gap.
- Thus 100% spin polarization occurs in minority spin channel.
- The calculated total magnetic moment (4 μB) and atom resolved magnetic moments indicate that Cr is more responsible for observed ferromagnetic character in CoZrCrZ.
- The figure of merit of 0.54, 0.48 and 0.23 is elucidated for CoZrCrAl, CoZrCrGa and CoZrCrIn, respectively.
- Besides, these results suggest that the studied Heusler alloys are potential candidates for possible spintronic and thermoelectric applications.