EPJ Web of Conferences **356**, 01021 (2026) https://doi.org/10.1051/epjconf/202635601021
ICC 2025

XRD simulation through vesta for the associated structure of Co_2MnSi and Co_2FeSi full-Heusler alloys

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Abstract. Among all the full-Heusler alloys, Co_2MnSi and Co_2FeSi alloys have been exhibited to be tremendous magnetic behavior such as high magnetic moment, half-metallicity and high Curie temperature. Magnetic moments are found to be highest value for the fully ordered sample and half-metallicity drastically reduces with disorder/swapping of elements. Hence, analysis of disorder/swapping is very trivial for achieving the highest magnetic moment and preserving half-metallicity in such type of alloys. Here, we have simulated the X-Ray Diffraction pattern using Vesta software for parent materials as well as associated with disordered and swapping with other elements. Super reflection peaks obtained from the simulated data are found to be very sensitive even for the small amount of swapping. Therefore, we have plotted the ratio of super reflection peaks and compared with the scattering factor data collected from the NIST, USA. Tetragonal distortion has also been revealed in the cubic structure; hence we have simulated the XRD pattern for the distorted sample also. Scaling of magnetization value have also been calculated from the Slater-Pauling rule and these values have compared with the experimental results available in the literature. This study will help researchers to understand and compare their experimental XRD results with simulated one.

1. Introduction

Heusler based magnetic materials have been found to be good candidate for making the magnetic based devices. Among the others, Co based alloys have attracted due to the highest magnetic moment and Curie temperature. Co_2MnSi and Co_2FeSi have shown the tremendous magnetic properties such as half-metallic character, spin caloric properties, high magnetoresistance etc. These Heusler alloys have been found to be stabilized in face centered cubic structure with three additional interpenetrating lattices with original cube along the

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body diagonal. In Co_2MnSi structure, Co (I) and Co (II) atoms occupy (¾, ¾, ¾) and (¼, ¼, ¼) while Mn and Si occupy (0, 0, 0) and (½, ½, ½) respectively.

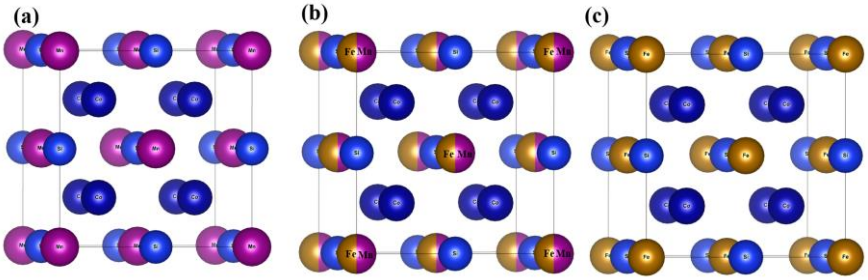

Fig. 1 Schematic diagram of unit cell of **(a)** Co_2MnSi, **(b)** $Co_2Mn_{0.5}Fe_{0.5}Si$ and **(c)** Co_2FeSi full-Heusler alloys.

Moreover, half-metallicity/spin polarization has been found to be reduced due to the anti-site disorder, temperature and stoichiometry in Co_2MnGe and Co_2MnSi alloys [1-3]. Large magnetoresistance (MR) ratio has revealed in Co_2MnSi epitaxial layer grown on Ag in both side and 67.2% at 110K temperature [4]. Magnetic electrode in magnetic tunnel junction has also been made from Co_2MnSi and tunneling magnetoresistance effect amplitude has found to be tuned with temperature [5]. Spin polarization has also verified experimentally and found to be 93% spin polarization at room temperature in Co_2MnSi [6]. Electrochemical behavior has also been studied for Co_2MnSi alloy [7]. Moreover, Co_2FeSi has revealed magnetic moment of $6\mu_B$ and 1100K Curie temperature which is the highest value so for in the family of Heusler materials and others also [8]. Thin film of Co-based full-Heusler alloys grown on different type of substrate layers have demonstrated the different properties. Co_2FeSi has grown on the Ga (001) interface shows the loss of half-metallic nature near the interface rather the its bulk side [9]. In order to achieve theoretical value of half-metallicity in Co_2FeSi alloy, highly ordered single crystal has grown and significant electrical behavior has determined which was attributed to the half-metallic nature [10]. Ball milling technique was used to prepare the nano particle of Co_2FeSi by crushing the bulk for 9h and optimized for 12h. These nano particles have exhibited the superparamagnetic behavior and saturation magnetization has been found to be reduced in comparison to their bulk structure due to the magnetically dead layer at the surface of the particles [11]. Anomalous magnetic behavior has revealed in Co_2FeSi microwires coated by glass and M-H curve and coercivity value have been found to be changed drastically [12]. The evolution of structural disorder and the impact of finite temperature have been identified as the primary causes of the disparity between theoretical predictions and experimental results [13]. Transition metal elements in these compounds tend to swap sites with each other due the similar size and most electronegativity differences attributed to the evolution of new states in the minority spin gap destroying half-metallic properties. The spin disorder that occurs at finite temperatures another cause of the destruction of half-metallic properties [13].

2. Result and Discussions

Further, due to the highly sensitive nature of magnetic properties of these alloys with the structural order, specific structure of these alloys plays a vital role for the specific magnetic properties. In order to analyze the structural order, we have simulated the each XRD pattern corresponding to every 5% substitution of Fe at Mn site in Co_2MnSi alloy.

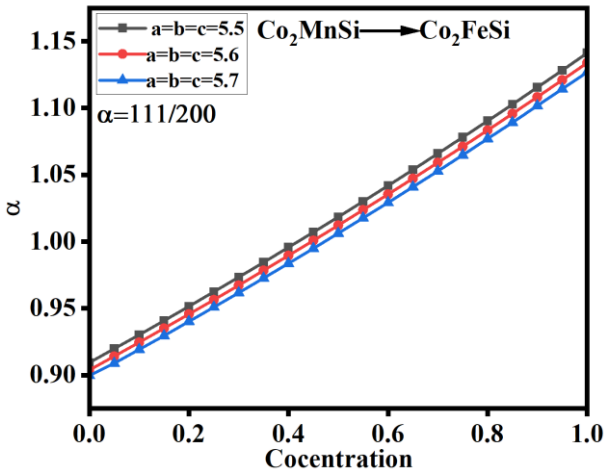

Fig. 2 Plot between the increasing concentration of Fe at Mn site in Co_2MnSi versus ratio of super reflection peaks (111 and 200).

Each XRD data contains a pair of peaks between 25-30 value of 2θ. These peaks determine the extent of anti-site disorder/swapping in the given structure. Relative intensities have been found to change with the concentration of Fe at Mn site. Therefore, we have taken the ratio of first super reflection peaks and plotted the curve between the ratio and the concentration of Fe as shown in Fig. 2. From this plot, we have found the linearly increasing behavior due to the higher scattering of Fe than Mn. The value of scattering factors for Fe and Mn has been found to be 25.26 e^-/atom and 24.69 e^-/atom respectively taken from the NIST, USA. We have also taken same data with different lattice parameter of unit cell of Co_2MnSi. Similar trend has obtained for 5.6Å and 5.7Å value of lattice parameters with reduced value. This decreased value of α with increasing lattice parameter directly suggests that compact structure has less probability of scattering. This might also be due to the tightly linked electrons with the atoms which do not respond to the X-rays. We have only used the experimentally acceptable value of lattice parameter from the several reports. Although, we have performed the similar study with the complete replacement of third atom in Co_2MnSi alloy which has briefly described below.

We have also plotted the value of α with changing the third element in Co_2Mn based full-Heusler alloys as shown in Fig. 3. From the plot, we have seen that both the curve has reduced between 60-80 value of atomic mass. In the inset of Fig. 3, scattering factor versus atomic mass have been plotted and found to be linear which is obvious due to increasing the number of electrons. However, α has exhibited its lowest value for Ga, Ge and As which might be attributed to the localization of the transition metal's electron by substituting these Ga, Ge and As at X position in Co_2MnX alloy. Localization of electrons lead to reduce the scattering factors as well as magnetic contribution also. After comparing both the curve in Fig. 3, we can say that tendency to localize the electrons would have the similar trend as α has demonstrated the variation with atomic masses.

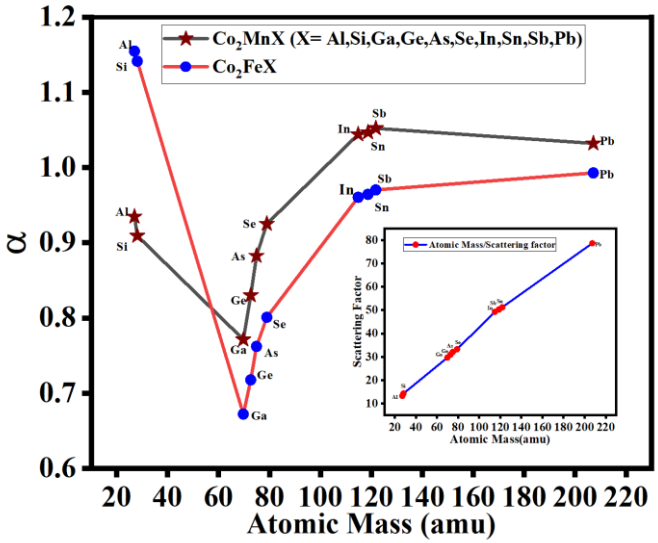

Fig. 3 Plot of the atomic mass of X atom in Co_2MnX and Co_2FeX (X=Al, Si, Ga, Ge, As, Se, In, Sn, Sb, Pb) versus ratio of super reflection peaks (α).

3. Conclusion

Substitution of Fe and Mn at X site in Co_2MnSi has been successfully implanted through Vesta software. Ratio of super reflection peaks have been noted for each percentage which was increased linearly and similar trend have found for increasing lattice parameter with lowering α value. Substitution of other elements at X site in Co_2MnX and Co_2FeX have obtained and found to be reduced for Ge, Ga and As which was explained on the basis of delocalization of electrons.

Acknowledgement

One of the Authors Bal Govind acknowledges financial support from CST UP, Lucknow (Reference no- CST/D-838).

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