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# A Systematic Review on Magnetic Properties of Mn-Ni Based Full-Heusler Alloys

**Shubham Pushkar*[2, 4], Rajesh Kumar Verma[2, 4], Bal Govind*[1,3]**
**[1]Kisan Post Graduate College, Bahraich, U.P. 271801, India.**
**[2]K. S. Saket P. G. College, Ayodhya, U.P. 224123, India.**
**[3]Maa Pateswari University, Balrampur, U. P. 271201, India.**
**[4]Dr. Rammanohar Lohia Avadh University, Ayodhya, U. P. 224001, India.**
**Corresponding Author's Email- spushkar346@gmail.com, balgovind@kisanpgcollege.ac.in**

**Abstract:**Magnetic materials are becoming high demanding due to their suitable application in spintronic devices. Among the several magnetic materials, Heusler alloys have exhibited a great interest mainly due to their half metallic behavior along with high magnetic moments. Here, we report the rigorous analysis of Mn based full-Heusler magnetic materials as magnetic moment in these materials are found to be highly around the Mn elements. Magnetic moment of Mn in different Mn-based alloys has been listed in the table for the comparison. Therefore, experimental findings specifically on $Mn_2NiSb$ have been critically reviewed in the subsequent section of this manuscript. However, several compensated ferrimagnetic and antiferromagnetic Heusler alloys have also been studied and few examples have also been given in order to show the multifunctionality of these alloys. Composites of half and full-Heusler have also been experimentally established with reducing their magnetic behavior.Effect of structure on the magnetic has also been revealed from the available literature. Specifically, structure of $Mn_2NiSb$ full-Heusler alloy in their cubic, tetragonal and hexagonal form has been simulated and X-Ray diffraction data are plotted for each. Since, the magnetic behavior of these materials are intrinsically linked to their crystal structure and their respective sites. Any small change in their structure has significantly change their magnetic behavior. Therefore, transition from low temperature austenite to high temperature martensite phase have been exhibited which has revealed in the magnetization versus temperature data in zero field cooled and field cooled measurements.

**Keywords-** Full-Heusler Alloys, Spintronic Application, Magnetic Moment, X-Ray Diffraction Data etc.

**Introduction-** Heusler alloys have been found be a good candidate in the field of magnetism which have attracted a remarkable interest for the spintronic devices. However, several challenges have been revealed in these alloys such as 100% spin polarization, swapping, disorder and defects [1-6]. Similar atoms have always possibility to swap from their respective position. Heusler alloys have generally divided into three categories depending

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upon the elements used to prepare a particular alloy and vacant sites. First is half-Heusler which contains 4 site available in their face centered cubic lattices, and out of these four sites, two of them are filled by two transition metals (XY) and one is filled be p-group elements (Z), and one site remains vacant [7]. With the same analogy, three sites are filled by two transition metals ($X_2Y$ or $Y_2X$) by repeating X or Y and one site is filled by p-group elements (Z) and we can prepare full-Heusler. All the four sites are completely filled in full-Heusler alloys [8]. Similarly, if all the four sites are filled by three different transition metals and one is p-group element, we can prepare quaternary Heusler alloys [9]. Schematic diagram of different type of Heusler alloys has been shown in Fig. 1 for the sake of convenience.

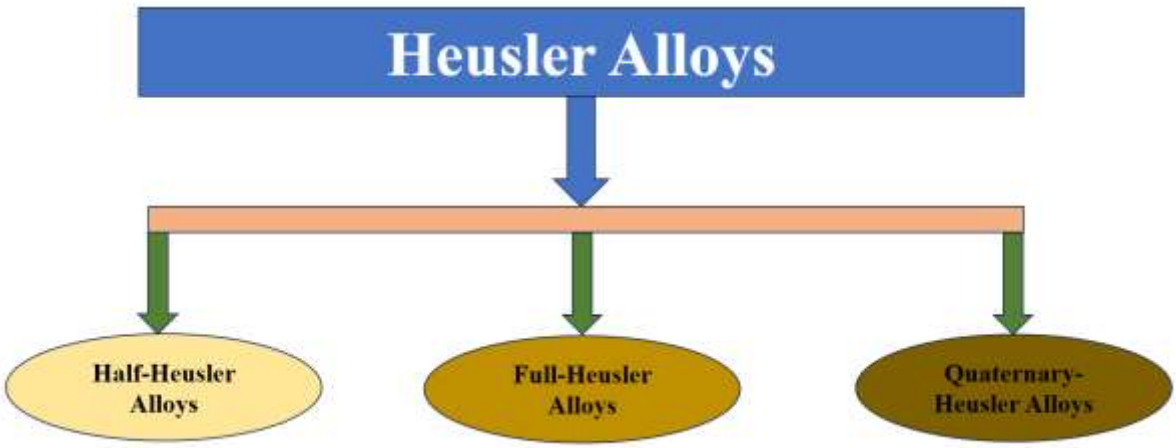


**Fig. 1** Schematic representation of classification of Heusler alloys.

Further, full-Heusler alloys have found to be stabilized in two prototype structure: one is $Cu_2MnAl$ prototype and other is $Hg_2CuTi$ prototype structure [10-11]. Depending upon the type of elements used in these alloys, we have classified these alloys in few types i.e. $Co_2YZ$, $Fe_2YZ$, $Ni_2YZ$ and $Mn_2YZ$ etc. In this article, we have focused on the $Mn_2YZ$ based Heusler alloys. $Mn_2YZ$ based full-Heusler alloys have been found to be more interesting due to the easily manipulating their spin [12-13]. Orientation of spin between Mn-Mn atoms have been found to be strongly related to the distance between them. If the distance between the two adjacent Mn atoms is maintained greater than 2.9Å then would be aligned in parallel direction schematically shown in Fig 2.

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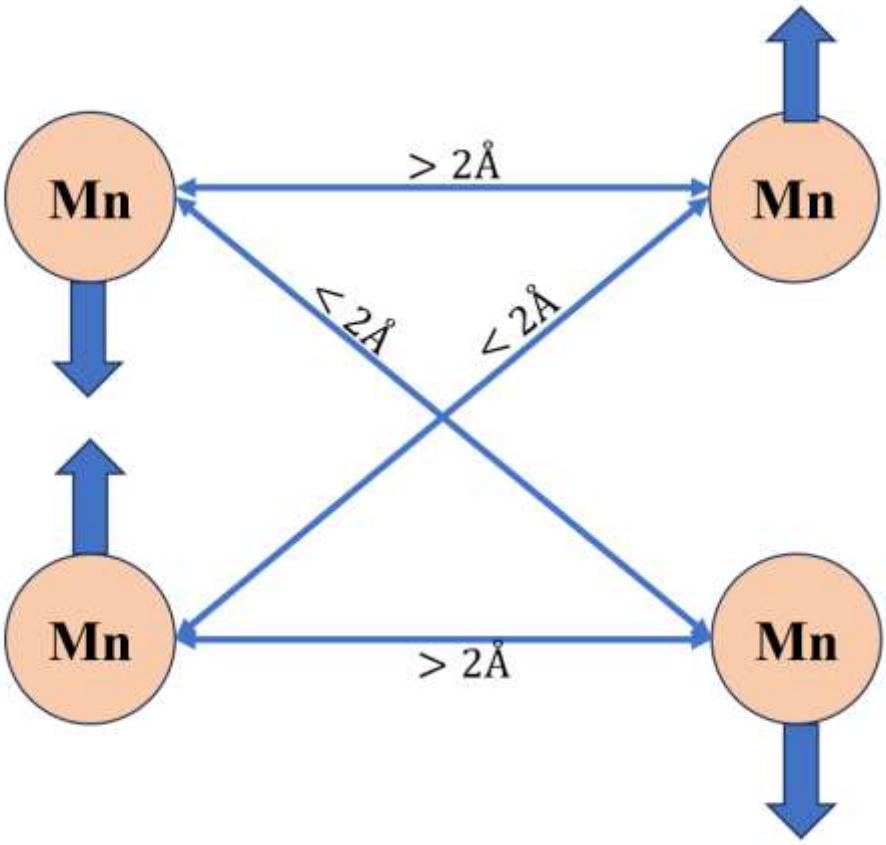


**Fig. 2** Parallel and antiparallel alignment of spin of Mn atom as a function of distance.

By taking the advantage of this property, one could make a strong ferromagnetic material. This could be achieved either through the direct interaction between Mn-Mn or through indirect interaction as by extra element substitution between the two adjacent Mn atoms. Later is applied in case of Heusler alloys. Among the others, $Mn_2NiSb$ have been widely explored due to their high magnetic moment and high Cuire temperature. These materials are found to be stabilized in both $Cu_2MnAl$ and $Hg_2CuTi$ prototype structure. Schematic diagram of unit cell of both the structures has been shown in the Fig. 3. In $Cu_2MnAl$ type, in case of $Mn_2NiSb$, Mn (I) and Mn (II) prefer to fill (0.25, 0.25, 0.25) and (0.75, 0.75, 0.75) position while Ni and Sb prefer to occupy the (0.5, 0.5, 0.5) and (0,0,0) respectively. In $Hg_2CuTi$ prototype, Mn (I) and Mn (II) prefer to fill (0,0,0) and (0.25, 0.25, 0.25) position while Ni and Sb prefer to occupy the (0.5, 0.5, 0.5) and (0.75, 0.75, 0.75) respectively. Experimentally, lattice parameters of the unit cell have been generally found to be greater than 6Å. Therefore, distance between nearest neighbors Mn atoms would be greater than 3Å in $Cu_2MnAl$ structure. However, it might be lees than 3Å in diagonal direction in case of $Hg_2CuTi$ prototype structure. Hence, less value of magnetic moment has been reported in $Hg_2CuTi$ prototype structure as compared to $Cu_2MnAl$ structure.

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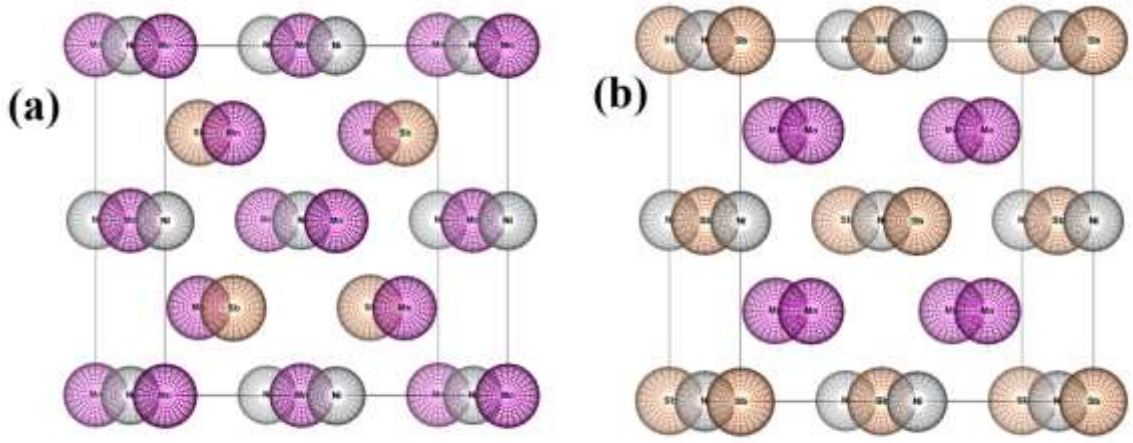


**Fig. 3 (a)** Schematic unit cell of $Mn_2NiSb$ in $Hg_2CuTi$ prototype structure and **(b)** in $Cu_2MnAl$ prototype structure.

We have simulated the X-Ray diffraction pattern for both the above structure which have shown in Fig 4. From this data, we can see the difference in both the pattern i.e. ratio between first two peaks is obtained to be different. These super reflections peaks (111 and 200) are highly sensitive for the swapping and disorder in the samples [14]. Any small change in the position of atoms significantly changes the relative ratio of these peaks. Hence, we can calculate the amount of swapping up two few extents. However, X-ray is not very sensitive for the similar atoms due to the equivalent scattering factors.

Moreover, we have also simulated the XRD pattern for tetragonal structure of $Mn_2NiSb$ because several Heusler alloys have been found to be stabilized in tetragonal structure also. Lattice parameters of the tetragonal unit cell and cubic cell used for the simulation are given in the table 1. In addition to the structural analysis, magnetic moments of the Heusler alloys could also be predicted from the Slater Pauling rule which is given as follows-

$M_T = N_V - 18$, for half-Heusler

$M_T = N_V - 24$, for full-Heusler

$M_T = N_V - 28$, for full-Heusler

Where $M_T$ is the total magnetic moment per unit cell and $N_V$ is the total valance electron count.

| Structure of $Mn_2NiSb$ | Prototype | Lattice parameters | angle |
|---|---|---|---|
| Cubic | $Hg_2CuTi$ | a=b=c= 6.0 | $\alpha = \beta = \gamma = 90^0$ |
| Cubic | $Cu_2MnAl$ | a=b=c= 6.0 | $\alpha = \beta = \gamma = 90^0$ |
| Tetragonal | ---------- | a=b=3.95, c= 7.0 | $\alpha = \beta = \gamma = 90^0$ |

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**Table 1.** Parameters used in the simulation of cubic and tetragonal XRD data.

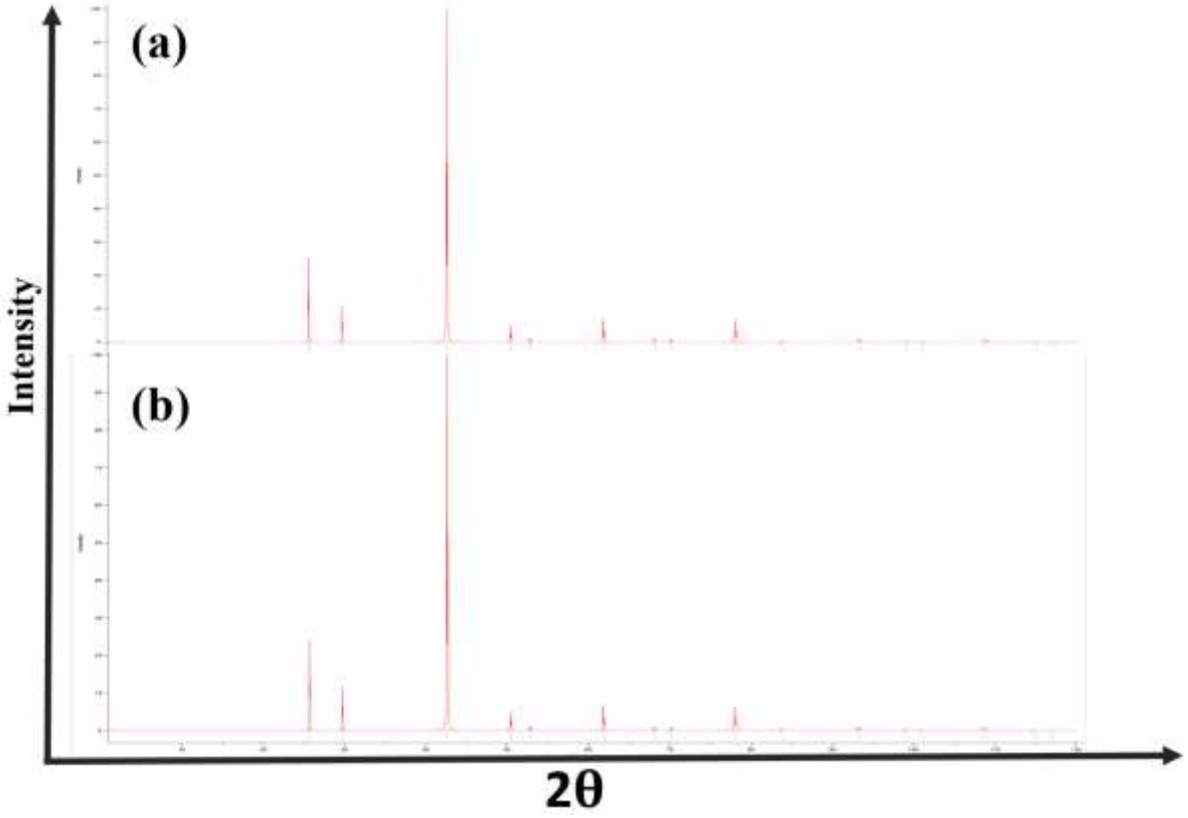
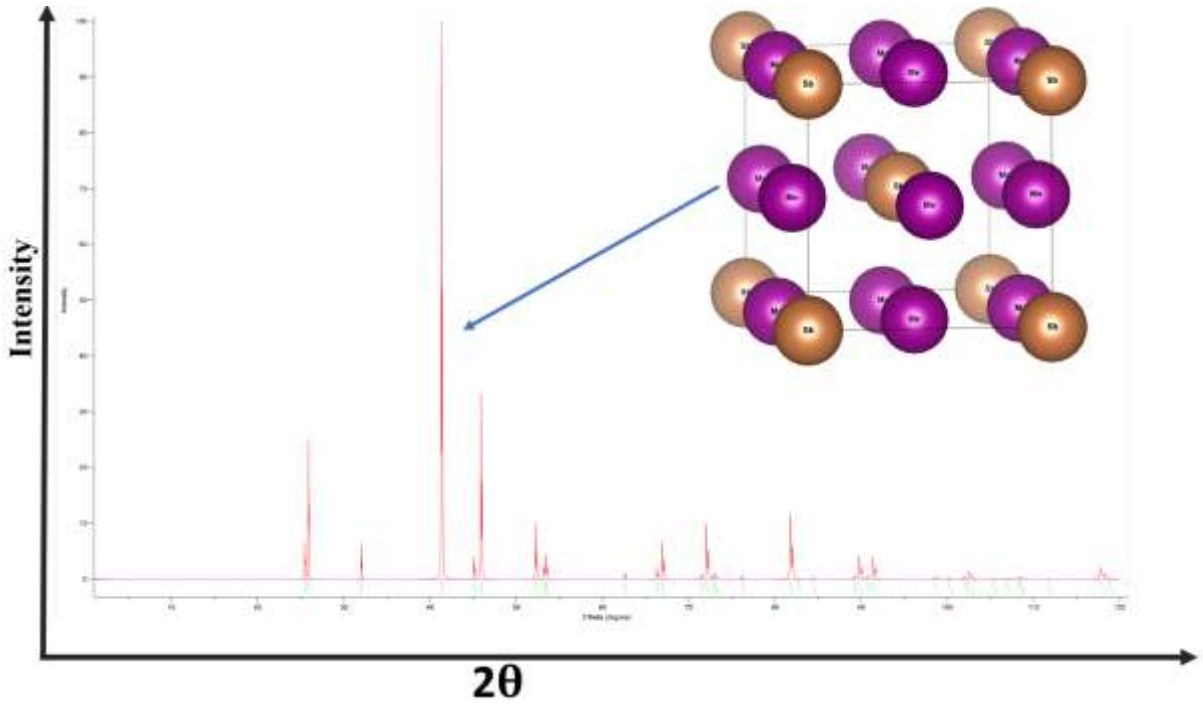



**Fig 4.** Simulated XRD pattern of Mn2NiSb in (a) $Hg_2CuTi$ and (b) $Cu_2MnAl$ structure.




**Conclusion-** We have successfully simulated the XRD data of Mn2NiSb in Hg2CuTi and Cu2MnAl prototype structure respectively and found to be the different relative height of super reflection peaks which indicated the level of sensitivity of these peaks in accordance

with the structure. We have also simulated the XRD graph for the tetragonal structure of $Mn_2NiSb$ also. These simulated XRD pattern will be useful for comparing the experimental XRD data and used as a standard data for the refinement of the XRD data also.

**Conflict of Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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