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Understanding Structural Differences Between Bulk $Mn_2CoFeGe_2$ Double Half-Heusler Alloy and Deposited Thin Films

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***Abstract:** We report preliminary findings from our study on a new alloy and its thin film form. A double half-Heusler $Mn_2CoFeGe_2$ alloy was prepared in an arc furnace, and a thin film was deposited on silicon (100) and glass substrates via thermal evaporation. The films were characterized to evaluate their surface morphology and crystal structure using scanning electron microscopy and diffraction analysis. Elemental composition was determined through X-ray spectroscopy. These results highlight the importance of maintaining precise stoichiometry to obtain the intended material properties.*
***Keywords:** $Mn_2CoFeGe_2$, Double Half-Heusler Alloy, Thin films, Magnetism*

I. INTRODUCTION

Heusler alloys form a broad family of materials, generally classified as Half Heusler (X_1Y_1Z), Full Heusler ($X_2Y_1Z_1$), Inverse Heusler, Binary, and Quaternary Heusler types. In these compositions, Z acts as the primary element, while X and Y are typically transition metals. What began as a topic of fundamental research has now evolved into a material class with meaningful technological relevance [1]. Today, Heusler alloys are gaining attention for use in sensors, energy conversion devices, magnetic shape-memory actuators, thermoelectric generators, and magnetic refrigeration systems**,** among other applications. Both Full and Half Heusler compounds have been widely explored, supported by extensive theoretical investigations as well as significant experimental studies[2]**.** The discovery of new functional materials remains a key focus in condensed matter physics, with manganese-based (Mn-based) Heusler alloys standing out for their remarkable physical properties and tunable structure. Their electronic and magnetic behavior can be tailored through doping, stoichiometry control, and structural adjustments. Notably, these alloys often exhibit strong ferromagnetism with high magnetic moments, making them suitable for applications such as magnetic sensors, permanent magnets, data storage, and advanced spintronic devices[3,4].

In this work, we focus on a newly synthesized material, $Mn_2CoFeGe_2$, and explore its fundamental characteristics. Early observations suggest that this alloy could be highly promising for magnetic applications. Classified as a double half-Heusler compound, it belongs to the wider Heusler family, well recognized for its flexible magnetic behavior and technological relevance. Changes in its crystal structure, driven by the substitution of Mn, Co, and Fe, are expected to strongly influence both its magnetic and structural properties. At the same time, the presence of Ge alters the bonding and coordination environment within the alley, further shaping its overall behavior [5].

II. EXPERIMENTAL TECHNIQUE.

Initially 1-gram $Mn_2CoFeGe_2$ alloy was synthesized using an arc furnace. High-purity elemental Manganese (Mn), Iron (Fe), Cobalt (Co), and Germanium (Ge) (≥99.99%) were weighed in stoichiometric amounts and melted together under a high-purity argon atmosphere. Since manganese is volatile, an extra 3% Mn was added to compensate for weight loss during melting. To ensure homogeneity, the resulting ingot was remelted several times, flipping it between melts. The total weight loss after the process was kept below 1%. For further compositional uniformity, the ingot was sealed in a quartz ampoule and annealed at 1000 °C for six hours in a tube furnace. Finally, the sample was allowed to cool naturally to room temperature before subsequent characterization.

For thin-film deposition, the $Mn_2CoFeGe_2$ ingot was first broken into smaller pieces and placed in a tungsten boat for thermal evaporation using an Advanced Processing Technologies (APT) system. The films were deposited onto silicon (Si (100)) and glass substrates, with the chamber pressure maintained at 5×10^{-6} Torr throughout the process.

After deposition, all samples underwent post-annealing at temperatures ranging from 100 °C to 400 °C for 30 minutes in a vacuum environment at a pressure of 5×10^{-3} Torr to improve structural uniformity and film quality[6].

Powder and Thin film samples were exposed to Cu-Kα radiation (1.54 Å) to obtain X-ray diffraction (XRD) patterns at room temperature using a Rigaku Smart Lab system (Japan). The composition of the sample was analyzed using a JEOL JIB-4700 FIB-SEM in energy-dispersive X-ray spectroscopy (EDS) mode, with EDS data acquired via scanning electron microscopy (SEM).

III. RESULTS AND DISCUSSION

A. X-ray Diffraction Studies

The structural characteristics of the alloy and films were examined using a high-resolution X-ray diffractometer with a Cu-Kα radiation source. The diffraction patterns were recorded in the 2θ range of 5º to 80º, as illustrated in Figure 1(a) for the powder sample and Figure 1(b) for the thin film samples. However, the thin films on the glass substrate did not exhibit any XRD peaks, likely due to the limitations of the thermal evaporation method. The XRD pattern of the synthesized $Mn_2CoFeGe_2$ powder confirms its crystallinity and shows a crystalline phase. This crystalline phase influences the properties of the material, potentially offering a combination of properties of the orthorhombic and cubic phases[7,8].

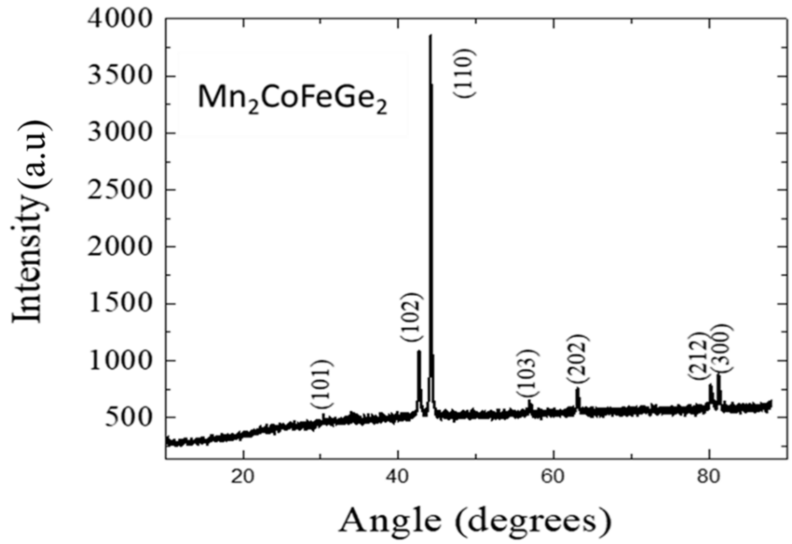

Figure 1(a). XRD patterns of powder sample of $Mn_2CoFeGe_2$

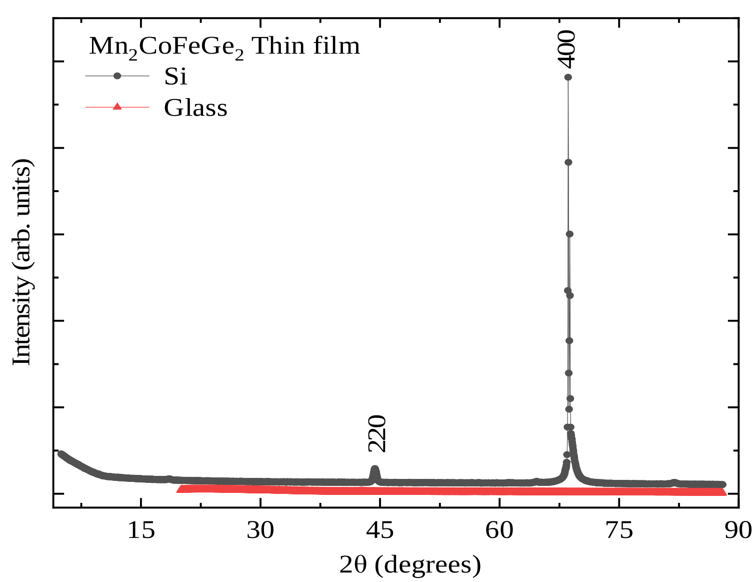

Figure 1(b). XRD patterns of thermally evaporated $Mn_2CoFeGe_2$ thin films

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B. Morphological Analysis

The surface microstructure was examined by FESEM images in Figure 3(a) for alloy samples and Figure 3(b) shows for thin film samples, and the EDS image is shown in Figure 4, thin film elemental distribution in the images, which are at the same scale of 0.1 µm. The film surface evolves into a continuous one. Figure 5, thin film elemental distribution in the images, on the Si (100) substrate. The film surface evolves into a continuous one.

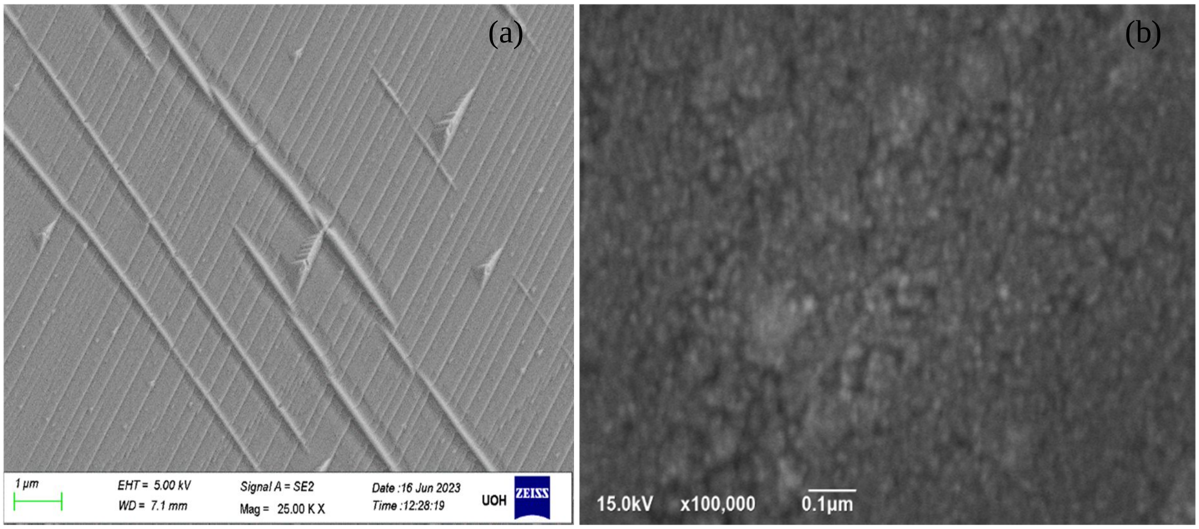

Figure 3(a). Surface morphology of $Mn_2CoFeGe_2$ alloy and Figure 3(b) Thin films on Si (100) captured using FESEM

The surface grains or granules could be because, as we grow film for less time, but cannot get enough time to form a continuous surface, and small grains can be seen all over the surface. With the increase in the deposition time, the merging of islands starts and creates a continuous type of surface structure[9].

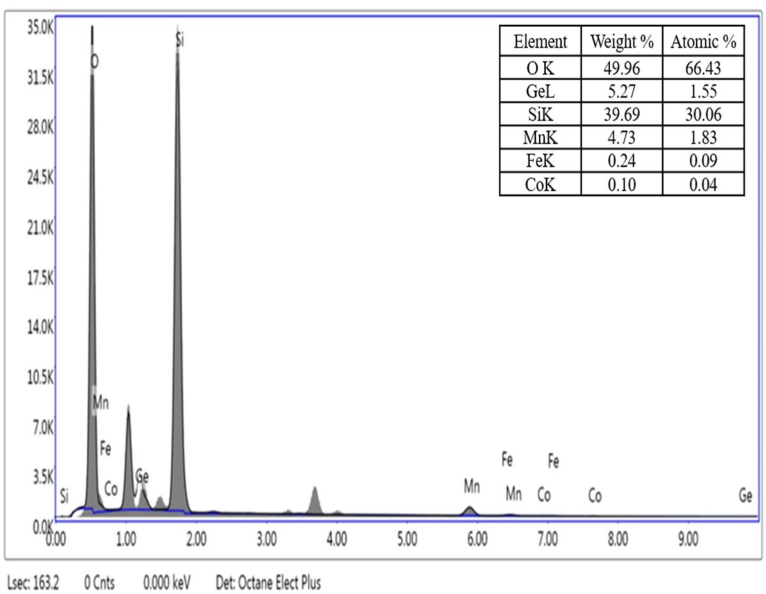

Figure. 4. EDS spectrum showing the elemental composition (Fe, Co, Mn, and Ge) of the $Mn_2CoFeGe_2$ thin film on a glass substrate.

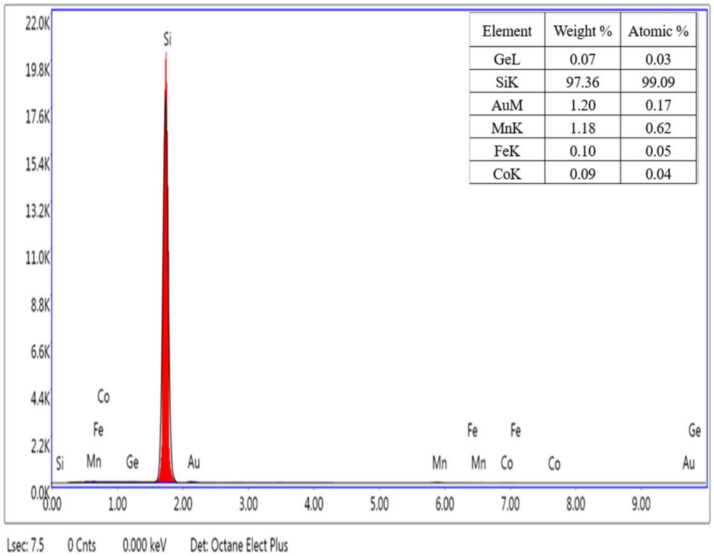

Figure 5. EDS spectrum showing the elemental composition (Fe, Co, Mn, and Ge) of the $Mn_2CoFeGe_2$ thin film on the Si (100) substrate.

Energy-dispersive X-ray spectroscopy (EDS) was used to determine the chemical composition of $Mn_2CoFeGe_2$, and the results presented in Figure 6. match the nominal composition. which was discovered to fit the nominal composition. The volume particles homogeneous of Mn, Fe, Co, and Ge were discovered through X-ray element mapping; no obvious inhomogeneities were discovered.

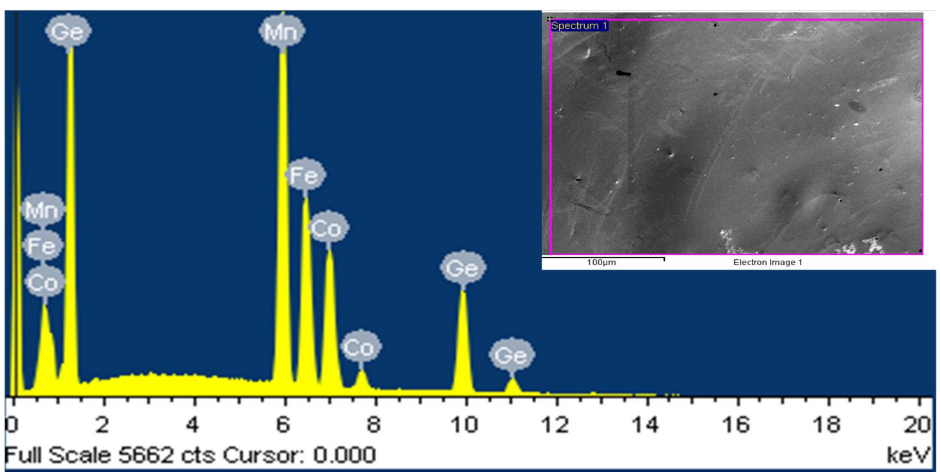

Figure. 6. EDS spectrum showing the elemental composition (Fe, Co, Mn, and Ge) of the $Mn_2CoFeGe$ alloy.

In Table 1. The atomic percentage ratio of 2:1:1:2 agrees with the values anticipated from the findings.

DHH alloy ($Mn_2CoFeGe_2$)	Manganese (Mn)		Cobalt (Co)		Iron (Fe)		Germanium (Ge)	
	Weight (%)	Atomic (%)	Weight (%)	Atomic (%)	Weight (%)	Atomic (%)	Weight (%)	Atomic (%)
Spectrum 1	29.23	32.77	16.14	16.87	15.71	17.33	38.92	33.03
Composition Ratio	2 : 1 : 1 : 2							

Table 1. Composition ratio for $Mn_2CoFeGe_2$ double half-Heusler alloy.

IV. CONCLUSION

In this study, we focused on the $Mn_2CoFeGe_2$ Heusler alloy and examined it in both bulk and thin-film forms. The bulk sample was prepared by arc melting, with repeated melting steps to ensure proper mixing and uniformity. Thin films of the same material were grown on Si (100) and glass substrates using a thermal evaporation process. To understand the structure and composition of the samples, we used X-ray diffraction (XRD) and energy-dispersive spectroscopy (EDS). These techniques helped us confirm the phase formation, crystal structure, and elemental distribution in both the powdered alloy and the thin films. XRD results gave us clear information about the crystalline behavior of $Mn_2CoFeGe_2$, while EDS confirmed the stoichiometry and elemental uniformity across the material. Using both techniques together allowed us to gain a better understanding of how the material's structure relates to its properties. This is particularly important for Heusler alloys, as their tunable magnetic and electronic behavior makes them promising for applications in areas such as spintronics, magnetocaloric devices, and thermoelectric systems.

A. Declaration of Competing Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

V. ACKNOWLEDGEMENTS

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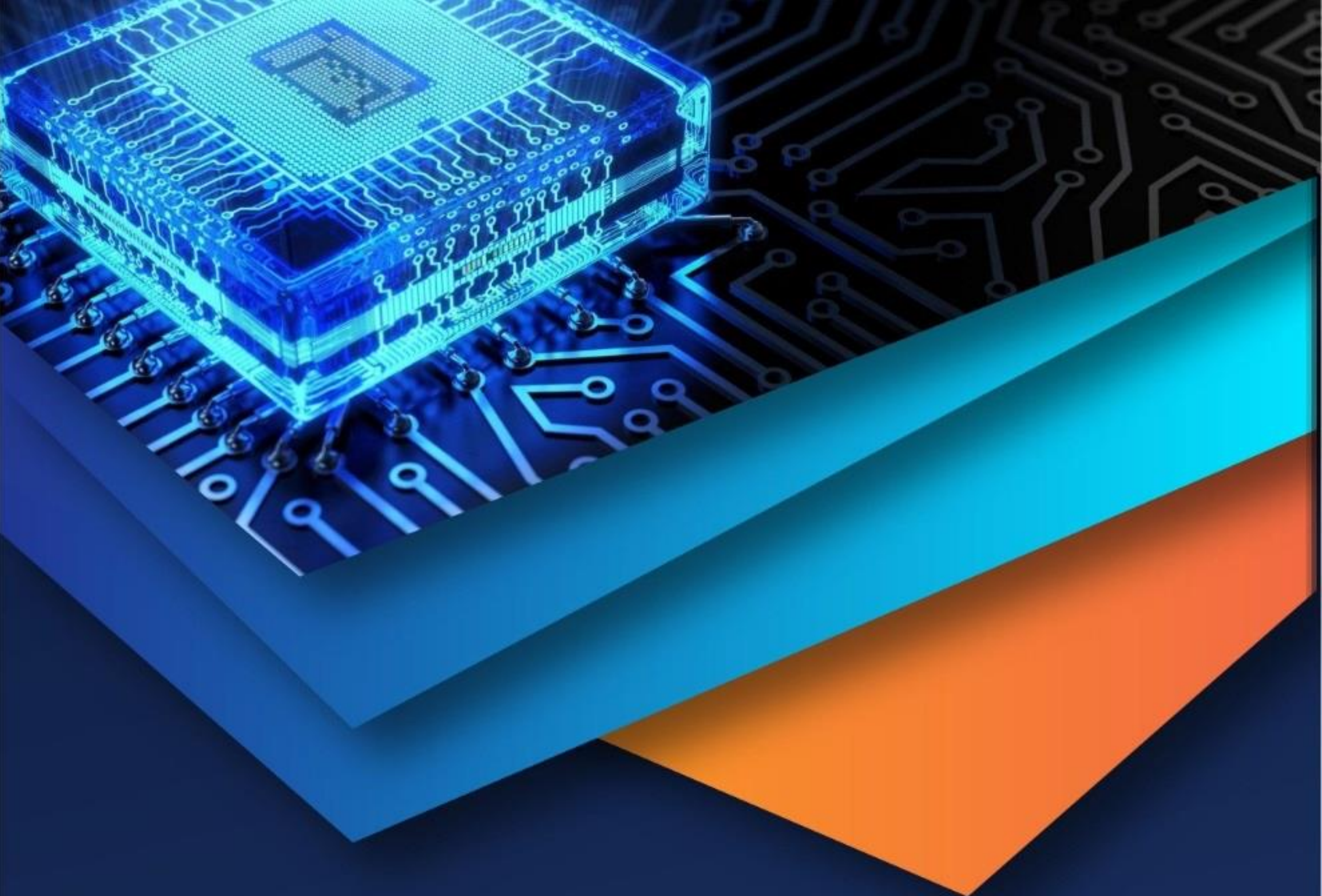

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