# Comparative study of $Co_2MnSi$ structural and surface morphological thin films on $Si/SiO_2$

**Rashmi Singh[1], Puneet Jain[1], Naresh Kumar[2], Rachana Kumar[3], Pramod Kumar[1*]**

[1]*Magnetic and Spintronics Laboratory, Department of Applied Science,*
*Indian Institute of Information Technology Allahabad, Allahabad 211012, India*
[2]*Department of Physics, Motilal Nehru National Institute of Technology Allahabad 211004, India*
[3]*National Physical Laboratory, New Delhi 110012, India*

[*]Corresponding author, Tel: (+91) 05-322922202; E-mail: pkumar@iiita.ac.in

**Received: 29 March 2016, Revised: 27 September 2016 and Accepted: 21 December 2016**

DOI: 10.5185/amp.2017/203
www.vbripress.com/amp

## Abstract

Thin films of $Co_2MnSi$ are grown on n-doped Si (100) and $SiO_2$ (100) substrates by RF sputtering. The deposition time to grow the films is varied, once for ten minutes and another for an hour at a particular substrate temperature 600°C and keeping all the other parameters same. The $Co_2MnSi$ thin films deposited on Si and $SiO_2$ are crystalline irrespective of the deposition time. The grains were round in the thin films deposited for 10 minutes and these grains are more consistently interconnected in the films deposited for 1 hour. This is supported by the surface roughness data from AFM. The rms roughness is found to be 4.82nm for Si for 10 minutes and 2.50nm for Si for 1 hour deposition that was observed over an area of $3 \mu m^2$. Copyright © 2017 VBRI Press.

**Keywords:** Heusler alloy, half-metallic ferro-magnets, $Co_2MnSi$, thin films, RF sputtering, XRD, AFM.

## Introduction

Heusler alloys are entitled after Friedrich Heusler. He exposed $Cu_2MnAl$ to be ferromagnetic, though the alloy comprised of simply non-magnetic elements **[1]**. Consequently, a Heusler alloy is well-defined as an intermetallic ferromagnetic metal alloy with general formulae $X_2YZ$ or XYZ. The form $X_2YZ$ is recognized as Full Heusler alloy while XYZ form is identified as Half-Heusler alloy. Usually X, Y and Z are elements of transition metal group while Z belongs to group III-V elements. The full Heusler alloys have $L2_1$ structure and the half Heusler alloys have $C1_b$ structure. A full Heusler alloy's unit cell has four interpenetrating fcc lattices, each occupied by one of the four constituents, while in case of half Heusler alloy there are three occupied and one free sub-lattice. The reason for ferromagnetism in many Heusler alloys is still not entirely unstated; however, it is attributed due to the complex unit cell of these kinds of materials **[2]**.

Heusler alloys have grown a lot of attention due to their flexible magnetic properties. Groot *et al.* have revealed that certain Heusler alloys show half-metallic character **[3]**. Half-metal means a material acts like a metal for the majority-spin electronic band structure and semiconductor for the minority-spin electronic band structure **[4]**. In various compounds the energy gap can be located instead in the majority-spin band **[5-7]**. This exceptional property made them smart for applications in newly developed sub- fields of electronics: spintronics and magneto-electronics **[8, 9]**. Spintronics is an evolving region that is converging on the blending of electron spin and its charge. The progress of such devices necessitates the optimization of ferri-magnetic and ferro-magnetic materials, displaying magnetic properties like high magnetization, high polarization, high coercive field, etc. Full-Heusler alloys have acquired much consideration in this direction as they have high Curie Temp. ($T_C$~1000K), and most of them are half metals **[2]**. Due to this half-metallic nature of Heusler alloys, they are also used as a test for the calculation of band structure in materials which have electronic correlations of moderate strength **[10]**. Using band structure methods, it has been predicted that many Heusler compounds have 100% spin polarized **[11]**.

Amongst the known half-metallic full-Heusler alloys, the most extensively considered are the ones that comprise cobalt **[12-14]**. Although $Fe_2MnZ$ type Heusler alloys have been projected to show half metallic ferromagnetism, but Brown *et al.* **[15]** showed that there is a very small spin-down density of states at the Fermi level, by neutron diffraction studies. Among these cobalt containing Heusler alloys, $Co_2MnSi$ has gained a lot of interest **[14]**. The first attention towards $Co_2MnSi$ has stimulated when Ishida *et al.* in 1998 **[16]** showed that the band structure of $Co_2MnSi$ shows half-metallic character, from the theoretical research. So we can conclude that $Co_2MnSi$ is a ternary Heusler alloy which comes in the group of Full Heusler alloys and also shows half metallic ferromagnetism. This half metallic means that there is an energy gap in the minority spin band at the Fermi energy. This leads to 100 % spin polarized conduction electrons, which would enable ideal spin-device performance to be obtained. Due to this half metallic ferromagnetism, there is a large energy gap in the minority band of ~0.4eV. Apart from half metallic ferromagnetism, $Co_2MnSi$ also a high Curie temperature of 985K, among the known Heusler alloys **[17-20]**. Moreover, $Co_2MnSi$ has a very high spin magnetic moment ($5\mu_B$ per formula unit) **[21]**.

$Co_2MnSi$ has $L2_1$ structure, as it is a full Heusler alloy. A unit cell of $Co_2MnSi$ has four interpenetrating fcc lattices in such a way that the two Co sub-lattices are at (0, 0, 0) and (1/2, 1/2, 1/2), while Mn sub-lattice is at (1/4, 1/4, 1/4) and this Si sub-lattice is at (3/4, 3/4, 3/4) **[2]**. So, Si and Mn atoms are surrounded by eight Co atoms, and each Co has four Si and four Mn atoms as next neighbors. The lattice constant of $Co_2MnSi$ is found to be a = 0.5670nm **[22]**.

Webster **[23]** studied bulk samples of $Co_2MnSi$ in terms of its microstructural behavior and magnetic behavior. For spintronics devices application, thin films (films having thickness in ~nm range) are required. These thin films of $Co_2MnSi$ were discussed independently by Geiersbach *et al.* **[24, 25]** and Raphael *et al.* **[26]**. For the first time, they fabricated $Co_2MnSi$ thin films and hence laid the foundation of our present work. In this present work, we have deposited $Co_2MnSi$ thin films on Si and $SiO_2$ wafers by varying the deposition temperature and deposition time, and tried to study how the structural and surface morphological properties of $Co_2MnSi$ thin film on Si and $SiO_2$ vary with deposition time.

## Experimental

### *Materials/ chemicals details*

$Co_2MnSi$ target is used. The target diameter is of two inches and its purity is 99.99%.

### *Material synthesis / reactions*

$Co_2MnSi$ (here after, CMS) thin films are deposited on Si and $SiO_2$ substrate using RF sputtering and are characterized by XRD and AFM for structural and morphological studies. Commercially available Si (n-type with 100 orientation) and $SiO_2$ wafers (n-type with 100 orientations) are cleaned using RCA cleaning. Thereafter, CMS thin films are grown using RF sputtering on these substrates. The base pressure in the chamber is kept $2.3\times10^{-6}$ mbar. Argon gas is used to produce the plasma in order to grow thin films of CMS. The substrate temperature and pressure of the chamber at the time of the deposition is kept 600ºC and $1.2\times10^{-2}$ mbar, respectively. The RF power is maintained at 100 watts. We deposited thin films by varying the deposition time. The deposition time has been kept as 10 minutes and 1 hour.

### *Characterizations / device fabrications / response measurements*

Ellipsometry, XRD and AFM imaging were performed to study the film thickness, structural and morphological properties.

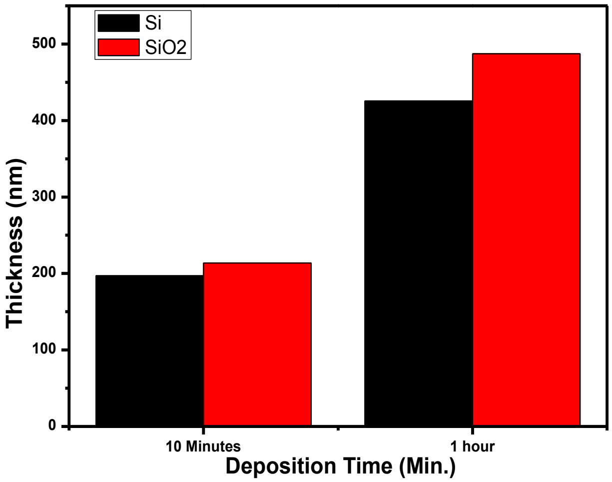

**Fig. 1**. Ellipsometry of CMS at different time intervals.

## Results and discussion

The thickness of the CMS thin film on Si and $SiO_2$ wafer has been measured using Ellipsometry and is shown in **Fig. 1**. The film is deposited at two different time intervals i.e. for 10 minutes and for 1 hour, keeping all the other parameters of pressure, temperature etc. same as discussed above in experimental section. The thickness of CMS on Si wafer for 10 minutes deposition and for 1 hour is 193.9nm and 425.4nm respectively and that on $SiO_2$ wafer is 213.8nm and 487.2nm respectively. This is in agreement with the expected result, as the film which has been deposited for 1 hour has a larger thickness, as compared to the film which has been deposited for only 10 minutes. There is a difference between the thicknesses of the deposited CMS for a same deposition time due to the fact that the wafer which is close to the target has a greater thickness as compared to the one which has a far from the target.

**Fig. 2** compares the XRD pattern of different CMS films deposited for 1 hour and 10 minutes on Si and $SiO_2$ wafers at 600˚C. As can be seen from the XRD pattern that the film deposited has a peak around (220) miller plane. This XRD pattern is in good agreement with Kijima *et al.* **[27]**. So here we can conclude that the CMS film deposited on Si and $SiO_2$ is crystalline irrespective of the deposition time. For both, *i.e.* 1 hour deposition and for 10 minutes deposition, structurally we got almost crystalline thin film. The intensities of the (220) peaks are increased as the deposition time is increased from ten minutes to an hour. In this sense, the crystal structure of the as-deposited CMS film was improved by the deposition time. Also, the substrate is being heated at 600ºC temperature continuously during the deposition.

This is another factor that should be considered for crystalline nature of the films.

Moreover, the lattice mismatch for depositing $Co_2MnSi$ over Si with same orientation is around 4% (bulk value). As the lattice mismatch is very large, growth of $Co_2MnSi$ on n-type Si (100) substrate did not come out with many orientations. However, the (220) oriented growth of Co2MnSi on n-type Si (100) substrates signifies that this growth does not depend on substrate orientation.

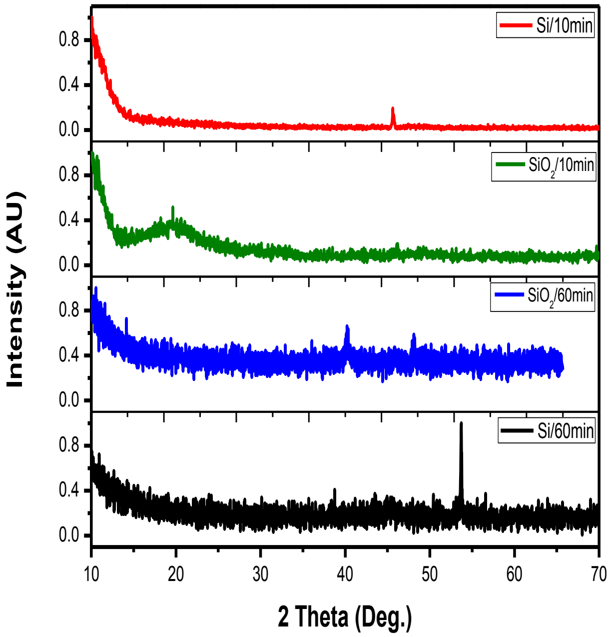

**Fig. 2**. XRD of CMS at different time intervals.

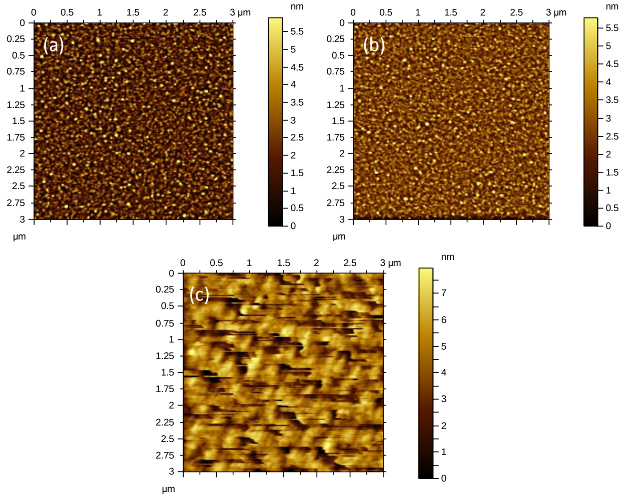

**Fig. 3.** AFM of $Co_2MnSi$ on (a) Si for 10 minutes, (b) $SiO_2$ for 10 minutes, and (c) Si for 1 hour deposition.

**Fig. 3** compares the atomic force microscopy (AFM) images of CMS on Si and $SiO_2$ wafer deposited for 10 minutes and 1 hour. AFM imaging is done for surface morphological studies. From **Fig. 3**, it is visible that for 10 minutes deposition, there is a grain size distribution ranging from 2-3nm on Si wafer and 3-4nm on $SiO_2$ wafer, but for 1 hour deposition the grain size distribution ranges from 7-8nm on Si wafer. So, we can conclude that the grain shape is nearly round and uniform for 10 minutes deposition, but for 1 hour deposition, the grains are interconnected with a string like pattern. This pattern has also been observed by Laura Jane *et al.* **[28]**.

As it is known that the surface roughness plays an important role affecting spin injection. Hence, the interface roughness is analyzed by AFM. The rms roughness is found to be 4.82nm for Si for 10 minutes and 2.50nm for Si for 1 hour deposition respectively which was observed over an area of $3\mu m^2$. As we find that increase in deposition time at a particular substrate temperature causes a decrease in surface roughness. This surface roughness gets decreased, probably, due to some chemical reactions occurring between CMS and Si leading grains to be interconnected.

## Conclusion

We have deposited CMS thin films on Si and $SiO_2$ wafer for 10 minutes and 1 hour, by RF sputtering. It has been found that irrespective of the deposition time, the deposited films are crystalline in nature. No significant difference can be found in the structure and morphological properties, between the CMS films grown on the two different substrates. Ellipsometry confirms that films deposited for 10 minutes have a lesser thickness as compared to the same films deposited for 1 hour. AFM reveals the morphology of the deposited films and confirms that the films deposited for 10 minutes, the grains were round but for the films deposited for 1 hour, the grains were more interconnected.

### Acknowledgements

One of the author (Dr. Pramod Kumar) acknowledges DST for financial support. I would like to acknowledge Dr. Hari K. Singh (National Physical Laboratory, New Delhi) for their support in characterization measurements of the samples.

### Author's contributions

All authors have equal contributions.

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