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Structural analysis of Fe_2VAl based full-Heusler alloys using vesta

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Abstract. Spontaneous orientation of magnetic moments in a particular direction gives rise to strong magnetization called ferromagnetism. The phenomenon of ferromagnetism in magnetic materials has been widely used in order to fabricate the magnetic based devices such as random-access memory, spin valves and spin switches. Although, several difficulties have been found to fabricate these materials due to the evolution swapping and disorder during the fabrication which significantly affects the magnetic behavior in the samples. In order to analyze the swapping, voids and disorders, we report the simulation of X-Ray diffraction (XRD) pattern of Fe_2VAl full-Heusler alloy with the implantation of swapping between the elements having equivalent electronegativity and atomic size, and substituting other elements at the Fe, V and Al site. First two peaks observed called superlattice peaks in the XRD pattern have been found to be very sensitive even for the small amount of swapping/disorder of the atoms. Therefore, we have plotted the intensity ratio of these two peaks corresponding to the systematic swapping between the atoms. These results suggested that the elements at their respective sites are responsible for the scattering of the X-Ray and scattering factors of any elements depends not only that particular elements but their chemical surrounding also. This study will help to analyze the experimental XRD data with the simulated one along with the swapping/disorder between the atoms up to some extent.

1 Introduction

Heusler alloys have made a fascinating material due to their multifunctional magnetic properties make it appropriate for spintronic devices. Although, several physical challenges are always here to fabricate the material and to achieve the theoretically predicated values. However, large number of studies have been performed for making Heusler alloys and significant properties have been achieved yet. Among the others, Fe based Heusler alloys have popular due to their magnetic as well as good thermoelectric properties. Fe_2VAl is the most studied alloy in the family of Fe based alloys. It is basically found to be stabilized in face centered cubic (FCC) structure and three more interpenetrating FCC lattices equally

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spaced along their body diagonal. Occupancy of Fe (I), Fe (II), V and Al are generally given at, (¼, ¼, ¼), (¾, ¾, ¾) (0, 0, 0) and (½, ½, ½) respectively in Cu_2MnAl prototype structure.

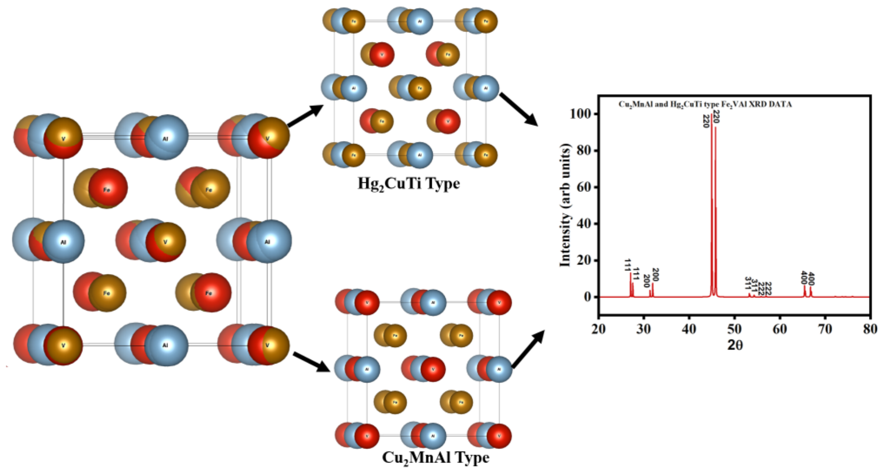

Fig. 1. Schematic diagram of Fe_2VAl in Hg_2CuTi and Cu_2MnAl prototype structure and combined XRD data simulated through Vesta.

Moreover, if the site preferences of Fe (I), Fe (II), V and Al are at (0, 0, 0) (¾, ¾, ¾), (¼, ¼, ¼) and (½, ½, ½) respectively then structure is called Hg_2CuTi prototype structure. Simulated XRD data have plotted as shown in figure 1. From the figure, we can see that height of intensities of 111, 200 and 220 are relatively changed for both the structures. Hence, we can measure the value of occupancy of atoms varies from their respective site by analyzing the relative changes in the intensities of XRD peaks. Here, we have reported the theoretical study of swapping/anti-site disorder of atoms from the respective site in Fe_2VAl. Moreover, Fe_2VAl alloy have been generally found in non-ferromagnetic ground state but swapping of Fe on V site have exhibited a local magnetic moment calculated by local density approximation technique and revealed spin glass nature for moderate Fe concentration on V site [1]. Al-rich Fe_2VAl have also studied theoretically and found to be weak magnetic with respect to Ni_2VAl. Figure of merit ZT have been obtained to be 0.02 and 0.05 for Ni and Fe respectively [2].Transition from cubic $L2_1$ structure to A_2 followed by B_2 disordered structure have been exhibited at 1080°C and 1100°C temperature respectively [3]. Recently, thermoelectric measurement has been performed on Fe_2VAl alloy through the band tuning and variation in charge carrier in order to improve power factor. However, quenched and prolonged annealed Fe_2VAl alloys have shown the reduction and conversely enhancement the anti-site disorder respectively. Quenching sample have revealed the enhancement in electrical conductivity and prolonged annealed sample has exhibited the reduction in the electrical resistivity [4]. Effect of pressure have been studied theoretically for Fe_2VAl and band structure near the Fermi level have modified which resulted the low value of electrical conductivity [5]. Substitution of heavy elements such as Ta or W on V site has been performed through simulation and thermal conductivity Fe_2VAl have been reflected five times larger than bare Fe_2VAl alloy [6]. Defects in Fe_2VAl alloy such as interstitials, vacancies have also been implemented in the study and found the associated magnetic nature due to the V-vacancies as well as due to the anti-site disorder of Fe at V site and vice versa [7]. Effect of sintering processes have been exhibited and enhancement of thermoelectric performance have found theoretically [8]. Self-substitution of V at Al has been used to analyzed and n-type and p-type of Fe_2VAl

have been studied. Electronic specific heat of n-type ($Fe_2V_{1.07}Al_{0.93}$) have found 1.9 times greater in comparison to p-type ($Fe_2V_{0.92}Al_{1.08}$) which in turn gives the enhancement of power factor in n-type Fe_2VAl alloy [9]. Another study on self-substitution in Fe_2VAl have demonstrated the non-trivial increase in lattice parameter which was suggested to be associated with the variations in interatomic charge transfer as proposed in Bader analysis but power factor was detected to be enhanced [10]. First principles calculation performed on Fe_2VAl has revealed the non-magnetic behavior for ordered structure and magnetic behavior for short range ordering by considering the excess portion of clusters [11]. Nanoparticles of $Fe_2V_{1.08}Al_{0.92}$ have been prepared via dispersion of Al_2O_3 and La_2O_3 followed by ball milling and size of $Fe_2V_{1.08}Al_{0.92}$ has been found to be 200nm and 100nm for the dispersion of Al_2O_3 and La_2O_3 respectively [12]. However, thermal conductivity has reduced in both the cases [12]. Thermal quenching from high temperature have enabled to systematically tune amount of anti-site disorder, systematically tuned disorder allows to drive the Anderson transition which shows the significant enhancement of thermoelectric performance of stoichiometric Fe_2VAl alloy [13]. Substitution of Co at Fe site in Fe_2VAl leads to induce the transition from non-magnetic to magnetic due to hybridization between Co-Co and ferromagnetic coupling between Fe and Co with V atoms at their respective site [14].

From the above discussion, we have seen that defect engineering, anti-site disorders, exerted pressure, substitution of heavier elements etc. are very important in order to enhance the thermoelectric properties of Fe_2VAl alloy. Hence, the careful analysis of anti-site disorders, associated vacancies/point defects is very crucial in order to link and scale the obtained/enhanced properties of the Fe_2VAl alloy. Therefore, we have performed the simulation of XRD pattern corresponding to each anti-site disorder between Fe and Al, V and Al, and Fe and V. Since, super-reflection peaks (111 and 200) are reported as very sensitive peaks for even the small amount of anti-site disorder. Therefore, we have calculated the ratio (α) of 111 and 200 and showed the variation of $\alpha$with amount of disorder.

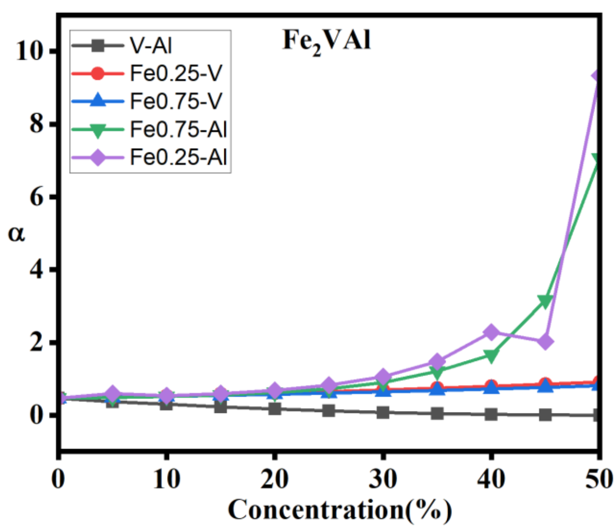

Fig. 2. Plot of ratio of 111 and 200 and concentration of possible anti-site disorder.

From above fig. 2, we have shown the anti-site disorder from their respective site to either site. We have implemented the anti-site disorder of Al at V site and vice-versa, Fe (I) at Al site and Fe (II) at Al site and vice versa and finally Fe (I) at V site and Fe (II) at V site and vice versa. Ratio α has been found to be for Fe (I) and Fe (II) at Al site and other plots have been found to be decreased for Fe (I) and Fe (II) at V site and V-Al site. This might be understood due to the different scattering factors of different elements. Although, scattering amplitude also depends on the chemical environment (surroundings) of particular atoms. Scattering factor can be seen in fig. 3 as given below.

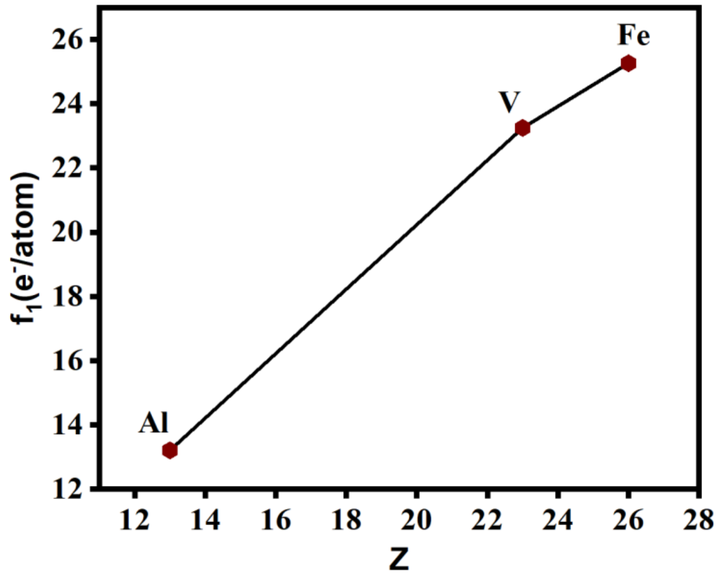

Fig. 3. Plot between the atomic number and scattering amplitude of the Al, V and Fe elements.

From fig. 3, we have seen that Fe has more scattering amplitude than V and V has more scattering amplitude than Al. Therefore, if we substitute Fe (I) at Al site, scattering amplitude from 111 plane increases due to the higher number of Fe contained in the that plane. Almost similar behavior has shown for the Fe (II) atoms at Al site due to the same reason. Moreover, if Fe is swapped by V then no any significant change has been obtained due to nearly equivalent scattering amplitude of Fe and V elements. Swapping between V and Al have decreased due to the less scattering amplitude of Al in comparison to V.

2 Conclusion and Future Aspects

We have successfully simulated the XRD data through Vesta for all the possible value of swapping between the atoms in Fe_2VAl and plotted all the data between the concentration and ratio of super reflection peaks. Analysis of all the curve have been performed through scattering amplitude of all the elements in Fe_2VAl alloy. Anti-site disorder between the atoms in Fe_2VAl have been found to be an important factor which play a vital role in order to enhance its thermoelectric properties and transition from non-magnetic to magnetic phase. This study will help to find the extent of anti-site disorder and to introduce a relationship between the disordering and thermoelectric performance for the future researchers.

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