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Structural, magnetic and transport properties of half-metallic ferrimagnet Mn_2VGa

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ABSTRACT

Polycrystalline Mn_2VGa samples were synthesized using an arc furnace. X-ray diffraction (XRD) pattern was analyzed using General Structural Analysis System (GSAS) package and the refined lattice parameter was found to be 5.905 Å. We found magnetic ordering in the system below 783 K and the spontaneous magnetization was observed to be following the Bloch $T^{3/2}$ law below 80 K. The magnetic moment per formula unit at 5 K was observed to be 1.88 μ_B. The temperature variation of the electrical resistance was found to follow the relation $R_n = R_{0n} + aT^{\alpha}$ ($\alpha = 1.616$) and (R_n—normalized electrical resistance) in the temperature range of 25–300 K and we observed almost a temperature independent variation of the electrical resistance below 25 K indicating the absence of spin-flip scattering.

1. Introduction

Half-metallic ferromagnets fall under an interesting class of materials in which the majority spin sub-band has a metallic character whereas the minority spin sub-band has an insulating or a semiconducting character which leads to, ideally, 100% spin polarization at the Fermi level. This peculiar asymmetry in the band structure was predicted by de Groot et al. [1] using band structure calculation on the half Heusler NiMnSb system. Ishida et al. have predicted that the full Heusler alloys of the type Co_2MnZ (Z = IIIb, IVb, Vb element) also exhibit half-metallicity [2]. Among the various classes of half-metallic ferromagnets (CrO_2, $La_{0.7}Sr_{0.3}MnO_3$, double pervoskites and transition metal chalcogenedies), Heusler alloys are attractive for magneto-electronic device applications [3–5] due to their higher magnetic ordering temperature and good lattice matching with zinc blende type semiconductors such as GaAs, GaN etc. [6,7].

Heusler alloys are ternary intermetallic compounds with X_2YZ or XYZ stoichiometry where X and Y are transition metals; Z is an element with sp valence electrons. Full Heusler alloys crystallize in $L2_1$ cubic structure with the space group $Fm\bar{3}m$ [8,9]. The formation and coupling of the magnetic moment studies in these systems were carried out by Kübler et al. [10]. The total spin magnetic moment per formula unit is given by the simple Slater–Pauling relation $M_s = (Z_t - 24)\,\mu_B$ (where Z_t is the total no. of valance electrons in the unit cell) in the case of full Heusler alloy and $M_s = (Z_t - 18)\,\mu_B$ for half Heusler alloys [3]. Recently, there have been a number of reports in literature predicting possible new half-metallic Heusler alloys based on band structure calculations [11–13]. However, there are only very few reports of experimental confirmations on these materials. Özdoğan et al. carried out *ab initio* electronic structure calculations for Mn_2VZ (Z = Al, Ge, Si, Ga, In and Sn) and found that with the exception of Z = Si and Ge all the other systems are ferrimagnetic at their equilibrium lattice constant. Moreover, they proposed that the formation of disordered compounds such as $Mn_2V_{1-x}Al_{1+x}$ and $Mn_2V_{1-x}Si_{1+x}$ leads to high spin polarization and stabilizes the ferrimagnetic ground state [13]. First-principle calculations on exchange interaction and Curie temperatures in Mn_2VZ (Z = Al, Ge) systems were carried out by Şaşioglu et al. [14]. Among the various Mn_2VZ systems that have been predicted to be half-metallic, experimental results are available in literature only on Mn_2VAl system. Neutron scattering experiments have confirmed ferrimagnetic ordering in Mn_2VAl system with Mn moment 1.5 μ_B

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and V moment −0.9 μ_B [15]. Magnetic and transport properties of Mn_2VAl system was reported by Jiang et al. [16]. Buschow et al. [17] reported the heat of formation, lattice parameter and saturation magnetization (at 5 K) for the compound Mn_2VGa. However, there is no experimental work reported in literature on probing the half-metallic character of the material Mn_2VGa. Our efforts to synthesize the stoichiometric compounds in the Mn_2VZ (Z = Ga, Ge, Si, In and Sn) systems revealed that only Mn_2VGa crystallizes in stable single phase form when prepared by conventional arc melting followed by vacuum annealing. In this report we present the results of our studies on the structural, magnetic and transport properties of Mn_2VGa compound.

2. Experimental details

All the compounds were prepared by arc melting the pure elements (Mn—99.99%, V—99.7%, Ga—99.99%) under argon atmosphere. Due to the volatile nature of the Manganese, 2.5 wt% of Mn was added in excess to compensate the weight loss during melting. The ingots were remelted several times and homogenized in vacuum (10^{-6} mbar) at 1075 K for a week. Structural characterization was carried out by taking the X-ray diffraction (XRD) pattern on powder samples using a PANalytical (X'pert PRO) X-ray diffractrometer employing Cu-K_α radiation. Experimental XRD data was analyzed by Rietveld refinement method using General Structural Analysis System (GSAS) package. The phase analysis was carried out using a scanning electron microscope with an energy dispersive X-ray spectrometer (EDS) attachment. Magnetic measurements were done using a vibrating sample magnetometer upto an applied field of 60 kOe in the temperature range 5–875 K. The spontaneous magnetization value was estimated from *M–H* plot by extrapolating the high field data to the zero field. The temperature variation of electrical resistance was carried out by conventional linear four-probe method in the temperature range 2.4–300 K.

3. Results and discussion

XRD pattern of Mn_2VGa powder sample showed only order-independent principal reflections: *h*, *k*, *l* all even with sum equal to 4*n* (Fig. 1). However, the superlattice peaks with $h+k+l = 4n+2$

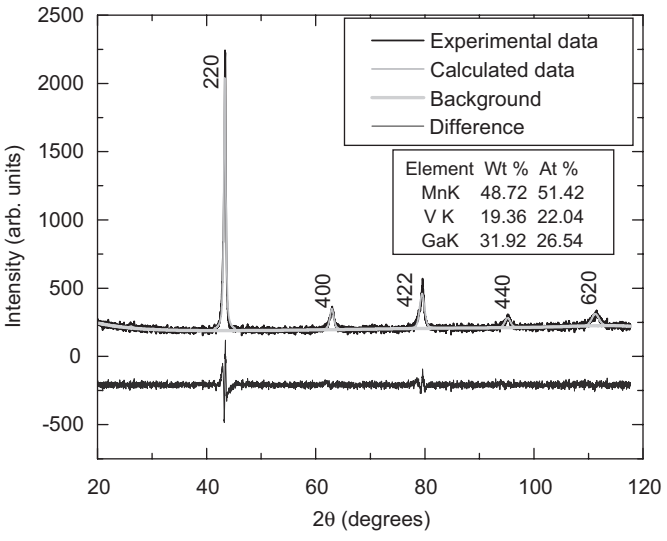

Fig. 1. Observed and calculated XRD pattern for the compound Mn_2VGa. Weighted Refined parameter was observed to be 0.0707. The inset box depicts the EDS data.

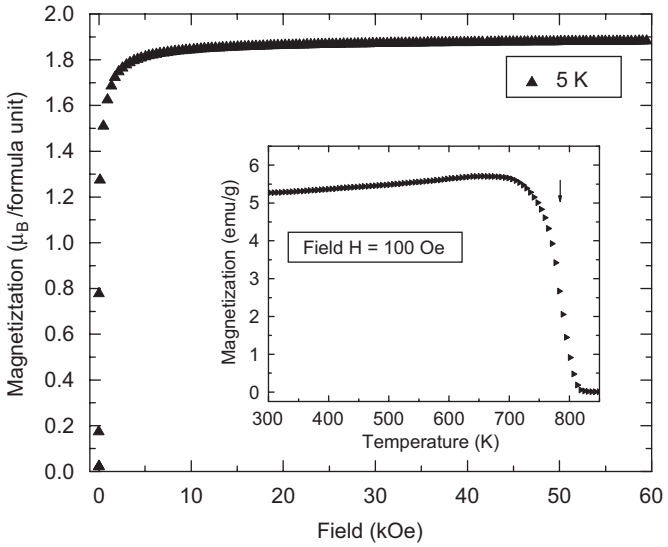

Fig. 2. Field variation of magnetization carried out at 5 K and the inset shows the magnetic moment variation as a function of temperature.

((2 0 0) type reflections) and *h*,*k*,*l* all odd ((1 1 1) type reflections) are absent as shown in Fig. 1. It is observed in many Heusler alloy systems that the atomic anti-site disorder, known as B2-type disorder, greatly reduces the intensity of the (2 0 0) and (1 1 1) type reflections [9]. This could be the reason for the absence/weak intensity of the order-dependent reflections. The refined lattice parameter was found to be 5.905 Å and this value is very critical in the perspectives of magnetic and half-metallic properties. The observed lattice parameter value is very close to the value suggested by Özdoğan et al. for the isostructural half-metallic ferrimagnetic Mn_2VAl system. The back-scattered electron image showed a single-phase micro-structure for the compound Mn_2VGa and the composition was estimated to be $Mn_{2.05}V_{0.88}Ga_{1.06}$ from EDS analysis. The temperature variation of magnetic moment was carried out at 100 Oe and the Curie temperature was observed to be 783 K (inset of Fig. 2). Since the isoelectronic elements occupying the *Z* site do not significantly affect the magnetic and half-metallic properties, it is worthwhile comparing our system with the Mn_2VAl compound that has been predicted as well as observed to be a half-metal. We observed a ~25 K increase in the Curie temperature compared with Mn_2VAl (760 K) system. This could be attributed to the decrease in the Mn–V (2.556 Å) bond length in the Mn_2VGa system. In the mean field approximation it is observed that the Mn–V antiferromagnetic exchange interaction is the dominant one among the possible Mn–V, Mn–Mn and V–V interactions, hence decrease in the Mn–V bond length enhances the Mn–V exchange interaction [14]. Our results on Mn_2VGa are compared with some of the earlier theoretical and experimental results on Mn_2VZ (Z = Al or Ga) systems (see Table 1). The room temperature saturation magnetization was found to be 43.3 emu/g and the value is well in agreement with the reported value [17]. The magnetic moment per formula unit was estimated from field sweep data recorded at 5 K and it was found to be 1.88 μ_B (see Fig. 2). The observed value is little less than the expected integer magnetic moment (2 μ_B) and this could be due to the slight variation in the stoichiometry of the compound. The total number of valance electrons for the $Mn_{2.05}V_{0.88}Ga_{1.06}$ system is found to be 22.14 and from the Slater–Pauling relation the magnetic moment per formula unit for the present investigation is observed to be 1.86 μ_B.

Half-metallic Heusler alloys are known to exhibit localized moment even with delocalized 3d electrons (itinerant electrons)