Study of Structural, Magnetic, and Mossbauer Properties of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ (0.0 ≤ x ≤ 1.0) Prepared via Arc Melting Process

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Abstract: Intermetallic compounds of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ (x = 0.0 to 1.00) were synthesized by arc melting. Samples were investigated for structural, magnetic, and hyperfine properties using X-ray diffraction, vibration sample magnetometer, and Mossbauer spectrometer, respectively. The Rietveld analysis of room temperature X-ray diffraction data shows that all the samples were crystallized in Th$_2$Fe$_{17}$ structure. The unit cell volume of alloys increased linearly with an increase in Nb content. The maximum Curie temperature $T_C$ ~523 K for $x = 0.6$ sample is higher than $T_C = 153$ K of Dy$_2$Fe$_{17}$. The saturation magnetization decreased linearly with increasing Nb content from 61.57 emu/g for $x = 0.0$ to 42.46 emu/g for $x = 1.0$. The Mössbauer spectra and Rietveld analysis showed a small amount of DyFe$_3$ and NbFe$_2$ secondary phases at $x = 1.0$. The hyperfine field of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ decreased while the isomer shift values increased with the Nb content. The observed increase in isomer shift may have resulted from the decrease in s electron density due to the unit cell volume expansion. The substantial increase in $T_C$ of thus prepared intermetallic compounds is expected to have implications in magnets used for high-temperature applications.

Keywords: permanent magnetic materials; 2:17 intermetallic; Mossbauer spectroscopy; Curie temperature; X-ray diffraction; Rietveld analysis

1. Introduction

Intermetallic compounds based on rare-earth elements (R) and 3d-transition elements (T) are important from a fundamental and a technological point of view as they possess outstanding magnetic properties because of their high saturation magnetization, $M_s$. R$_2$Fe$_{17}$ (2:17) alloy has the most Fe-content among all R-iron intermetallic and hence they have the highest $M_s$ in the class of intermetallic magnets. However, these compounds have relatively low Curie temperature, $T_C$. For example, $T_C$ ~473 K for Gd$_2$Fe$_{17}$ and 370 K for Dy$_2$Fe$_{17}$, along with low magnetic anisotropies [1]. Various strategies have been employed to address issues related to improving magnetic anisotropy, magnetization, and Curie temperature of R$_2$Fe$_{17}$ compounds. Efforts in this direction include insertion of metalloids, hydrogen, nitrogen, and carbon in the R$_2$Fe$_{17}$ matrix [2–5]. An improvement in the $T_C$ value of Ce$_2$Fe$_{17}$ [6], Gd$_2$Fe$_{17}$ [7,8], Dy$_2$Fe$_{17}$ [9,10], Pr$_2$Fe$_{17}$ [11], Nd$_2$Fe$_{17}$ [12], Er$_2$Fe$_{17}$ [13], Tm$_2$Fe$_{17}$ [14], Lu$_2$Fe$_{17}$ [15,16], Ho$_2$Fe$_{17}$ [17], Sm$_2$Fe$_{17}$ [18] have been reported by adding metallic atoms like Si, Cr, Mn and metalloids like Ga on Fe sites. The substitution of non-magnetic atoms to Fe sites has been reported to increase the ferromagnetic coupling, leading to an increase in the $T_C$ value [19,20] and magneto-crystalline anisotropy [9] of the compound. Improvements in the $T_C$ of R$_2$Fe$_{17}$ with substitution of a non-magnetic atom Ga have been reported for Ce$_2$Fe$_{17}$–xGax [21], Sm$_2$Fe$_{17}$–xGax [22] compounds, where the maximum in $T_C$ ~462 K was observed for Dy$_2$Fe$_{16}$Ga$_1$ [9].

Low substitution of Ga content has been identified to increase the $T_C$ of rare-earth intermetallic compound [9]. Additional phases are reported for a higher content of Ga.

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substitution [9]. More recently, replacing one Fe atom with one Nb atom has increased $T_c$ up to 460 K for Dy$_2$Fe$_{16}$Nb$_1$ [23]. Based on these reports, we proposed studying the co-substitution of Ga and Nb in the Dy$_2$Fe$_{17}$ compound to increase $T_c$ values further. The study is critical in developing futuristic applications demanding high-temperature operation of magnets such as fast-breeder reactors, ion propulsion engines for spacecraft.

2. Experimental

The raw materials of Dy, Fe, Ga, and Nb metals with 99.9% purity were purchased from Sigma Aldrich (St. Louis, MO, USA). The parent alloys Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ ($x = 0.0, 0.2, 0.4, 0.6, 0.8$ and $1.0$) with a stoichiometric amount of elements above were prepared by arc melting under a high purity argon atmosphere. A high degree of homogeneity was ensured by melting the ingots several times. The X-ray diffraction measurement was carried out with CuK$_\alpha$ (1.5406 Å) radiation on a Bruker (D8 Advance) X-ray diffractometer via a Vantec detector. Diffraction patterns were collected from $20^\circ$–$70^\circ$ with a step of 0.02 degrees. Room temperature (RT) magnetic properties were investigated using a vibrating sample magnetometer (VSM), and Curie temperature, $T_c$, was measured using Thermal Gravimetric Analysis (TGA) equipped with a permanent magnet. The RT $^{57}$Fe Mössbauer spectra were collected in transmission geometry using 25 mCi $^{57}$Co in Rh matrix $\gamma$-ray source (SEE Co. Mössbauer Spectrometer, Minneapolis, MN, USA). All the isomer shifts were measured relative to $\alpha$-iron at RT used for calibration. The hyperfine parameters, viz. hyperfine field, $HF$, isomer shift, $IS$, and quadrupole shift, $QS$, were extracted by fitting the Mössbauer spectra using WMoss software (SEE Co. Minneapolis, MN, USA) [24].

3. Results and Discussion

Figure 1 represents the XRD patterns of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ ($0.0 \leq x \leq 1.0$) samples. The spectra show that the samples had Th$_2$Ni$_{17}$ structure (hexagonal, space group, P$6_3$/mmc) without any impurity; however, a small additional peak of NbFe$_2$ and DyFe$_3$ was detected for $x = 1.0$. The Rietveld [25] refined XRD patterns are shown in Figure 1b. The refined profile shows an excellent match between observed and calculated profiles. During the refinement process, all structural and lattice parameters, peak shift, background profile function, thermal parameters, etc., were refined until the observed profile functions matched with the calculated profile. The initial crystal structure parameter used for the refinement was adapted from Laio et al. [26]. The lattice parameters $a$ and $c$ of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ ($0.0 \leq x \leq 1.0$) are shown in Figure 2, and the corresponding data are listed in Table 1. It is observed from Figure 2 that the unit cell volume increases with the increase in the Nb content, $x$. The increase in the unit cell volume is due to Nb ionic radius (~0.86 Å) is greater than the ionic radius of Ga (0.62 Å) [27]. The linear increase in the $c/a$ ratio indicates that the unit cell’s expansion along the $c$-axis is greater than that along the $a$-axis. Considering the fact that the $6c(4f)$ dumbbell site is located along the $c$-axis, the $c$-axis expansion could affect the $T_c$ value of the 2:17 compound [1]. The $c/a$ ratio deviates at higher Nb concentrations ($x = 1.0$) due to the formation of secondary phases. In addition, it is observed from Table 1 that the average bond distance between each site changes with the concentration of both Nb and Ga ($6c(4f-4f) \approx 2.42$ Å, $12k-12k \approx 2.43$ Å, $12j-12j = 2.46$ Å). The $12j$ sites show that both Ga and Nb prefer to stay in the same sites.
Figure 1. (a) X-ray diffraction patterns of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ compounds. (b) Rietveld refinement profile for Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$. 
Table 1. Lattice parameters, volume, site occupancy, Ms, and Tc of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$.

| $x$ | $a$ (Å) | $c$ (Å) | Volume (Å$^3$) | $c/a$ | 6c(4f-4f) (Å) | 6g-12j (Å) | 6g-12k (Å) | 12j-12j (Å) | 12k-12k (Å) | Ms (emu/g) | Tc (K) |
|-----|---------|---------|---------------|------|---------------|-----------|-----------|------------|------------|------------|-------|
| 0.0 | 8.463(4)| 8.290(2)| 514.01(3)     | 0.979| 2.4166(53)    | 2.4312(12)| 2.4799(21)| 2.4589(31) | 2.4102(22) | 61.5(7)    | 488(3) |
| 0.2 | 8.486(3)| 8.324(9)| 519.15(9)     | 0.981| 2.4181(22)    | 2.4322(18)| 2.4956(18)| 2.4609(27) | 2.4281(32) | 61.1(9)    | 489(5) |
| 0.4 | 8.471(0)| 8.340(0)| 519.94(1)     | 0.988| 2.4195(32)    | 2.4335(14)| 2.5312(16)| 2.4625(9)  | 2.4299(35) | 53.2(8)    | 502(8) |
| 0.6 | 8.481(6)| 8.330(9)| 520.34(6)     | 0.982| 2.4286(42)    | 2.4344(21)| 2.6901(15)| 2.4656(21)| 2.4325(32) | 47.8(7)    | 523(7) |
| 0.8 | 8.498(2)| 8.359(6)| 520.56(7)     | 0.986| 2.4289(37)    | 2.4343(7) | 2.7521(12)| 2.4673(18)| 2.4375(27) | 44.5(9)    | 481(7) |
| 1.0 | 8.509(3)| 8.305(4)| 520.86(2)     | 0.976| 2.4293(4)     | 2.4355(21)| 2.8801(23)| 2.4732(32)| 2.4399(29) | 42.6(6)    | 489(6) |

Figure 3 shows the room temperature $M$ vs. $H$ magnetization plot for Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$. The $M$ vs. $H$ plot shows that the $M$$_s$ decreases with the increase in the Nb content. The $M$$_s$ as a function of Nb content, $x$, of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ is plotted in Figure 4. From Figure 4, it is observed that the Ms of Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ decreases at the rate of $-3.7$ emu/g per Nb atom. The decrease in the magnetization of substituted R$_2$Fe$_{17}$ compounds can be understood based on 3d band model. Inherently R$_2$Fe$_{17}$ compounds are weak ferromagnets because both spin-up and spin-down bands are filled incompletely. The reduction in the Fe magnetic moment upon non-magnetic atom substitution results from the transfer of valence electrons of the substituted atom to the 3d band of Fe [28,29], which progressively fills the 3d band and moves the Fermi level up. A decrease in Fe magnetic moment is due to the electronic hybridization effect in R$_2$Fe$_{17}$M$_x$, with M = Ga, Al, and Si is well reported in the literature [30,31]. This decrease in Fe moment with the substitution is due to Fe ([Ar]3d$^6$4s$^2$–Ga([Ar]4s$^2$4p$^1$), Fe–Al ([Ne]3s$^2$3p$^1$) and Fe–Si ([Ne]3s$^2$3p$^2$) electronic hybridizations. The decrease in the magnetic moment in Nb substituted Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$ compound is due to indirect (3d-4s-4d) hybridization between Fe ([Ar]3d$^6$4s$^2$), Ga([Ar]4s$^2$4p$^1$), and Nb ([Kr]4d$^4$5s$^1$), which reduces the spin polarization of Fe-3d states, resulting in a net decrease in the magnetic moment. In a study reported by Lekdadri et al.; on Co$_{1-x}$Nb$_x$ alloy, cobalt
moment was observed to decrease with increasing Nb content in the alloys due to a similar hybridization effect [32].

![Saturation Magnetization (emu/g)](image)

**Figure 3.** RT magnetization plot for Dy$_{2}$Fe$_{16}$Ga$_{1-x}$Nb$_{x}$.

![Saturation Magnetization (emu/g)](image)

**Figure 4.** Room temperature (RT) saturation magnetization, $M_s$, as a function of $x$, Nb content.

The Curie temperature, $T_c$, of Dy$_{2}$Fe$_{16}$Ga$_{1-x}$Nb$_{x}$ as a function of Nb content is shown in Figure 5. It is observed that Curie temperature of Dy$_{2}$Fe$_{16}$Ga$_{1-x}$Nb$_{x}$ alloys increases with increase in Nb concentration from 488 K ($x = 0.00$) to a maximum of 523 K ($x = 0.6$) and then decreases to 460 K ($x = 1.00$). The achieved $T_c$ for Dy$_{2}$Fe$_{16}$Ga$_{0.4}$Nb$_{0.6}$ is 35 K higher than that of Dy$_{2}$Fe$_{17}$Ga$_{1}$ and 153 K higher than that of Dy$_{2}$Fe$_{17}$ [10]. In general, $T_c$ in rare-earth intermetallic compound is due to three kinds of exchange interactions, namely the 3d-3d exchange interactions, i.e., between the magnetic moment of the Fe sub-lattice ($J_{FeFe}$), 4f-4f exchange interaction, i.e., the interaction between the magnetic moment within the R sub-lattice ($J_{RR}$), and the inter sub-lattice 3d-4f exchange interaction ($J_{RF}$). It is reported that the $T_c$ increases with an increase in the $J_{FeFe}$ [33]. The interactions between the rare-earth spins (4f-4f) are assumed to be weak and negligible compared to the other
two types of interactions. Thus, the $T_c$ in the $R_2Fe_{17}$ intermetallic compound is mainly dictated by $J_{FeFe}$. The strength of Fe–Fe exchange interaction highly depends on interatomic Fe–Fe distance [34,35]. Accordingly, the exchange interactions between iron atoms situated at distances smaller (greater) than 2.45–2.50 Å are negative (positive). In the $R_2Fe_{17}$, the majority of Fe–Fe distances favor the negative interaction [9]. The negative exchange interaction can be reduced either by volume expansion or by reducing the number of Fe–Fe pairs with negative exchange interactions. The low $T_c$ observed in the parent Dy$_2$Fe$_{17}$ compound is believed to result from the antiferromagnetic coupling of Fe–Fe moments at the 6c(4f) sites [36]. Their Fe–Fe distance separation is less than 2.45 Å needed for the ferromagnetic ordering Table 1, [37]. An increase in $T_c$ has been reported earlier with Ga substitution ($x = 1$) [9] but with a concomitant decrease in magnetization due to the magnetic dilution effect. However, the simultaneous substitution of non-magnetic Ga and Nb atoms enhances the intermetallic Curie temperature without significantly lowering the saturation magnetization. It is noted from Table 1 that 4f–4f distances steadily increase with the Nb content, thus making $J_{FeFe}$ more positive with a steady improvement in the $T_c$ value.

![Figure 5. Curie temperature as a function of $x$, Nb content.](image)

Figure 6 shows the room temperature fitted Mössbauer spectra for Dy$_2$Fe$_{16}$Ga$_{1-x}$Nb$_x$. The hyperfine parameters viz. hyperfine field, HF, and isomer shift, IS, extracted from the fits are plotted in Figure 7 and listed in Table 2. Dy$_2$Fe$_{17}$ compounds have a basal magnetization that needs eight magnetic sextets to fit their Mössbauer spectra [38]. The fitting of spectra, shown in Figure 7, was carried out with eight magnetic sextets assigned to 4f, 6g, 12j, and 12k sites in Dy$_2$Fe$_{17}$ [21,39–41]. The Mössbauer spectral analysis was carried out with magnetic sextets assigned to the 4f, 6g, 12j, and 12k sites in Dy$_2$Fe$_{17}$–x Nb$_x$. The 12j and 12k sites were further split into two, corresponding to the site occupancies of Fe atoms in the crystal structure of $R_2Fe_{17}$ with planar anisotropy. The intensities of the six absorption lines of each sextet were assumed to follow the 3:2:1 intensity ratio expected for randomly oriented powder samples in zero magnetic fields, and a single common linewidth was assumed for all the seven sextets. The isomer shifts ($\delta$) for the magnetically inequivalent sites were constrained to be the same, whereas the hyperfine fields were expected to vary at pairs of magnetically inequivalent sites due to variations in the dipolar and orbital contributions to the magnetic hyperfine fields [42]. Doublets were used for additional phases for $x = 1.0$ to include paramagnetic phases DyFe$_3$ and NbFe$_2$ during Mössbauer fitting. It was found that the additional doublet covered 8.86% of the area. This is in confirmation of the additional phases observed in the x-ray diffraction pattern. From Table 2, it is evident that the HF follows a 4f(6c) > 6g(9d) > 12(18f) > 12k(18h) sequence, which is similar to the sequence observed in other similar RE$_2$Fe$_{17}$ compounds [43,44].
Figure 6. RT Mössbauer fitted spectra for Dy2Fe16Ga1−xNbx.

Figure 7. RT Mössbauer hyperfine parameters and isomer shift plots as a function of x, Nb content.
From Figure 7, it is observed that the HF decreases with an increase in Nb content which is in agreement with the reduction in the magnetic moment. On the other hand, the isomer shift value increases with the Nb content. The isomer shift value reflects s-electron charge density at the Fe nucleus. With the unit cell volume expansion upon Nb substitution, the s-electron charge density at the Fe nucleus decreases, resulting in a concomitant increase in the isomer shift value.

Table 2. The RT hyperfine parameters, hyperfine field (HF) (kOe), isomer shift (IS) (mm/s), quadrupole shift (QS) (mm/s), and area (%) of the Dy2Fe16Ga1−xNbx.

| x   | 4f     | 4e     | 6g1   | 6g2   | 12/1 | 12/2 | 12k1 | 12k2 | Doublet |
|-----|--------|--------|-------|-------|------|------|------|------|---------|
| HF (kOe) |        |        |       |       |      |      |      |      |         |
| 0.0  | 278.7  | 249.7  | 230.1 | 214.9 | 260.0 | 218.1 | 196.4 | 220.0 | 9.5     |
| 0.2  | 274.1  | 256.2  | 230.8 | 215.0 | 255.7 | 196.3 | 174.4 | 198.4 | 9.5     |
| 0.4  | 264.2  | 250.0  | 224.1 | 210.8 | 248.6 | 191.4 | 176.7 | 190.3 | 9.5     |
| 0.6  | 262.0  | 247.1  | 234.2 | 214.8 | 253.3 | 192.1 | 170.1 | 191.5 | 9.5     |
| 0.8  | 248.0  | 251.01 | 234.2 | 207.9 | 256.0 | 202.9 | 165.9 | 192.7 | 9.5     |
| 1.0  | 240.0  | 248.2  | 240.2 | 210.1 | 246.8 | 200.1 | 169.4 | 190.0 | 9.5     |
| IS (mm/s) |        |        |       |       |      |      |      |      |         |
| 0.0  | 0.126  | 0.301  | −0.209 | −0.309 | −0.209 | −0.422 | −0.422 | −0.254 | −0.254 |
| 0.2  | 0.166  | 0.059  | −0.097 | −0.097 | −0.173 | −0.173 | 0.019  | 0.019  | 0.019  |
| 0.4  | 0.210  | 0.119  | −0.092 | −0.092 | −0.175 | −0.175 | 0.081  | 0.081  | 0.081  |
| 0.6  | 0.264  | 0.152  | −0.117 | −0.117 | −0.191 | −0.191 | −0.015 | −0.015 | −0.015 |
| 0.8  | 0.171  | 0.301  | −0.117 | −0.117 | −0.16  | −0.16  | −0.028 | −0.028 | −0.028 |
| 1.0  | 0.080  | 0.220  | −0.124 | −0.124 | −0.159 | −0.159 | −0.093 | −0.093 | −0.211 |
| QS (mm/s) |        |        |       |       |      |      |      |      |         |
| 0.0  | 0.158  | 0.010  | 0.133  | 0.259  | −0.418 | −0.48  | 0.259  | −0.58  |         |
| 0.2  | 0.27   | 0.216  | 0.04683 | 0.088  | −0.198 | 0.166  | 0.246  | 0.264  |         |
| 0.4  | 0.206  | 0.060  | 0.07976 | 0.124  | −0.119 | 0.080  | 0.200  | 0.153  |         |
| 0.6  | 0.384  | 0.154  | −0.0932 | 0.137  | −0.129 | 0.046  | 0.024  | 0.156  |         |
| 0.8  | 0.320  | 0.33   | −0.0683 | 0.313  | −0.156 | −0.286 | 0.102  | 0.190  |         |
| 1.0  | 0.420  | 0.081  | −0.0349 | 0.297  | −0.381 | −0.153 | 0.039  | 0.089  | 0.035  |
| Area (%) |        |        |       |       |      |      |      |      |         |
| 0.0  | 13.70  | 14.90  | 20.00  | 21.00  | 10.53  | 5.59  | 10.9  | 3.93  |         |
| 0.2  | 9.14   | 8.68   | 19.63  | 20.24  | 15.74  | 15.82 | 2.39  | 8.25  |         |
| 0.4  | 8.55   | 5.92   | 18.46  | 20.00  | 16.12  | 15.05 | 5.87  | 9.66  |         |
| 0.6  | 3.42   | 4.64   | 19.73  | 22.70  | 8.92   | 15.96 | 8.43  | 15.93 |         |
| 0.8  | 6.33   | 2.14   | 17.02  | 26.60  | 7.15   | 14.83 | 10.8  | 15.24 |         |
| 1.0  | 4.27   | 6.02   | 12.14  | 26.80  | 8.22   | 17.75 | 8.46  | 16.42 | 8.86    |

4. Conclusions

In the present study, single phase Dy2Fe16Ga1−xNbx intermetallics were successfully synthesized using arc melting. The X-ray powder diffraction (XRD) results and the Rietveld refinements show that the samples have a Th2Ni17-type structure (space group, P63/mmc). The XRD patterns show the presence of impurities phases DyFe3 and NbFe2 at higher Nb content (x > 0.80) only, which is also confirmed by Mossbauer spectral analysis. Rietveld analysis shows a linear unit-cell volume expansion with increasing Nb content. The reduction in Ms of Dy2Fe16Ga1−xNb at 300 K with an increase in Nb content is attributed to the hybridization effect. For Dy2Fe16Ga0.4Nb0.6, maximum Tc was observed to 523 K, which is 35 K higher than the Dy2Fe16Ga compound and 153 K more elevated than its parent compound Dy2Fe17. The hyperfine fields, HF, of Dy2Fe16Ga1−xNb decrease upon Nb substitution, reflecting moment reduction. The enhancement in the Curie temperature of thus prepared Dy2Fe16Ga1−xNb compound with a judicious choice of Ga and Nb content can be helpful in areas demanding the high-temperature operation of magnets.

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