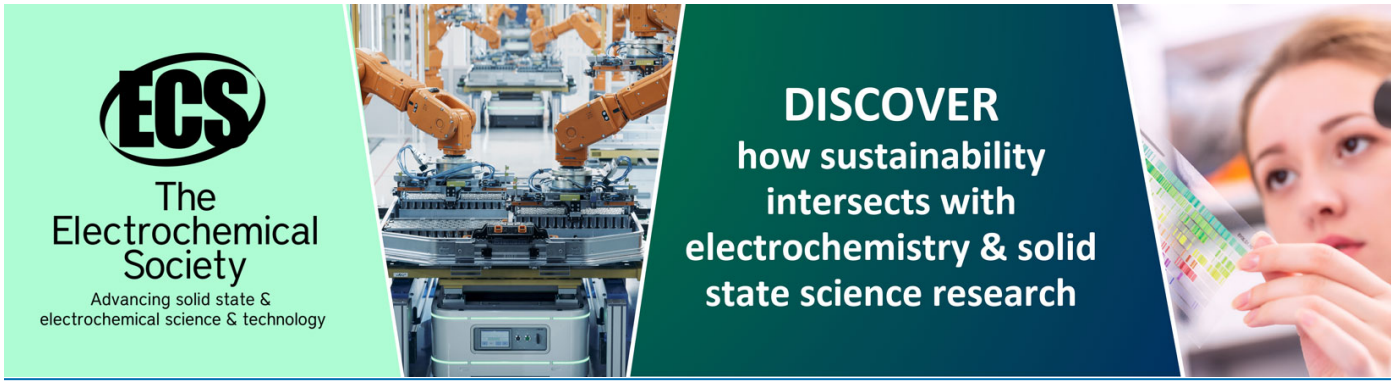
Mössbauer effect, magnetic and electrical properties studies of $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ intermetallics



Journal of Physics: Conference Series **217** (2010) 012130 doi:10.1088/1742-6596/217/1/012130

Mössbauer effect, magnetic and electrical properties studies of $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ intermetallics

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Abstract. Synthesis, X-ray analysis (300K) and Mössbauer effect studies in the intermetallic compounds $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ are reported. Cubic Laves phase $MgCu_2$ - type, were observed across the series. Lattice parameter is linearly increased with Gd concentration. The lattice parameters of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series are compared to data previously observed for the $R(Fe_{1-x}Co_x)_2$ series (R= Y, Dy, Gd). ^{57}Fe Mössbauer effect measurements for the series were realized at 4.2 and in the temperature range around the magnetic ordering temperature. Curie temperatures of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series were determined using both electrical resistivity and Mössbauer effect measurements. The magnetic hyperfine field and Curie temperature increases with Gd content. The obtained magnetic hyperfine field and Curie temperatures for the series $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ are related to the data known for the $R(Fe_{1-x}Co_x)_2$ series (R= Y, Dy, Gd).

1. Introduction

The intermetallic series $R(Fe_{1-x}Co_x)_2$ (R - heavy rare earth) with a C15 cubic Laves phase structure are intensely studied for their fundamental interest and their practical applications [1,2]. From Mössbauer effect studies it was found, that a magnetic hyperfine field observed at ^{57}Fe nuclei as a function of composition for the $R(Fe_{1-x}Co_x)_2$ (R =Y, Gd, Dy, Ho) intermetallic series, behaves similarly to the Slater - Pauling curve, in analogy to the 3d metal-3d metal alloys [3,4] with a maximum field for the $R(Fe_{0.7}Co_{0.3})_2$ compound. Usually substitution of one transition metal/another transition metal in the RM_2 system (M - transition metal) is adopted as a driving force to change across the series the number n of 3d electrons (n calculated per transition metal atom) in the transition metal sublattice and thus to change band properties and related to them magnetic and hyperfine interaction properties [4,5].

Magnetic ordering temperature observed across the exemplary $R(Fe_{1-x}Co_x)_2$ (R=Y, Dy, Gd) series can be treated as a certain replica of the magnetic hyperfine field [6-8]. Namely, the Curie temperatures increases with x and a maximum value is approached in the area of the $R(Fe_{0.7}Co_{0.3})_2$ (R =Y, Gd, Dy) compounds. Further Fe/Co substitution strongly reduces the Curie temperatures.

Yttrium, which lacks a well localized electron magnetic shell, is often used in intermetallics instead of rare earths to probe the influence of 4f electrons on their properties [7]. Gd^{3+} ions are characterized by maximal spin of 4f shell and highest de Gennes factor (G) [9]. It would be interesting to test the influence of the yttrium and gadolinium atoms on the 4f-4d(5d)-3d hyperfine interactions and magnetism of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series.

2. Materials and structures

The polycrystalline compounds $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ (x=0, 0.1,...,0.8 and 0.9) were prepared by arc melting in a high purity argon atmosphere using appropriate amounts of Y (99.95% purity) with Gd (99.95% purity), Fe and Co (all 99.99% purity) as starting materials. As a next step, the synthesized ingots were annealed in a vacuum (10^{-6}Pa) at 850ºC for 10h and then allowed to cool down along with the furnace at approximately 250K/h.

Crystal structures were tested with a standard X-ray powder diffraction procedure using CuK_α radiation. The good quality X-ray diffractograms obtained for these materials were analysed using the Rietveld-type method adopting both the $K_{\alpha1}$ (wave length α_1=1.540560 Å) and $K_{\alpha2}$ (α_2=1.544390 Å) lines [10,11]. Pure cubic, Fd3m, $MgCu_2$ - type (C15) crystal Laves phases were observed for all prepared compounds of the studied series. Figure 1 shows diffractogram for exemplary compound $(Y_{0.2}Gd_{0.8})(Fe_{0.7}Co_{0.3})_2$. Since additional X-ray reflexes caused by a long range order have not been observed, thus a random distribution of Fe, Co atoms in the transition metal sublattice and Y, Gd atoms in the rare earth sublattice can be expected to exist. The C15 Laves phase has been previously described in detail elsewhere [12].

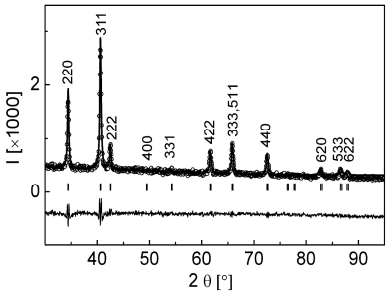

Figure 1. X-ray powder diffraction patterns observed for the exemplary compound $(Y_{0.2}Gd_{0.8})(Fe_{0.7}Co_{0.3})_2$. Fitted differential pattern is added below each diffractogram.

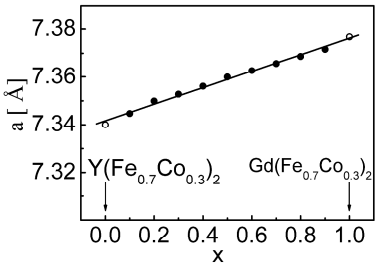

Figure 2. The unit cell edge a observed for the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ intermetallics (300K). The literature data is added [6,7].

Becouse the atomic radius of Gd atom is higher than the corresponding radius of Y atom (r_{Gd}=2.54 Å, r_Y=2.27 Å) [13] the unit cell parameter "a" is linearly increased with the gadolinium content x (Figure 2). A numerical formula a(x)=(0.035x+7.342) Å , the result of a least squares fitting, properly describes experimental points (Figure 2). The experimental points for the series $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ are compared to data known from the literature for $Y(Fe_{0.7}Co_{0.3})_2$ compound [7] and $Gd(Fe_{0.7}Co_{0.3})_2$ compound [6].

3. Mössbauer effect

The Mössbauer effect measurements were performed at 4.2K and in the temperature range around the magnetic ordering temperature using a standard transmission technique with a source of ^{57}Co in Rh. The collected ^{57}Fe Mössbauer effect spectra of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ intermetallics are presented in Figure 3. The experimental spectra are composed of a number of subspectra and this complexity arises from the different nearest neighbourhoods of the observed Fe-atoms. The problems in determining the number of nearest neighbour surroundings, the number of subspectra, the probabilities of the particular subspectra and the fitting procedure of the experimental spectra in the case of three elements, with

randomly distributed atoms, in the transition metal sublattice, have been discussed elsewhere for an analogous intermetallic series [14]. It can be added that the n.n. surrounding is composed of n_1 Fe atoms and n_2 Co atoms. The probabilities P(6; n_1, n_2) of the particular n.n. surroundings were calculated using the Bernoulli formulae [15]. As mentioned above $l = n_1 + n_2 = 6$ is the number of n.n. in the transition metal sublattice surrounding the studied Fe atom. The Fe and Co atoms are randomly populated with probabilities of $p_1 = 0.7$, $p_2 = 0.3$, because is no change of stoichiometric proportions Fe and Co atoms in the transition metal sublattice. Therefore, all experimental spectra are fitted using seven subspectra, which the starting amplitudes follow the probabilities P(6; n_1, n_2).

The average values of the hyperfine interaction parameters at 4.2 K, determined from the fitting procedure i.e., the isomer shift IS (with respect to pure iron metal, at 300 K), the magnetic hyperfine field $\mu_0 H_{hf}$ and the quadrupole interaction parameter QS obtained for the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series, are presented in Figure 4 (μ_0 is the magnetic permeability, QS as defined in [16]). The isomer shift decreases with x and experimental points are described by a numerical equation: IS (x) =(0.015x + 0.055) mm/s (curve 1). The magnetic hyperfine field $\mu_0 H_{hf}$ increases across the series with the Gd-content x. The experimental points tally well with the fitted formula: $\mu_0 H_{hf}(x) = (0.79x + 24.15)$T (curve 2).The quadrupole interaction parameter increases slightly with x and the experimental points follow the fitted formula: QS (x) = (0.030x + 0.021) mm/s (curve 3). The literature data for x=1 (open points in Figure 4) is also presented [17].

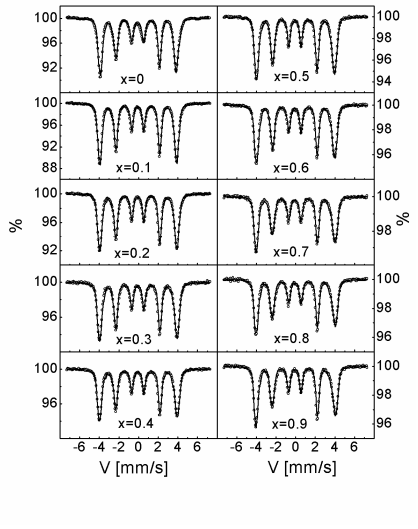

Figure 3. ^{57}Fe Mössbauer effect spectra of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ intermetallics (4.2K).

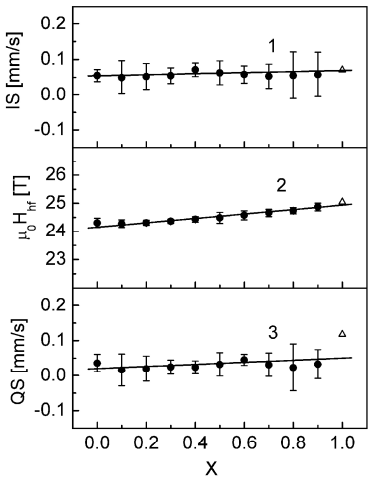

Figure 4. Hyperfine interaction parameters of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series: 1– the isomer shift, 2 – the magnetic hyperfine field and 3 – the quadrupole interaction parameter.

4. The Slater–Pauling and Curie temperature dependencies

It is interesting to situate the obtained magnetic hyperfine fields of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series among the magnetic hyperfine fields already known for the series $R(Mn_{1-x}Fe_x)_2$ and $R(Fe_{1-x}Co_x)_2$, where R= Y, Dy, Gd [7]. The magnetic hyperfine fields of these series, treated as a function of the average number n of 3d electrons (number n calculated per transition metal atom) and the de Gennes factor G [9] are presented in Figure5.

Figure 6 shows the $T_C(n,G)$ dependence for the $Y(Fe_{1-x}Co_x)_2$ (curve 1) [7], $Dy(Fe_{1-x}Co_x)_2$ (curve 2) [8], $Gd(Fe_{1-x}Co_x)_2$ (curve 3) [6] and $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ (curve 4). Curie temperatures of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ series were determined using both electrical resistivity (curve 4, black points) and Mössbauer effect measurements (curve 4, open points). The methods described elsewhere [6,8,18]

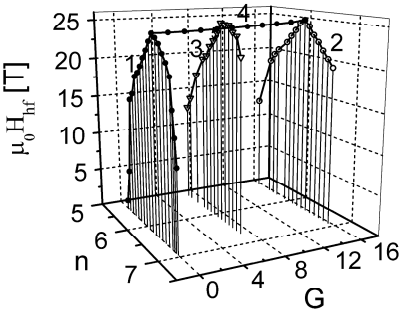

Figure 5. The hyperfine field $\mu_0 H_{hf}(n,G)$ dependencies of the intermetallic series.

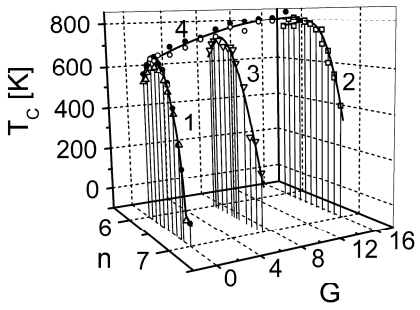

Figure 6. The Curie temperature $T_C(n,G)$ dependencies of the intermetallic series.

5. Conclusion

The intermetallics series $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ were prepared by arc melting in a high purity argon atmosphere. X-ray diffraction patterns confirm the formation of a cubic $MgCu_2$ type structure. ^{57}Fe Mössbauer studies indicate that the magnetic hyperfine field slightly increases with Gd increasing addition. The Curie temperatures of the $(Y_{1-x}Gd_x)(Fe_{0.7}Co_{0.3})_2$ are found to increase with increasing Gd addition. The above dependencies are attributed to the additional 4f–5d exchange interaction (Gd–Gd) introducing parallel alignment of the localized magnetic moment 4f and the band 5d magnetic moment. Correspondingly, the 5d–3d exchange interaction (Gd–Fe), (Gd–Co) introduces an antiparallel alignment between the 5d and 3d band magnetic moments. Moreover the 3d–3d exchange interactions establish the parallel order in the transition metal subsystem.

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