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Mössbauer study of Laves phase $Y(\text{Fe}_{0.8}\text{Mn}_{0.2})_2$

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Abstract. A ternary $Y(\text{Fe}_{0.8}\text{Mn}_{0.2})_2$ compound with a Laves structure has been studied by Mössbauer spectroscopy. The magnetic transition temperature of the sample is found to be 454 ± 3 K. As compared to the binary $Y\text{Fe}_2$ compound, it is found that the addition of Mn element in the sample does not change either the crystalline structure or the electric field gradient at Fe sites. However, it is found to strongly influence the hyperfine fields at Fe sites, the magnetic-transition temperature and the phonon spectrum in the magnetic phase transition region.

1. Introduction

Over the past two decades, a great many investigations have been reported on the binary compounds $R\text{Fe}_2$ (where R is a rare earth element) with large magnetostrictive coupling constants [1]. Although Y is not a rare earth, it has been found to be a good rare earth substitute [2]. The $Y\text{Fe}_2$ compound has a cubic Laves structure. The Y ions are situated on a diamond sublattice and the Fe ions on a corner-sharing network of regular tetrahedra. The site symmetry of the Fe ions is $3m$ with each being crystallographically equivalent and the threefold axis in the (111) direction. Recently, it was found that the $Y\text{Mn}_2$ compound with the same Laves structure undergoes a first-order phase transition with a large volume anomaly [3]. Since then there has been much interest in the structure and magnetic properties of this compound [4–9]. In comparison with the binary compounds $Y\text{Fe}_2$ and $Y\text{Mn}_2$, only a few investigations have so far been performed on the ternary $Y(\text{Fe}, \text{Mn})_2$ compound. In this work, a ternary compound $Y(\text{Fe}_{0.8}\text{Mn}_{0.2})_2$ is studied by Mössbauer spectroscopy. The effect of the addition of Mn element on the magnetic properties of Fe sites in the ternary compound is presented.

2. Experimental details

For the preparation of the ternary compound $Y(\text{Fe}_{0.8}\text{Mn}_{0.2})_2$, Y (99.9%), Fe (99.5%) and Mn (99.5%) were mixed to a nominal composition and melted in an arc furnace several times in an Ar atmosphere. To obtain a more homogeneous sample, the polycrystalline $Y(\text{Fe}_{0.8}\text{Mn}_{0.2})_2$ alloy was further annealed at 1223 K for one week.

Mössbauer spectra of the sample were recorded in a conventional spectrometer with constant-acceleration transmission geometry. The single-line source consisted of 50 mCi ^{57}Co in a Rh matrix. All isomer shift values are given relative to the centre of the α -Fe at room temperature. For measurements at 4.2 K, a He cryostat with a superconducting magnet was used. For measurements at temperatures higher than 300 K, heating took place

in a vacuum of 10^{-5} Torr. The sample temperature, with stability better than 1 K during the measurement, was measured using a thermocouple. In order to determine the magnetic transition temperature (T_0) of the sample, the zero-velocity thermal scan method was used [10], since for the sample in the paramagnetic state one of the Mössbauer resonant lines happened to almost overlap with the source line at zero velocity. The integrated counts were accumulated for a fixed time of 120 s while the temperature was raised from 410 K to 480 K.

3. Results and discussion

3.1. The structure of the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound

Due to the limited solid solubility of elements Fe and Mn in each other and the different crystal structures, it is necessary to add a third element, for example Y and rare earth elements, to achieve a solid solution of both elements Fe and Mn. The structure of the $Y(Fe_{0.8}Mn_{0.2})_2$ sample was examined by x-ray diffraction measurement. A single cubic Laves structure was found in the sample.

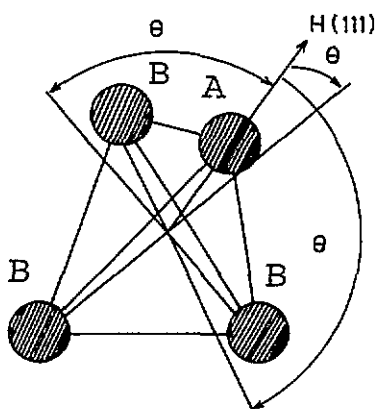


Figure 1. An illustration of the location of the Fe atoms in the tetrahedra in the Laves phase relative to the (111) axial direction. The Fe atom in site A has $\theta = 0^\circ$ and the Fe atoms in sites B have $\theta = 70.5^\circ$.

Table 1. Mössbauer parameters for the four components at 4.2 K: hyperfine field (H), isomer shift (is), quadrupole splitting (qs), line width (LW) and relative area (RA) in the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound.

Component	H (kOe)	is ($mm\ s^{-1}$)	qs ($mm\ s^{-1}$)	LW ($mm\ s^{-1}$)	RA (%)
1	216	0.044	0.127	0.315	19
2	199	0.032	-0.518	0.320	6
3	195	0.055	0.043	0.532	25
4	164	0.053	0.000	0.690	50

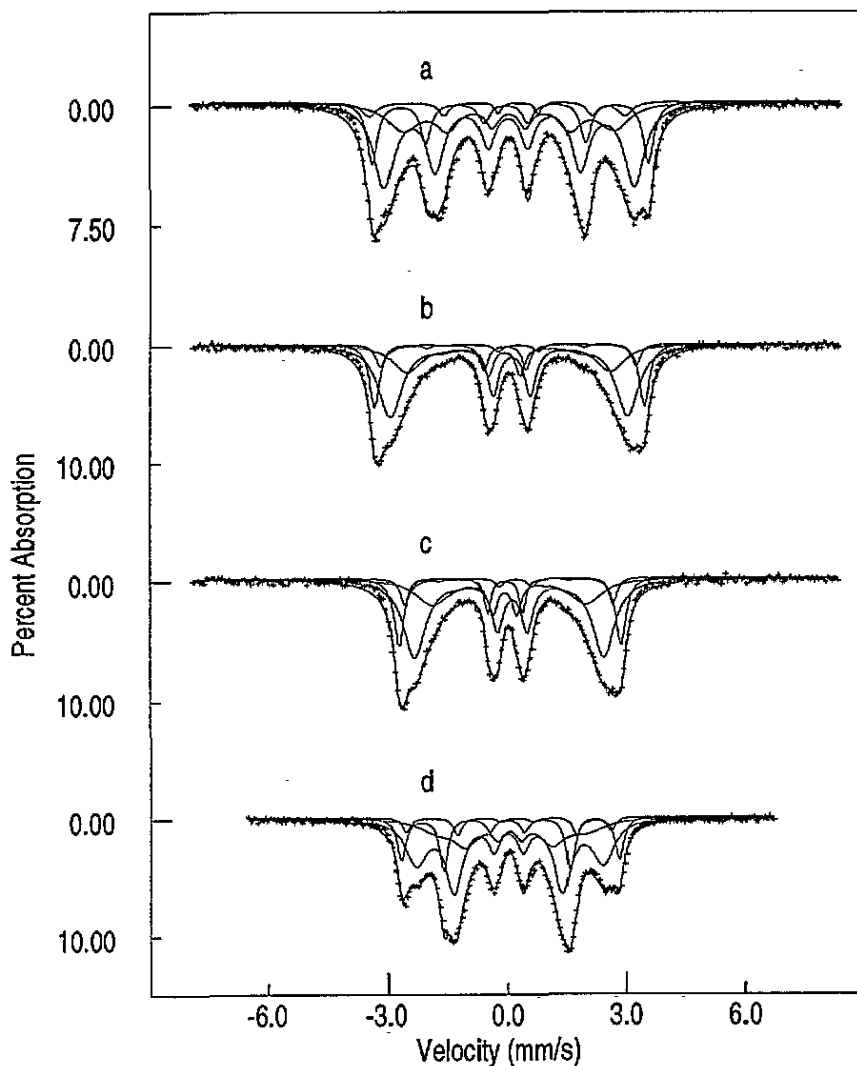


Figure 2. Mössbauer spectra for the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound at 4.2 K: no field (spectrum a); 1 T field parallel to γ -ray propagation (spectrum b); 5 T field parallel to γ -ray propagation (spectrum c) and 5 T field perpendicular to γ -ray propagation (spectrum d).

The Mössbauer spectrum of the YFe_2 alloy at 4.2 K has been previously described by two magnetic splittings [11]. In the cubic Laves structure all Fe atoms are crystallographically equivalent. However, the local threefold symmetry axes of electric field gradient (EFG) at the Fe site produce inequivalent magnetic fields at Fe nuclei due to different angles θ between the EFG axes and the direction of the Fe moment. The easy direction of the Fe moment is (111) in the YFe_2 compound. An illustration of the location of the Fe atoms in the Laves phase relative to the (111) axial direction is shown in figure 1. In this case, there are two angles with $\theta = 0^\circ$ and 70.5° . The intensity ratio occupying these positions is 1:3. Mössbauer spectra of the $Y(Fe_{0.8}Mn_{0.2})_2$ sample at 4.2 K are shown in figure 2. In the ternary compound $Y(Fe_{0.8}Mn_{0.2})_2$ some Fe atoms are substituted by Mn atoms. The Mn substitution process has an influence on the hyperfine field due to the existence of various

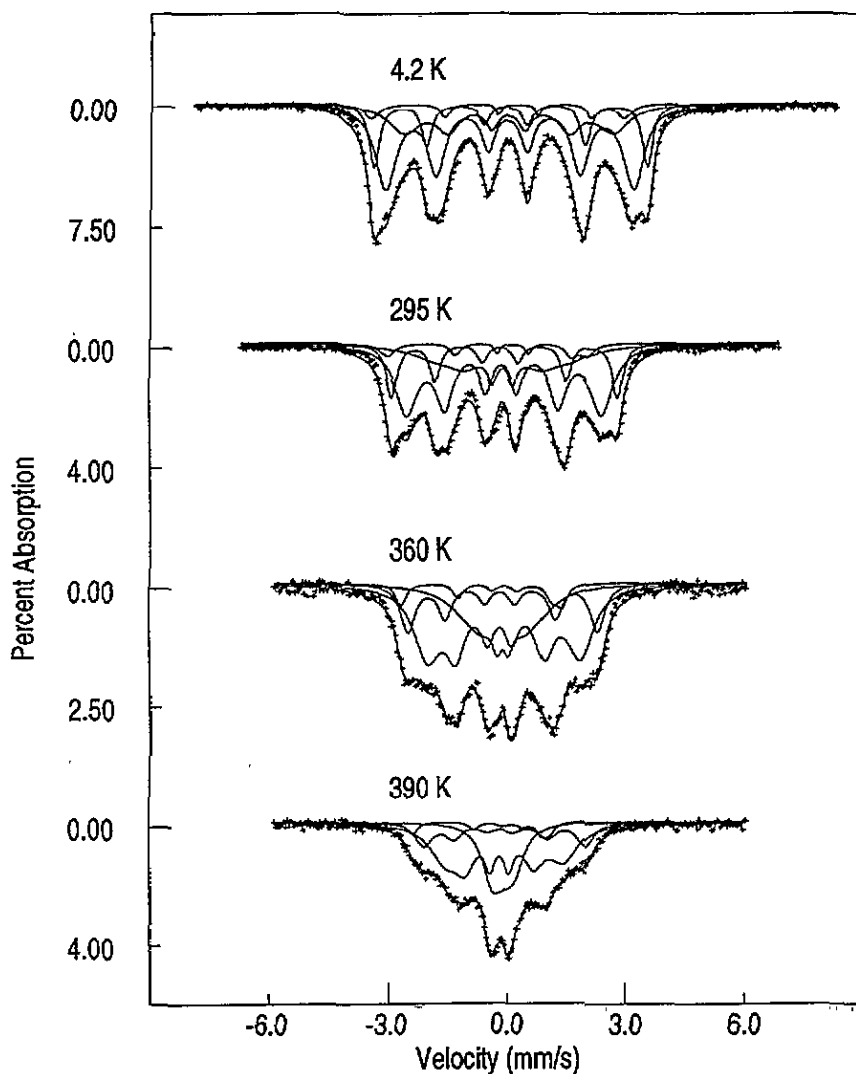


Figure 3. Mössbauer spectra for the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound in the temperature range of 4.2–390 K.

nearest-neighbour configurations of the Fe atom in the ternary compound. The outmost resonant absorptions in the spectrum (figure 2(a)) are asymmetric, which means that more than one subspectrum is needed to fit this spectrum. Two subspectra were used to fit the spectrum. However, a good fit to the spectrum cannot be achieved. Before we describe the details of the fitting process, one result obtained by investigating magnetic properties on $Y(Fe, Mn)_2$ samples should be mentioned [12]. Hilscher [12] found that in the $Y(Fe, Mn)_2$ samples magnetic clusters were formed; this was caused by the concentration fluctuations. In the first approximation the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ system may be composed of two parts: one is the YFe_2 phase with a negligible amount of Mn and the other the $Y(Fe_{0.75}Mn_{0.25})_2$ phase. The latter gives two possibilities for the location of the Mn atom in the tetrahedra. One is the Mn atom located at the A site. There is only one Fe site in the $Y(Fe_{0.75}Mn_{0.25})_2$

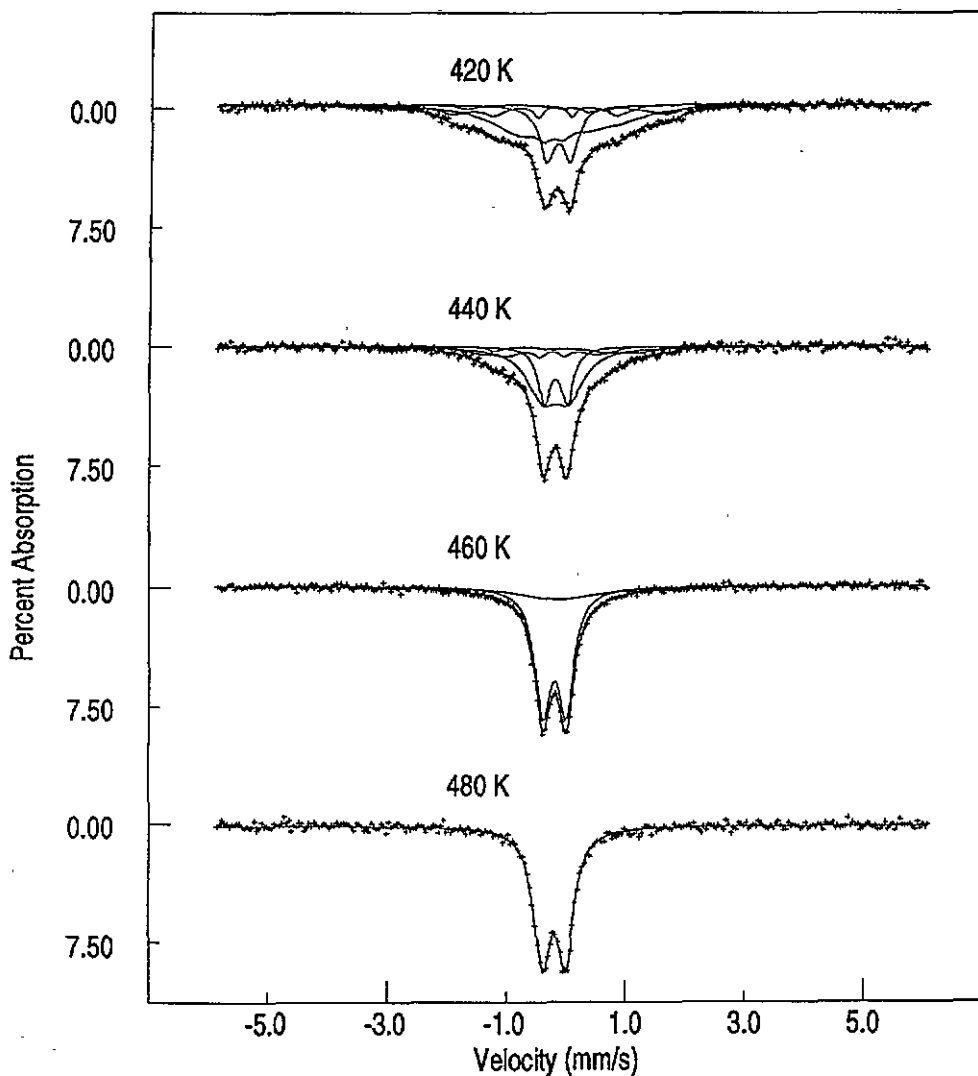


Figure 4. Mössbauer spectra for the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound in the temperature range of 420–480 K.

phase. However, by using this configuration a good fit to the spectrum in figure 2(a) cannot be obtained. The other is the Mn atom located at any one of the B sites. In this case, there are two different Fe sites in the $Y(Fe_{0.75}Mn_{0.25})_2$ phase. By using this configuration the fit to the spectrum is remarkable. The Mössbauer parameters for the four subspectra (or components) are listed in table 1. The first two components are attributed to the Fe sites with a negligible influence of Mn addition, which are similar to those in pure YFe_2 . The other two components, 3 and 4, are attributed to the A and B Fe atoms in the $Y(Fe_{0.75}Mn_{0.25})_2$ phase, respectively. In order to examine the validity of the four-subspectra model, the high-field Mössbauer spectra were recorded for the $Y(Fe_{0.8}Mn_{0.2})_2$ sample in the geometry with the direction of the applied field parallel to the γ -ray propagation. Fe moments in the sample rotate toward the direction of the applied field, which means that the intensity

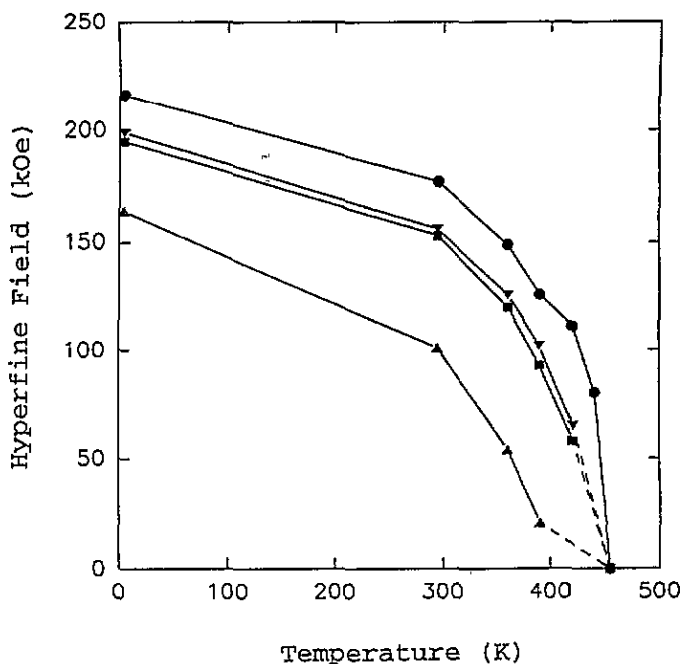


Figure 5. The temperature dependence of hyperfine fields corresponding to the four subspectra in the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound in the temperature range of 4.2–460 K: ●, for component 1; ▼, for component 2; ■, for component 3 and ▲, for component 4.

of the second (or fifth) line will be reduced with increasing field. The spectrum can be easily fitted due to the smaller overlap between the first line and second line (or the sixth line and fifth line). As we see in figure 2, spectra b and c, these spectra can be also well fitted by using the above model. After fitting it was found that the canting angle between the Fe moment and the direction of the applied field is $14.2^\circ \pm 0.5^\circ$ for an applied field of 1 T and $10.5^\circ \pm 0.5^\circ$ for 5 T. Furthermore, a high-field Mössbauer measurement was performed in the geometry with the direction of the applied field perpendicular to the γ -ray propagation as shown in figure 2, spectrum d. The four-subspectra model can again fit the spectrum well. The canting angle between the Fe moment and the direction of the applied field was obtained to be $10.8^\circ \pm 0.5^\circ$. Since the sample is powder, the canting angle should be the same in figure 2, spectra c and d. Therefore, after fitting the spectra c and d the same canting angle obtained within the experimental error suggested again that the above four-subspectra fitting model can approximately approach the Fe atomic configurations in the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound.

3.2. Temperature-dependence Mössbauer measurements

Figures 3 and 4 show some of the recorded Mössbauer spectra of the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound in the temperature range of 4.2–480 K. All spectra in figure 3 were fitted by using the four-subspectra model. The temperature dependences of four hyperfine fields corresponding to these four subspectra are plotted in figure 5. When the temperature rises, hyperfine field values decrease, especially for component 4. When the temperature is above 390 K, the four components cannot be clearly separated from each other because relaxation in all four components exists. The magnetic transition temperature of the ternary

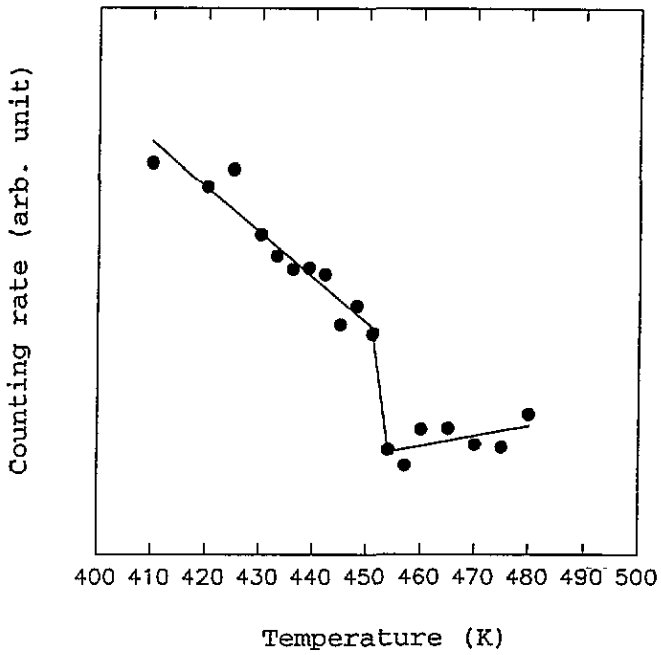


Figure 6. The counting rate of the 14.4 keV γ -ray at zero velocity as a function of the temperature for the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound.

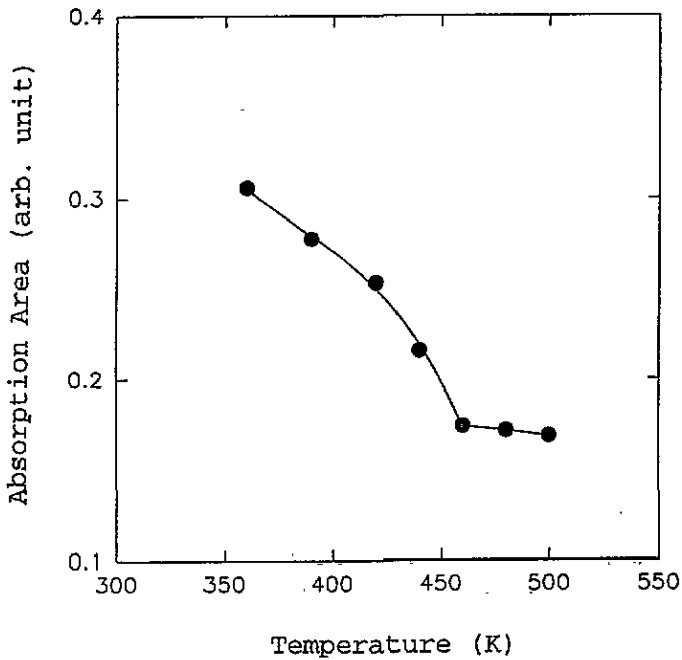


Figure 7. Absorption areas of the Mössbauer effect as a function of the temperature for the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound.

$Y(Fe_{0.8}Mn_{0.2})_2$ compound was found from figure 5 to be about 460 K. A more accurate value of the magnetic transition temperature was found to be 454 ± 3 K by using the zero-velocity thermal scan measurement. The result of the measurement for the sample in the temperature range of 410–480 K is shown in figure 6. T_0 is significantly lower than 540 K for the binary YFe_2 compound [11]. This large difference of the magnetic transition temperature between the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ and binary YFe_2 compounds may be explained by the dilution of the Fe magnetic moment by the adjacent element Mn [12].

The spectrum recorded at the temperature of 480 K, well above T_0 , in figure 4 shows pure quadrupole splitting with $QS=0.392$ mm s⁻¹. The corresponding EFG reflects the asymmetry of the environment of the Fe sites. In principle, the spectrum should be fitted with at least two doublets, which are responsible for the two compounds YFe_2 and $Y(Fe_{0.75}Mn_{0.25})_2$, respectively. However, one quadrupole doublet already gives a satisfactory fit and the value of the quadrupole doublet of the ternary compound is in good agreement with the reported value of the binary YFe_2 compound [11]. These results indicated that the substitution of Mn atoms for Fe atoms has no large influence on the EFG at Fe sites. This differs from the effect of the Mn atom substitution for Fe atoms on the magnetic transition temperature.

Absorption areas of the Mössbauer effect in a temperature range of 350–500 K for the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound are shown in figure 7. Since the sample used was not very thick (~ 0.2 mg cm⁻² ⁵⁷Fe), the area under the absorption curves is approximately proportional to the value of the recoil-free fraction $f(T)$. It is clear that two temperature ranges can be distinguished: one is below 460 K and the other above 460 K. In the latter $f(T)$ slightly decreases with increasing temperature, but in the former $f(T)$ rapidly increases when temperature decreases. The rapid enhancement of $f(T)$ can be linked with spin fluctuation. As we know, when the temperature is below 454 K, the sample becomes magnetic. Then, the magnon–phonon coupling may enhance the Mössbauer recoil-free fraction $f(T)$. In the magnetic phase transition region a discontinuity of $df(T)/dT$ occurs. However, it was previously reported that there is no discontinuity of $df(T)/dT$ in the binary YFe_2 compound [13]. This leads us to believe that the observed phenomenon is to be associated with the addition of the Mn element in the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound.

According to the above analyses, it can be concluded that by the addition of the Mn element to the binary YFe_2 compound the cubic Laves structure still remains and the EFG at Fe sites does not change, but hyperfine fields at Fe sites, the magnetic transition temperature of the sample and the phonon spectrum in the phase transition region are greatly influenced by the substitution of Mn atoms for the Fe atoms in the ternary $Y(Fe_{0.8}Mn_{0.2})_2$ compound.

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