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Mössbauer studies of spin reorientations in $Er_{2-x}Gd_xFe_{14}B$

Anna Wojciechowska, Bogdan F. Bogacz, Antoni T. Pędziwiatr

Abstract The $Er_{2-x}Gd_xFe_{14}B$ (x = 0.5, 1.0, 1.5) polycrystalline compounds have been investigated with ^{57}Fe Mössbauer spectroscopy in the 80–330 K temperature range. The spin reorientation phenomena (changes from planar to axial spin arrangements) have been studied extensively by a narrow step temperature scanning in the neighbourhood of the spin reorientation temperature. From the analysis of the spectra it was deduced that in the region of transition each subspectrum was split into two Zeeman sextets, which were characterized by different hyperfine magnetic fields and quadrupole splittings. A consistent way of describing the Mössbauer spectra in the wide range of temperatures was proposed. The composition and temperature dependencies of hyperfine interaction parameters and subspectra contributions were derived from experimental spectra. The transition temperatures were determined for all the compounds studied.

Key words Mössbauer effect • spin reorientation

Introduction

The studies of spin reorientation phenomena in the Er-based $R_2Fe_{14}B$ (R = rare earth) systems are important because they establish the temperature region of uniaxial anisotropy which is crucial for permanent magnet applications. In these compounds, the magnetocrystalline anisotropy changes from planar (basal plane) to axial (along the c-axis) with increasing temperature.

The easy magnetisation direction of $Er_{2-x}R_xFe_{14}B$ depends on the temperature induced competition between the uniaxial Fe sublattice anisotropy [2] and the basal plane (Er, R) sublattice anisotropy [4].

The $Er_{2-x}Gd_xFe_{14}B$ crystallize in a tetragonal structure with the $P4_2/mnm$ space group. Iron atoms occupy six non-equivalent crystal sites ($16k_1$, $16k_2$, $8j_1$, $8j_2$, 4e, 4c), the rare earth ions occupy 4f and 4g crystallographic sites and boron is located at 4g site [3].

In this study, the polycrystalline $Er_{2-x}Gd_xFe_{14}B$ (x = 0.5, 1.0, 1.5) isostructural compounds have been investigated by ^{57}Fe Mössbauer spectroscopy in order to establish the spin reorientation temperatures, T_{SR}, the influence of reorientation on hyperfine interaction parameters and to establish the influence of gadolinium on transition.

Experimental

The $Er_{2-x}Gd_xFe_{14}B$ (x = 0.5, 1.1, 1.5) alloys were obtained by a standard procedure of induction melting under flowing high purity argon and subsequent annealing at 900°C for two weeks. The X-ray and thermomagnetic analyses proved the single phase integrity of materials. The ^{57}Fe Mössbauer

A. Wojciechowska, B. F. Bogacz, A. T. Pędziwiatr✉
M. Smoluchowski Institute of Physics,
Jagiellonian University,
4 Reymonta Str., 30-059 Kraków, Poland,
Tel.: + 48 12/ 663 55 05, Fax: +48 12/ 663 70 86,
e-mail: ufpedziw@if.uj.edu.pl

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transmission spectra were recorded in the temperature range 80–330 K. The spin reorientation phenomenon near T_{SR} has been studied extensively by narrow step (even 2 K) temperature scanning using a ^{57}Co(Rh) source and a computer – driven constant acceleration mode spectrometer. A high purity iron foil was used to calibrate the velocity scale. Isomer shifts were established with respect to the centre of gravity of the room temperature iron Mössbauer spectrum.

Data analysis

Several experimental Mössbauer spectra of the $Er_{0.5}Gd_{1.5}Fe_{14}B$ alloy are shown in Fig. 1. The "exponential" approximation [1] of the transmission integral and a simultaneous fitting of several spectra was applied to describe the investigated Mössbauer spectra and obtain consistent fits. For temperatures outside the transition region, the Mössbauer spectra were analysed using six Zeeman subspectra with relative intensities in agreement with iron occupation of crystallographic sublattices (4:4:2:2:1:1). For temperatures inside the region of reorientation each subspectrum splits into two parts.

All subspectra were characterized by the following hyperfine interaction parameters: magnetic field, B; isomer shift, IS; quadrupole splitting, QS (defined as $[(V_5 - V_6) - (V_2 - V_1)]/2$ where V_i are the velocities corresponding to Mössbauer line positions). It is significant that spectra below spin reorientation region (described by "low temperature" Zeeman sextets) and above (described by "high temperature" Zeeman sextets) have different values of B and QS. There is a coexistence of the "low" and "high temperature" Zeeman sextets in the region of reorientation. Both kinds of Zeeman sextets exchange gradually (between themselves) their contributions C_l, C_h to the total spectrum. The weak, systematic changes of B and QS with temperature were taken into account for spectra below and above spin reorientation region. A common linear temperature dependence of IS caused by second order Doppler shift effect was assumed for "low" and "high temperature" Zeeman sextets.

Results and discussion

Figures 2 and 3 show the behaviour of B and QS in the $Er_{0.5}Gd_{1.5}Fe_{14}B$ compound. It is visible that hyperfine field

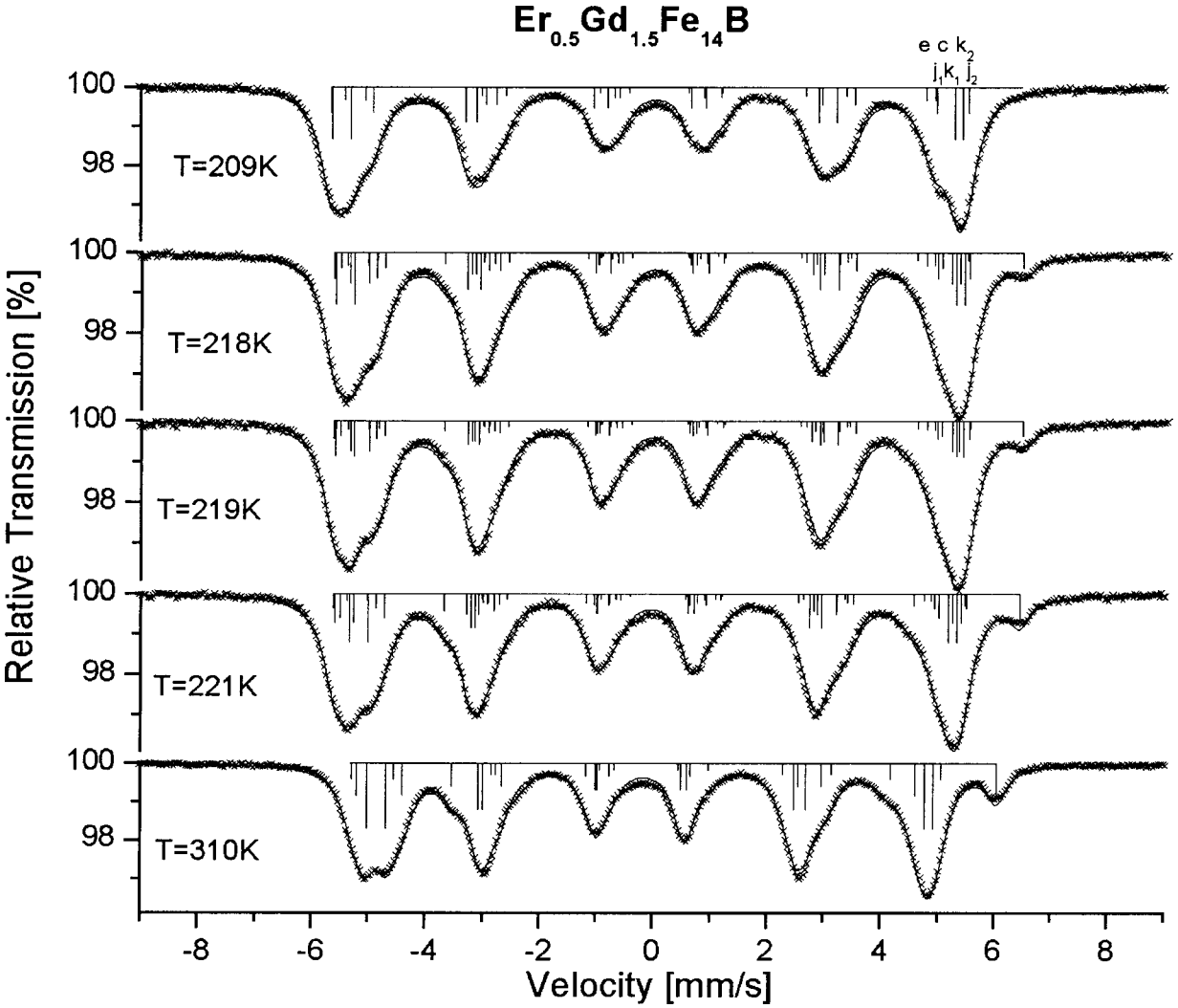

Fig. 1. Selected ^{57}Fe Mössbauer transmission spectra for the $Er_{2-x}Gd_xFe_{14}B$ (x = 1.5) intermetallic compound. The solid lines are fits to the data. The stick diagrams show the line positions and relative intensities.

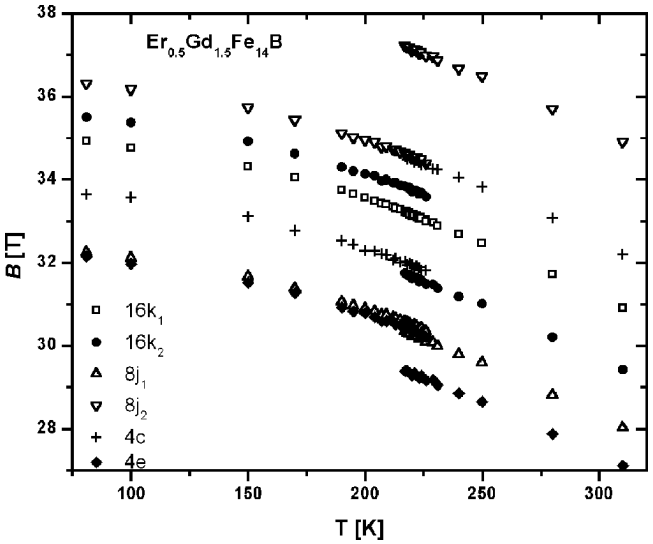

Fig. 2. Temperature dependence of the hyperfine magnetic field, B, $Er_{0.5}Gd_{1.5}Fe_{14}B$. The average error is 0.1 T.

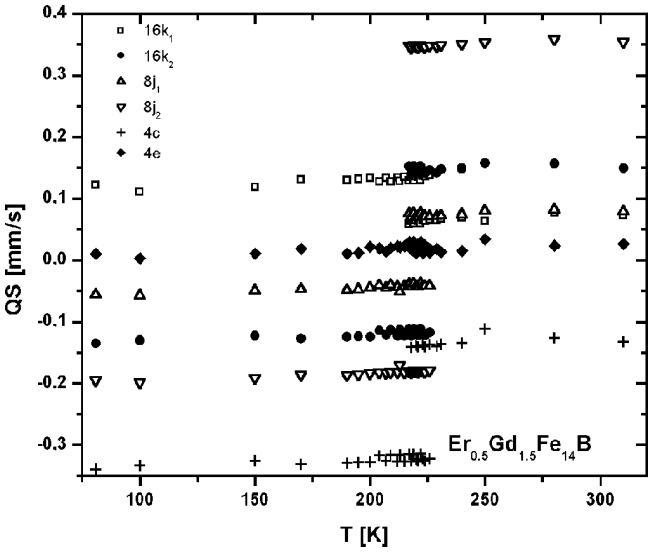

Fig. 3. Temperature dependence of the quadrupole splitting, QS, for different crystal sities of the $Er_{0.5}Gd_{1.5}Fe_{14}B$. The average error is 0.01 mm/s.

decreases with increasing of temperature, whereas the quadrupole splitting behaves inversely. Moreover, in the region of reorientation each subspectrum is characterized by two Zeeman sextets and hence by different B and QS.

The contributions C_l, C_h of both "low" and "high temperature" Zeeman sextets for $Er_{0.5}Gd_{1.5}Fe_{14}B$ compound are shown in Fig. 4. From this plot, the T_{SR} (assumed to be at the intersection point of C_l and C_h curves) was

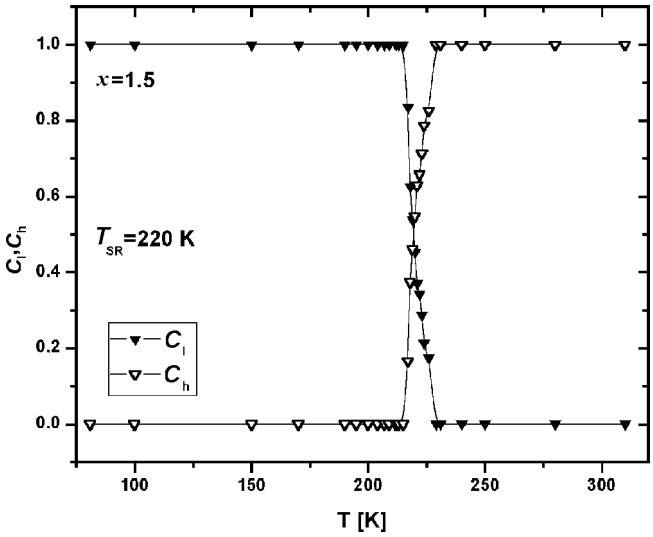

Fig. 4. Temperature dependencies of subspectra contributions for both C_l – "low temperature" (solid triangle) and C_h – "high temperature" (open triangle) Zeeman sextets for $Er_{0.5}Gd_{1.5}Fe_{14}B$. The average error is 1 K.

Table 1. Spin reorientation temperatures, T_{SR}, for $Er_{2-x}Gd_xFe_{14}B$. T_{SR} error is ±1 K.

Compound	T_{SR} [K]
X = 0.0	325 [5]
X = 0.5	306
X = 1.0	273
X = 1.5	220

derived. The T_{SR} values for all studied compounds are given in Table1. It was found that the substitution of Gd for Er causes a decrease of T_{SR}.

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