

05,07

Magnetic phase transformations and hyperfine interactions in a multicomponent system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ ($0 \leq x \leq 1$)

© Z.S. Umkhaeva¹, V.S. Rusakov², T.V. Gubaidulina², A.Yu. Karpenkov³, I.S. Tereshina², N.Yu. Pankratov², I.M. Aliev¹

¹ Kh. Ibragimov Complex Institute of the Russian Academy of Sciences, Grozny, Russia

² Moscow State University, Moscow, Russia

³ Tver State University, Tver, Russia

E-mail: zargan.umhaeva@yandex.ru

Received July 2, 2024

Revised September 14, 2024

Accepted September 16, 2024

This paper presents the results of the study of structural and magnetic properties, as well as hyperfine interactions in a multicomponent system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, where $x = 0, 0.2, 0.4, 0.6, 0.8, 1.0$. It is established that all the obtained alloys are single-phase and possess atomic-crystalline structure of cubic symmetry of the type of Laves C15 phase. For alloys of the system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ the values of Curie temperatures, saturation magnetisation σ_s , have been determined, the values of magnetic moment coming to the iron atom μ_{Fe} have been calculated. The studies of the Mössbauer effect on ^{57}Fe nuclei at room temperature have been carried out. The values of hyperfine parameters of Mössbauer spectra for all alloys of the system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ have been determined. The dependences of structural and magnetic parameters on the concentration of yttrium (a non-magnetic analogue of rare-earth elements) have been analysed and the features related to magnetic phase transformations in the studied system have been revealed.

Keywords: Laves phases, magnetization, Curie temperature, magnetic moment, Mössbauer effect, hyperfine fields, isomeric shift, quadrupole coupling constants, easy magnetisation axis.

DOI: 10.61011/PSS.2024.10.59629.176

1. Introduction

The rare-earth intermetallic compounds based on iron $R\text{-Fe}$ (R — atoms of rare-earth elements (REE)) are suitable objects to study the interaction of two types of magnetoactive atoms, namely R atoms with $4f$ -electron shell located deep and screened by above laying electron layers, and so having weak reaction to the external effect, and Fe atoms, in which $3d$ -electron shell is rather strongly subjected to the effect of crystal and exchange fields. That's why study of properties of the alloys $R\text{-Fe}$ is rather actual and associated, mainly, with search of new compounds with predictable or regulated set of functional parameters and properties.

Currently, as we known, the multi-component alloys are actual based on rare earth element having one of structure of Laves phase. Our studies [1–4] executed previously showed that multi-component Laves phase based on rare-earth metals $(R_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ (where $R = \text{Gd}, \text{Tb}, \text{Dy}$ and Er), are rather interesting objects of study both due to fundamental, and practical (high efficient magnetostriction alloys) points of view. Using complex type of substitution in rare-earth sublattice, as well as changing temperature and values of external magnetic fields we can actively affect their

magnetic and magnetostriction properties, as well as to observe some unique magnetic transformations including magnetic compensation of rare-earth sublattice and Fe sublattice, as well as spin re-orientation of magnetic moments.

It was interested also to study the similar $(R_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ system of alloys with Ho, as all previously studied systems [1–4] are rare-earth intermetallic compounds, that additionally to light rare-earth element samarium comprise also heavy REEs. Holmium is one of them and has maximum magnetic moment $10 \cdot \mu_{\text{B}}$. So, synthesis and study of the system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ can expand works relating study of the multi-component alloys $(R_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ with structure of Laves phase, this ensures further analysis and forecast, including theoretically, the regions of concentration of components where we can obtain compounds with most optimal magnetic characteristics in specified range of temperatures and magnetic fields.

Selection of the exactly such $(R_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ compound of alloys is due to that compounds of type $R\text{Fe}_2$ with heavy REEs are ferrimagnetics in wide range of temperatures of magnetic orderings. This means that intersublattice $R\text{-Fe}$ exchange is negative, and magnetic moments of rare-earth and $3d$ -sublattices are directed

antiparallel [5]. The compound SmFe_2 is ferromagnetic, as Sm relates to light REEs and intersublattice exchange Sm-Fe in it is positive. When substituting atoms of heavy rare earth element R initially atom of light rare earth element Sm with fixed concentration (for example, 20 at.%), an then Y with different value of substitution parameter (for example, $x = 0, 0.2, 0.4, 0.6, 0.8, 1.0$), in system alloys the competition of intersublattice exchange interactions in pairs Sm-Fe and R -Fe (R — heavy REE) will occur depending on concentration of weak magnetic yttrium.

Note that signs of magnetic anisotropy constants, and signs of magnetostriction constants in alloys $R\text{Fe}_2$ with light and heavy REE can differ. As a result, in multi-component alloys of type $(R_{1-x}Y_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, where R — heavy REE, we can observe also inversion of signs of these constants.

Competition of exchange interactions in alloys of new multi-component system with holmium of type $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ can ensure in the obtained alloys some magnetic transformations, including, for example, phenomenon of magnetization compensation of rare-earth sublattice and Fe sublattice [6] not only by compound, but by temperature, due to high magnetic moment Ho^{3+} .

Together with magnetometric methods of properties study of magnetic materials the hyperfine interactions are sensitive to changes in sign and type of exchange and crystal interactions between magnetoactive atoms of REE and Fe, such interactions are studied, as a rule, using Mössbauer effect of ^{57}Fe .

Study of properties of rare-earth intermetallic compounds of type $R\text{Fe}_2$ with structure of Laves phases has great practical value. Currently these compounds are widely used in various areas of science and engineering as magnetostrictors, and detectors and sensors of movement [7]. This study will ensure scope expansion of such materials, for example, by creation based on them of the temperature transmitters and other devices.

In connection with the above the main aim of this work was detail investigation of atomic-crystal structure, magnetic properties and hyperfine interactions in multi-component alloys based on holmium, samarium and yttrium, namely of system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

2. Sample preparation and methods

In this paper we for the first time synthesized the system of multi-component alloys based on heavy rare-earth metal holmium $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ with substitution parameter $x = 0, 0.2, 0.4, 0.6, 0.8, 1.0$.

The $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ samples were prepared from high-purity constituting metals in an induction furnace under a purified atmosphere of argon. The so-obtained ingots with weight of 10–20 g were wrapped in nickel-iron foil, sealed in an evacuated quartz tube with an argon pressure of 70 kPa and annealed in a resistive furnace. The annealing regime contains the following stages: heating with rate $7^\circ\text{C}/\text{min}$ up to 800°C , dwelling for 40 hours. Finally, all

samples were quenched in water. The presence of noble gas, argon, in the tube prevented alloy component evaporation during annealing.

X-ray diffraction analysis was performed for all samples using DRON-7 diffractometer using $\text{Cu-K}\alpha$ radiation ($\lambda = 0.1540598 \text{ nm}$) at room temperature in the angle range $2\theta = 15\text{--}105^\circ$. To determine structural properties, the diffraction patterns were analyzed using the spectrum fitting procedure. The diffraction patterns were analyzed by a whole pattern fitting procedure to determine the structural properties. Each structural model was refined to convergence and the best results were chosen based on the agreement factor and stability of the refinement. A refinement of the lattice parameter of a unit cell was determined by the Rietveld Method.

To measure field dependences of magnetization of the obtained samples the automated vibration magnetometer was used. Measurements were performed in wide temperature range of 85 to 750 K in fixed magnetic fields up to 1.5 T.

The Mössbauer spectra were recorded in transmission geometry using MS-1104Em spectrometer in constant acceleration mode. ^{57}Co gamma radiation source in Rh matrix and with activity $\sim 20 \text{ mCi}$ was used for the experiment. The spectrometer was calibrated at room temperature using $\alpha\text{-Fe}$ reference standard. Spectra were processed using SpectrRelax software [8,9].

3. Experimental results and discussion

System of multi-component alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, obtained by us, comprises 6 samples, namely, three-component $\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ and $\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, and four-component $(\text{Ho}_{0.8}\text{Y}_{0.2})_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, $(\text{Ho}_{0.6}\text{Y}_{0.4})_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, $(\text{Ho}_{0.4}\text{Y}_{0.6})_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, and $(\text{Ho}_{0.2}\text{Y}_{0.8})_{0.8}\text{Sm}_{0.2}\text{Fe}_2$. Figure 1 presents the diffraction spectra of above alloys, obtained at room temperature (at $T = 290 \text{ K}$).

According to X-ray diffraction phase analysis of the obtained spectra were identified that all alloys of the system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ are practically single-phase and have atomic-crystal structure of cube symmetry of Laves phase type C15 (sp. gr. $Fd\bar{3}m$). The literature data analysis shows that this atomic-crystal structure is rather well studied. Its features are described in detail in many papers relating structural studies of both binary compounds $R\text{Fe}_2$, and multi-component alloys, including, similar one studied in this paper [5,6,9–11].

It is known, for example, that at Curie temperature there is magnetic structural phase transition associated with different distortions of the cube structure depending on direction alignment of magnetic moments.

Parameter calculation of cubic lattice for all obtained samples ensures determination that in the system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ at room temperature with yttrium concentration increasing the lattice parameter steadily increase from 0.7321 nm in compound $\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ (i.e. at $x = 0$) to 0.7368 nm in compound $\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ (i.e.

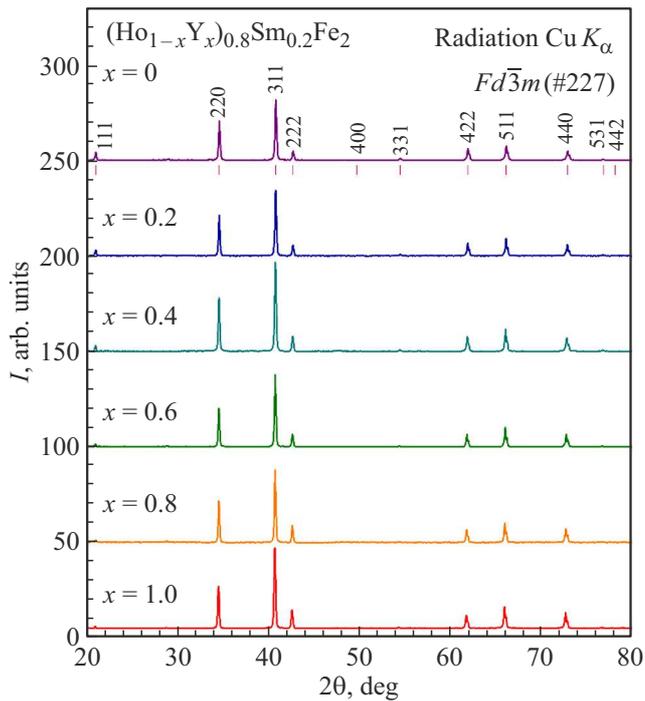


Figure 1. X-ray reflection spectra of system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ at various values of substitution parameter x , obtained at $T = 290$ K.

at $x = 1.0$) (Figure 2). But, in Figure 2 we observe the deviation of dependence $a(x)$ from the Vegard linear law. Such behaviour can be determined, as per our opinion, by two basic reasons. Firstly, at room temperature all alloys of this system are in magnetic ordered state. As it was stated above, in Laves phases the transition over the Curie temperature is accompanied by not only occurrence of spontaneous magnetic moment, but also by spontaneous magnetostriction, which can be one of the reasons of such behaviour. Secondly, we rather well know the phenomenon of „lanthanide“ contraction in row of REEs [6], which leads to the fact that the greater the atomic number of rare earth element is the lower its ionic radius is. So in Ho, which is practically at the end of row of heavy REEs, the ionic radius is less the radius of Y ions introduced into its sublattice. So, concentration increasing of larger Y ions in the system leads to abrupt rise of lattice parameters of alloys.

For comparison note that in the binary compounds YFe_2 , SmFe_2 and HoFe_2 , as per known literature data [12] the parameters of cubic lattice are 0.7363, 0.7401 and 0.7287 nm, respectively.

Note that while in alloy $\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, the lattice parameter is rather close to appropriate value for the binary compound YFe_2 (within experimental and calculation error), and in alloy $\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ the lattice parameter a differs from value for the binary compound HoFe_2 . This fact can be associated with the presence and, on the contrary, with absence of significant in value magnetic moment in atoms of holmium and yttrium, respectively.

One of the main parameters of magnetic-ordered state is the Curie temperature. For system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ Curie temperature was determined using thermomagnetic analysis, which assumes measurement and analysis of the temperature dependence of specific magnetization in external magnetic field. In our study curves $\sigma(T)$ were obtained for all studied samples in wide range of temperatures $T = 85\text{--}700$ K in magnetic field $\mu_0 H = 1$ T and are represented in Figure 3. Values of Curie temperature were determined by plotting the derivative of magnetization with respect to temperature, at which $d\sigma/dT$ has minimum values.

During the experiment we determined (see Figure 3, insert) that Curie temperature of system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ decreases from $T_C = 595$ K for alloy $\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ (i.e. at $x = 0$) to $T_C = 501$ K for $\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ (i.e. at $x = 1$).

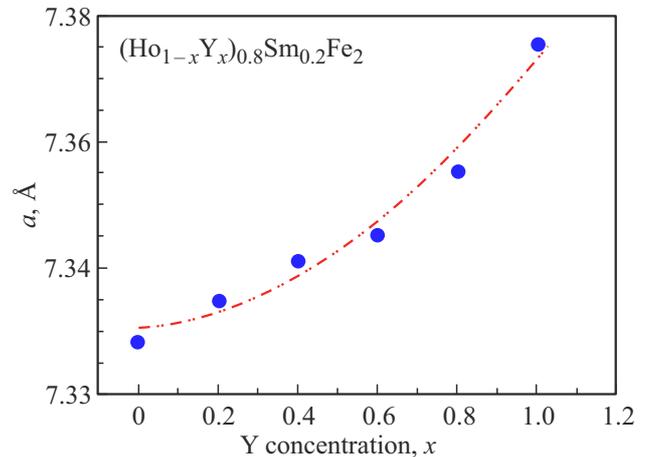


Figure 2. Crystal lattice parameter vs. substitution parameter x in system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

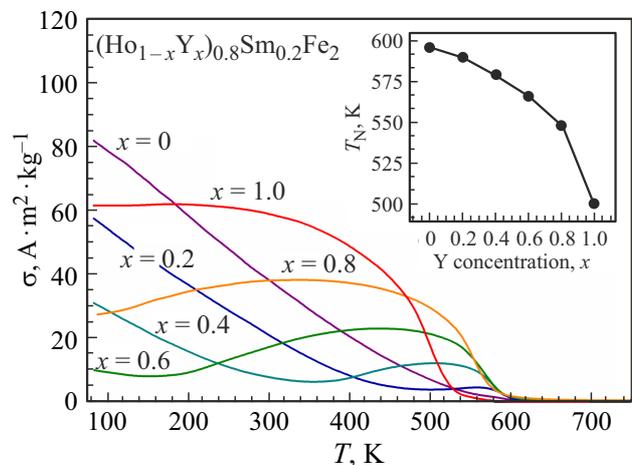


Figure 3. Specific magnetization of system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ vs. temperature in external magnetic field 1 T. Insert: Curie temperature vs. substitution parameter x in system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

So, we see from Figure 3 (Figure 3, insert), that while yttrium concentration increases the Curie temperature of studied alloys steadily decrease, this is explained by magnetic moment absence, and, hence, by absence of magnetic contribution into T_C from yttrium atoms. At the Curie temperature the magnetic phase transformation takes place in alloys — transition of type „order-disorder“. This phase transformation according to Landau theory of phase transition [13] occurs as second-order phase transition. At temperatures above and below T_C the alloys are in para- and ferrimagnetic state, respectively. Only compound $Y_{0.8}Sm_{0.2}Fe_2$ is ferromagnetic with typical form of dependence $\sigma(T)$ (see Figure 3, curve for compound $x = 1.0$). In ferro- and ferrimagnetic state the alloys demonstrate rather high magnetization. For the ferrimagnetics the curves $\sigma(T)$, as a rule, can have more complex form (this is observed in Figure 3), which is associated with feature of behaviour of the temperature dependences of individual magnetic sublattices.

The field dependences of magnetization $\sigma(H)$ were measured at room temperature in magnetic fields below 1 T (Figure 4). By extrapolating the $\sigma(H)$ curves extrapolation to region of high fields we determined values of saturation magnetization σ_s for compounds $(Ho_{1-x}Y_x)_{0.8}Sm_{0.2}Fe_2$. It was identified that the saturation magnetization abruptly decreases from $40.79 \text{ Am}^2/\text{kg}$ for compound $Ho_{0.8}Sm_{0.2}Fe_2$ (i. e. at $x = 0$) to $\sigma_s = 8.38 \text{ Am}^2/\text{kg}$ at values of substitution parameter $x = 0.4$. Then the saturation magnetization again increase to $59 \text{ Am}^2/\text{kg}$ at $x = 1$ for compound $Y_{0.8}Sm_{0.2}Fe_2$. Thus, in the yttrium concentration range $0.4 \leq x \leq 0.5$ we can expect the mutual magnetic compensation of magnetic moments of rare-earth sublattice and Fe sublattice.

It is known that compound at which compensation is observed is called compensation compound. Such composition can be determined using calculations, in particular, under model of collinear magnetic moments.

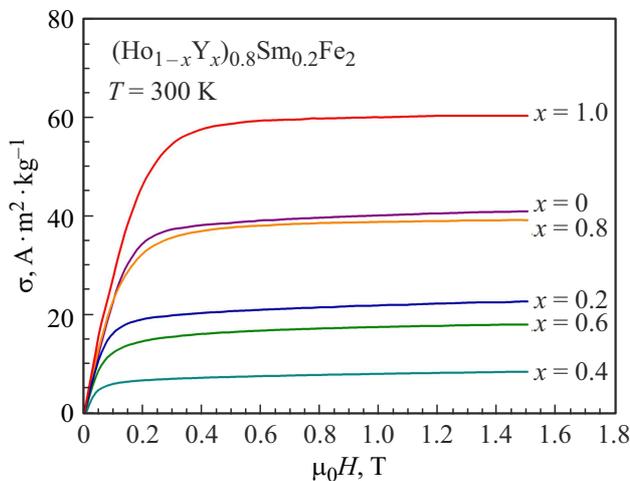


Figure 4. Specific magnetization of system alloys $(Ho_{1-x}Y_x)_{0.8}Sm_{0.2}Fe_2$ vs. external magnetic field at temperature 300 K.

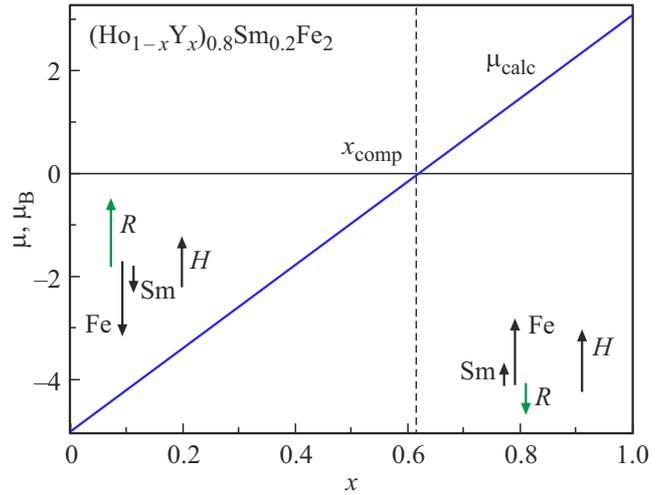


Figure 5. Calculated dependence of complete magnetic moment on yttrium concentration for compounds $(Ho_{1-x}Y_x)_{0.8}Sm_{0.2}Fe_2$.

The made calculations showed that in range of temperatures near the absolute zero the compensation compound is compound with yttrium concentration $x_{comp} = 0.62$ [14]. In our calculations, the full magnetic moment was calculated using the following equation

$$\mu_{calc} = 2\mu_{Fe} + 0.2\mu_{Sm} - 0.8(1 - x)\mu_{Ho}$$

Here $\mu_{Fe} = 1.45 \mu_B/\text{at}$. — magnetic moment of Fe determined from magnetization of compound YFe_2 ; $\mu_{Ho} = 10 \mu_B/\text{at}$. and $\mu_{Sm} = 0.7 \mu_B/\text{at}$.

Remember that signs in the above equation are given considering direction of magnetic moments of iron, holmium and samarium. The total magnetic moment of the compounds under study $(Ho_{1-x}Y_x)_{0.8}Sm_{0.2}Fe_2$ depends linearly on the substitution parameter x (see Figure 5). In range of calculation concentration $x_{comp} = 0.62$ in range of low temperatures there shall be equality of the directed antiparallel magnetic moments of atoms of iron and samarium with magnetic moments of holmium atoms.

Note that some incompliance of the experimentally determined yttrium concentration x , at which mutual compensation of magnetic sublattices of REE and Fe with the theoretically calculated value is observed, also occurred for same system $(Er_{1-x}Y_x)_{0.8}Sm_{0.2}Fe_2$, studied by us [15]. In both cases as per our assumptions said fact can be associated with several factors, including — violation of collinearity of magnetic structure, and different path of temperature dependences of magnetizations of $4f$ - and $3d$ -sublattices.

We performed experimental studies of magnetization in range of low temperatures, they showed that phenomenon of mutual compensation of magnetic sublattices in system $(Ho_{1-x}Y_x)_{0.8}Sm_{0.2}Fe_2$ in region of low temperatures, namely at $T = 85 \text{ K}$, is observe near compound with $x_{comp} = 0.6$, i. e. near yttrium concentration calculated a per theoretical model.

The main magnetic properties of system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ at 85 K

Substitution parameter	Compound	σ_s , emu/g	M_s , $\mu_B/\text{f. u.}$	μ , $\mu_B/\text{at. Fe}$
$x = 0$	$\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$	81.99	4.02	2.01
$x = 0.2$	$\text{Ho}_{0.64}\text{Y}_{0.16}\text{Sm}_{0.2}\text{Fe}_2$	57.56	2.70	1.35
$x = 0.4$	$\text{Ho}_{0.48}\text{Y}_{0.32}\text{Sm}_{0.2}\text{Fe}_2$	31.15	1.39	0.70
$x = 0.6$	$\text{Ho}_{0.32}\text{Y}_{0.48}\text{Sm}_{0.2}\text{Fe}_2$	10.32	0.44	0.22
$x = 0.8$	$\text{Ho}_{0.16}\text{Y}_{0.64}\text{Sm}_{0.2}\text{Fe}_2$	27.8	1.12	0.56
$x = 1$	$\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$	61.55	2.35	1.17

Basic magnetic characteristics of the system alloys obtained at $T = 85$ K are presented in Table.

Important feature of the system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ is dependence of magnetic moment on iron atom μ_{Fe} on yttrium concentration (for $T = 85$ K see Table). In compounds $R\text{Fe}_2$ and substitution alloys on their basis it is accepted that magnetic moment on Fe atom is practically constant (within experiment error) and equal to $\mu_{\text{Fe}} = 1.45 \mu_B$, like in ferromagnetic compound YFe_2 [12].

Calculations of the magnetic moment on Fe atom conducted using the saturation magnetization μ_s determined from experiment showed that μ_{Fe} for alloys of the system under study varies and depends on the yttrium content in REE sublattice. In initial compound $\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ ($x = 0$) the experimentally determined value μ_{Fe} is $1.00 \cdot \mu_B$ at room and $2.01 \cdot \mu_B$ at nitrogen temperatures, respectively. During complete substitution of Ho atoms by Y atoms (alloy $\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$) the magnetic moment $\mu_{\text{Fe}} = 1.13 \cdot \mu_B$ and $1.17 \cdot \mu_B$ at same temperatures, respectively.

So, it is determined that value μ_{Fe} in system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ is below value in binary YFe_2 and depends on yttrium content in REE sublattice. Therefore, we studied the Mössbauer effect and found hyperfine magnetic fields indirectly associated with magnetic moments of Fe atoms [16,17].

Mössbauer spectra on ^{57}Fe nuclei in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, obtained at room temperature (Figure 6), were analyzed within the tensor description of magnetic hyperfine interactions [18,19]. Spectra were processed in the SpectrRelax software [8,9] using techniques based on model fitting of spectra „Laves“ described in detail in papers [20,21]. The model consists of four Zeeman sextets with hyperfine parameters whose bonds consider the local magnetic inhomogeneity of Fe atom sites in compounds of type $R\text{Fe}_2$ with collinear magnetic and cubic (sp.gr. $\text{Fd}\bar{3}\text{m}$) atomic structures and are based on relationships (19)–(30), given in Ref. [20].

As a result of this model application in the process of minimizing the chi-square functional, it is possible to find the optimal values of the physical quantities of interest to us: the isomer shift δ , quadrupole coupling constants

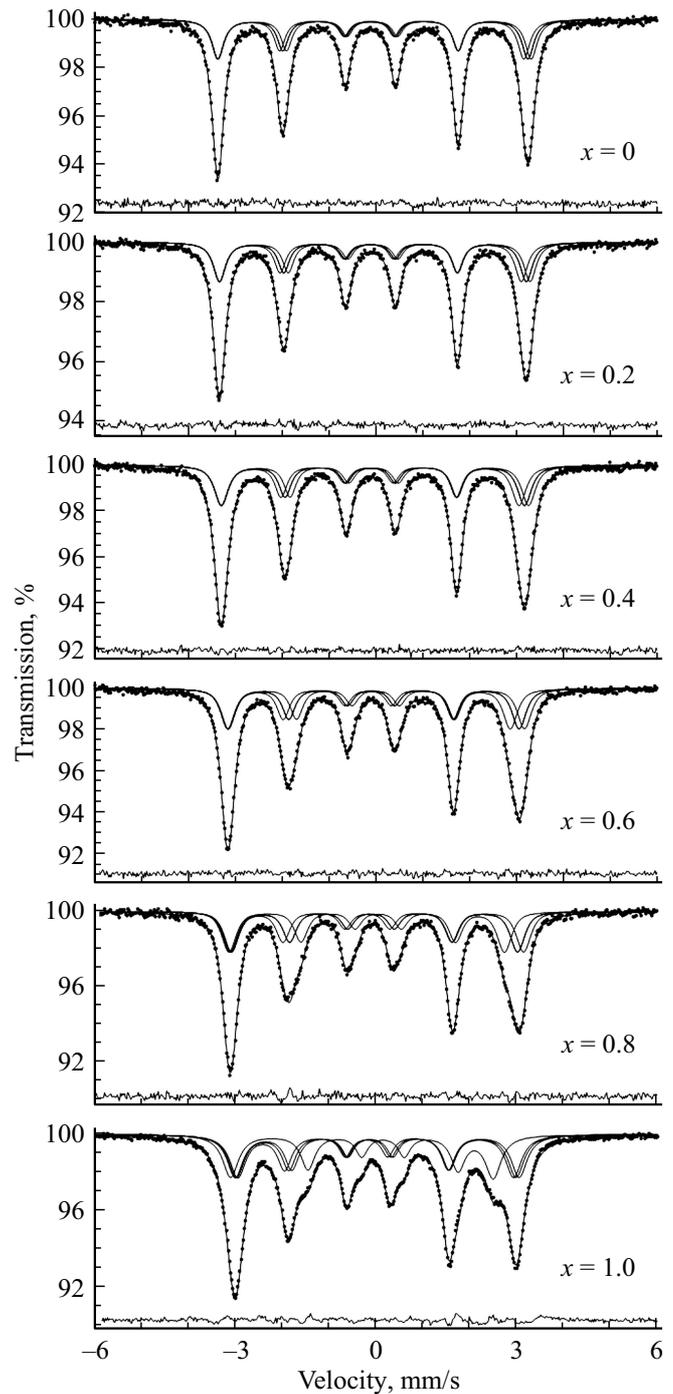


Figure 6. Model interpretation of spectra of ^{57}Fe nuclei in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

e^2qQ of isotropic H_{is} and anisotropic H_{an} magnetic fields, azimuthal φ and polar ϑ angles specifying orientation of easy magnetic axis (EMA) relative to crystallographic axes.

Figure 6 shows that use of „Laves“ model provides good description of the obtained ^{57}Fe nuclei spectra of alloys system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

Dependence of the spectrum shift δ on Y atom concentration obtained by means of model interpretation is

shown in Figure 7. It is shown that the δ , that is equal to the sum of the isomer shift due to the electron density in the nucleus and of the temperature shift due to the dynamic properties of nucleus, increases almost linearly with Y concentration. The observed increase in the shift by 0.023(6) mm/s with full substitution of Ho atoms by Y atoms (Figure 7) is primarily associated with increase in the isomer shift due to the decrease in the electronic density on the nucleus with increase in the lattice parameter (see Figure 2) and, therefore, in the interatomic distance with Ho atoms substitution by Y atoms.

Figure 8 presents behavior of quadrupole coupling constant e^2qQ in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ upon substitution of Ho atoms by Y atoms according to value of substitution parameter x . Figure 8 shows that in this alloys system value (absolute value) of quadrupole coupling constant remains practically unchanged with some oscillations within range (1.0–1.1) mm/s.

In system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ Ho atoms substitution by Y atoms the decrease by 21.4(4) kOe in

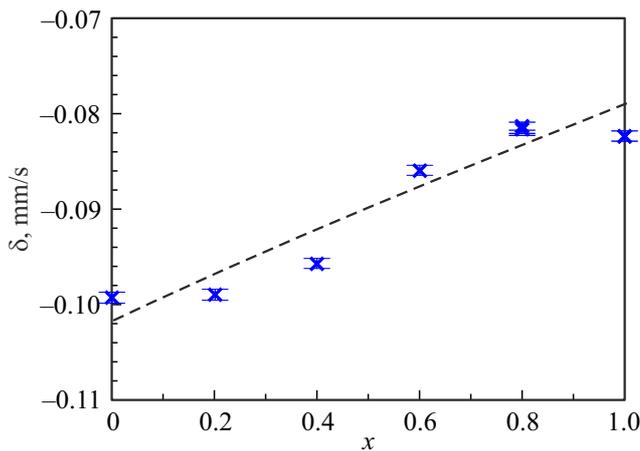


Figure 7. Spectrum shift δ of ^{57}Fe nuclei depending on Y concentration in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

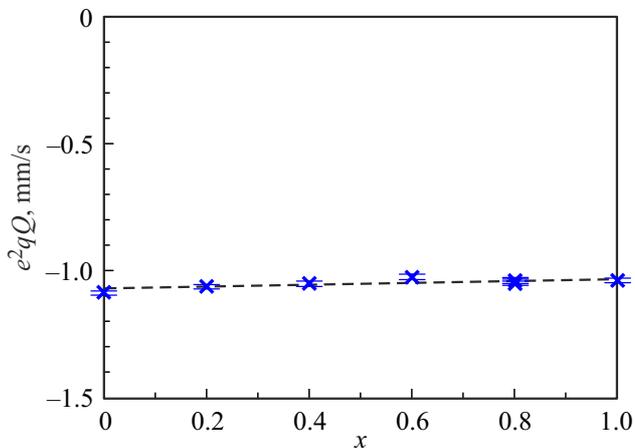


Figure 8. Quadrupole coupling constant e^2qQ of ^{57}Fe nuclei vs. Y concentration in the system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

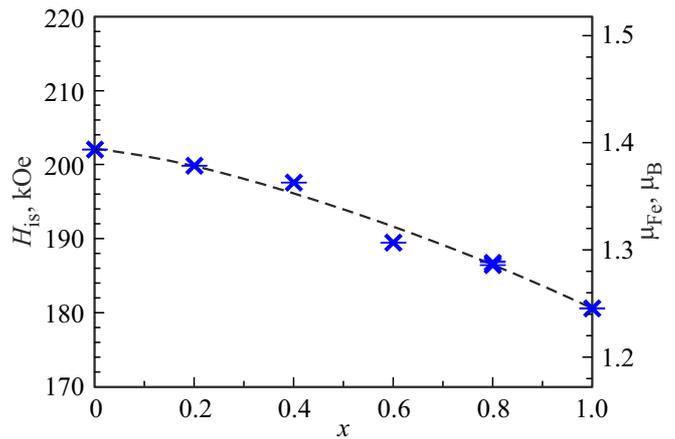


Figure 9. Isotropic field H_{is} on ^{57}Fe nuclei and magnetic moment μ_{Fe} of Fe atom depending on Y concentration in system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

the isotropic magnetic field in region of nucleus location (Figure 9) is observed. According to the density of state calculation of the rare-earth Laves phases $R\text{Fe}_2$ [22,23] the hybridization of $3d-5d$ electron shells in the positive local $4f-5d$ interaction results in increase in Fe ion spin (and magnetic moment) with increase in the rare earth spin. Such increase in the Fe ion spin, in turn, results in increase in the main contribution into the isotropic field — Fermi contribution H_{Fermi} . According to the theoretical calculations [24], the Fermi contribution into the isotropic field depend linear on the magnetic moment of $3d$ -shell of iron atom. For crystalline and amorphous rare earth — iron alloys, the aspect ratio between the hyperfine magnetic field strength and magnetic moment of iron atom equal to 145 kOe/ μ_B is commonly used [16,17]. Using the isotropic field data, the magnetic moment of iron atom in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ may be estimated at room temperature. For this, in Figure 9, besides the y axis for the isotropic field, an axis for magnetic moment of Fe atoms is provided. It can be seen that values μ_{Fe} , obtained from value H_{is} , are somewhat higher the values obtained by the magnetometer method, like system $(\text{Dy}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ [25].

For anisotropic hyperfine magnetic field H_{an} , dependence on Y concentration similar to that of the isotropic field H_{is} is observed: anisotropic field strength (absolute value) decreases by 4.9(4) kOe when Ho atoms are substituted by Y atoms (Figure 10). According to [26,27], contribution into the anisotropic field due to the conduction electrons, polarized by magnetic dipole field of the localized magnetic moments of atoms, has the same sign as the dipole-dipole contribution.

Both contributions to the anisotropic field, either dipole-dipole contribution from the localized magnetic moment of the lattice atoms or the contribution from the conduction electrons, decrease with Ho atoms substitution by Y atoms,

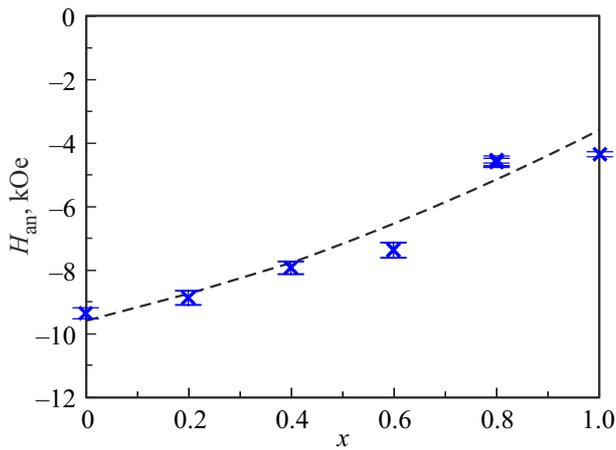


Figure 10. Anisotropic field H_{an} on ^{57}Fe nuclei in system alloys depending on Y concentration in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

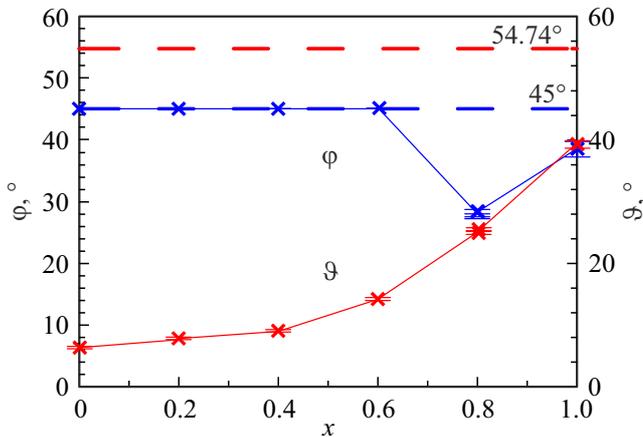


Figure 11. Azimuthal φ and polar θ angles, specifying orientation of easy magnetic axis relative to crystallographic axes vs. Y concentration in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$.

because the mean magnetic moment of rare-earth atoms decreases and the interatomic distance increases.

Interpretation of spectra of the system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ in the „Laves“ model allowed the EMA orientation to be defined depending on the degree of Ho atoms substitution by Y atoms (Figure 11). The spectra processing showed that until yttrium concentration $x = 0.6$ the azimuthal angle $\varphi = 45^\circ$, i.e. EMA lies in plane $(1\bar{1}0)$, at that with increase in concentration x the polar angle θ (angle between EMA and direction $[001]$) increases from $6.3 \pm 0.2^\circ$ at $x = 0$ to $14.2 \pm 0.3^\circ$ at $x = 0.6$. At concentration $x = 0.8$ there is abrupt EMA exit from plane $(1\bar{1}0)$ — azimuthal angle φ decreases to $27.9 \pm 0.7^\circ$, at that the polar angle θ continues its increasing and becomes equal to $24.9 \pm 0.5^\circ$. For last compound $\text{Ho}_{0.2}\text{Y}_{0.8}\text{Fe}_2$ ($x = 1$) the polar angle θ is more larger ($39.4 \pm 0.7^\circ$), and azimuthal angle φ , equal to

$38.6 \pm 1.4^\circ$, indicates that EMA stays beyond the plane $(1\bar{1}0)$.

So, at room temperature EMA does not coincide with crystallographic directions in the crystal. Such deviations of the EMA orientation from the crystallographic directions at room temperature were observed in RFe_2 in Refs. [27–29].

4. Conclusion

The findings show that yttrium introduced into the rare-earth sublattice of system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, significant effects the basic magnetic characteristics and parameters of hyperfine interaction. The substitution parameter x increasing leads to an increase in the lattice parameter, and, hence, interatomic distances, this is frequently accompanied by competition of intersublattice exchange interactions in pairs Ho-Fe and Sm-Fe. Considering the change in the interatomic distances in the rare earth sublattice, we obtain the system with competing exchange interactions, both intersublattice and intrasublattice. This in turn causes phenomena, such as decrease in the Curie temperature of alloys (from $T_C = 587\text{ K}$ in compound $\text{Ho}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ to $T_C = 501\text{ K}$ for $\text{Y}_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ with increase in Y concentration). Additionally, there is mutual compensation of magnetic moments of rare-earth and $3d$ -sublattices at yttrium concentration $x = 0.6$. This can also include the dependence of magnetic moment on Fe atoms (μ_{Fe}) on the value of the substitution parameter x in multi-component system $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, in contrast to the generally accepted concept that (μ_{Fe}) keeps its value in the RFe_2 stoichiometry.

The model interpretation of Mössbauer spectra of system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ showed that the isomer shift δ increases almost linearly with the concentration of Y atoms. The observed increase in the isomeric shift by $0.023(6)\text{ mm/s}$ with complete Ho atoms substitution by Y atoms is primarily due to the decrease in the electronic density on the nucleus with increase in the lattice cell parameter, therefore, in the interatomic distance (similar to systems with Tb, Ho and Er).

The quadrupole coupling constant e^2qQ of ^{57}Fe nuclei with electric field gradient tensor, provided by localized charges of ions and Basic magnetic characteristics by polarized conductivity electrons in system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$, practically does not change upon Ho atoms substitution by Y and is equal in absolute value to $1.05(4)\text{ mm/s}$.

In system alloys $(\text{Ho}_{1-x}\text{Y}_x)_{0.8}\text{Sm}_{0.2}\text{Fe}_2$ upon Ho atoms substitution by Y atoms there is a decrease in both the isotropic magnetic field H_{is} and the anisotropic magnetic field H_{an} (H_{is} decreases by $21.4(4)\text{ kOe}$, and H_{an} decreases in magnitude by $4.9(4)\text{ kOe}$).

Azimuthal φ and polar θ angles specifying orientation of easy magnetic axis relative to crystallographic axes are determined, and their dependence on Y concentration is determined. It is shown that in this alloys system

EMA direction does not coincide with the crystallographic direction in any of system alloys.

This study will facilitate creation of new multi-component alloys with optimal physical and chemical parameters for various applications.

Acknowledgments

The authors thank the Lomonosov Moscow State University for upgrading the scientific research equipment used in the study and the Magnetic Materials Laboratory of the the Center for Collective Use of Tver State University of the Tver State University for conducting the synthesis and magnetization studies of the alloys of this system.

Funding

This study was supported by grant provided by the Russian Science Foundation No. 22-22-00313, <https://rscf.ru/project/22-22-00313/>

Conflict of interest

The authors declare that they have no conflict of interest.

References

- [1] A.S. Ilyushin, I.S. Tereshina, N.Yu. Pankratov, T.A. Aleroeva, Z.S. Umkhaeva, A.Yu. Karpenkov, T.Yu. Kiseleva, S.A. Granovsky, M. Doerr, H. Drulis, E.A. Tereshina-Chitrova. *J. Alloys and Compounds* **847**, 155976 (2020).
- [2] Z.S. Umkhaeva, A.S. Ilyushin, T.A. Aleroeva, T.V. Kiseleva, I.S. Tereshina. *Journal of Physics: Conference Series* **1753**, 012079 (2021).
- [3] Z.S. Umkhaeva, I.S. Tereshina, N.Yu. Pankratov, I.M. Aliev, M.R. Khomenko, A.Yu. Karpenkov. *Crystallogr. Rep.*, **68**, 3, 446 (2023).
- [4] N.Yu. Pankratov, A.Yu. Karpenkov, V.S. Rusakov, T.V. Gubaidulina, Z.S. Umkhaeva, I.S. Tereshina. *Journal of Magnetism and Magnetic Materials* **595**, 171643 (2024).
- [5] A.S. Ilyushin. *Vvedenie v sructurnuyu fiziku intermetallicheskih soedinenij*. MGU, M. (1984), 99 p. (in Russian).
- [6] K.A. Gschneidner, L. Eyring. *Handbook on the Physics and Chemistry of Rare Earths*, Elsevier, Vol. 1:Metals (1978), 894 p.
- [7] K.P. Belov. *Magnetostriction Phenomena and Their Technical Application*, Nauka, M. (1987), 159 p. (in Russian).
- [8] M.E. Matsnev, V.S. Rusakov. *AIP Conference Proceedings* **1489**, 178 (2012).
- [9] M.E. Matsnev, V.S. Rusakov. *AIP Conference Proceedings* **1622**, 40 (2014).
- [10] T.A. Aleroeva, I.S. Tereshina, Z.S. Umkhaeva, T.P. Kaminskaya, A.V. Filimonov, A.S. Ilyushin. *FTT* **61**, 12, 2471 (2019). (in Russian).
- [11] Z.S. Umkhaeva, I.S. Tereshina, I.M. Aliev, A.Yu. Karpenkov, Z.Sh. Gatsaev. *Vestnik KNII RAN. Seriya „Estestvennye i tekhnicheskie nauki“* **2**, 101 (2022). (in Russian).
- [12] K.N.R. Taylor, M.I. Darby. *Physics of rare earth solids*. Chapman and Hall: London (1972). 308 P.
- [13] K.P. Belov. *Magnitnye prevrascheniya*. Fizmatgiz, M. (1959). 259 P. (in Russian).
- [14] Z.S. Umkhaeva, I.S. Tereshina, N.Yu. Pankratov, I.M. Aliev, F.S.A. Said-Akhmatova. *Izvestiya ChGU* **2**, 7 (2022). (in Russian).
- [15] Z.S. Umkhaeva, A.Yu. Karpenkov, I.S. Tereshina, N.Yu. Pankratov, I.M. Aliev. *Bulletin of the Russian Academy of Sciences: Physics* **88**, 5, 779 (2024).
- [16] J. Chappert, J.M.D. Coey, A. Lienard, J.P. Rebouilliat. *J. Phys. F: Metal Phys.* **11**, 2727 (1981).
- [17] K.H.J. Buschow, Van der A.M. Kraan. *J. Magn. Magn. Mater.* **22**, 220 (1981).
- [18] V.I. Nikolaev, V.S. Rusakov, T.B. Solodchenkova. *Izv. AN SSSR. Ser. Fizicheskaya* **54**, 9, 1681 (1990). (in Russian).
- [19] V.S. Rusakov. *Messbauerovskaya spektroskopiya lokalno neodnorodnykh sistem*. Almaty: IYaF NYaTs RK. (2000). 431 s. (in Russian).
- [20] V.S. Rusakov, V.S. Pokatilov, T.V. Gubaidulina, M.E. Matsnev. *Phys. Metals Metallogr.* **120**, 4, 339 (2019).
- [21] M.E. Matsnev, V.S. Rusakov. *Phys. Met. Metall.* **124**, 3, 279 (2023).
- [22] M.S.S. Brooks, O. Eriksson, B. Johansson. *J. Phys.: Cond. Matter* **1**, 5861 (1989).
- [23] M.S.S. Brooks, L. Nordstrom, B. Johansson. *J. Appl. Phys.* **69**, 8, 5683 (1991).
- [24] R.E. Watson, A.J. Freeman. *Phys. Rev.* **123**, 2027 (1961).
- [25] Z.S. Umkhaeva, V.S. Rusakov, T.V. Gubaidulina, A.Yu. Karpenkov, I.S. Tereshina, N.Yu. Pankratov, I.M. Aliev. *Phys. Solid State* **66**, 1, 94 (2024). (in Russian).
- [26] U. Atzmony, M.P. Dariel. *Phys. Rev. B.* **10**, 5, 2060 (1973).
- [27] P. Ray, S.K. Kulshreshtha. *J. Physique* **41**, 12, 1487 (1980).
- [28] C. Meyer, F. Hartmann-Boutron, Y. Gros, Y. Berthier. *J. Physique* **42**, 4, 605 (1981).
- [29] E.R. Bauminger, H.T. Savage. *J. Appl. Phys.* **52**, 3, 2055 (1981).

Translated by I.Mazurov