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LATTICE EFG TENSORS AT THE RARE-EARTH METAL SITES IN $RBa_2Cu_3O_7$

Parameters of the tensors of the electric field gradient (EFG) created by lattice ions at the rare-earth metal (REM) sites in $RBa_2Cu_3O_7$ (R is Pr, Nd, Sm, Eu, Gd, Dy, Y, Tm or Yb) have been determined by means of $^{155}Eu(^{155}Gd)$ emission Mossbauer spectroscopy. The EFG tensors at the REM sites have been calculated in the point charge approximation. The experimental and calculated EFGs are shown to be in good agreement when holes are supposed to be mainly in sublattices of the chain oxygen for $RBa_2Cu_3O_7$. It is shown that the anomalous behavior of the compound $PrBa_2Cu_3O_7$ is caused by antistructural substitution of Pr^{3+} for Ba^{2+} at its orthorhombic lattice.

Keywords: Mossbauer spectroscopy, the electric field gradient.

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ТЕНЗОР КРИСТАЛЛИЧЕСКОГО ГЭП В УЗЛАХ РЕДКОЗЕМЕЛЬНЫХ МЕТАЛЛОВ В РЕШЕТКАХ $RBa_2Cu_3O_7$

Параметры тензора градиента электрического поля (ГЭП), создаваемого ионами кристаллической решетки в узлах редкоземельных металлов (РЗМ) в $RBa_2Cu_3O_7$ (R = Pr, Nd, Sm, Eu, Gd, Dy, Y, Tm или Yb), были определены методом эмиссионной мессбауэровской спектроскопии на изотопе $^{155}Eu(^{155}Gd)$. Тензор ГЭП в узлах РЗМ был рассчитан в приближении точечных зарядов. Экспериментальные и рассчитанные значения ГЭП находятся в хорошем согласии, если предположить, что дырки, как правило, находятся в подрешетке цепочечного кислорода решеток $RBa_2Cu_3O_7$. Показано, что аномальное поведение соединения $PrBa_2Cu_3O_7$ объясняется антиструктурным замещением Pr^{3+} на Ba^{2+} в его орторомбической решетке.

Ключевые слова: мессбауэровская спектроскопия, градиент электрического поля.

1. Introduction

The spatial distribution of charges among sites in ionic lattices can be determined comparing the experimental and calculated parameters of the electric field gradient (EFG) tensors [9]. Generally, the U_{pp} components of the diagonalized EFG tensor at a nucleus consist of two parts

$$eQU_{pp} = eQ(1 - \gamma)\, V_{pp} + eQ(1 - R_0)\, W_{pp}\,, \qquad (1)$$

where V_{pp} and W_{pp} are tensor components of the EFG created by lattice ions (lattice EFG) and by valence electrons related to the nucleus (valence EFG), respectively; γ and R_0 are the Sternheimer coefficients, p is the Cartesian coordinate.

The lattice EFG may be calculated using the point charge model, whereas the valence EFG is given by various quantum-mechanical methods [9]. The validity of the results of the latter might evoke some doubt, and, therefore, probe atoms with spherical electron shells, i.e. without valence contribution to equation (1), are preferable for measuring of EFG. The ^{67}Cu(^{67}Zn) emission Mossbauer spectroscopy was suggested as the technique for the experimental determination of the EFG tensor at the copper-based high-temperature superconductors (HTSCs) [1 - 4, 7]. In this technique a Zn^{2+} ion with a spherical $3d^{10}$ electron shell, and thus without valence EFG, appears at a copper site after the decay of the parent ^{67}Cu nucleus [9].

The above described technique allowed us to find the effective charges of oxygen ions for $YBa_2Cu_3O_7$ with certain assumptions made for the cation charges [5, 7]. The agreement between the calculated and experimental parameters of the lattice EFG tensors for $YBa_2Cu_3O_7$ may be achieved using two kinds of models. Both imply the presence of a hole in the immediate vicinity of the chain copper, either at the chain oxygen (model *A*) or at the bridging (apical) oxygen (model *B*). Additional evidence is necessary to choose the model. The present work proposes ^{155}Eu(^{155}Gd) emission Mossbauer spectroscopy as a source of the necessary additional evidence for $RBa_2Cu_3O_7$ compounds (R is a rare-earth metal (REM) or Y).

2. Experimental details

The principle of the used technique consists in extraction of a carrier-free preparation of the ^{155}Eu parent activity followed by synthesis of ^{155}Eu-doped ceramic samples and by ^{155}Eu (^{l55}Gd) emission Mossbauer spectra recording. ^{155}Eu has been considered to occupy the REM sites in the substances mentioned above. It is supported by the chemical similarity of all rare-earth metals. Therefore, the ^{155}Gd Mossbauer probe produced after the decay of ^{155}Eu should also reside at a regular REM site [6, 8]. The carrier-free ^{155}Eu preparation allows low Mossbauer impurity concentrations and enables one to use structural data for undoped $RBa_2Cu_3O_7$ to analyze the results.

Typical for the Gd^{3+} ion is the $^6S_{7/2}$ state with a half-filled spherical $4f^7$ shell. Due to this reason the EFG at ^{155}Gd nuclei is expected to be created only by lattice ions.

The ^{l55}Eu activity was produced by the ^{154}Sm(n, γ)^{155}Sm reaction followed by β decay of ^{155}Sm. The carrier-free ^{155}Eu preparation was separated chromatographically, since the half-lives of ^{155}Eu and the intermediate nucleus ^{155}Sm are 4.96 years and 23 min, respectively. The separation was carried out in six months after the reactor irradiation for the decay of the residual activity of ^{156}Eu with a half-life of 15 d.

Ceramic samples of $RBa_2Cu_3O_7$ (R is Pr, Nd, Sm, Eu, Gd, Dy, Y, Yb or Tm) were prepared sintering the corresponding oxides. The ^{155}Eu activity was added to the starting mixture. Test samples of $RBa_2Cu_3O_7$ had an orthorhombic structure and critical temperatures T_c of about 85 K.

The Mossbauer spectra (86.5 keV transition) were recorded at 80 K using a singlet $GdPd_3$ absorber. The 86.5 keV radiation was detected by a NaI(Tl) detector with a Pb critical filter that

suppressed the 60 keV and 105 keV radiation of ^{155}Eu and the rest of the 89 keV radiation of ^{155}Eu. For this reason the ^{155}Gd 86.5 keV spectra were recorded predominantly. The ^{155}Gd 105 keV spectra were additionally suppressed due to the high measuring temperature. The ^{155}Gd 60 keV spectra were not observed in the velocity range used because of their large line width of about 30 mm/s.

Typical spectra are shown in figures 1. The results of the processing of the spectra are shown in figures 2.

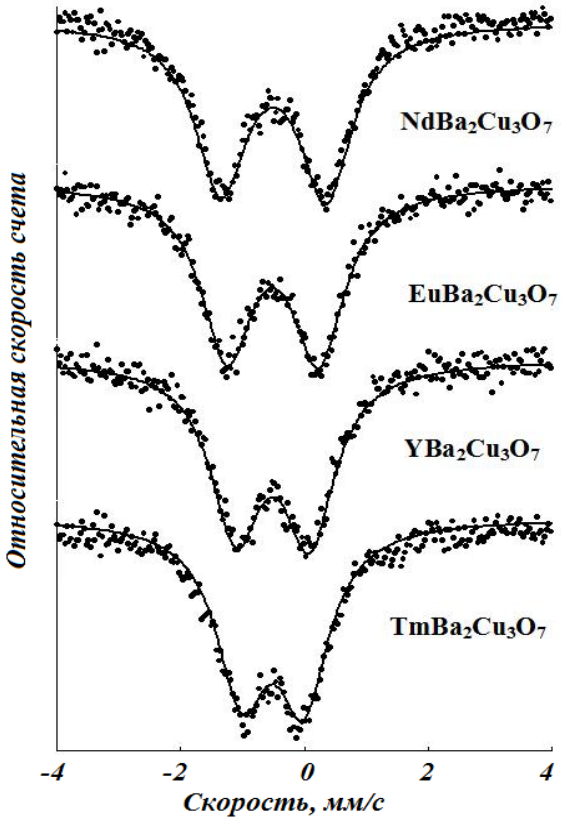

Fig. 1. ^{155}Eu(^{155}Gd) emission Mossbauer spectra of $RBa_2Cu_3O_7$

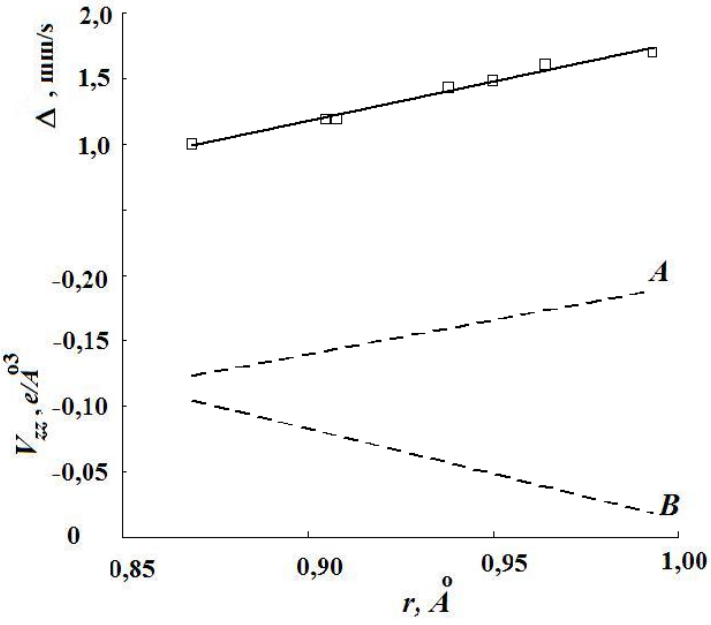

Fig. 2. Dependence of the quadrupole splitting Δ of the $RBa_2Cu_3O_7$:^{155}Eu Mossbauer spectra on the rare-earth ion radius r and dependences of the calculated principal components V_{zz} of the lattice EFG tensors at the REM sites of the $RBa_2Cu_3O_7$ compounds on r for models A and B.

3. Experimental results and discussion

3.1. $RBa_2Cu_3O_7$ (R is Nd, Sm, Eu, Gd, Dy, Y, Tm or Yb) compounds

The emission Mossbauer spectra of the $RBa_2Cu_3O_7$:^{155}Eu samples are quadrupole doublets. It points to a non-cubic environment of the REM sites. The isomer shifts of all spectra correspond to Gd^{3+}. The fact that the quadrupole splitting Δ increases with increasing radius *r* of the REM ion (see figure 2) is important to mention. The quadrapole splitting of the ^{155}Gd Mossbauer spectra is determined by the ground state of the nucleus (spin $I = 3/2$, quadrupole moment $Q = 1.59$ b) and is described by the equation:

$$\Delta = \frac{1}{2}\left|eQU_{zz}\right|\left(1+\frac{\eta^2}{3}\right)^{1/2}, \qquad (2)$$

where U_{zz} is the principal component of the total EFG tensor at the ^{155}Gd nucleus; $\eta = (U_{xx} - U_{yy})/U_{zz}$ is the asymmetry parameter of the total EFG tensor. For the tensor components the inequality $|U_{xx}| \le |U_{yy}| \le |U_{zz}|$ should be valid.

Thus, the value of Δ is proportional to $|U_{zz}|$ which is determined by the lattice EFG for the Gd^{3+} probe

$$U_{zz} \approx (1-\gamma)\, V_{zz}, \qquad (3)$$

where V_{zz} and γ relate to the REM sites and Gd^{3+} ion, respectively.

We have calculated the lattice EFG tensor components V_{pp} for all sites of the $RBa_2Cu_3O_7$ lattices using the point charge approximation. The lattice was considered as a superposition of eight sublattices according to the structural formula $RBa_2Cu(1)Cu(2)_2O(1)_2O(2)_2O(3)_2O(4)$. Since various versions of oxygen site numbering are accepted in the literature, our designations are shown in figure 3. The structural parameters used in calculation of the lattice EFG for the $RBa_2Cu_3O_7$ compounds were taken from [10]. All the calculated EFG tensors proved to be diagonal in the crystal axes.

Previously [11] we used the results of the lattice EFG calculations for the Cu(1), Cu(2), O(1), O(2) and O(4) sites in $YBa_2Cu_3O_7$ as well as the parameters of the quadrupole coupling tensors for ^{67}Zn at the copper sites and for ^{17}O at the oxygen sites to determine the charge distribution among the sites for both A and B models

$$R^{3+}Ba_2^{2.05+}Cu(1)^{2.16+}Cu(2)_2^{2.15+}O(1)_2^{2.17-}O(2)_2^{2.01-}O(3)_2^{1.90-}O(4)^{1.38-}, \qquad (A)$$

$$R^{3+}Ba_2^{3.25+}Cu(1)^{1.32+}Cu(2)_2^{1.48+}O(1)_2^{1.49-}O(2)_2^{2.02-}O(3)_2^{1.90-}O(4)^{2.98-}. \qquad (B)$$

Then the lattice EFG tensors were calculated at the REM sites using both charge distributions. Figure 2 shows the slopes of the calculated $V_{zz}(r)$ dependences having opposite signs for models *A* and *B*. The *z*-axes of the calculated EFG tensors are also different for different models. The *z*-axis coincides with the crystal axes *c* and *a* for models *A* and *B*, respectively. Unfortunately, our ^{155}Eu(^{155}Gd) data for ceramic samples are insensitive to the direction of the *z*-axis. A qualitative agreement between, the measured $\Delta(r)$ dependence and the calculated $V_{zz}(r)$ one is found only for model *A*. Thus, the ^{155}Eu(^{155}Gd) emission Mossbauer data support model A for the $RBa_2Cu_3O_7$ compounds.

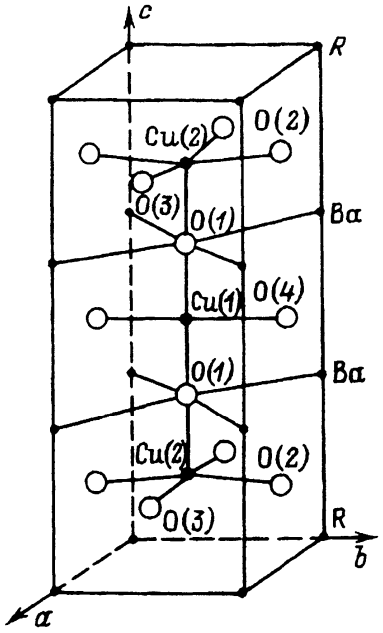

Fig. 3. The unit cells of $RBa_2Cu_3O_7$

However, this conclusion is valid only if the EFG at the Gd^{3+} probe nuclei is created solely by the lattice ions. To examine this condition we have plotted the dependence of Δ on $\Delta_{cr} = \frac{1}{2} V_{zz} \left(1 + \frac{\eta_{cr}^2}{3} \right)^{1/2}$, where $\eta_{cr} = \frac{V_{xx} - V_{yy}}{V_{zz}}$ η_{cr} is the asymmetry parameter. Figure 4 shows that for model *A* this dependence is satisfactorily described by a straight line. An extrapolation of the latter to $\Delta_{cr} = 0$ gives the value $\Delta_0 = -(0.09 \pm 0.02)$ mm/s. Compared with the experimental values of Δ this value is small. Therefore, in figure 4 the dependence could be considered as an approximately direct proportionality.

The quadrupole splitting of the ^{155}Gd Mossbauer spectra is described by the following equation derived from equations (1) and (2)

$$\Delta = \frac{1}{2} \left| eQ \right| \left| (1-\gamma) V_{zz} + (1-R_0) W_{zz} \right| \left(1 + \frac{\eta^2}{3} \right)^{1/2}, \qquad (4)$$

where $\eta = \frac{(1-\gamma) V_{zz} \eta_{cr} + (1-R_0) W_{zz} \eta_{val}}{(1-\gamma) V_{zz} + (1-R_0) W_{zz}}$.

Here, γ and R_0 are the Sternheimer coefficients for Gd^{3+}, η_{val} is the asymmetry parameter of the valence EFG tensor. From equation (4) it can be seen that the direct proportionality in figure 4 gives evidence of the small valence EFG at the ^{155}Gd nuclei. The valence contribution $eQ(1 - R_0)W_{zz} > 0$, since $V_{zz} < 0$ and $\Delta_0 < 0$. Its magnitude can be estimated by the quantity $|\Delta_0/eQ| = 0.13 \pm 0.10$ e×Å^{-3}. The slope of the straight line in figure 4 corresponds to the Sternheimer coefficient for the Gd^{3+} ion $\gamma = -(24 \pm 2)$, which gives the values of the lattice contribution $(1-\gamma)$ V_{zz} in the range from −2.45 to − 4.60 e×Å^{-3} for the investigated compounds $RBa_2Cu_3O_7$. It should be mentioned that the value $\gamma = -24$ is only a rough estimation. For instance, it is considerably less than the value $\gamma = -60.87$ resulted from quantum-mechanical calculations [9].

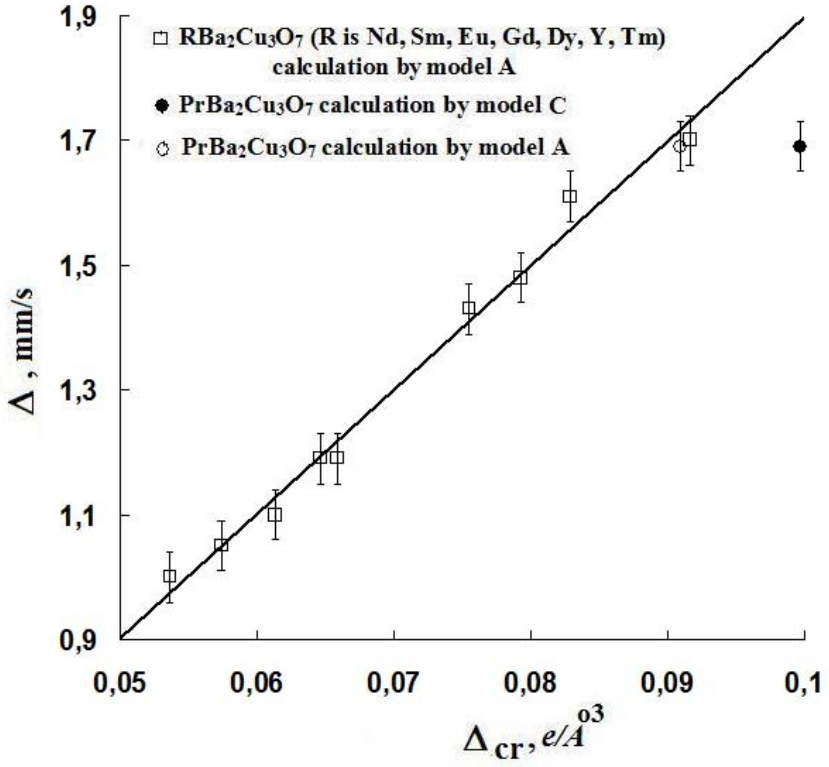

Fig. 4. Dependence of the quadrupole splitting Δ of the $RBa_2Cu_3O_7$: ^{155}Eu Mossbauer spectra on the parameters of the calculated lattice EFG tensor Δ_{cr} at the REM sites. The experimental data of $PrBa_2Cu_3O_7$ were taken from Ref. 11

3.2. Charge distribution in the $PrBa_2Cu_3O_7$ lattice

$RBa_2Cu_3O_7$ compounds (R is a rare-earth metal or yttrium) with the perovskite structure are superconductors with a transition temperature $T_c \sim 90$ *K*. An exception to the rule is $PrBa_2Cu_3O_7$, and its anomalous behavior is connected either with Pr being tetravalent, or with partial mutual substitution of the Pr^{3+} and Ba^{2+} ions. $^{155}Cu(^{155}Gd)$ Mossbauer emission spectroscopy data obtained by us for the $R_{1-x}Eu_xBa_2Cu_3O_7$ solid solutions (R is Nd, Sm, Eu, Gd, Dy, Y, Tm or Yb, with $x < 10^{-3}$) and ^{155}Gd Mossbauer absorption measurements made for $GdBa_2Cu_3O_7$ (Ref. 12) and for gadolinium impurity atoms in Pr sites of the $PrBa_2Cu_3O_7$ orthorhombic lattice [10] permit one to decide between these two models.

The crystal-field EFG tensor can be calculated in the point charge approximation using the lattice constants *a, b*, *c*, and the coordinates of atomic planes in the unit cell [*z*(Ba), *z*(Cu2), *z*(O1), *z*(O2, O3)] which are known. Such data are available for $RBa_2Cu_3O_7$ compounds [10] (R = Tm, Y, Dy, Gd, Eu, Sm, Nd) with the orthorhombic structure, while for orthorhombic $PrBa_2Cu_3O_7$ only lattice constants are known [6]. To determine the atomic coordinates in the orthorhombic cell of $PrBa_2Cu_3O_7$, we assumed a linear relation between the atomic-plane coordinates and the ionic radius of R^{3+} ions. This assumption is supported by the fact that extrapolation of the dependences of the parameters *a, b,* and *c* on *r* to the ionic radius of Pr^{3+} (r = 1.013 Å) yields a = 3.870 Å, b = 3.916 Å, and c = 11.75 Å, that is in excellent agreement with the values [6] a = 3.874 Å, b = 3.912 Å, and c = 11.74 Å (Fig. 5). We treated the data [10] on atomic-plane coor-

dinates by the least-squares technique and extrapolated the straight lines thus constructed to the ionic radius of Pr^{3+} to obtain for the $PrBa_2Cu_3O_7$ lattice z(Ba) = 0.1831, z(Cu2) = 0.3511, z(O1) = 0.156, and z(O2, O3) = 0.371 (Fig. 5).

Necessary for calculation of the crystal-field EFG tensor the charge distribution over the lattice sites in $RBa_2Cu_3O_7$ was taken (A). Figure 4 presents the dependence of the experimental value of Δ^{exp} on the calculated value of $\Delta_{lat} = V_{zz}(1 + \eta^2/3)^{1/2}$ for $RBa_2Cu_3O_7$ compounds (R = Tm, Dy, Y, Gd, Eu, Sm, Nd). This dependence is described by the straight line, as expected for the $^{155}Gd^{3+}$ probe, which feels only the EFG generated by lattice ions. Only the corresponding to $PrBa_2Cu_3O_7$ point falls off of the linear relationship.

We have calculated the crystal-field EFG tensor at Pr sites of the $PrBa_2Cu_3O_7$ lattice for the model assuming partial mutual substitution of the Pr^{3+} and Ba^{2+} ions:

$$\left[\mathrm{Pr}_{0.9}^{3+}\,\mathrm{Ba}_{0.1}^{2.05}\right]\left[\mathrm{Ba}_{1.9}^{2.05}\mathrm{Pr}_{0.1}^{3+}\right]\mathrm{Cu(1)}^{2.16+}\mathrm{Cu(2)}_2^{2.15+}\mathrm{O(1)}_2^{2.17-}\mathrm{O(2)}_2^{2.01-}\mathrm{O(3)}_2^{1.90-}\mathrm{O(4)}^{1.38-} \qquad (C)$$

(charge states of the copper and oxygen atoms remain unchanged). As it is seen from Fig. 4, the calculated data agree with experiment for the $PrBa_2Cu_3O_7$ compound. The assumption that Pr^{4+} ions are stabilized in the structure of $PrBa_2Cu_30_7$ (with the corresponding change of the charge state of the O(4) atoms to O^{2-}) results in an increase of Δ_{lat} and in a disagreement between experimental and calculated values for the $PrBa_2Cu_3O_7$ compound.

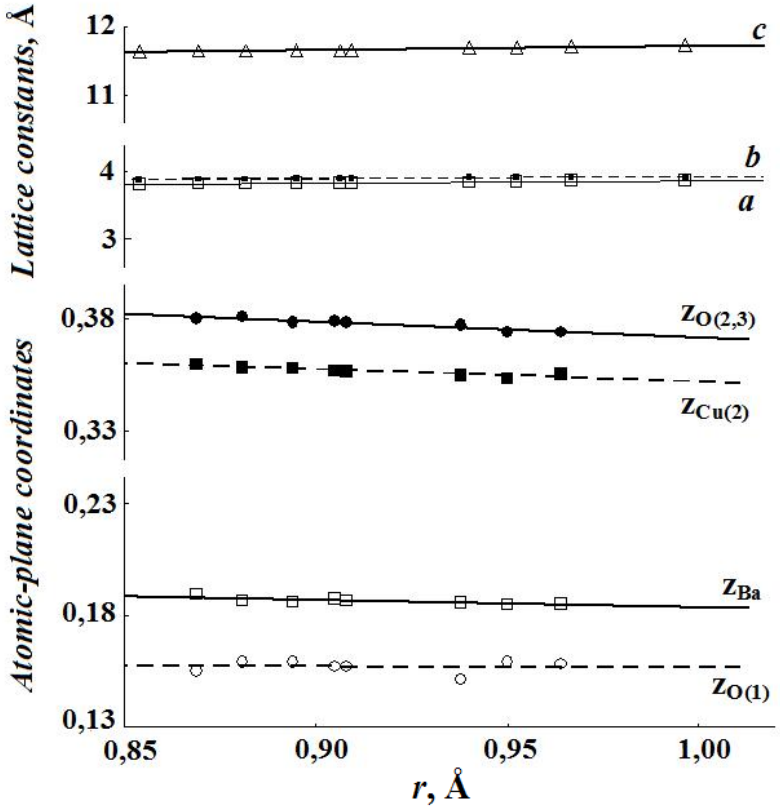

Fig. 5. Dependence of the lattice constants and atomic-plane coordinates on the rare-earth ion radius r

4. Conclusions

$^{155}Eu(^{55}Gd)$ emission Mossbauer spectroscopy has been shown to be applicable for determining the parameters of the lattice EFG tensor at the REM sites of $RBa_2Cu_3O_7$. The experimental EFG can

be fitted by the calculated values if the holes are placed mainly at the chain and Cu-O plane oxygen sites of the $RBa_2Cu_3O_7$ lattices.

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USING THE $^{57m}Fe^{3+}$ MÖSSBAUER PROBE TO DETERMINE THE EFG TENSOR PARAMETERS IN THE COOPER SITES TO THE LATTICES OF CuO And $La_{2-x}Sr_xCuO_4$

Mössbauer emission spectroscopy of the $^{57}Co(^{57m}Fe)$ isotope has shown that the impurity iron atoms appearing at the CuO-lattice cation sites after the decay of $^{57}Co^{2+}$ are donors and can become stabilized in two charge states, $^{57m}Fe^{3+}$ and $^{57m}Fe^{2+}$. A satisfactory agreement between the calculated and experimental values of the quadrupole splitting in Mössbauer spectra has been obtained for the $^{57m}Fe^{3+}$ centers. This permits one to consider the results obtained in the $^{57}Co(^{57m}Fe)$ Mössbauer emission spectroscopy study of cuprates as reliable experimental data on the lattice electric-field gradient (lattice EFG) tensor parameters at copper sites. The parameters of the lattice EFG tensor at the copper sites in the $La_{2-x}Sr_xCuO_4$ lattice (the main component of the EFG tensor V_{zz} and the asymmetry parameter) were determined experimentally by emission Mössbauer spectroscopy with $^{57}Co(^{57}Fe)$ isotopes. A comparison of the experimental and calculated dependences of V_{zz} on x shows that the holes arising from the substitution of La^{3+} by Sr^{2+} are localized mainly at the oxygen sites in the Cu-O_2 plane.

Keywords: Mössbauer emission spectroscopy, electric field gradient tensor.