Application Of Mössbauer Spectroscopy To Determine The Parameters Of The EFG Tensor At Barium Nodes For YBA2CU3O7-X

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ABSTRACT
The method of the Messbaur emission spectroscopy on the Ba-133 isotope, the parameters of the electric field gradient (EFG) tensor are determined. It is established that the discrepancy between the experimental and calculated values of eqxp is explained by the imperfection of the models used to calculate eqxp.

KEYWORDS
Electric field gradient, tensor, frame, nuclear quadrupole resonance, isotope, the waking nucleus, spin, spectrum, quadrupole splitting, asymmetry parameters, experimental value, semiconductor, superconductor.

INTRODUCTION
When studying the structural properties of HTSCs, there are many problems, the solution of which is mandatory. In this aspect, one of the main problems in HTSC physics is the problem of determining the location of hole localization, which determine the phenomenon of superconductivity. The most reliable method for identifying holes in HTSC
lattices is considered to be a comparison of the experimentally determined parameters of the electric field gradient tensor (EFG) with the results of their theoretical calculation. This method is most effective when measuring and calculation of the parameters of the EFG tensor. All HTSCs, as a rule, contain copper, and the parameters of the EFG tensor at copper sites are most sensitive to the charges of atomic centers. This work is devoted to the consideration of the experimental and theoretical results of determining the parameters of the EFG tensor in the copper nodes of the UBa2Cu3O7-x ceramics.

MATERIALS AND METHODS

The combination is one of the most typical high-temperature superconductors and is distinguished by a relative prostate synthesis, high values of the temperature of transition to the superconducting state Tc, and the ability to regulate Tc by changing x. It is these features that explain the fact that the overwhelming number of studies on comparing the calculated and experimental parameters of the EFG tensor refers to UBa2Cu3O7-x. Ceramics UBa2Cu3O7-x is characterized by a variable composition (0≤x≤1). The maximum value of Tc (~ 91K) was found for UBa2Cu3O7 (x = 0). As x increases, Tc decreases and compositions with x> 0.65 do not exhibit superconductivity. The experimental determination of the parameters of the electric field gradient (EFG) tensor at the lattice sites of UBa2Cu3O7-x is an urgent problem. This is primarily due to the possibility for the specified ceramics to compare the experimental and calculated parameters of the EGF and, as a result, the ability to assess the validity of those initial assumptions within which the calculation of the lattice sums is performed. The most complete information on the parameters of the EFG at the sites of the crystal lattice can be obtained by the methods of nuclear quadrupole resonance (NQR) and Mössbauer spectroscopy. However, as applied to UBa2Cu3O7-x, both methods refer either to copper centers (NQR on 63Cu and 65Cu isotopes [1]) or to impurity centers in the position of copper atoms (Mössbauer effect on 57Fe (57Co) 119Sn and 67Zn (67Cu) isotopes), or to the centers of rare earth metals in the position of yttrium atoms (the Mössbauer effect on the isotopes 151Eu, 155Gd, 161Dy, 166Er, 169Tm, and 170Yb). Without touching here on the problem of extracting information about eqcr from the experimental values of e2qQ. We only note that there are practically no direct measurements of the parameters of the EFG tensor at the sites of barium atoms for ceramics UBa2Cu3O7-x (here eQ is the quadrupole moment of the nucleus under study, eq is the main component of the EFG tensor on the nucleus under study, eqcr is the main component of the EFG tensor created by lattice ions at this node).

This is due to both the difficulties of measuring the NQR spectra on the isotopes 135Ba, 137Ba, and the absence of stable Mössbauer isotopes of barium.

In this work, it is proposed to use emission Mössbauer spectroscopy on the 133Ba (133Cs) isotope to determine the parameters of the EFG tensor at barium nodes. Electron capture in the 133Ba mother nucleus leads to the formation of an excited 81-keV level of 133Cs, and the recoil energy during neutrino emission in this case does not exceed 1 eV, so that the daughter cesium atom is in the position of barium atoms. The isomeric transition in 133Cs occurs between states with spins 5/2 and 7/2, so that when a cesium atom is in a crystal field...
whose symmetry is below cubic, eight lines of different intensities should appear in the Mössbauer spectrum. However, taking into account the values of the quadrupole moments of the nucleus $^{133}\text{Cs}$ in the ground and excited states ($Q_{\text{OCCH}} = -0.003 \times 10^{-24}\text{cm}^2$, $Q_{\text{exc.}} = -0.22 \times 10^{-24}\text{cm}^2$ [2]), the degeneracy is actually lifted only for the excited nucleus of $^{133}\text{Cs}$, so that three lines should be observed in the Mössbauer spectrum, the relative position of which with the velocity spectrum allows, in principle, to determine the value of $e2qQ$, its sign and the value of the asymmetry parameter. Finally, the daughter atom of cesium in its chemical compounds exhibits only valency $+1$ (electronic configuration $4d^{10}$), which makes it possible to determine the value of $eqcr$ from the experimental values of $eq$, and as a result, to compare the experimental and calculated values of $eqcr$. Samples $U^{133}\text{Ba}_2\text{Cu}_3\text{O}_7$ were prepared by sintering the corresponding oxides in air, samples $U^{133}\text{Ba}_2\text{Cu}_3\text{O}_6$ were obtained by heating $U^{133}\text{Ba}_2\text{Cu}_3\text{O}_7$ with vacuum pumping. Samples $\text{YBa}_2\text{Cu}_3\text{O}_7$ had a rhombic structure and for them $T_c\approx85\text{ K}$. Samples $\text{YBa}_2\text{Cu}_3\text{O}_6$ had a tetragonal structure and they were semiconductors at $T\geq4.2\text{ K}$. Mössbauer spectra were recorded at $4.2\text{ K}$ with an absorber $\text{CsCl}$ with a surface density of $350\text{ mg/cm}^2$.

RESULTS AND DISCUSSIONS

As a preliminary stage, we measured the emission Mössbauer spectrum of $^{133}\text{BaO}$ (Fig. A) - it is a single line with the width ($\text{HEXP.} = 0.90\pm0.02\text{ mm/s}$) slightly exceeds the doubled natural width $81\text{- keV}$ of the $^{133}\text{Cs}$ level ($2\text{Gest.} = 0.54\text{ mm/s}$). Since BaO has a NaCl-type lattice, we considered that the difference between HEXP. and $2\text{Gest.}$ caused only by instrumental effects and later on, $0.90\text{ mm/s}$ was taken as the instrumental width of the spectral line (i.e., when the experimental Mössbauer spectra of $U^{133}\text{Ba}_2\text{Cu}_3\text{O}_7\times$ were decomposed into quadrupole multiplets, it was assumed that the width of the components could not be less than $0.90\text{ mm/s}$). The Mössbauer spectrum of superconducting ceramics $\text{YBa}_2\text{Cu}_3\text{O}_7$ is a single broadened line (see Fig. B and table), which corresponds to $^{133}\text{Cs}\times$ centers at barium sites. In the structure of $\text{YBa}_2\text{Cu}_3\text{O}_7\times$, barium atoms occupy a single position, and therefore the broadening of the experimental spectrum is associated with unresolved quadrupole splitting. The table shows the values of $e2qQ$ determined from the spectrum in Fig. B. For semiconductor ceramics $\text{YBa}_2\text{Cu}_3\text{O}_6$, the Mössbauer spectrum is also a single line, but its width will noticeably increase (see Fig. C and table). This spectrum also corresponds to $^{133}\text{Cs}\times$ centers at barium sites; the $e2qQ$ values for them are given in the table.

From the experimental values of $eq$ according to the relation $eq = (1-\gamma)eqcr$. (here $\gamma$ is the Sternheimer coefficient for $\text{Cs} + \gamma = -121.3$), were obtained $eqcr$ values. [3]. As can be seen from the table, the transition from the orthorhombic to the tetragonal modification $\text{YBa}_2\text{Cu}_3\text{O}_7\times$ is accompanied by an increase in $eqcr$. And there is a qualitative agreement between the experimentally determined and calculated values of $eqcr$. Although there is no quantitative agreement. As an illustration, Fig. the dashed line shows the theoretical Mössbauer spectrum for the $U\text{Ba}_2\text{Cu}_3\text{O}_6$ sample, and the value of $eqcr$ given in [4] was used for the calculation.

CONCLUSION

It can be seen that, in contrast to the experimental spectrum, a distinct structure
and significant broadening are observed for the theoretical spectrum. We believe that the discrepancy between the experimental and calculated values of eqcr. is explained by the imperfection of the models used to calculate eqcr.

Table. Parameters of the emission Mössbauer spectra of $\text{YBa}_2\text{Cu}_3\text{O}_7-x$

| Соединение          | Центр      | $|e2qQ|$, МГц | $|eq\text{экр}|$, e/Å³ |
|---------------------|------------|-------------|-----------------|
| $\text{Y133Ba2Cu3O7}$ | 133Cs+     | 45±5        | 0.048±0.002     |
| $\text{Y133Ba2Cu3O6}$ | 133Cs+     | 65±5        | 0.069±0.002     |

Fig. Emission Mössbauer spectra of 133BaO [a], YBa2133Cu3O7 [b], and YBa2133Cu3O6 [c] at 4.2 K. For spectrum [c], the theoretical spectrum is shown (eqcr (Ba) = 0.150 e/Å³)
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