Application Of Mössbauer Spectroscopy To Determine The Parameters Of The EFG Tensor At Barium Nodes For УBA2CU3O7-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 eqкр is explained by the imperfection of the models used to calculate eqкр.

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 $UBa_2Cu_3O_{7-x}$ 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 T_c, and the ability to regulate T_c 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 $УBa_2Cu_3O_{7-x}$. Ceramics $УBa_2Cu_3O_{7-x}$ is characterized by a variable composition ($0 \le x \le 1$). The maximum value of T_c (~ 91K) was found for $УBa_2Cu_3O_7$ (x = 0). As x increases, T_c 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 $УBa_2Cu_3O_{7-x}$ 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 $УBa_2Cu_3O_{7-x}$, both methods refer either to copper centers (NQR on ^{63}Cu and ^{65}Cu isotopes [1]) or to impurity centers in the position of copper atoms (Mössbauer effect on ^{57}Fe (^{57}Co) ^{119}Sn and ^{67}Zn (^{67}Cu) isotopes) , or to the centers of rare earth metals in the position of yttrium atoms (the Mössbauer effect on the isotopes ^{151}Eu, ^{155}Gd, ^{161}Dy, ^{166}Er, ^{169}Tm, and ^{170}Yb). 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 $УBa_2Cu_3O_{7-x}$ (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 ^{135}Ba, ^{137}Ba, and the absence of stable Mössbauer isotopes of barium.

In this work, it is proposed to use emission Mössbauer spectroscopy on the ^{133}Ba (^{133}Cs) isotope to determine the parameters of the EFG tensor at barium nodes. Electron capture in the ^{133}Ba mother nucleus leads to the formation of an excited 81-keV level of ^{133}Cs, 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 ^{133}Cs 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 133Cs in the ground and excited states (QOCH = -0.003 • 10-24cm2, Qexc. = - 0.22 • 10-24cm2 [2]) the degeneracy is actually lifted only for the excited nucleus of 133Cs, 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 4d10), 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 U133Ba2Cu3O7 were prepared by sintering the corresponding oxides in air, samples U133Ba2Cu3O6 were obtained by heating U133Ba2Cu3O7 with vacuum pumping. Samples УBa2Cu3O7 had a rhombic structure and for them Tc - 85 K. Samples УBa2Cu3O6 had a tetragonal structure and they were semiconductors at T≥4.2 K. Mössbauer spectra were recorded at 4.2 K with an absorber Cs≤CI with a surface density of 350 mg / cm2.

RESULTS AND DISCUSSIONS

As a preliminary stage, we measured the emission Mössbauer spectrum of 133BaO (Fig. A) - it is a single line with the width (HEXP. = 0.90 ± 0.02 mm / s) slightly exceeds the doubled natural width 81 - keV of the 133Cs level (2Gest. = 0.54 mm / s). Since BaO has a NaCl-type lattice, we considered that the difference between HEXP. and 2Gest. caused only by instrumental effects and later on, 0.90

mm / s was taken as the instrumental width of the spectral line (i.e., when the experimental Mössbauer spectra of U133BaCu3O7-x were decomposed into quadrupole multiplets, it was assumed that the width of the components could not be less than 0.90 mm / s). The Mössbauer spectrum of superconducting ceramics УBa2Cu3O7 is a single broadened line (see Fig. B and table), which corresponds to 133Cs + centers at barium sites. In the structure of УBa2Cu3O7-x, 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 УBa2Cu3O6, the Mössbauer spectrum is also a single line, but its width will noticeably increase (see Fig. C and table). This spectrum also corresponds to 133Cs + 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-γ) eqcr. (here γ is the Sternheimer coefficient for Cs + γ = -121.3), were obtained eqcr values. [3]. As can be seen from the table, the transition from the orthorhombic to the tetragonal modification УBa2Cu3O7-x 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 UBa2Cu3O6 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 УBa2Cu3O7-x

Соединение	Центр	$|e2qQ|$, Мгц	$|eq_{экр}|$, $e/\mathring{A}^3$
У133Ba2Cu3O7	133Cs+	45±5	0.048±0.002
У133Ba2Cu3O6	133Cs+	65±5	0.069±0.002
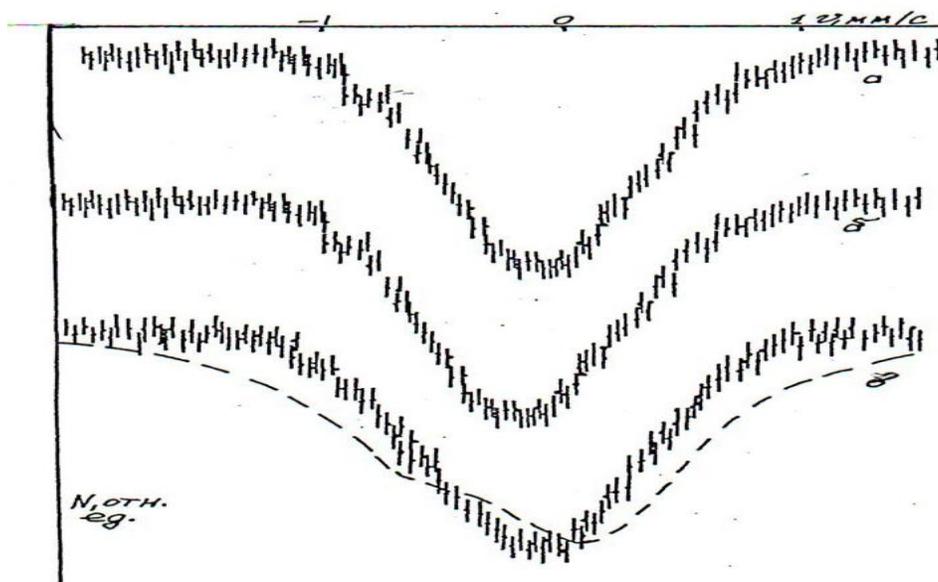
Fig. Emission Mössbauer spectra of 133BaO [a], YBa2133Cu3O7 [b], and YBa2133Cu3O6 [c] at 4.2 K.

For spectrum [c], the theoretical spectrum is shown (eqcr (Ba) = 0.150 e / Å3)

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