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DETERMINATION OF LOCALIZATION OF HOLES IN LATTICES OF HIGH-TEMPERATURE SUPERCONDUCTORS

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ABSTRACT:

Using the method of Mossbauer's emission spectroscopy on Cu-57 isotopes in samples of complex copper's metal oxides, information about the parameters of the tensor of electric field gradient (EFG) has been obtained, and theoretical calculations of the EFG's tensor parameters by the method of point charges by the Hartree-Fock method have been performed. By comparing the calculated and experimental values of the parameters of the EFG's tensor, the locations of the infected particles were determined by studying the values of the charge states of the atoms.

KEYWORDS: Mossbauer's spectroscopy, superconduction, localization, charging state, atoms, copper oxides.

INTRODUCTION:

One of the main problems of modern solid state physics is the experimental and theoretical determination of the parameters of the electric field gradient tensor (EFG) at the lattice sites of a high-temperature superconductor. Also, a number of works [1-3] are devoted to the problem of determining effective charges and the spatial distribution of charge states in lattices of high-temperature superconductors (HTSC).

The study of the structure and charge state of atoms in complex copper metal oxides makes it possible to determine some parameters of the so-called high-temperature superconductors, which are the main objects of physicists [4].

Determination of the indicated quantities is necessary both for constructing a theory of HTSC and for creating the technological foundations for obtaining HTSC.

Determination of the boundary of the transition to the superconducting state, as well as the study of the charge state of atoms in superconducting materials and during the transition to the semiconducting state were the main problems of this study.

RESEARCH METHODOLOGY:

Two groups of experimental methods are used to study impurity atoms in solids. One of them is insensitive to the electronic structure of impurity centers (for example: electrical conductivity, photoconductivity, Hall effect, and others). [five]

The second group of methods (the method of electron paramagnetic resonance (EPR), the method of nuclear quadrupole resonance (NQR), the method of nuclear gamma-resonance spectroscopy (NGRS)) are sensitive to the electronic structure of impurity centers and these methods make it possible not only to identify the nature of impurity centers, but also to interpret results directly in terms of electronic structure. [6].

The most promising method for solving the problem of determining charges is the method of comparing the experimentally determined parameters of the electric field gradient tensor (EFG) with the results of their theoretical calculation. [7]

Therefore, we tried to formulate the requirements for Mössbauer spectroscopy on

impurity atoms when it is used as a method for identifying the charges of atomic centers in crystals. We have implemented these requirements for the case of the most typical high-temperature superconductors.

The theoretical calculation of the EFG tensor can be carried out within the framework of the model of point charges, by the Hartree-Fock method and molecular orbitals, by the method of plane waves in the local density approximation.

Experimental information on the parameters of the EFG tensor can be obtained by NGRS and NMR methods. [eight]

In this work, we used the emission Mössbauer spectroscopy on isotopes Cu - 57 in samples of complex copper metal oxides. [nine]

$YBa_2Cu_3O_7$ samples were prepared by sintering oxides in an oxygen atmosphere.

RESULTS:

X-ray structural analysis showed one-phase control samples with orthorhombic structure parameters. The superconducting transition temperature was Tc ~ 85K. The Cu - 67 isotope was introduced into the charge in the chemical form $CuCl_2$. At T ≥ 85 K, the samples remained in the semiconducting state.

The emission Mösbauer spectra of YBa2Cu3O7 represent the superposition of two quadrupole triplets of different intensities (Fig. 1).

Based on the ratio of the populations of the Cu - (1) and Cu - (2) positions, the more intense triplet is assigned to the 67 Cu + 2 atom in the Cu - (2) sites, and the less intense one to the 67 Cu + 2 atom in the Cu - (1).

To theoretically calculate the value of the principal component of the EFG tensor at copper sites in $YBa_2Cu_3O_7$ lattices, the EFG tensor parameters were calculated with the selection of the contribution to the total EFG from individual sublattices by the method of point charges [10].

Thus, the results obtained on the basis of theoretical calculations of the parameters of the electric field gradient tensor by the method of point charges, as well as the experimentally determined parameters of the EFG tensor using emission Mössbauer spectroscopy on Cu-57 isotopes makes it possible to compare and, on their basis, determine the location of charged particles in the HTSC lattice.

The localization of holes in the lattice of a high-temperature superconductor was determined by comparing the calculated and experimental values of the EFG tensor parameters [11].

The temperature of the transition to the superconducting state is found to be Tc ~ 85K. At T> 85K, the samples passed into the semiconducting state.

Copper atoms have also been determined in a high-temperature superconductor; it turns out to be in two charge states, and in a semiconductor sample, only in one state, based on the ratio of the occupancy of the Cu - (1) and Cu - (2) positions.

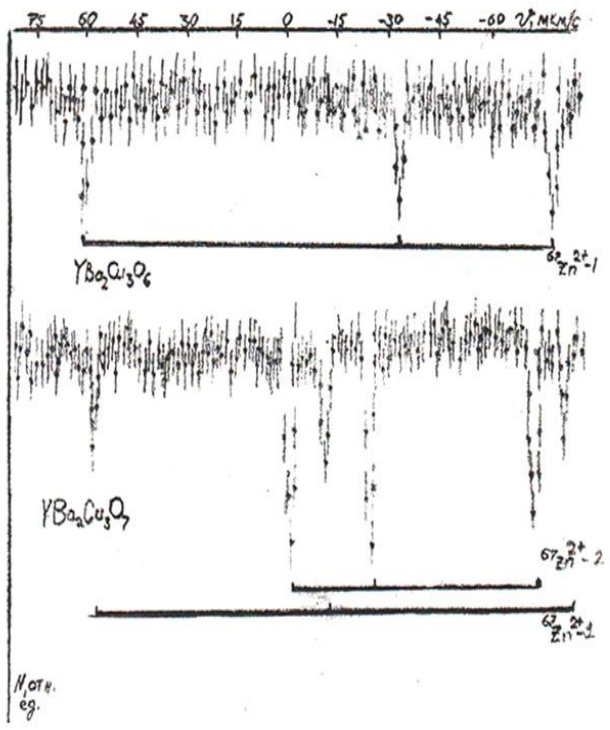

Fig. 1. Emission Mössbauer spectra of $YBa_2Cu_3O_6$ and $YBa_2Cu_3O_7$ at 80K.

CONCLUSION:

The hole in this ceramic is localized mainly at the sites of the bridging oxygen O (4), although a partial transfer of the hole to the O (2) and O (3) sites is possible.

The hole localization in $YBa_2Cu_3O_7$ ceramics was determined by studying the value of the charge states of atoms. The charge state of atoms in ceramics is (4).$Y^{3,14+}$ $Ba_2^{2,09+}$ $Cu(1)^{1,89+}$ $Cu(2)_2^{1,89+}$ $O(1)_2^{2,09-}$ $O(2)_2^{1,93-}$ $O(3)_2^{1,81-}$ $O(4)^{1,34-}$ The smallest value of the charge of the fourth oxygen indicates the possibility of localization of the hole in the sites of the bridging oxygen O

REFERENCES:

1) F.S.Nasredinov, E.Yu. Turaev, P.P. Seregin, H.B. Rakhmatullaev, and Bakhadirkhanov M.K. Mechanism of Two-Elektron Exchange between Neutral and Ionized Centres of Tin in $PbS_{1-x}Se_x$ Solid Solutions. Phys. stat. sol. (a) 121. 571, 1990
2) Turaev E.Yu. The Application of Messbauer spectroscopy in the study of copper oxides. International Journal of Advanced Research in Science, Engineering and Technology (IJARSET), Volume 6, Issue 10, October 2019, p.11060-11062, India
3) Seregin P.P., Turaev E.Yu. Application of the Mossbauer effect in the physics of amorphous semiconductors, Tashkent, Science, 1989.
4) Turaev E.Yu., Niyazova O.A. Determination of localization of holes in lattices of High-temperature superconductors. International Journal of Advanced Research in Science, Engineering and Technology (IJARSET), Volume 6, Issue 10, October 2019, p.11041-11043, India.