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Determination of Localization of Holes in Lattices of High-Temperature Superconductors

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ABSTRACT: The charges of atomic centers in high-temperature superconducting crystals have been identified through using emission Mössbauer spectroscopy. The location of charged particles was determined by studying the values of the charge states of atoms.

KEYWORDS: high-temperature superconductor, effective charge, lattice, hole, solid, electronic structure, impurity center, single-phase, spectrum.

I.INTRODUCTION

One of the main problems of modern physics is the problem of determining the effective charges and spatial distribution of electronic defects in lattices of high-temperature superconductors.

The determination of these values is necessary both for constructing the theory of HTSC, and for creating the theoretical foundations of the technology for producing HTSC.

II. RELATED WORKS

Two groups of experimental methods are used to study impurity atoms in solids. One of them is not sensitive to the electronic structure of impurity centers (for example: electrical conductivity, photoconductivity, Hall effect, and others) [1].

The second group of methods (EPR, NQR, NGRS) are sensitive to the electronic structure of impurity centers and these methods not only identify the nature of impurity centers, but also interpret the results directly in terms of the electronic structure [2].

III. METHODS

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

X-ray diffraction analysis showed the single-phase nature of the control samples with the parameters of the orthorhombic structure. The temperature of the transition to the superconducting state was $T_c{\sim}85K$. The $Cu-67$ isotope was introduced into the charge in the chemical form $CuCl_2$. At $T\geq 85\ K$, the samples remained in a semiconductor state.

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IV. ALGORTHMS USED

The Mesbauer emission spectra of $YBa_2Cu_3O_7$ represent the superposition of two quadrupole triplets of different intensities (Fig. 1). Based on the ratio of the populations of the positions *Cu - (1)* and *Cu - (2)*, the more intense triplet is assigned to the $^{67}Cu^{+2}$ atom at the *Cu - (2)* sites, and the less intense triplet is assigned to the atom $^{67}Cu^{+2}$ at the *Cu - (1)* sites.

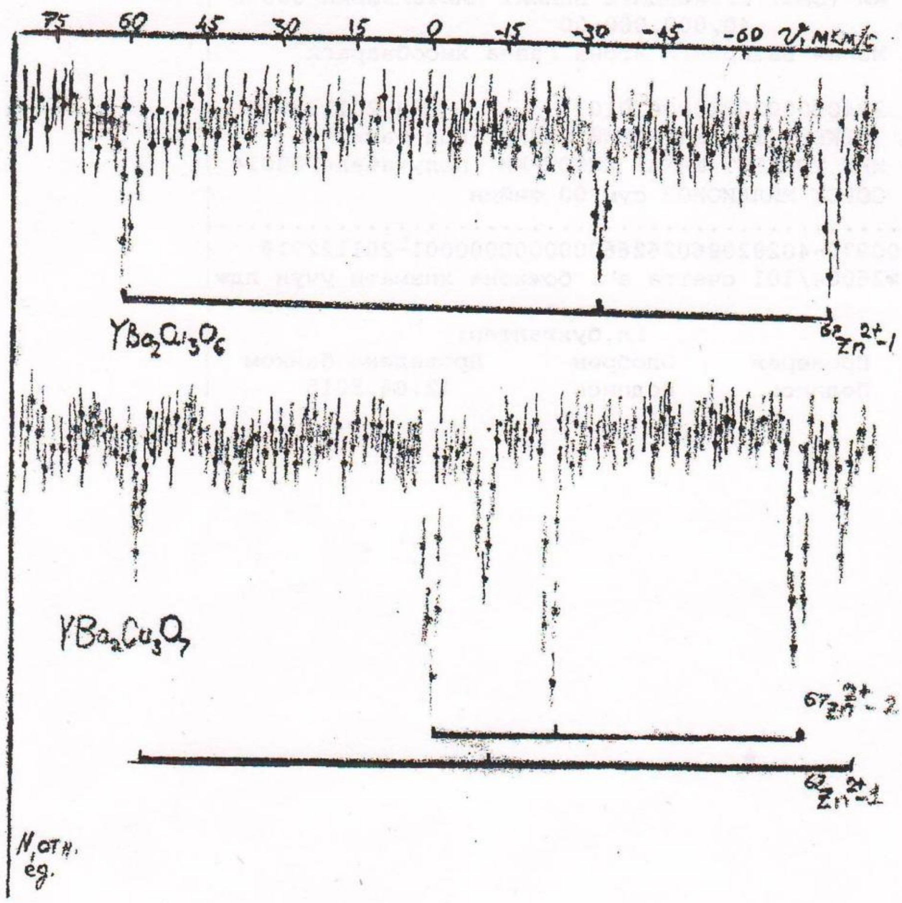

Fig. 1, Mesbauer emission spectra $YBa_2Cu_3O_6$ and $YBa_2Cu_3O_7$ are at a temperature of 80 K.

To theoretically calculate the values of the main component of the EFG tensor in copper sites in $YBa_2Cu_3O_7$ lattices, the parameters of the EFG tensor were calculated with the contribution of the point charge to the total EFG from individual sublattices [3].

V. RESULTS

By comparing the calculated and experimental values of the parameters of the EFG tensor, the localization of holes in the lattices of a high-temperature superconductor was determined [4].

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

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VI. CONCLUSION

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

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