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The Application of Messbauer Spectroscopy in the Study of Copper Oxides

Turaev Ergash Yuldashevich

The Professor of Termez State University

ABSTRACT: In order to determine the effective atomic charges in the lattices of high-temperature superconductors, we used the method of comparing the experimentally determined parameters of the electric field gradient tensor (HEP) with the results of their theoretical calculation. It has been established that, with a decrease in temperature below the Neel temperature, a fine structure appears, indicating a magnetic ordering of the sub lattice.

KEYWORDS: Messbauer spectroscopy, pure materials, impurity atoms, impurity centers, radioactive isotopes, high-temperature superconductors, charge, tensor, gradient, isotope, quadrupole split, iron centers, lattice.

I.INTRODUCTION

Pure materials have only academic interest and only alloying opens up the possibility of their practical use.

The 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].

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 implemented these requirements for the case of the most typical copper metal oxides by introducing the C_o - 57 radioactive isotopes by synthesis. Studying the structure and charge states of atoms in copper oxides allows us to determine some parameters of the so-called high-temperature superconductors that are currently the main objects of physicists. High-temperature superconductors (HTSC) are an urgent task of modern physics.

One of the main problems of modern physics is the problem of determining the effective charges of atoms and the spatial distribution of electronic defects in HTSC lattices. The determination of these values is necessary both to create the theoretical foundations of the technology for producing HTSC with a given set of electrophysical properties [3].

The most perspective method for solving the problem of determining charges is the method of comparing experimentally determined parameters of tensor of the electric field gradient (EFG) with the results of their theoretical calculation. The theoretical calculation of the EFG tensor can be carried out within the framework of the point charge model, using the Hartree – Fock method and molecular orbitals, by the plane wave method in the local density approximation [4].

The experimental information on the parameters of the EFG tensor can be obtained by NMR, NQR, and NGRS. The experimental data refers either to the centers of copper, oxygen and REM, or to impurity atoms in copper sites [5].

In this work, we used Mössbauer emission spectroscopy on C_o - 57 isotopes.

We were faced with the task of methodologically substantiating the possibilities of emission Mössbauer spectroscopy on the indicated isotope to study the structures of complex copper metal oxides.

The spectra of CuO: (Co - 57) samples at 295 k were quadrupole doublets corresponding to Fe (2+) centers (Fig. 1).

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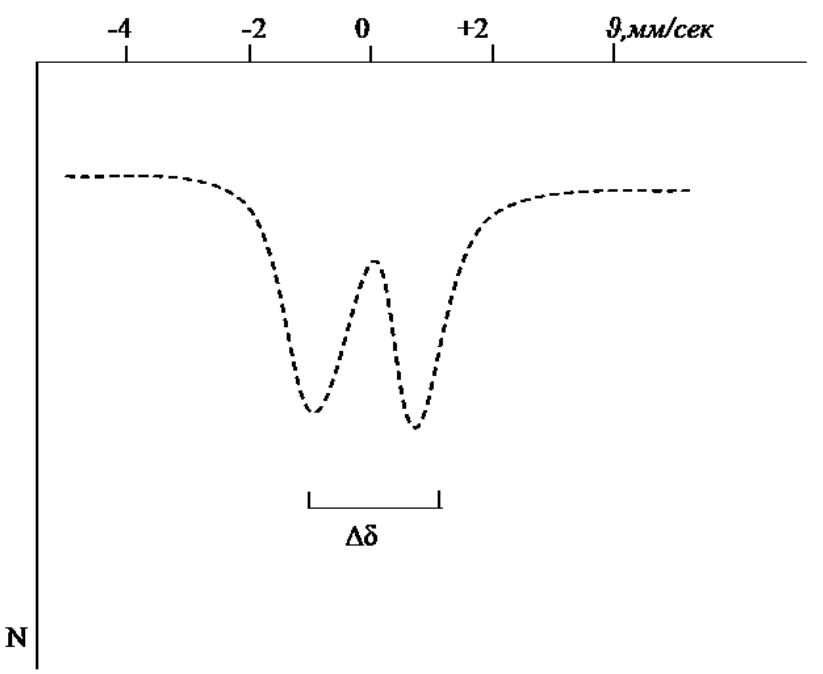

Fig. 1

As the temperature decreases below the Néel temperature, the resolution of the spectrum deteriorates and a fine structure appears, indicating the magnetic ordering of the sublattice in which impurity atoms are localized.

This fact led to the conclusion about the stabilization of impurity atoms Fe (2+) at the sites of the crystal lattice of copper, and the substitution of Cu (2+) ions by Fe (2+) should not lead to the appearance of compensation centers.

The crystalline EFG tensor was calculated for cationic CuO sites, and the lattice was written as Cu (2+) O (2-)

The calculated quadrupole splitting of the CuO: (Co - 57) spectrum is 2.32 mm / s, which is significantly different from the experimental value of 1.56 mm / s. This discrepancy is explained by the fact that, for Fe (2+) centers, HEPs on Fe - 57 nuclei are created both by ions of the crystal lattice and by the valence electrons of the iron center (1), while the calculation takes into account only the crystalline component of the EFG. Thus, although the isovalent substitution of Cu (2+) ions by Fe (2+) ions in the CuO lattice leads to a well-described model, however, the theoretical calculation of the EFG tensor is impossible for it.

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