



Application of Mössbauer Spectroscopy in the Study of Copper Oxides

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Annotation: 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 the lattices of HTS. The definition of these values is necessary both to create the theoretical foundations of the technology for obtaining HTS with a given set of electrophysical properties

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

To study impurity atoms in solids, a group of experimental methods is used. 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, JCR, JAGRS) are sensitive to the electronic structure of impurity centers and these methods allow not only to identify the nature of impurity centers, but also to interpret the results directly in terms of electronic structure [2].

So we tried to formulate the requirements for Mössbauer spectroscopy on impurity atoms when it was used as a method for identifying the charges of atomic centers in crystals. These requirements were implemented by us for the case of the most typical copper metal oxides when radioactive isotopes of ^{67}Co were introduced by synthesis. The study of the structure and charge states of atoms in copper oxides makes it possible to determine some parameters of the so-called high-temperature superconductors, which are the main objects of physicists at the present time. High-temperature superconductors (HTS) 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 the lattices of HTS. The definition of these values is necessary both to create the theoretical foundations of the technology for obtaining HTS with a given set of electrophysical properties [3].

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

Experimental information on the parameters of the GEO tensor can be obtained by NMR, NMR and JAGS methods. Experimental data refers either to the centers of copper, oxygen and rare earth metals, or to impurity atoms in copper nodes [5].

In the present work, emission Mössbauer spectroscopy on isotopes of ^{67}Co is used.



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We were faced with the task of methodological substantiation of the possibilities of emission Mössbauer spectroscopy on this isotope for the study of the structures of complex copper metaloxids

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

With a decrease in temperature below the Neel temperature, the resolution of the spectrum deteriorates and a thin structure appears, indicating the magnetic ordering of the sublattice in which impurity atoms are localized.

This fact made it possible to conclude that impurity Fe atoms (2+) in the nodes of the copper crystal lattice are stabilized, and the replacement of Cu (2+) ions with Fe (2+) should not lead to the appearance of compensation centers.

The crystalline GEO tensor for cationic nodes of CuO was calculated, and the lattice was recorded in the form of Cu(2+)O(2-).

The calculated value of the quadrupole splitting of the CuO spectrum: (Co - 57) 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 the centers of Fe (2+) the GEO on the Fe nuclei - 57 is created as ions of the crystal rib, and valence electrons of the center of iron (1), while the calculation takes into account only the crystalline component of the GEO. Thus, although the isovalent substitution of Cu(2+) ions with Fe (2+) ions in the CuO lattice results in a well-written model, a theoretical calculation of the GEO tensor for it is impossible.

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