THE DETERMINATION OF CASES OF CURRENT CONDUCTORS IN HIGH TEMPERATURE CONDUCTORS ON THE BASIS OF COMPARISON OF PARAMETERS OF ELECTRIC FIELD GRADIENT TENSOR

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ABSTRACT

The cases of current carriers in high-temperature superconductors were determined on the basis of mutual comparison of experimentally and theoretically determined values of the parameters of the electric field gradient tensor using nuclear quadrupole resonance and nuclear gamma resonance methods.

Key words: Nuclear quadrupole resonance, nuclear gamma resonance, charge state, isotope, tensor, superconductor, current carriers, theoretical calculations.

It is known that after the discovery of high-temperature superconductors in 1986, theoretical and experimental research work in this field has greatly increased. Due to the fact that high-temperature superconducting materials are structurally complex copper oxides, many types of high-temperature superconductors have been identified, and very accurate data on their physical properties have been obtained and scientific articles have been published [1].

This paper is devoted to the study of the physical properties and structure of the first detected YBa2Cu3O7-x compound of high-temperature superconductors, and certain conclusions are made on the basis of comparing the results obtained using spectroscopic methods with previously obtained theoretical data. The YBa2Cu3O7-x compound is a typical representative of high-temperature superconductors, characterized by its ease of synthesis and the fact that the transition temperature to the superconducting state is much higher. Due to these properties, the results of experiments comparing theoretical and experimental scientific results in this compound have been extensively studied [2].

YBa2Cu3O7-x ceramics have a variable composition ($0 \le x \le 1$) and the maximum value of transition to superconductivity Tc = 91 K was observed in the composition x = 0 in this system. As the value of X increases, the transition temperature of Ts decreases and the compound loses its superconducting properties when it contains $x \ge 0.65$ [3].

The YBa2Cu3O7-x compound has an orthorombic structure in which the copper atoms are in the two structural equivalents, Si (1) and Si (2). Oxygen atoms, on the other hand, are present in four structural equivalent states, O (1), O (2), O (3), and O (4). Therefore, the structural formula of the compound can be written as UVa_2Si (1) Si (2) $_2O$ (1) $_2O$ (2) $_2O$ (3) $_2O$ (4). The two Si (1) and Si (2) states of the copper atoms in the compound were found to be in a 1: 2 ratio to each other [4].

In the system, a compound with x = 1 has a tetrogonal structure $UVa2Si3O_6$ and exists in two states with copper atoms Si (1) and Si (2), while the state O (4) in the compound does not exist or in other words disappears spontaneously. Therefore, this compound has the following formula: UVa_2Si (1) Si (2) $_2O$ (1) $_2O$ (2) $_2O$ (3) $_2$ and the Si (1) and Si (2) states of the copper atoms are in a 1: 2 ratio [5].

The complete experimental data on the parameters of the electric field gradient tensor can be obtained using the methods of nuclear quadrupole resonance and nuclear gamma resonance (Messbauer spectroscopy). However, since there are no isotopes of copper atoms used in Messbauer spectroscopy, compound atoms are used to study the YBa2Cu3O7-x compound using the Messbauer spectroscopy method.

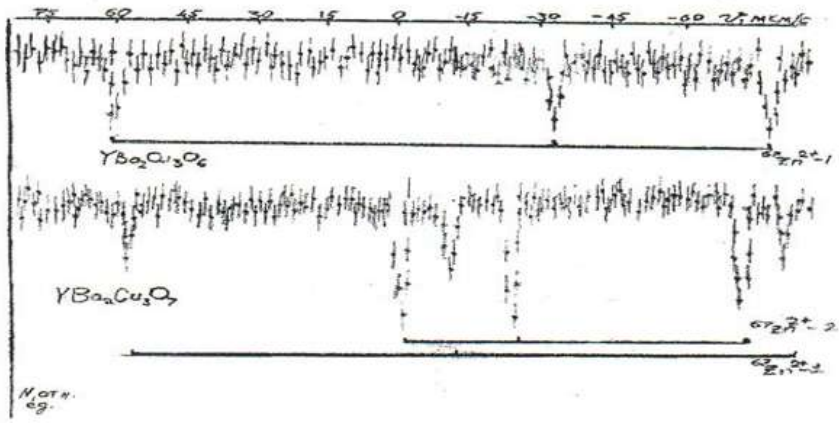
The isotope Fe57 is used as the compound atoms, and it is assumed that these isotope atoms are located in place of the Si (1) and Si (2) atoms, and that its Messbauer spectra provide information about the local state of the copper atoms [6].

Messbauer transitions in the Fe^{-57} isotope occur between 3/2 and 1/2 spin levels, and the Messbauer spectrum of Fe57 is divided into two components. Also, in the emission variant of Messbauer spectroscopy, the isotope Si^{-67} (Zn^{-67}) was used to determine the parameters of the electric field gradient tensor in the bonds Si (1) and Si (2) in the $UVa_2Si_3O_{7-x}$ compound.

The Messbauer spectrum of the compound $UVa_2Si_3O_7$ consists of a combination of two quadrupole triplets, the intensity of which is 1: 2 (Figure 1 (a)).

Taking in consideration, the probability of filling of the cases Si (1) and Si (2), the low-intensity part of the spectrum was considered to belong to the Zn^{+2} centers in the Si (1) bond, and the high-intensity part of the spectrum to the Zn^{+2} centers in the Si (2) bond. The Messbauer spectrum of the compound $UVa_2Si_3O_6$ consists of a single quadrupole triplet and belongs to a single state of centers Zn^{+2}.

It is known that in T≤420 K in the case of Si (2) in the form of antiferromagnetically ordered for $UVa_2Si_3O_6$, it becomes clear that the spectrum in Fig. 1 (b) belongs to the centers Zn^{+2} of the bond Si (1). Thus, using Messbauer spectroscopy, it is possible to determine the parameters of the electric field gradient tensor in the nuclei of Zn^{-67}, in which case it is possible to observe that the theoretical and experimental values do not fully match.



Picture 1.

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