ISSN (Online): 2455-3662
EPRA International Journal of Multidisciplinary Research (IJMR) - Peer Reviewed Journal
Volume: 7 | Issue: 4 | April 2021|| Journal DOI: 10.36713/epra2013 || SJIF Impact Factor 2021: 8.047 || ISI Value: 1.188

PROBLEMS OF COMPARING THE EXPERIMENTAL AND CALCULATED VALUES OF THE ELECTRIC FIELD GRADIENT TENSOR PARAMETERS FOR IMPURITY ATOMS $^{57}Co(^{57M}Fe)BCuO$ AND Cu_2O

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ANNOTATION

The article is devoted to the study of high-temperature conductors and the physical processes occurring in them using Mossbauer spectroscopy.

KEY WORDS: ***electric field gradient, high-temperature superconductors, Mossbauer spectra, nuclear charge density operator.***

Impurity Mossbauer spectroscopy 12 is widely used to study high-temperature superconductors. This is primarily due to the peculiarities of the nuclear parameters of isotope 21, which make it possible to measure Mossbauer spectra in a wide temperature range, and in this case, Mossbauer spectroscopy makes it possible to reliably determine the charge state of impurity atoms and the parameters of the EFG tensor (electric field gradient) at the location of the probe nucleus. It is assumed that impurity iron atoms replace copper atoms at the lattice sites of high-temperature superconductors (HTSC), so that the experimentally determined values of the quadrupole splitting of the Mossbauer spectra can be compared with the results of their theoretical calculation within the framework of the point-charge model, and based on this comparison, conclusions about the nature of the local environment of copper centers. Of course, such a comparison requires independent proofs of the finding of impurity iron atoms precisely in the copper lattice sites. Unfortunately, in many cases it is impossible to determine the location of impurity atoms only from Mossbauer experiments; this leads to ambiguity in the interpretation of experimental Mossbauer spectra ^{57}Fe in HTSC lattices.

However, even if an impurity iron atom replaces a copper atom, an equally complex problem arises related to the alivalence of the impurity atom (i.e., the valences of the impurity atom and the replaced lattice atom do not coincide). The alivalence of the impurity atom should lead to the appearance of compensating centers in the lattice, which are localized in the vicinity of the impurity atom, and this significantly changes the parameters of the EFG tensor on the nucleus under study.

That is why it seemed to us expedient to compare the experimental and calculated parameters of the EFG tensor for the case of impurity iron atoms in the lattices of simple copper oxides (CuO, Cu_2O).These oxides are typical representatives of compounds of two and monovalent copper, and it is these valence states that are characteristic of HTSC structures. At least for CuO, it is possible to draw a conclusion about the location of impurity atoms from the Mossbauer spectra: copper oxide is an antiferromagnet with a Neel temperature of $T_N = 230K$ and therefore it was expected that if the impurity iron atoms enter copper sites, then at $T < 230K$ the Mössbauer spectra will represent a magnetic sextet (or superposition of several sextets), and at $T > 230K$ - a quadrupole doublet (or superposition of several quadrupole doublets).

As a rule, cobalt in its compounds exhibits a valency of +2, and we expected that the daughter atoms ^{57M}Fe formed after the decay of $^{57}Co^{2+}$ would also be stabilized in the $^{57M}Fe^{2+}$ state. Iron in its compounds exhibits two characteristic valences (+2, +3), and it was expected that under conditions of oxidative

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synthesis, iron will stabilize in the $^{57}Fe^{3+}$ state. Depending on the valence state of copper (+1 at Cu_2O and +2 at CuO), compensation for the excess charge of impurity iron atoms should be accompanied by the appearance of a different number of cationic vacancies (which have an effective charge equal in magnitude to the charge of the copper cation, but opposite in sign).

The Hamiltonian describing the interaction between the nucleus and the surrounding electrostatic field has the form:

$$H = \int P(r_k)U(r_k)dV_k \qquad (1.1)$$

$P(r_k)$ is the operator of the charge density of the nucleus, $U(r_k)$ is the electrostatic potential arising from all charges, except for the nucleus under consideration, dV_k is the element of the volume of the nucleus, r_k is the radius vector between the center of gravity of the nucleus and dV_k. In the vicinity of the center of the nucleus $(r_k = 0)$, the potential $U(r_k)$ changes little and can be expanded in a series. The first term of such expansion is the electrostatic energy of the point nucleus and by choosing the origin of the energy reference, it can be considered equal to zero. The second term describes the dipole interaction, and since $P(r_k)$ is an even function, this term is also zero. The third term of the expansion can be represented as the sum of two terms:

$$H = E_R + H_Q \qquad (1.2)$$

Term E_R describes the interaction of a nuclear charge with an electron cloud and causes the isomeric shift of the Mossbauer spectra. The isomeric shift for most isotopes makes it possible to determine the charge state of the studied atom.

Term H_Q describes the interaction of the electric quadrupole moment of the nucleus with an inhomogeneous electric field (a measure of this inhomogeneity is the electric field gradient tensor, EFG):

$$H_Q = \frac{1}{6}\sum_{ij} Q_{ij}U_{ij} \qquad (1.3)$$

where U_{ij} are the components of the EFG tensor, Q_{ij} are the components of the quadrupole moment tensor of the nucleus.

Due to the axial symmetry of the nuclear charge distribution, all off-diagonal components of the nuclear quadrupole moment tensor are equal to zero ($Q_{ij} = 0$ at $i = j$). For the diagonal components, the Laplace equation is valid

$$Q_{xx} + Q_{yy} + Q_{zz} = 0 \qquad (1.4)$$

and for axial symmetry the tensor can be specified in terms of one component $Q_{xx} = Q_{yy} = -2Q_{zz}$, which is called the quadrupole moment of the nucleus (here x, y, z are the principal axes of the tensor of the quadrupole moment of the nucleus).

The quadrupole moment of the nucleus characterizes the degree of deviation of the nuclear charge distribution from spherical symmetry. The quadrupole moment of the nucleus has the dimension of area and is measured in barns (1 barn =10^{-24}sm^2).

For nuclei with spin $I = 0$ or $I = \frac{1}{2}$, the quadrupole moment of the nucleus is zero. For nuclei with spin $I > \frac{1}{2}$, the quadrupole moment can be nonzero, and for nuclei oblate along the quantization axis $Q > 0$, and for nuclei elongated along the quantization axis $Q < 0$. Here are the Q values for some of the cores that are most often encountered in this work:

$^{17}O - 0,026$ barn, $^{63}Cu - 0,211$, $-0,18$, $-0,16$ barn (the most reliable value is considered to be $-0,211$ barn), $^{139}La + 0,21$ barn.

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If at the location of the core the EGF is created by external charges with axial symmetry, then the EFG tensor can be reduced to a diagonal form, and the Laplace equation (1.4) is valid for the components of the tensor U_{xx}, U_{yy}, U_{zz}. Therefore, the EFG tensor can be specified by two parameters:

$eq = U_{zz}$ is the main component of the EFG tensor,

$$n = \frac{(U_{xx} - U_{yy})}{U_{zz}} \text{ - asymmetry parameter} \quad (1.5)$$

and the choice of the principal axes of the EFG tensor (x, y, z) is based on inequality $|U_{xx}| < |U_{yy}| < |U_{zz}|$.

Replacing components U_{ij} and Q_{ij} in expression (1.3) with parameters q, n, I, Q leads to the expression for the Hamilton operator for the nuclear quadrupole interaction in the axes of the EFG tensor:

$$H_Q = \left[(e^2 Qq) / (4I(2I-1) \right] \cdot \left[3I_z^2 - I(I+1) + n(I_+^2 - I_-^2) \right] \quad (1.6)$$

where $I(+,-) = I_x + iI_y$ is the raising and lowering operators, I is the spin of the nucleus, and e^2Qq is the constant of the quadrupole interaction.

Thus, as a result of the quadrupole interaction, the nuclear level splits into several components, and the levels that differ only in the sign of the magnetic quantum number remain degenerate.

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