CALCULATION OF THE CRYSTALLINE EFG TENSOR FOR LATTICE NODES $YBa_2Cu_3O_{7-x}$

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The tensors of the crystal EFG (electric field gradient) at the cationic and anionic sites of the $YBa_2Cu_3O_{7-x}$ lattices were calculated in the approximation of the model of point charges. Lattice $YBa_2Cu_3O_7$ was written as $YBa_2Cu(1)Cu(2)_2O(1)_2O(2)_2O(3)_2O(4)$ and grating $YBa_2Cu_3O_6$ as $YBa_2Cu(1)Cu(2)_2O(1)_2O(2)_2O(3)_2$.

The tensor components for the n-node were written in the form

$$V_{gpkn} = \sum_i e_k^* U_{gpkn}$$

$$V_{gpkn} = \sum_i \frac{(3(g_{ikn}^2 / r_{ikn}^2) - 1)}{r_{ikn}^5} \quad (1)$$

$$V_{gpkn} = \sum_i \frac{3 g_{ikn} p_{ikp}}{r_{ikp}^5}$$

where k is the index of summation over sublattices $(k=1-y, k=2-Ba, k=3-Cu(1), k=4-Cu(2), k=5-O(1), k=6-O(2), k=7-O(3), k=8-O(4))$ e_k^* is the effective charge of ions, k is the sublattice, i is the index of summation over sites inside the sublattice, r_{ikn} is the distance from the i site of the k sublattice to site n is the sublattice, gp — Cartesian coordinates.

To calculate the components of the EFG tensor of the $YBa_2Cu_3O_6$ lattice, the structural parameters were taken from the work [1], and for the calculation of the EFG tensor of the $YBa_2Cu_3O_7$ lattice, from the work [1]. Some of the calculations were made using the structural data of the authors [2]. For each specific case, we indicate the source of the structural data. We only note that the results of calculations using various structural data are very close. Lattice sums U_{gg} and U_{gp} were calculated on a computer; summation was carried out inside a sphere of radius 30 $\overset{0}{A}$. The tensors of the lattice sums from all sublattices turned out to be diagonal in the crystallographic axes. The main component of the crystalline EFG tensor was determined after substituting the values of e_k^* into (1). The asymmetry parameter of the EFG tensor was calculated from the ratio

$$n_{cr} = \frac{V_{xxcr} - V_{yycr}}{V_{zzcr}}$$

moreover , the principal axes of the tensor of crystalline EFG $\{x, y, z\}$ were chosen proceeding from inequality $|V_{zzcr}| > |V_{yycr}| > |V_{zzcr}|$.

Table 1 shows the results of calculations of the crystal EGF tensor at sites $Cu(1)$ and $Cu(2)$ for the most commonly used models of charge distribution over lattice sites $YBa_2Cu_3O_{7-x}$.

TABLE 1. PARAMETERS OF THE CRYSTALLINE EFG TENSOR FOR COPPER LATTICE NODES $YBa_2Cu_3O_{7-x}$

Charge distribution model	eq_{cr3}, e/A^{03}	n_{cr3}	eq_{cr4}, e/A^{03}	n_{cr4}
$Y^{3+}Ba_2^{2+}Cu(1)^{+}Cu(2)_2^{3+}O_7^{2-}$	0,997	0,02	0,552	0,16
$Y^{3+}Ba_2^{2+}Cu(1)^{2+}Cu(2)_2^{2+}O_7^{2-}$	1,162	0,40	0,700	0,13
$Y^{3+}Ba_2^{2+}Cu(1)^{+}Cu(2)_2^{2+}O_6^{2-}$	-1,252	0,00	0,669	0,00
$Y^{3+}Ba_2^{2+}Cu(1)^{3+}Cu(2)_2^{2+}O_6^{2-}$	-1,569	0,00	0,816	0,00

Литература:

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