Characteristics of the Oxygen Function in High T_c Copper Oxide Superconductors

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Abstract: Comments on the studies of the oxygen functions in high T_c copper oxide superconductors and the effects of isotope were made. And the characteristics of the oxygen functions in high T_c copper oxide superconductors were discussed on the basis of the dual-body structure model of superconductors. It is pointed out that the characteristics of the oxygen functions in high T_c copper oxide superconductors are that they influence the crystal structure and the carriers density and participate in the electron phonons coupling.

Key words: High T_c copper oxide superconductors, electrongetivity equalization principle, crystal structure, electrons phonons coupling.

1. Introduction

Since the discovery of the high T_c superconductivity [1], the study of the micro mechanisms of this new type high T_c copper oxide superconductors has attracted great attention in this field [2-4]. On the basis of some results of experiments, many theoretical models have gradually been set up. But none of the theories have so far been used to make a thorough and comprehensive explanation of the origin of high T_c superconductivity [5-8]. In addition to the key and indisputable results to be obtained, it is more important to analyze and study the change temperature T_c on the superconductors in the high T_c copper oxide superconductors, changes of parameter a of isotopic effects, correlated crystal structure and the decisive factors of the substitution effects which the blending chemical elements should possess. The oxygen elements are only one kinds element in high T_c copper oxide superconductors. The oxygen element and

copper element are completely different in their properties. Moreover, they are formed chemistry bonds and electrons transfer. So, there is a very important question of the oxygen element function in high T_c copper oxide superconductors. The characteristics of oxygen functions in high T_c copper oxide superconductors will be discussed in this paper.

2. Methods

The component particles of superconductivity materials may be separated into two groups: One is closely related to the superconductivity that is the superconductive part, marked is $1 - \omega = N_s/N$ of the total; the other parts, marked is $\omega = N_n/N$ of the total and the two part, $N_s = N_n = N$, are of the same volume and interaction. The particle numbers ω and $1 - \omega$ are irrelative to the temperature, but are decided by the structure and property of the superconduction materials. Note that ω and $1 - \omega$ are relative to the phase formed and to the phase component. The J_c of superconductive materials is determined by the part of $1 - \omega = N_s/N$. The T_c of the superconductivity material is relative to both ω and $1 - \omega$ [9].

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3. Results and Discussion

3.1 Property Characteristics of Oxygen Element

Oxygen element lies in the 11 cycle in the chemical element period table in the IV main clan, belonging to those in sp zone. The atomic electronic structure is $1s^2 2s^2 2p^4$, the usual exhibited valence state is -2 and the ionic electronic structure is $1s^2 2s^2 2p^6$, the electronegativity defined by Puling is 3.5, the radius of ion is 132 pm, the polarizability of ion is $a = 2.4$ (a equals the dipole moment functioned by ions the unit electric field in the numerical value). Since oxygen is of larger electric negativity (paling) [10], in the common chemical reactions electronic charge obtained is -2. Because of the larger polarizability of ions, a polarizing effects are caused when they meet with the positive ions of the smaller radius and high electric charge. Thus, feedback bonds are formed. In many oxides, the distributing number of electric charge on the oxides is smaller than 2, as shown in Table 1.

The characteristics of bond state in the high T_c

copper oxide superconductors Cu and O are $d\pi$ coordination band, whose state has a close relationship with T_c . And its characteristics and bond type depend on the distribution of the oxygen's electric charge on Cu-O bond, as shown in Table 1 [11].

3.2 Study of the Oxygen Effects in the High T_c Copper Oxides Superconductors

There are two stable phases in the $YBa_2Cu_3O_{7-y}$ system of high T_c superconductors, one is perpendicular phase and the other is a square phase. They are decided by the amount of oxygen contained in the samples. When $0.0 < Y < 0.5$, it is the perpendicular phase of high T_c superconductivity and its space group p_{mm} . $0.0 \leq y \leq 0.2$, T_c near 90 K, it approximates a constant, and $0.0 \leq Y \leq 0.4$, T_c will sharply drop to 60 K. When $0.5 < y < 1$, it will change into a square phase and its space group will be P_4/mmm , axis a and b will be in complete symmetry and have no superconductivity. After a through comparison study of $YBa_2Cu_3O_y$ superconductors, it

Table 1 Some of the electric charge in the oxygen in the solid oxides [11].

Compounds	$-\delta_o$	Compounds	$-\delta_o$	Compounds	$-\delta_o$	Compounds	$-\delta_o$
Cu ₂ O	0.41	HgO	0.27	Ca ₂ O ₃	0.19	CO ₂	0.11
Ag ₂ O	0.41	ZnO	0.29	Ti ₂ O ₃	0.21	GeO ₂	0.13
Li ₂ O	0.80	CdO	0.32	In ₂ O ₃	0.23	SnO ₂	0.17
Na ₂ O	0.81	CoO	0.32	B ₂ O ₃	0.24	PbO ₂	0.18
K ₂ O	0.89	BeO	0.36	Al ₂ O ₃	0.31	SiO ₂	0.23
Rb ₂ O	0.92	PbO	0.36	Fe ₂ O ₃	0.33	MnO ₂	0.29
Cs ₂ O	0.94	SnO	0.37	Cr ₂ O ₃	0.37	TiO ₂	0.39
FeO	0.40	CoO	0.40	Sc ₂ O ₃	0.47	ZrO ₂	0.44
NiO	0.40	MnO	0.41	Y ₂ O ₃	0.52	HfO ₂	0.45
CaO	0.55	MgO	0.50	La ₂ O ₃	0.56	-	-
SrO	0.60	BaO	0.68	-	-	-	-

Table 2 Partial electric charges on oxygen of high T_c superconductors Cu-O bond.

No.	superconductor	$-\delta_o$	T_c/K
1	La _{1.85} Ba _{0.15} CuO _{3.93+x}	0.494	26
2	La _{1.85} Sr _{0.15} CuO _{3.93+x}	0.491	37
3	LaBa ₂ Cu ₃ O _{6.5+x}	0.455	75
4	Y _{0.5} La _{0.5} Ba ₂ Cu ₃ O _{6.5+x}	0.451	82
5	YBa ₂ Cu ₃ O _{6.5+x}	0.447	94
6	Tl ₂ Ca ₂ Ba ₂ Cu ₃ O _{10+x}	0.395	125
7	Bi _{1.6} Pb _{0.3} Sb _{0.1} Sr ₂ Ca ₂ Cu ₃ O _{9.85+x}	0.386	132

is concluded that the change of y is very wide, $y = 6.0$ to 7.0 , and at the same time it is found that different numbers of y decide different T_c , even whether it has superconductivity [12, 13]. Guskov, et al. [14] used the air pressure measuring method to decide the deviation from stoichiometry study of y in $\text{YBa}_2\text{Cu}_3\text{O}_y$ system and they found that although y is between $6.30\sim 6.85$, great change have taken place in the quality of materials, from insulators to superconductors. Idemoto, et al. [15] obtained the following conclusions through their studies of the crystal structure of $(\text{Nd}_{0.675}\text{Ce}_{0.325})_2(\text{Ba}_{0.664}\text{Nd}_{0.336})\text{Cu}_{3.00}\text{O}_y$, T_c and oxygen contents.

(1) There is a superconductivity of materials between $y = 9.12\sim 9.14$ and the average valence state of T_c and Cu element is related to y ;

(2) The changes of the bond length of Cu-O on Cu_2O plane is related with the changes of Δy while in the superconductive state CuO_2 plane bond angle is not related with Δy ;

(3) Except for the Cu-O on the CuO_2 plane, other changes of the length of M-O, the changes of the position of M and the moving-away changes of CuO_2 plane increase with the increases of Δy ;

(4) T_c of superconductors is related with the average valence state of Cu on CuO_2 plane which explains Cu and on CuO_2 plane is the key factor to the creation of the superconductivity of the materials.

After Higgins, et al. [16] made the study of the effects of oxygen in $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_{4+\delta}$ electronic

impurified type superconductors, they pointed out that oxygen functions as other high T_c copper oxide superstores.

3.3 Studies of the Isotope Effects of Cu and O

While a study of high T_c copper oxide superconductivity was being conducted, a large number of studies on the effects of the oxygen isotope were made. At the initial stage, the oxygen isotope effects parameter α of La system and Y system was between $0.0\sim 0.02$ [17-20]. As a result, it was popularly believed the origin of high T_c copper oxide superconductivity was different from the description of BCS theory. With the progress of the studies and the improvements on the experimental methods, some new experimental results have appeared. No matter whether they are oxygen or copper, their isotopic effects α are closely related with oxygen contents. It is usually found that the value α of the isotopic effects in the underdoped region is large. And while it is intended to become small to the optimum doped region, the over being-doped becomes abnormally negative.

3.4 The Functioning Properties of Oxygen in High T_c Copper Oxide Superconductors

Through the discussions in Sections 3.2 and 3.3 and combined with the physics model of superconductors' dual body [9], such a conclusion can be drawn as follows: the functions of oxygen in the high T_c copper oxide superconductors are: (1) Oxygen is the sole

Table 3 The values of isotope effects in high in high T_c copper oxide superconductors [21].

Superconductor	α_0	α_{cu}	T_c (K)
La-Sr-Cu-O	$\alpha_0 \approx 0.2$	-	-35
Y-Ba-Cu-O	$\alpha_0 \approx 0.1$	-	-90
Y-Ba-Cu-O	-	$\alpha_{\text{cu}} = 0.01$	-90
$\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$	$X < 0.15$, $\alpha_0 \approx 0.4\sim 0.6$ $X \geq 0.5$, $\alpha_0 \approx 0.1$	-	-
$\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$	$X = 0.15$, $\alpha_0 = 0.15$ $X = 0.125$, $\alpha_0 = 0.91$	$\alpha_{\text{cu}} = 0.1$ $\alpha_{\text{cu}} = 0.93$	-
$\text{Y}_{0.7}\text{Pr}_{0.3}\text{Ba}_2\text{Cu}_3\text{O}_{6.97}$	$\alpha_0 = 0.2\sim 0.24$	-	-
$\text{YBa}_2\text{Cu}_3\text{O}_y$ ($y \approx 6.6$)	-	$\alpha_{\text{cu}} = 0.37$	-

negative ion in the high T_c copper oxide superconductors to participate in structuring the crystals. Thus, oxygen contents influence the crystal structure; (2) The characteristics of the oxygen properties decide Cu-O bond state characteristics in high T_c copper oxide superconductors, forming feed-back $d\pi$ matching bond. (3) The oxygen phonons on CuO_2 plane in the superconductors join in the electrons coupling phonons. (4) The oxygen outside the CuO_2 plane in the superconductors play an important role in regulating the interactions of the carriers reservoir and conducting layers, regulating all the structures of the electrons in the conducting layers and $d\pi$ coordination bonds and influencing the changes of phonon models and further changes of T_c [22]. Piers Coleman's purpose in his presentation in raising the superconductive changing temperature is to seek for the best combination between the superconductors' conducting layers (CuO_2) and carrier reservoirs in the insulating layers [23].

4. Conclusions

By commenting on the studios of the oxygen functions in the high T_c copper oxide superconductors and of the isotopic effects. The functioning characteristics of oxygen in the high T_c copper oxide superconductors have been understood which is beneficial to the exploration the original mechanism of high T_c copper oxide superconductors.

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