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CRYSTAL STRUCTURE AND SUPERCONDUCTIVITY OF $Ba_2YCu_3O_{9-x}$ COMPOUND

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The crystal structure and superconductivity of the compound $Ba_2YCu_3O_{9-x}$ are reported in this paper. The compound has an orthorhombic distorted perovskite structure cell with a=3.892Å, b=3.824Å and c=11.64Å. The temperature at the middle point of superconducting transition is 93.6K.

High T_c superconductivity exists on BaO-Y_2O_3-CuO system.[1] We have studied the phase diagram and phase relations of the system. In the region of rich CuO (>=50mol%) of the system, there are at least three phases whose stoichiometric formulas are close to $Y_{2-x}Ba_xCu_2O_5$ (x=0.03), BaY_2CuO_5 and $Ba_2YCu_3O_{9-x}$ respectively. The single phase sample of $Ba_2YCu_3O_{9-x}$ have been obtained and superconductivity of the compound has been measured.

Y_2O_3(Lb purity), $BaCO_3$(A.R) and CuO(A.R) were used as starting materials. The materials were mixed, ground and pressed into pellets. Then the pellets were sintered at 950°C-1000°C in air about 10h.

The resistivity measurment was carried out by the standard four-probe method. A.C. magnetic susceptibility was measured by the mutual-indutance method and output signals were detected by a PAR-124A lock-in amplifier with reference frequency 314Hz and time constant of 300ms. Phase analysis was made by using Guinier-de Wolff monochromatic focusing camera. X-ray diffraction data were collected with Ru-1000 rotating anode diffractometer. CuK_α radiation was used with pure Si powder as an inner standard and the slit systems 0.5°, 0.5°, and 0.3mm.

The diffraction lines of the compound $Ba_2YCu_3O_{9-x}$ can be indexed with an orthorhombic system of a=0.3892nm, b=0.3824nm and c=1.164nm. The results are listed in table 1. For (hkl) type diffraction, no systematic extinction occurs, so the lattice is preliminary and the possible space group is one of Pmmm, Pmm2 or P222.

The lattice constants of $Ba_2YCu_3O_{9-x}$ are $a \doteq b$ and $c \doteq 3a \doteq 3b$. We can imagine that three possible arrangements of ions and vacancies can give rise the long period along Z direction: (1) ordered arrangement of oxygen vacancies, (2) an ordered arrangement of Ba++ and Y+++, (3) both oxygen vacancies and cations having ordered arrangements. If both the oxygen vacancies and cations together have ordered arrangements, the projection

of the crystal structure along X-Z diection will be that shown in fig.1. In the superconductive phase, because of the electron exchange between Cu+++ and Cu++, the distribution of them may be disordered. According to electrostatic interaction, we consider that the low valence cations Ba++ may gather near the oxygen vacancy layer or have an ordered arrangement, so the lattice distortion takes place and the structural unit cell deviates from the perovskite cubic cell.

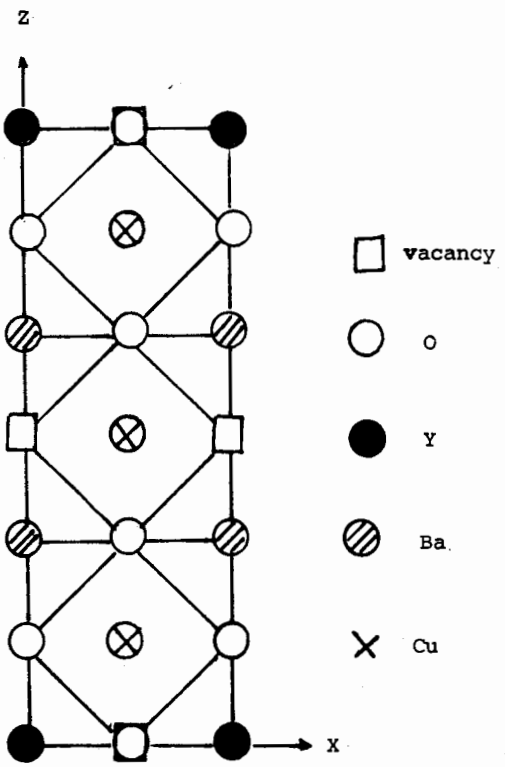

Fig.1 Projection of the imagined crystal structure along X-Z direction.

Because of the oxygen vacancies exist in the crystal structure, Cu coordination polyhedra might be CuO_6 octahedra, CuO_5 pyramid and CuO_4 regular planar. The precise positions of cations and the distribution of oxygen vacancies are now being studied in detail in our laboratory.

The onset of diamagnetism is 91.3K. Temperature at middle piont of zero resistivity transition is 93.6K(fig.2). The compound is an excellent superconductor.

The experimental results indicate in Ba-Y-Cu-O system, in a rather wide region of Y_2O_3 <=30mol%, BaO =10-45mol% and CuO >=50mol%, the superconductive samples with Tc around 90K can be obtained, although compositions and phases in the samples are different.

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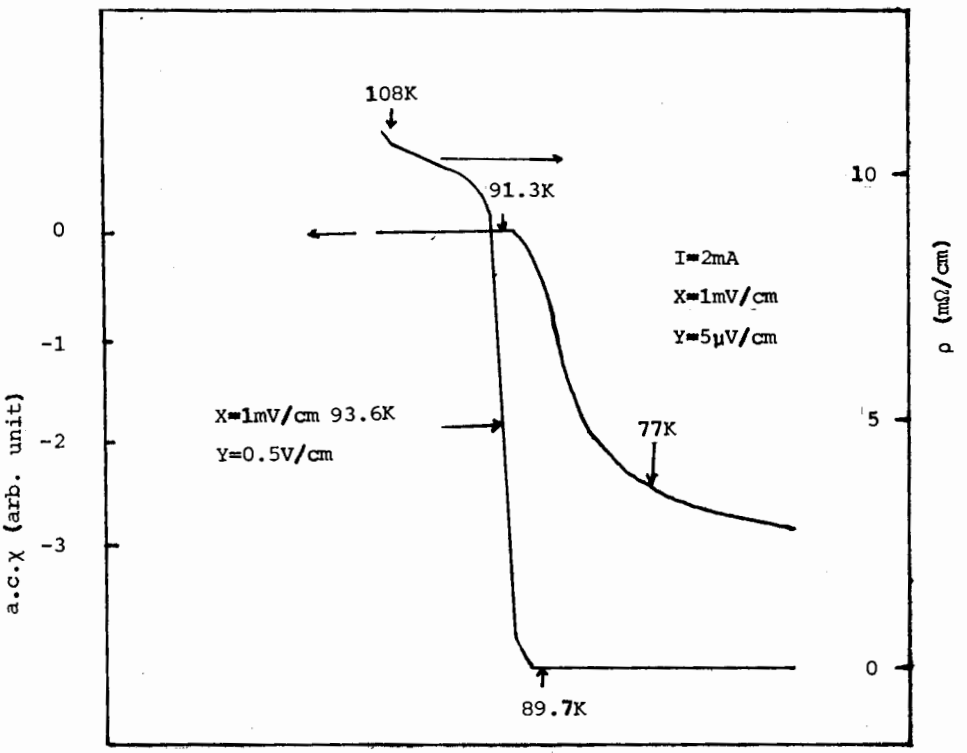

Fig.2 Temperature dependence of Resistivity and A.C.magnetic susceptibility of the compound $Ba_2YCu_3O_{9-x}$.

Table 1

hkl	I/Imax	d(obs)
001	vw	11.65
100(003)	33	3.910
010	2	3.827
102	3	3.264
012	3	3.209
103	82	2.757
110(013)	100	2.730
013	4	2.706
104(005)	10	2.330
113	22	2.238
105(114)	8	1.994

hkl	I/Imax	d(obs)
200(006)	5	1.947
201(020)	21	1.914
115	5	1.778
203(106)(210)	7	1.744
120(211)(023)	4	1.717
007(212)	17	1.670
212	4	1.644
213(116)	44	1.586
123	15	1.571
205(214)	4	1.497
124(025)	4	1.473
117	7	1.426
206	13	1.377
220(108)(026)	25	1.366
302(207)	4	1.263
310(109)(019)	6	1.229
130(033)	7	1.213

REFERENCES

1. ZHAO Zhongxian et al., KEXUETONGBAO, No.6(1987), in press.
2. J.G.Bednorz and K.A.Muller, Z.Phys.B64(1986)189.
3. CHE Guangcan et al., KEXUETONGBAO, in press.
4. XIE Sishen et al., in press.