

10-Physical and Chemical Properties of Materials in Relation to Structure (Superconductors, Fullerenes, etc)

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The degradation in YBCO ceramic can be explained in terms of the formation of non superconducting products by the reaction of YBCO with CO₂, H₂O, etc. from the atmosphere, and in terms of breakage of weak intergrain links.

PS-10.01.26 THE STRUCTURE AND SUPERCONDUCTIVITY OF Nd_{1-x}Y_xBa₂(Cu,Al)₃O_{8+y} SINGLE CRYSTALS. By O.A. Usov*, N.F. Kartenko, I.V. Rozhdestvenskaya, S.I. Goloschapov, S.G. Konnikov, Yu.G. Nosov and V.N. Osipov, A.F. Ioffe Physico-Technical Institute, Academy of Sciences of Russia, Polytechnical str., 26, 194021 St.-Petersburg, Russia.

Isostructural superconducting single crystals: NdBa(2)Cu(2.86)Al(0.34)O(8.5) (I), Nd(0.35)Y(0.65)Ba(2)Cu(2.70)Al(0.30)O(7.0) (II), space group P4/mmm, Z=1, studied by X-ray diffraction method (diffractometer P2/1 Siemens, MoK α). Parameters: a=b=3.914(1), c=11.826 Å, for 323 observed reflections final R=0.058; (II) a=b=3.885(1), c=11.805(2) Å, for 331 observed reflections final R=0.089. The superconductivity properties were measured by the field modulated microwave absorption method in low magnetic field, critical temperature T(c): (I) 10 K, (II) 7 K, weak signal being seen to 50 K. The Al atom was shown to occupy only Cu(1) positions that increases the oxygen contents and connects with the tetragonal symmetry. The large anisotropy of thermal parameters observed for "bridge" oxygen atoms could be interpreted as static displacement. The T(c) were considered to correlate with plane CuO(2) hole density (Tokura, Torrance, Huang & Nazzari, 1988), calculated by the bond valence sum method. For superconductors with low T(c) the hole density was shown to be very sensitive to the rare-earth site occupation factor.

References. Tokura, Y., Torrance, J. B., Huang, T. C. & Nazzari, A. I. (1988). Phys. Rev. B38, 7156-7159.

PS-10.01.27 NEUTRON INVESTIGATION OF La₂CuO₄ AND (Nd,Ce)₂CuO₄ SINGLE CRYSTALS. By A.M. Balagurov, S.N. Barilo, A.I. Beskrovnyi, N.N. Bydanov, K.V. Gamayunov, E.E. Rider, V.A. Sarin*, Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Obninsk Branch of Karpov Physical Chemistry Institute, Obninsk, Russia.

The purpose of this work was to study regularities of the structure defects caused by nonstoichiometry, to determine fine cationic and anionic distributions. The investigations of regularities of the reciprocal lattice, the definitions of twinning law, check of crystal quality were fulfilled on the time-of-flight diffractometer DN-2 with the help of position sensitive detector at the pulsed reactor IBR-2 in Dubna. The neutron diffraction measurements for precise structure calculations were done on the 4-circle diffractometer Syntex PIN at the reactor VVR in Obninsk ($\lambda = 1.167$ Å, $\sin \theta/\lambda = 0.81$).

There were two samples of La₂CuO₄. The sample S1 was annealed and quenched at 1150 °C, the sample S2 - at 400 °C. Neutron experiments for these samples were done at 18 °C and 300 °C. The parameters of elementary cell are

		SP.GR.	a, Å	b	c	V, Å ³
18 °C	S1	C mca	5,369 (3)	13,144 (9)	5,389 (3)	380,3 (5)
	S2	C mca	5,363 (2)	13,147 (13)	5,398 (2)	380,6 (5)
300 °C	S1	I4/mmm	3,811 (2)		13,208 (8)	191,8 (3)
	S2	I4/mmm	3,810 (2)		13,214 (8)	191,8 (3)

L.S. refinement of structure parameters at 300 °C gave R-factors 0,025 for 141 independent reflections for S1 and 0,028 for 143 independent reflections for S2 and next results. In position (c,4mm) parameters z/c are for La 0,36119(6) and for O1 0,1833(1) as for S1 and S2. Site occupations for all atoms in S1 and S2 are exactly 1. But the parameters of thermal vibrations are systematically higher for all atoms in S1

		B eq., Å ²	B11	B22	B33
La	S1	1,10 (1)	1,22 (2)	B11	0,87 (3)
	S2	0,92 (2)	1,04 (3)	B11	0,68 (4)
Cu	S1	0,98 (2)	0,66 (3)	B11	1,62 (4)
	S2	0,79 (2)	0,48 (3)	B11	1,43 (4)
O1	S1	2,56 (3)	3,24 (5)	B11	1,20 (5)
	S2	2,33 (3)	3,01 (6)	B11	0,97 (6)
O2	S1	1,52 (3)	0,69 (4)	1,37 (4)	2,52 (5)
	S2	1,32 (3)	0,47 (5)	1,22 (5)	2,28 (6)

Two samples with the composition Nd_{2,05}Cu_{0,95}O_x (N1) and Nd_{1,90}Ce_{0,18}Cu_{0,92}O_x (N2) were investigated at 18 °C. The parameters of elementary cell are

		SP.GR.	a, Å	c	V, Å ³
N1		I4/mmm	3,9450 (8)	12,170 (3)	189,4 (1)
N2		I4/mmm	3,8480 (1)	12,093 (4)	188,5 (2)

L.S. refinement of structure parameters gave R-factor 0,027 for 139 independent reflections for N1 and 0,028 for 139 independent reflections for N2. The main results are

		x/a	y/b	z/c	B eq., Å ²	site occupation
Nd	N1	0,0	0	0,35098 (8)	0,63 (1)	1,002 (5)
	N2	0	0	0,3515 (2)	0,47 (5)	0,965 (5)
Cu	N1	0	0	0	0,68 (2)	1,00
	N2	0	0	0	0,57 (7)	1,00 (3)
O1	N1	0	0,5	0	0,94 (2)	0,993 (7)
	N2	0	0,5	0	0,96 (9)	1,00 (3)
O2	N1	0	0,5	0,25	0,85 (2)	0,995 (7)
	N2	0	0,5	0,25	0,74 (3)	0,985 (6)

Because the lengths of neutron scattering for Nd and Ce are different but for Nd and Cu are approximately equal we can propose from our experimental results and compositions the next crystal chemistry formula for N1: Nd₂(Cu_{0,95}Nd_{0,05})O_{3,91} and for N2: (Nd_{0,91}Ce_{0,09})₂(Cu_{0,92}Nd_{0,08})O_{3,94}

PS-10.01.28 STUDY ON THE TWINNING OF YBCO-123 PHASE SUPERCONDUCTOR BY USING DIFFERENTIAL INTERFERENCE MICROSCOPE. By Shen Jinchuan Prof. and Wang Wenkui Prof., China University of Geosciences(Wuhan), Wuhan 430074, P.R.China.

A set of wonderful photos showing // {110} twinning of YBCO-123 phase are successfully taken by using differential interference microscope. The YBCO-123 phase crystal grew on the base of microcrystalline corundum. Some of (001) face of YBCO-123 crystal are roughly parallel to the stage of microscope. We select crystal with such orientation and adjust carefully to make the (001) face strictly coincide with the stage plane. twinning striation on the (001) face will show clearly in different interference colors. Changing wave length will cause interference color changed. Combined