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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 CO<sub>2</sub>, H<sub>2</sub>O, etc. from the atmosphere, and in terms of breakage of weak intergrain links.

PS-10.01.26 THE STRUCTURE AND SUPERCONDUCTIVITY OF Nd<sub>1-x</sub>Y<sub>x</sub>Ba<sub>2</sub>(Cu,Al)<sub>3</sub>O<sub>8+y</sub> 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 $\alpha$ ). 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 La<sub>2</sub>CuO<sub>4</sub> AND (Nd,Ce)<sub>2</sub>CuO<sub>4</sub> 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 ( $\lambda = 1,167 \text{ \AA}$ ,  $\sin \theta/\lambda = 0,81$ ).

There were two samples of La<sub>2</sub>CuO<sub>4</sub>. 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 <sup>3</sup>
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 <sup>2</sup>	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<sub>2,05</sub>Cu<sub>0,95</sub>O<sub>x</sub> (N1) and Nd<sub>1,90</sub>Ce<sub>0,18</sub>Cu<sub>0,92</sub>O<sub>x</sub> (N2) were investigated at 18 °C. The parameters of elementary cell are

		SP.GR.	a, Å	c	V, Å <sup>3</sup>
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 <sup>2</sup>	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: Nd<sub>2</sub>(Cu<sub>0,95</sub>Nd<sub>0,05</sub>)O<sub>3,91</sub> and for N2: (Nd<sub>0,91</sub>Ce<sub>0,09</sub>)<sub>2</sub>(Cu<sub>0,92</sub>Nd<sub>0,08</sub>)O<sub>3,94</sub>

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

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optical property observation with the structure study, the relations between tetragonal, pseudo-tetragonal and orthorhombic YBCO phases could be explained properly. Since the planes along (110) and (1-10) are rather similar to each other in orthorhombic phase structure, so its {110} twinning is very commonly developed. because the difference between a and b in orthorhombic structure is very small ( $\Delta = 0.0517$ ), the reciprocal lattice of two individuals in {110} twin almost coincide with each other. It is often mis-recognized as a tetragonal phase.

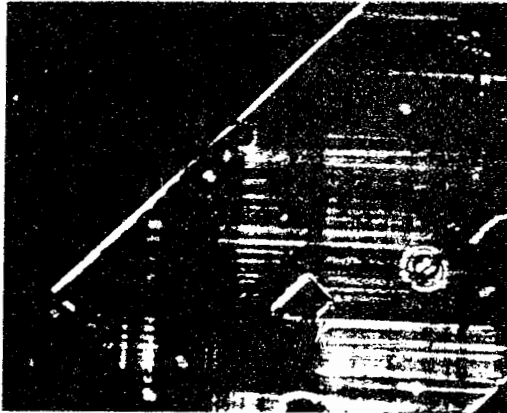


Fig.1 Photo showing // {110} twinning of YBCO-123 phase taken by differential interference microscope

PS-10.01.29 SINGLE CRYSTAL STRUCTURAL ANALYSIS OF YBCO-123 SUPERCONDUCTOR BY USING HIGH POWER X-RAY SINGLE CRYSTAL DIFFRACTOMETER. By Shen Jinchuan Prof. and Wang Yongzai, The Test Centre of Rocks and Minerals, China University of Geosciences(Wuhan), Wuhan 430074, P.R.China.

A crystal structure Analysis of  $YBa_2Cu_3O_{7-x}$  orthorhombic superconducting phase has been done. Sample being tested is prepared by our research group in China University of Geosciences. 892 raw data were collected by using RASA-SRP high power four circles single crystal X-ray diffractometer. Cell parameters are as follows:  $a_0 = 3.8231$ ;  $b_0 = 3.8748$ ;  $c_0 = 11.6721\text{\AA}$ ,  $\alpha = \beta = \gamma = 90^\circ$ , S.G. Pmmm. Coordinates, site occupancies, anisotropic thermal vibration factors, bond lengths and bond angles for all atoms are given in the table below,  $R = 0.06$ .

Table 1 basic data of the YBCO-123 phase structure

A.	COORDINATE			S.O.F.	A.N.	T.F.			P.H.
	X/A	Y/B	Z/C			U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	
Ba	0.0	0.0	0.3140	0.2500	2	0.0145	0.0058	0.0035	723
	0.0	0.0	0.0002	0.0		0.0012	0.0009	0.0010	
Y	0.0	0.0	0.0	0.1250	1	0.0151	0.0055	0.0001	481
	0.0	0.0	0.0	0.0		0.0030	0.0022	0.0022	
Cu(1)	0.5000	0.5000	0.5000	0.1250	1	0.0233	0.0120	0.0001	323
	0.0	0.0	0.0	0.0		0.0044	0.0033	0.0027	
Cu(2)	0.5000	0.5000	0.1431	0.2500	2	0.0111	0.0026	0.0008	362
	0.0	0.0	0.0004	0.0		0.0021	0.0018	0.0021	
O(1)	0.5000	0.0	0.5000	0.0842	0.67	0.0284	0.0048	0.0015	52
	0.0	0.0	0.0	0.0170		0.0352	0.0257	0.0246	
O(2)	0.5000	0.5000	0.3378	0.2500	2	0.0357	0.0181	0.0001	66
	0.0	0.0	0.0023	0.0		0.0164	0.0127	0.0102	
O(3)	0.5000	0.0	0.1242	0.2500	2	0.0177	0.0042	0.0001	64
	0.0	0.0	0.0021	0.0		0.0137	0.0112	0.0098	
O(4)	0.0	0.5000	0.1212	0.2500	2	0.0243	0.0138	0.0007	55
	0.0	0.0	0.0021	0.0		0.0150	0.0126	0.0098	

Table 2 Bond lengths and angles

Ba-O(1) × 2 2.893(2)Å (1 Å = 10 <sup>-10</sup> m)	Cu(1)-O(1) × 2 1.937	90°
Ba-O(2) × 4 2.736(3)	Cu(1)-O(2) × 2 1.893(26)	
Ba-O(3) × 2 2.926(17)	Cu(2)-O(2) × 1 2.273(27)	66.5° (0.5°)
Ba-O(4) × 2 2.969(19)	Cu(2)-O(3) × 2 1.950(3)	
Ba-O(2) 2.736(3)	Cu(2)-O(4) × 2 1.929(3)	89.1° (0.1°)
Y-O(3) × 4 2.399(14)	Cu(2)-O(2) 2.273(27)	
Y-O(4) × 4 2.399(14)		97.6° (0.7°)
		69.1° (0.3°)

PS-10.01.30 TWO SOLID SOLUTIONS OF  $K_2NiF_4$ -TYPE IN NEW THREE-PHASE REGION OF  $LaO_{1.5-x}SrO-CuO$  SYSTEM. By R.S. Bubnova\*, A.S. Novikova, S.K. Filatov, Institute of Chemistry of Silicates, Sankt-Petersburg University, St. Petersburg 199034, Russia.

By X-ray powder diffraction analysis at temperatures below 1150°C a new three-phase region is discovered, in which coexist two solid solutions  $La_{2-x}Sr_xCuO_{4-\sigma}$  (tetragonal cell,  $K_2NiF_4$ -type), (one of which is enriched with La, the other one with Sr), and the solid solution  $La_{2-x}Sr_{1+x}Cu_2O_{6-\sigma}$  (tetragonal cell,  $Sr_3Ti_2O_7$ -type). The values of cell parameter a are similar for both  $La_{2-x}Sr_xCuO_{4-\sigma}$  phases, therefore in powder X-ray patterns of hardened samples, corresponding peaks with small values of the index l for both phases superimpose and practically coincide, making it difficult to separate them. Peaks with large values of l are resolved, as values of the c cell parameters are not identical in both phases. E.g., phases  $La_{2-x}Sr_xCuO_{4-\sigma}$  of a sample of composition  $40LaO_{1.5}/25SrO/35CuO$  after synthesis (950°C) have cell parameters  $a = 3.774(1)$  and  $3.767(1)\text{\AA}$ ,  $c = 13.225(3)$  and  $12.912(4)\text{\AA}$  while the parameters of the phase  $La_{2-x}Sr_{1+x}Cu_2O_{6-\sigma}$  in the same sample have the values  $a = 3.8540(5)$ ,  $c = 20.088(3)\text{\AA}$ . Therefore the chemical composition of solid solutions in the three-phase region at different temperatures was estimated according to the value of a parameter from their elementary cells. At 950°C the three-phase region is made of the solid solutions  $La_{1.5}Sr_{0.54}Cu_{0.96}O_{4-\sigma}$ ,  $La_{0.78}Sr_{1.22}CuO_{4-\sigma}$  and  $La_{1.8}Sr_{1.2+\epsilon}Cu_{2-\epsilon}O_{6-\sigma}$  (value of  $\epsilon$  not exceeding 0.1). With a raise of temperature, the three-phase region narrows due to expanding limits of isomorphous substitutions La-Sr. The structure of the phase  $La_{2-x}Sr_xCuO_{4-\sigma}$  separated by La includes an additional quantity of Sr. Analogously, the phase separated by Sr includes additional La. These phases are registered according to the changes of their lattice parameters.

The result of expansion of the limits of isomorphous substitutions La-Sr is homogenization of solid solutions  $La_{2-x}Sr_xCuO_{4-\sigma}$ , which is registered at temperatures below 1150°C. Due to the homogenization, the three-phase region disappears and the two-phase one expands correspondingly, the latter containing solid solutions  $La_{2-x}Sr_xCuO_{4-\sigma}$  and  $La_{2-x}Sr_{1+x}Cu_2O_{6-\sigma}$ . With the further raise of temperature, the two phase region starts transition to one-phase region of existence of the solid solution.  $(La,Sr)_{2-y}Cu_{1+y/2}O_{4-\sigma}$  of the type  $K_2NiF_4$ . But in fact, the homogenization process is not completed, because there starts disintegration of the phase of the type  $K_2NiF_4$ , which possibly begins with the appearance of the liquid phase. At 1200°C in some samples, beside this phase of a somewhat different composition, there appear traces of the phases of univalent copper  $SrCu_2O_2$  and  $Cu_2O$ , and then the system should be considered a four-component one.