

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

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.

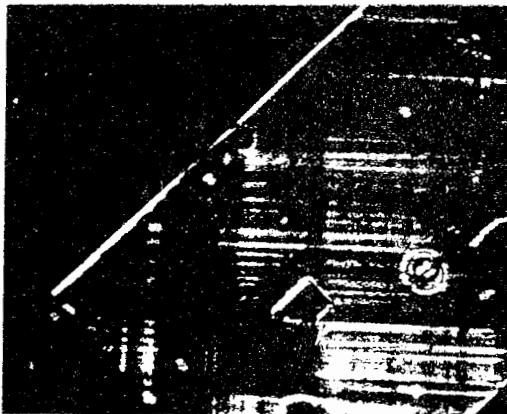


Fig.1 Photo showing // {110} twinning of YBCO-123 phase taken by differential interference microscope

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)	89.1° (0.1°)	
Y-O(3) × 4 2.399(14)	Cu(2)-O(4) × 2 1.929(3)		
Y-O(4) × 4 2.399(14)	Cu(2)-O(2)	2.273(27)	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.