

ESRF

	Experiment title: Phase separation in cuprate superconductors	Experiment number: HS45 (HC 362)
Beamline: BL18/BM29	Date of experiment: from: 12 October 96 to: 18 October 96	Date of report: 25 February 97
Shifts: 18+9	Local contact(s): A. Filliponi, P. Loeffen	<i>Received at ESRF:</i> 8 SEP. 1997

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Report:

We have measured the x-ray absorption-fine-structure (EXAFS) at the Y-K edge of **YBa₂Cu₃O_x** for x=6.806, 6.886, 6.947, 6.986, 6.984 at T=20-300 K. Optimum doping is found to be a notable point in the x-T phase diagram, also concerning the c-axis related displacements of the planar O_{2,3} and Cu₂ atoms. The O_{2,3}-Cu₂ spacing along c is found to be largest at **x_{opt}**. In the underdoped regime doping reduces the Cu₂-O_{2,3} spacing by displacing the O_{2,3} layer towards the Cu₂ layer. In the overdoped regime doping reduces the Cu₂-O_{2,3} spacing by displacing the O_{2,3} layer towards the Cu₂ layer [1,2]. Further we wish to emphasize the following details of the local structure and its vibrational dynamics:

- 1.) The **Y-Cu₂** bondlengths are independent on doping. In the normal phase the **Y-Cu₂** pairs vibrate harmonically, but in the superconducting phase the **Y-Cu₂** vibrations freeze out. On doping the **Cu₂** atoms shift along the c directions towards the Ba layer.
- 2.) The Y-O_{2,3} pairs exhibit strong anharmonicities. The degree of non-Gaussian disorder and the strong anharmonic vibrational dynamics depend significantly on the oxygen concentration. The **Y-O_{2,3}** mean squared deviations do not freeze out in the superconducting phase as the **Y-Cu₂** vibrations. But the mean-cubic deviations of the

Y-O_{2,3} pairs are large, depend on doping, and exhibit a clear singularity at T_c.

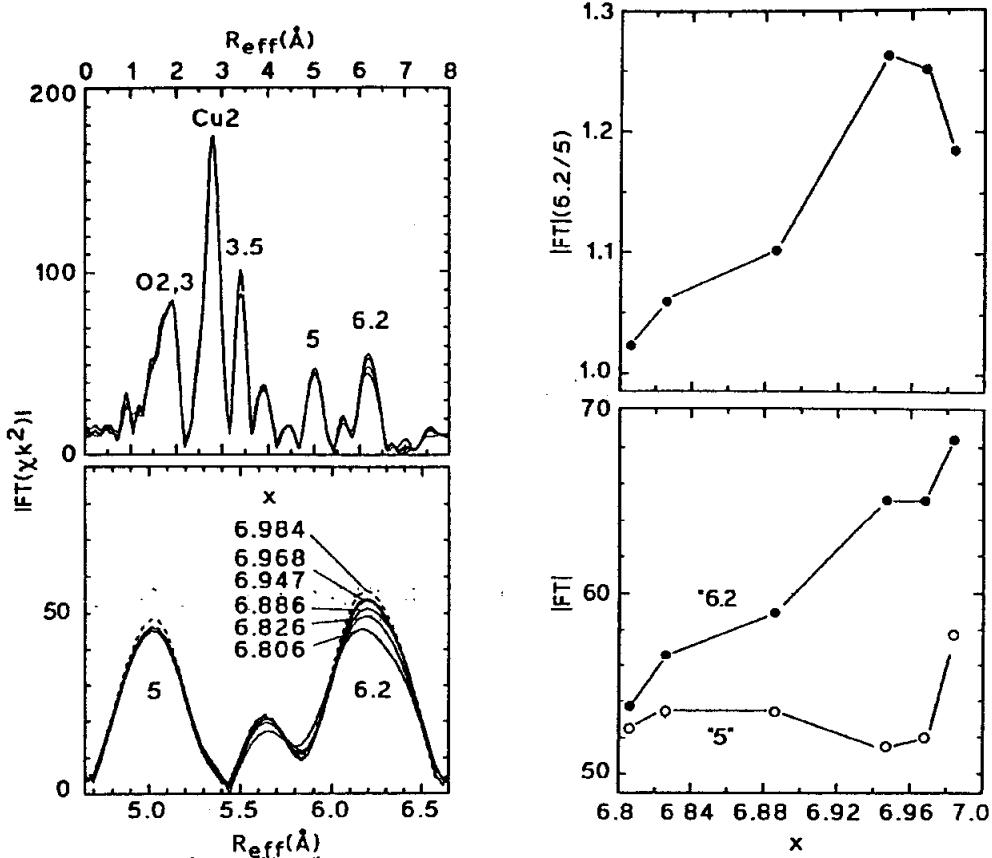


Fig 1. The underdoped-overdoped transition in YBa₂Cu₃O_x. *Left:* Fourier transform spectra of the Y-K EXAFS as a function of oxygen concentration at 90 K. Zoomed are the important Y-O_{2,3}-Ba (“5”) and Y-Cu₂-Ba (“6.2”) multiple scattering peaks, which yield the O_{2,3}-Cu₂ spacing of the dimpled CuO₂ planes. *Right:* The peak heights “6.2” and “5” monitor the c-axis related displacements of the Cu₂ and O_{2,3} layers, respectively. Its ratio clearly exhibits the O_{2,3}-Cu₂ spacing to be largest at optimum doping.

References

- [1] J. **Röhler**, P.W. Loeffen, S. **Müller**, K Conder, E. Kaldis in: “Material Aspects of High Tc Superconductivity: 10 years after the Discovery”, NATO Advanced Study Institute (ASI Series), Eds. E Liarokapis, E. Kaldis. Kluwer (Dordrecht) 1997. 33 pages, 20 Figs. In the press. Also available as electronic preprint: COND-MAT/9701208
- [2] J. Rohler, P.W. Loeffen, K. Conder, E. Kaldis, in: Proc. of the 5th Int. Conf. on Materials and Mechanisms of Superconductivity (Beijing), Physica C, 1997 (invited).

Acknowledgements - We are grateful to J. Jensen, A. Filliponi for the kind help during the data collection. Part of this work has been performed during a stay of J. Rohler as a visiting scientist at the **ESRF**. **He is grateful to B. Lengeler and to the staff of the ESRF for support.**