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Report:

We have measured the x-ray absorption-fine-structure (EXAFS) at the Y-K edge of $YBa_2Cu_3O_x$ 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 O2,3 and Cu2 atoms. The O2,3-Cu2 spacing along c is found to be largest at x_{opt}. In the underdoped regime doping reduces the Cu2-O2,3 spacing by displacing the O2,3 layer towards the Cu2 layer. In the overdoped regime doping reduces the Cu2-O2,3 spacing by displacing the O2,3 layer towards the Cu2 layer [1,2]. Further we wish to emphazise 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-O2,3 pairs exhibit strong anharmonicities. The degree of non-Gaussian disorder and the strong anharmonic vibrational dynamics depend significantly on the oxygen concentration. The Y-O2,3 mean squared deviations do not freeze out in the superconducting phase as the Y-Cu2 vibrations. But the mean-cubic deviations of the

Y-O2,3 pairs are large, depend on doping, and exhibit a clear singularity at T_c.

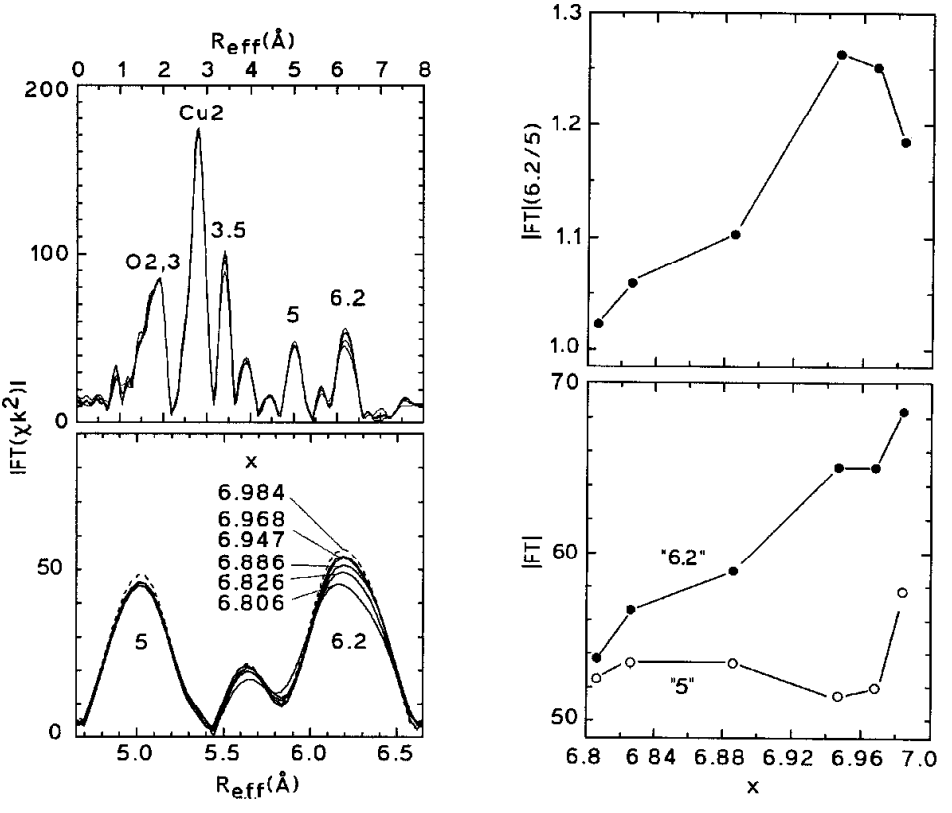

Fig 1. The underdoped-overdoped transition in YBa2Cu3Ox. Left: Fourier transform spectra of the Y-*K* EXAFS as a function of oxygen concentration at 90 K. Zoomed are the important Y-O2,3-Ba ("5") and Y-Cu2-Ba ("6.2") multiple scattering peaks, which yield the O2,3 Cu2 spacing of the dimpled CuO_2 planes. Right: The peak heights "6.2" and "5" monitor the c-axis related displacements of the Cu2 and 023 layers, respectively. Its ratio clearly exhibits the O2,3-Cu2 spacing to be largest at optimum doping.

References

[l] J. Rohler, P.W. Loeffen, S. Müllender, K. Conder, E. Kaldis in: "Material Aspects of High T_c Superconductivity: 10 Years after the Discovery", NATO Advanced Study Institute (AS1 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).

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