ESRF	**Experiment title:** **Phase Separation in Cuprate Superconductors: $Y_{1-y}Ca_yBa_2Cu_3O_{6.98}$ (y=0.02-0.2)**	**Experiment number:** **HS 533**
Beamline: BM 29	**Date of experiment:** from: 9. Febr. 98 to: 17. Febr. 98	**Date of report:** **25-8-98**
Shifts: 21	**Local contact(s):** D. Bowron	***Received at ESRF:*** 03 SEP. 1998

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Report:

Access to the overdoped regime in the phasediagram of the the high-T_c superconductor $YBa_2Cu_3O_x$ may be achieved by full oxygenation of the chain system (x>6.95) and/or by partial substitution of the separating Y^{3+} layer by Ca^{2+}. Although both types of doping, cation substitution in the separating layer, and oxygenation of the so-called insulating layer, increase the hole concentration, n_h, in the conducting CuO_2 layers, they have different effects on the electronic and atomic structure of the compound. For instance it is still a matter of controversy if $Y_{1-y}Ca_yBa_2Cu_3O_6$ (y>0.l), i.e. the completely deoxygentated but homogenously Ca doped compound is superconducting or not. To avoid the poorly defined physical states arising from the usual dual doping (where Ca and 0 doping are considered to be equivalent), we have taken special care to ensure the highest possible oxygenation (x=6.96-6.98) of the compund throughout the complete range accessible by Ca doping (y= 0-0.2) Thus we have been able to extend our systematic investigations of structural and electronic phase separation phenomena far into the o v e r d o p e d regime at most precise chemical conditions.

We have measured the local atomic structure of $Y_{1-y}Ca_yBa_2Cu_3O_6$ (x=6.96-6.98; **y=O**-0.2) by EXAFS beyond the Y-K edge (k < 20 $Å^{-1}$) at low temperatures (20-60 K).

The strongly dampened EXAFS amplitudes ("amorphization") found in some of the previous runs are most probably due to an incorrect thermal treatment. Fig.1 exhibits the dimpling of the CuO_2 planes vs. the Ca concentration as determined from the analysis of

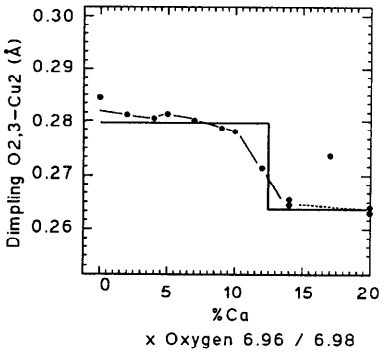

Fig.1
Dimpling in the CuO_2 planes of Ca doped $(Y,Ca)Ba_2Cu_3O_{6.98}$. The step-function indicates the behaviour expected from the critical percolation of the Ca-clusters at $0.09<y<0.16$, T=25 K.

the two nearly collinear multiple scattering paths Y-02,3-Ba (5) and Y-Cu2-Ba (6.2). While the average crystallographic structure (from neutron diffraction) indi-cates that increasing Ca content decreases the dimpling monotonously, the Y-probe of the local structure yields the dimpling to be independent on Ca-doping up to 9%. A step-like decrease by about 0.015 Å occurs around 10% Ca. Obviously the dimples in the CuO_2 planes located next to the Y sites remain unaffected up to a critical Ca concentration. Fig. 2 exhibits schematically (assuming the perfectly ordered case) the percolation of the Ca clusters (white) for 4, 9, 16, and 25 % Ca. Assuming that the divalent Ca atoms distort only the *nn* Y-cells, ≈10% Ca turns out to be the critical concentration for the percolation path connecting the Ca clusters and isolating the Y clusters. We conclude that the additional charge introduced by Ca^{2+} remains essentially localized at the Ca site, and thus the compound tends to decompose into two different electronic phases.The existence of two different electronic phases is also evidenced from a recent analysis of the Meissner effect exhibiting two superconducting transitions: one with T_c= 92 K indepen-dent on Ca substitution, and a second one with strongly decreasing T_c upon increasing Ca content.

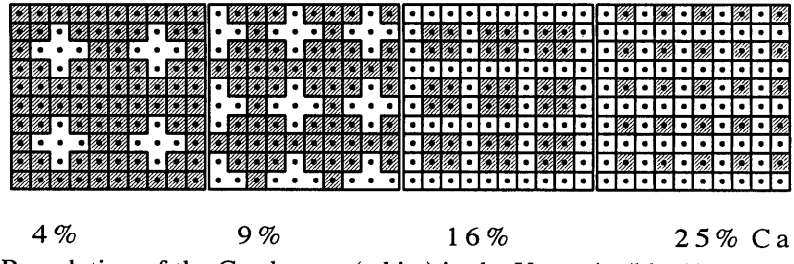

Fig.2: Percolation of the Ca clusters (white) in the Y matrix (black), schematic.