

Local and Electronic Structure of Brominated $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ Determined by Polarized Cu K-edge XAFS

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Beamline(s): X23A2

Introduction: The recovery of superconductivity in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$ (YBCO) by exposure to bromine is a long-standing unresolved problem. Whether Br is chemically substituted the system or if it causes a local decomposition reaction to occur, liberating oxygen, and re-oxygenating underdoped regions remains in dispute.

Methods and Materials: We have performed polarized Cu K-edge XANES and XAFS measurements on brominated YBCO(Br/Cu~1/30, $y\sim 0.6$) sowing $T_c\sim 88\text{K}$. All data were collected in FY using a PIPS detector at 300K.

Results: Polarized Cu K-edge XANES. Cu K-edges of normal and brominated YBCO ($y\sim 0.6$) measured in $\mathbf{E}\parallel\mathbf{c}$ and $\mathbf{E}\parallel\mathbf{ab}$ geometry are shown in Fig. 1. Major changes in the XANES spectra are similar to those observed for oriented powders of YBCO as y goes from 0.23 to 1 [1].

c-axis polarized Cu K-edge XAFS. The FT spectra of the normal and brominated samples are very different (Fig. 2). For Br_YBCO the first peak (due to Cu-O bonds) gets narrow and higher and is shifted to higher r . Fits to the filtered Cu-O XAFS were performed in terms of three constrained models, which differs on number of Cu-O shells. Model 1S implies a single Cu-O bond that has a mean distance for a complex Cu-O pair distribution, possibly a multiphase sample. Model 2S corresponds to YBCO in $\mathbf{E}\parallel\mathbf{c}$ geometry: two Cu(1,2)-O(4) distances and corresponding coordination factors are allowed to vary, while the numbers of the pairs are fixed to 2. Finally, model 3S assumes a mixture of two phases (one has Cu(1,2)-O(4) pairs as in the YBCO family, another one is characterized by an average Cu-O bond of unknown length) is considered. The best fit was achieved for the 3S model. The extracted structural parameters shed some light on the restoration of superconductivity in brominated sample: (i) Cu(1,2)-O(4) distances and corresponding DW factors associated with parent YBCO phase are similar to those expected in optimally doped crystals ($y\sim 0.9-1$); (ii) The unknown Cu-O distance was found to be $1.95\pm 0.01\text{ \AA}$. It is remarkably similar to Cu(1)-O(1) Cu(2)-O(2) and Cu(2)-O(3) distances which were reported to be equal to 1.928, 1.936 and 1.955Å in YBCO($y=0.51$). Note that in $\mathbf{E}\parallel\mathbf{c}$ geometry there should be no contribution from the above bonds into Cu-O XAFS unless these bonds are misalign with respect to the c-axis of the brominated crystal. Therefore, the Cu-O bonds of 1.95 Å should be viewed as constituting the secondary phase incorporated into the "host" crystalline YBCO lattice.

Conclusions: Combining Cu K-edge founding with our Br K-, Y K- and Ba L_3 -edge results [2], the brominated YBCO crystal becomes heterogeneous on an atomic length scales [3]. Heterogeneity brings about unusual structural and electronic properties of the normal state. Our results are consistent with the decomposition mechanism for recovery of T_c .

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References:

- [1] J. M. Tranquada *et al.*, *Phys. Rev. B* **38**, 8893 (1988).
 [2] See also 2001 Reports on Beamlines X11B and X18B for Y K- and Br K-edge XAFS data.
 [3] L. Dieng *et al.*, submitted to *Phys. Rev. B* (2002)

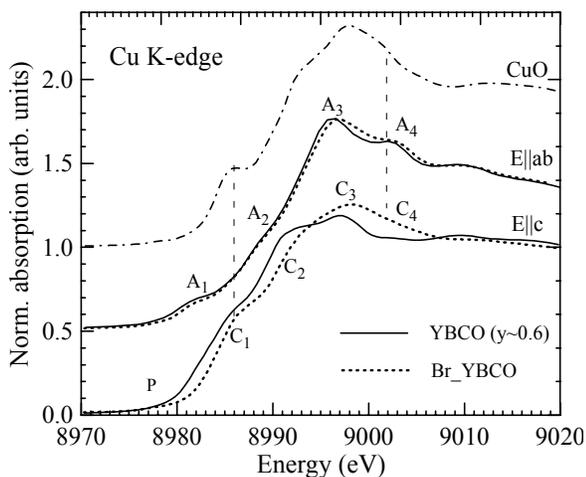


Fig. 1. Polarized Cu K-edge XANES spectra of normal and brominated YBCO.

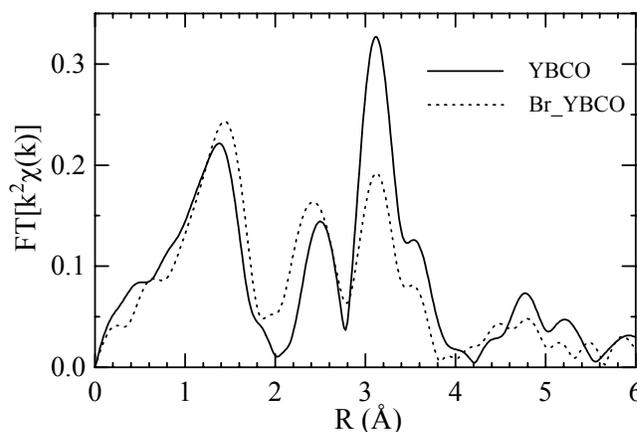


Fig. 2. FT of c-axis polarized $k^2\chi(k)$ spectra of normal and brominated YBCO.