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Role of Br in Brominated Single-Crystal $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ Determined by Polarized Br K -edge XAFS

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Beamline(s): X18B

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 incorporated in one of the crystallographic sites dopes 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 Br K -edge measurements on brominated YBCO ($\text{Br}/\text{Cu} \sim 1/30$, $y \sim 0.6$) with a $T_c \sim 88$ K. All data were collected in FY, using a 13-element Ge detector at 300 K.

Results: Fourier transformed (FT) XAFS data (Fig. 1) clearly show a multiple shell structure about Br. Br K -edge data reveal that Br does not enter substitutionally or interstitially into the *perfect* lattice. However, Br does occupy the Cu(1) site into the fragmented (discontinued) lattice forming Br-O(4)-Ba-Cu₂(1)Cu(2) nano-clusters in which Br-X pairs retain the 3-D structure of pristine YBCO. From the polarized measurements these nano-clusters are almost randomly orientated with respect to the "host" crystal and probably are the nucleus of the decomposed phase. Brominated YBCO gets *heterogeneous* on atomic length scales [1] that 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] See also 2001 Reports on Beamlines X11B and X23A2 for Y K - and Cu K -edge XAFS data.

[2] L. Dieng *et al.*, submitted to *Phys. Rev. B* (2002).

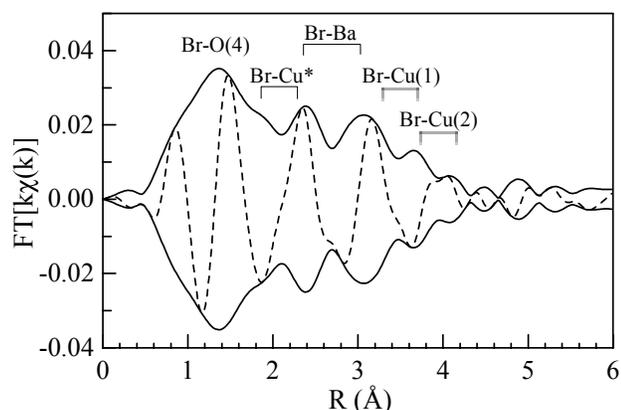


Fig. 1. FT of brominated YBCO. FT range is 2.9-11.4 Å square window. Peak assignment is based on multiple-shell model shown in Fig. 2.

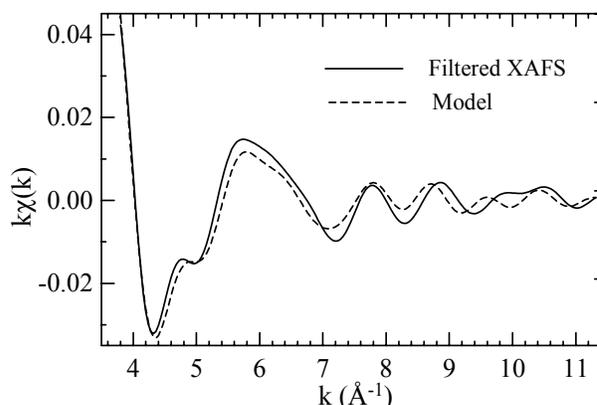


Fig. 2. Comparison of the Fourier-filtered data (solid line) with model involving Br - (O, Ba, Cu) pairs (dashed line). Structural parameters will be provided in [2].