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XANES and EXAFS Study of Au-Substituted $YBa_2Cu_3O_{7-\delta}$

Mark W. Ruckman
Brookhaven National Laboratory
Upton, New York

and

Aloysius F. Hepp
Lewis Research Center
Cleveland, Ohio

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Mark W. Ruckman
Brookhaven National Laboratory, Upton, NY 11973-5000

Aloysius F. Hepp
NASA Lewis Research Center, Cleveland, OH 44135

ABSTRACT

The near-edge structure (XANES) of the Au L_3 and Cu K edges of $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$ has been studied. X-ray diffraction suggests that Au goes on the Cu(1) site and XANES shows that this has little effect on the oxidation state of the remaining copper. The gold L_3 edge develops a white line feature whose position lies between that of trivalent gold oxide (Au_2O_3) and monovalent potassium gold cyanide ($KAu(CN)_2$) and whose intensity relative to the edge step is smaller than in the two reference compounds. The L_3 EXAFS for Au in the superconductor resembles that of Au_2O_3. However, differences in the envelope of the Fourier filtered component for the first shell suggest that the local structure of the Au in the superconductor is not equivalent to Au_2O_3.

INTRODUCTION

Substitution of many metals in $YBa_2Cu_3O_{7-\delta}$ (abbreviated as 123 in the following)[1-5] usually depresses the transition temperature T_c and has other negative effects on the superconducting properties. Trivalent metal ions like Fe, Co, or Al replace linear chain site copper, the Cu(1) site, and depress T_c more slowly than Zn and Ni which replaces copper located on the CuO_2^{2-} sheets, the Cu(2) site. XANES studies[6-8] indicate that transition metal substitutions on the Cu(1) site usually effect the oxidation state of the Cu(2) site and its associated oxygen, but substitution of zinc has little effect on the oxidation state.[9]

Noble metals like gold and silver are exceptional in that considerable amounts of Ag can be put into 123 before T_c begins to decrease[10], Au/123 junctions have a small contact resistance[11,12] and show little evidence of solid state reaction[13]. This is of obvious practical benefit in the fabrication of any device requiring a junction with a normal metal. Streitz et al.[14] examined the microstructure of Au/123 composites and found that separate Au and 123 phases exist after heat treatment in oxygen. They also determined that a small amount of Au ($x < 3$ atomic %) went into the orthorhombic 123 phase.[14] Hepp et al. came to a similar conclusion for $YBa_2(Au_xCu_{1-x})_3O_{7-\delta}$.[15]

We report results of an examination of the Cu K and Au L_3 edges for $YBa_2(Au_xCu_{1-x})_3O_{7-\delta}$. Gold substitution of 8 mole % has little effect on the oxidation state of Cu in 123. The appearance of the L_3 edge suggests that the oxidation state of Au is lower in the superconductor than Au_2O_3 and that Au has fewer unoccupied d-states in 123 than in the trivalent oxide. The appearance of the extended x-ray absorption fine structure (EXAFS) of the Au L_3 edge supports earlier findings that Au is incorporated in the lattice at this concentration.

EXPERIMENTAL

The samples used in this investigation were synthesized and characterized as previously discussed.[15] For $YBa_2(Au_xCu_{1-x})_3O_{7-\delta}$, x-ray diffraction (XRD) and x-ray photoemission (XPS) data suggest that trivalent Au goes into the Cu(1) site. When this occurs, the a and b axes remain unchanged but the c axis expands from 11.69 to 11.75 Å. This is in accord with the well known structural chemistry of Au (i.e., Au(III) forms square planar complexes).[15]

No evidence was found for the formation of secondary phases in the XRD patterns for Au substitutions less than 10 mole %; formation of a second phase was readily detected in the XRD data when more than 10 mole % was put in 123. T_c was observed to be 89 K for an 8 mole % gold containing material and 91 K for the parent 123 material made without Au_2O_3. Very similar conclusions were drawn in a recent study by Cieplak et al.[16], but they were unable to produce single-phase material when substituting Au for Cu. We were only able to obtain single-phase material, as determined by XRD and microscopy when using BaO_2 in the synthesis of the material.[15]

X-ray absorption measurements were made in the transmission mode using powdered samples dispersed on adhesive tape. Au or Cu foil absorbers were placed after the samples to run in conjunction with the samples to maintain a calibrated energy scale. The work was done at the X-11A beamline at the Brookhaven National Synchrotron Light Source).[17] The monochromator resolution is estimated to be 1.0 eV at the Cu K-edge and 1.2 eV at the Au L_3 edge. Samples were crushed into powder, screened through 400 mesh and dispersed onto adhesive tape.

The near-edge and EXAFS data for the Cu K and Au L_3 edges was analyzed using standard procedures.[18] A linear background was removed from the edge before normalization. To extract the EXAFS, the atomic absorption background was approximated by a spline curve. The $\chi(k)$ data was converted from energy space to k-space assuming an E_0 for Cu of 8992 eV and 11,919 eV for Au. The Fourier transforms were computed using a Gaussian window function to obtain a quantity related to the radial distribution function around the absorbing atom.

RESULTS AND DISCUSSION

The Cu K edges for the 123 material (solid line) and the 8 mole percent Au sample (dashed line) are shown in Fig. 1. The Cu K edge is complex and several interpretations of it exist.[19-23] XANES results are now available for highly oriented powders or single crystal materials using polarized x-rays and these provide more reliable data on the Cu K edge.[24-27] The Cu K near-edge structure arises from dipole transitions from the Cu 1s core level to the low-lying copper valence or conduction band states with p or π symmetry and to transitions from the Cu 1s to continuum final states that are modified by multiple scattering (shape resonances). The transitions to bound final states are related to the electron density of states and are sensitive to changes in the chemical state of the Cu while the shape resonances are sensitive to structural modification. Heald et al.[24] examined the Cu K edge from 123 powders oriented such that the x-ray polarization

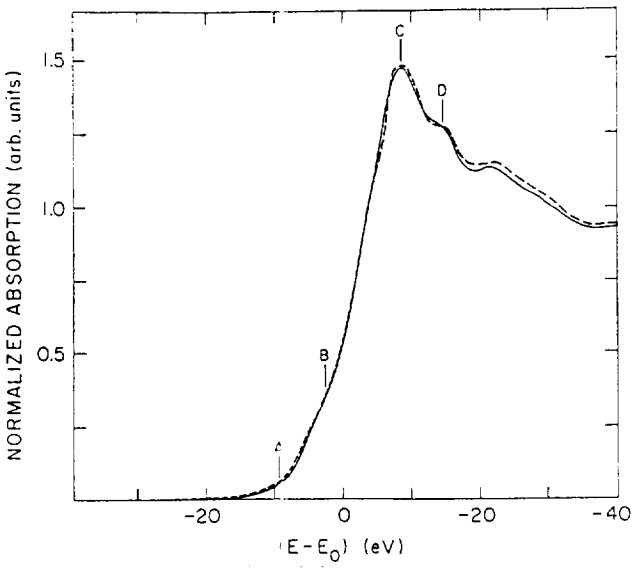

Fig. 1. Cu K edge XANES: $YBa_2Cu_3O_{7-\delta}$ (solid curve) and $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$ (dashed curve). The energy reference was maintained using a copper foil.

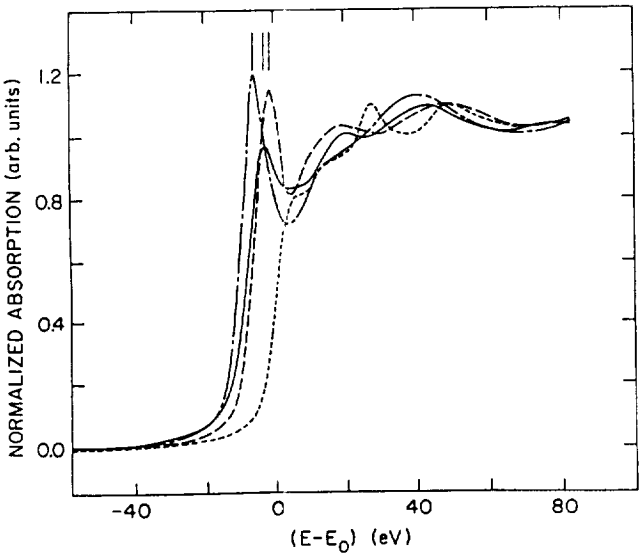

Fig. 2. The Au L_3 absorption edges for Au (dotted curve), a monovalent gold compound - $KAu(CN)_2$ (dashed curve), trivalent gold oxide - Au_2O_3 (dot- dashed curve) and $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$ (solid). A consistent energy reference was maintained by examining the L_3 edge of gold foil simultaneously.

vector ê was either parallel or perpendicular to the c axis. The position of a weak pre-edge feature marked "A" due to 1s to 3d quadrupole transitions is marked on figure 1 and it is directly related to the valence of the Cu. In oxygen deficient 123 material, this peak grows in proportion to the removal of holes from the Cu site and the formation of Cu.[28,29] Peak "B" is due to transitions from the 1s to $4p\pi$ band (Cu(1) and Cu(2) sites) accompanied by shake down transitions ($4p\pi^*$) and peak "C" contains contributions from the 1s to $4p\pi$ and 1s to $4p\sigma$ transitions from the Cu(2) and the Cu(1) sites. The feature marked "D" is identified as a shape resonance. Figure 1 shows the Cu K edges of $YBa_2Cu_3O_{7-\delta}$ and $YBa_2(Au_xCu_{1-x})_3O_{7-\delta}$ to be virtually identical. This suggests that Au substitution has little or no effect on the valence of copper on either site and that the Cu is still formally divalent.

The Au L_3 edges for $YBa_2(Au_xCu_{1-x})_3O_{7-\delta}$, Au foil, monovalent $KAu(CN)_2$ and trivalent Au_2O_3 are shown in figure 2. The spectra for the reference compounds and Au substituted 123 have been normalized to the edge step of the Au absorption edge. The near-edge structure of the L_2 and L_3 edges in 5d transition metal compounds is dominated by $2p_{1/2}$ to $5d_{3/2}$ and $2p_{3/2}$ to $5d_{1/2}$ transitions (white line feature).[30,31] The L_3 edge also has a contribution from the $2p_{3/2}$ to $5d_{3/2}$ but it is much weaker than the $2p_{1/2}$ to $5d_{3/2}$ and

$2p_{3/2}$ to $5d_{1/2}$ transitions. The intensity of this feature is thought to provide a good probe of the 5d-band occupation.[32] For Au (small dashed curve), the 5d band is filled and no white line feature is observed at the L_3 edge. The oxidation of Au to the mono- or trivalent state creates the white line feature. We find that the white line area is a little larger for Au_2O_3 (dot-dashed line) than $KAu(CN)_2$ (dashed line) and also find that the white line feature shifts to lower photon energy when the oxidation number increases from +1 to +3. It should be noted that the ratio of the white line areas for Au_2O_3 and $KAu(CN)_2$ is less than the ratio of d-electron removal suggested by the valence. This means that the actual d-band occupation changes less than expected from simple electron counting. The white line area for Au in 123 (solid line) is smaller than either of the reference compounds and the white line lies at lower energy than $KAu(CN)_2$.

From Au L_3 near-edge data presented for $YBa_2(Au_{0.1}Cu_{0.9})_3O_{7-\delta}$, it is clear that the electronic structure of Au in 123 differs from that of Au in trivalent Au_2O_3. Hepp et al.[15] made an assignment of the trivalent state for Au in the 123 material using XPS measurements of the Au 4f core level. We believe the L_3 near-edge data shows that oxidation state of Au in the 123 material is not equivalent to that of Au in the formally trivalent oxide. Au may be "formally" trivalent in this material but significant departures in the 5d band occupation seem to be taking place. Trivalent Fe also replaces Cu on the chain site. However, substitution of the same amount of Fe depresses T_c by 55 K[33] rather than the 2 K found for Au. Yang et al.[6] found that the Fe substitution modifies the O K edge and reduces the number of 2p holes on the oxygen. We speculate that the reduction in the apparent number of unoccupied Au 5d states for Au in 123 when compared to Au in Au_2O_3 and the small Au induced change in T_c implies that little or no change occurs in the number of the oxygen 2p holes. This is supported by our data for the Cu K edge which shows no change in the Cu-O bonding like that observed when the high T_c material becomes oxygen deficient and holes are removed from the copper and oxygen.[28] We also speculate that the placement of holes on the oxygen nearest neighbors reduces the hybridization of Au 5d states[32] and this is responsible for the smaller L_3 white line area for Au in 123 when compared to Au(III) oxide.

The $\chi(k)$ data extracted from the L_3 edge is shown in figure 3 for $YBa_2(Au_{0.1}Cu_{0.9})_3O_{7-\delta}$ (a), Au_2O_3 (b), and Au (c) . The data are k^2 -weighted to enhance the amplitude of high-k oscillations. The Au L_3 EXAFS functions for Au substituted 123 and Au_2O_3 look similar and are very different from that obtained for Au. The reduction in the strength of the EXAFS oscillations as a function of k suggests that the Au in the superconductor is coordinated by light elements like oxygen rather than a heavy element like Au.[33]

The appearance of the Au L_3 EXAFS provides support for our interpretation of the Au L_3 edge discussed earlier. The reduced strength of the white line could be rationalized by assuming that the L_3 edge is the sum of an oxidized Au component and metallic Au. However, a significant fraction of the Au would have to be in the metallic phase to account for the XANES result. If the Au particles are so small as to preclude getting EXAFS from the Au, it is difficult to see how the gold could have the metallic electronic structure.[34] Hence,

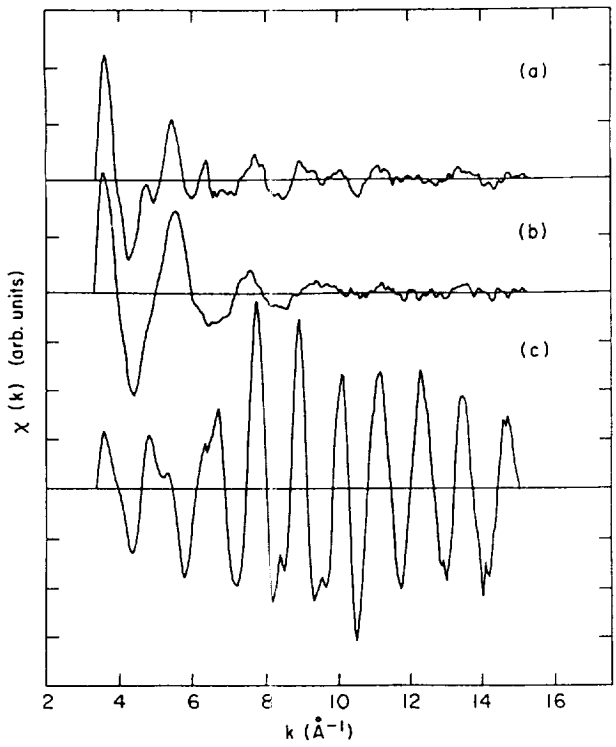

Fig. 3. Au L_3 $\chi(k)$ data for (a) $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$, (b) gold oxide, and (c) metallic gold. The chi data has been weighted by k^2 to enhance the oscillations at large k.

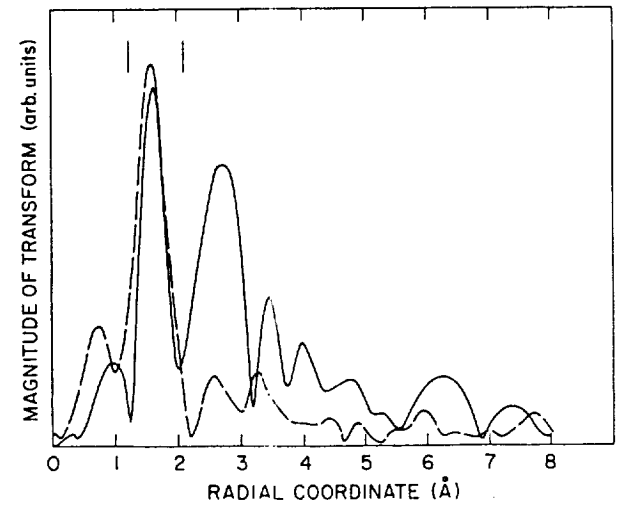

Fig. 4. The Fourier transforms of L_3 edge $k^2\chi(k)$ for Au_2O_3 (dashed curve) and $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$ (solid curve).

we conclude that the gold has not formed a separate metallic component as seen during the formation of 123/Au composites.

In figure 4, the Fourier transforms of the k^2-weighted L_3 $\chi(k)$ data for $YBa_2(Au_{0.1}Cu_{0.9})_3O_{7-\delta}$ (solid line) and Au_2O_3 (dashed line) are shown. The Fourier transformed EXAFS for both $YBa_2(Au_{0.1}Cu_{0.9})_3O_{7-\delta}$ and Au_2O_3 shows a peak located at a radial coordinate of 1.6 Å. This value is close to the first shell radial coordinate measured for copper by a number of groups[35-37] and ourselves for 123 (not shown); detailed analysis of the copper EXAFS[35] indicates a Cu-O spacing of 1.9 Å for the Cu(1)-O bond. Hepp et al.[15] found Au substitution causes little change in the a and b lattice constants and we think the Au-O spacing is nearly equal to that of Cu-O. Detailed analysis of the Au L_3 EXAFS data is hampered by the lack of a suitable Au-O standard.[38] To the best of our knowledge, a detailed structural study of Au_2O_3 has not been performed. We think that Au_2O_3 is highly disordered because the Fourier transformed EXAFS for Au_2O_3 shows only the single peak corresponding to the first shell. Figure 4 shows a second peak at 2.7 Å for the Au-substituted 123 material. X-ray[39] and neutron scattering[40] studies of the structure of $YBa_2Cu_3O_7$ indicate that Ba atoms are located 3.43 Å from the Cu(1) site and the next Cu(1) atom is located at 3.86 Å. Fourier transformed EXAFS

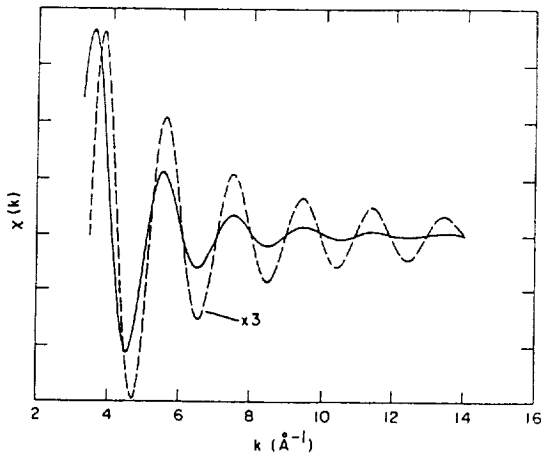

Fig. 5. The Fourier filtered components attributed to the first shells of Au_2O_3 (solid curve) and $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$ (dashed curve).

data for the Cu K edge shows a peak between 2 and 3 Å containing contributions from a higher order shell containing Ba.[35-37]

Figure 5 shows the Fourier filtered first shell contribution to EXAFS for the Au_2O_3 and $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$. The first shell contribution was obtained by back-transforming the region marked by vertical lines in figure 4. The $\chi(k)$ damps out rapidly for Au_2O_3; this can be attributed to the rapid decrease in backscattering amplitude of the oxygen nearest neighbors.[33] The static Debye-Waller term may also serve to diminish the EXAFS signal at higher k values. The $\chi(k)$ term does not decrease as rapidly for $YBa_2(Au_{0.1}Cu_{0.9})_3O_{7-\delta}$, this suggests that the Au-O first shell in 123 is less disordered or has a smaller Debye-Waller factor.

SUMMARY AND CONCLUSIONS

XANES and EXAFS features support earlier studies[15] which concluded that small amounts of gold can be incorporated in $YBa_2Cu_{7-\delta}$ at the Cu(1) site. The gold shows significantly less 5d involvement in the Au-O bond in the superconductor than in Au_2O_3. This could be related to the doping of the oxygen with holes and this is similar to the change in the number of holes on the copper-oxygen component when the material is made superconducting by hole doping. Au has less effect on the superconducting properties than Fe presumably because the gold does not localize holes on itself. There are no obvious changes in the Cu K edge and we conclude that Au substitution has little or no effect on the chemical state of copper or oxygen. Our EXAFS data show that Au is coordinated by oxygen and is in a more ordered environment than Au_2O_3. The lack of a good Au-O standard hinders a more through analysis of the Au L_3 EXAFS. The Cu K edge EXAFS is virtually identical to that published for $YBa_2Cu_3O_{7-\delta}$.

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16. Abstract

The near-edge structure (XANES) of the Au L_3 and Cu K edges of $YBa_2Au_{0.3}Cu_{2.7}O_{7-\delta}$ has been studied. X-ray diffraction suggests that Au goes on the Cu(1) site and XANES shoes that this has little effect on the oxidation state of the remaining copper. The gold L_3 edge develops a white line feature whose position lies between that of trivalent gold oxide (Au_2O_3) and monovalent potassium gold cyanide ($KAu(CN)_2$) and whose intensity relative to the edge step is smaller than in the two reference compounds. The L_3 EXAFS for Au in the superconductor resembles that of Au_2O_3. However, differences in the envelope of the Fourier filtered component for the first shell suggest that the local structure of the Au in the superconductor is not equivalent to Au_2O_3.

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