The Investigation of the Structure Distortion in the Single Crystals of $Sr_2YRu_{1-x}Cu_xO_6$

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$Sr_2YRu_{1-x}Cu_xO_6$ (SrY2116 for brevity) solid solutions have been found to be superconducting [1] while the parent compound without Cu is and antiferromagnetic insulator [2]. Single crystals of SrY2116 (x = 0-0.5) were grown from high temperature solutions of PbO-PbF_2 and found to exhibit a diamagnetic transition indicative of superconductivity [3]. Since X-ray absorption spectroscopy (XAS) measurements are sensitive to the electronic states and the structural symmetry of the sites of the absorbing atoms it is a powerful tool in determining the electronic properties of materials. We have used x-ray absorption near-edge structure (XANES) to explain the magnetic and superconducting properties of these crystals

XANES measurements were performed at the beamline 11-A1 (Dragon beamline) and 20A (HSGM) of NSRRC. Total-electron-yield (TEY) mode was used for data collections

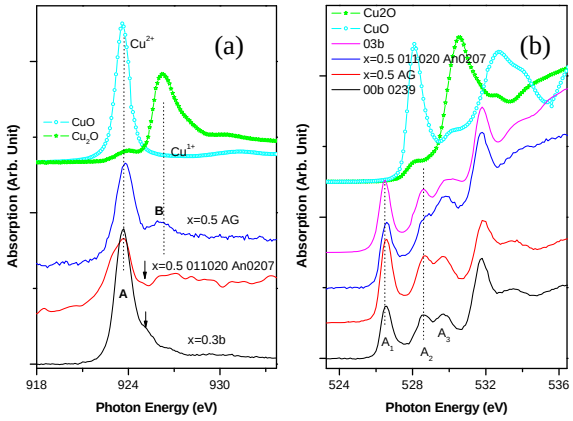

Figure 1. The XANES spectra of SrY2116 crystals (a) Cu L_3-edge (b) O K-edge

Fig. 1 (a) These spectra are related to the Cu 3d unoccupied stated, which are in good agreement with published results[4]. These two peaks correspond to the electronic valence state of Cu(II) and Cu(I) respectively in all the samples. A small feature observed between A and B peak. It has been attributed to the empty state of the Cu-O band bonding residing in the $3d^9\underline{L}$ ligand state, where a hole is located in the oxygen ions surrounding 'doped Cu site' ($\underline{L}$, a ligand hole, we may be tentatively labeled $3d^8$-like). The hole carrier concentration is found to increase in the annealed crystals.

The Fig 1(b) shows the O K-edge spectra recorded at room temperature. the octahedral crystal field splitting the t_{2g} and e_g bands are observed at 528.6 (A_1) and 529.7eV (A_2, A_3). It is not easy to separate the contributions from the 3d (Cu) and the 4d $t_{2}g$ (Ru) in the A_1 complex peak. The A_2 and A_3 peak are attributed to the splitting of Ru 4d e_g band. They correspond to the perovskite structural distortion due to Jahn-Teller effect. The energy of J-T splitting ($\Delta E_{J\text{-}T}=E_{A3}-E_{A2}$) is found to increase from 1eV of x=0.5 AG to 1.2eV of x=0.5 An crystal. The e_g band is more sensitive to the environment of the central atom. In the presence of Cu, x and y axis shrink and the z axis elongates resulting in a structural distortion. The orbital orientation in the transition metal 4d (Ru) interchange with the 3d (Cu) as a result of the crystal distortion and result in the oxygen holes in the annealed samples.

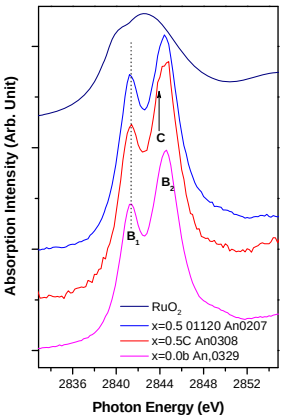

Figure 2. Ru L_3-edge spectra of SrY 2116 x=0.5 (a) AG and (b) An along with RuO_2 standard

The Fig. 2 shows the Ru L_3-edge spectra along with RuO_2 standard. Peak B_1 and B_2 are basically assigned to 4d t_{2g} and e_g band, respectively. The peak B_2 is observed as a shoulder C between the B_1 and B_2. This is a further confirmation of the crystal structure distortion (i. e. the structure extend/shorten in a-b/c axis of the octahedral symmetry) on Cu doping.

Taking into the transport properties of the bulk and crystals in the light of the above discussion, it may be concluded that the resistive transition seen in these is a result of the superconductivity brought about by the Ren-Wu model [5] and not from the presence of minor phases.

Reference:

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