Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: XPS investigation of the YBa_2CuO_3O_7-6
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DOI: https://doi.org/10.5169/seals-116119

XPS INVESTIGATION OF THE $YBa_2Cu_3O_{7-\delta}$

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In the latest years many papers reported about XPS investigations on $YBa_2Cu_3O_{7-}$ (YBCO) samples [1]. Most of these reports dealt with Cu 2p and/or O 1s lines in $\delta \approx 0$ samples. Very few papers reported XPS spectra of all the four YBCO elements and, in our knowledge, none of them in both the semiconductor and superconductor phases. On the contrary, we think very important to study the spectra of all the four elements and their evolution with the stoichiometry to try to find possible correlations helpful in the understanding of the superconductive behaviour.

In this preliminary report we show the most relevant peaks of Cu, O, Ba and Y in samples with values of $\delta \approx 0$ and $\delta \approx 1$.

Samples were syntered ceramic disks annealed for 12 hours at 500 C in flowing oxygen. After the introduction in the UHV system they were scraped before each measurement. They were also exposed to oxygen at increasing exposures between 10 and 1000 Langmuir (1L=1s at 10^{-6} torr). Some samples were sputtered with Ar ions at 5 KeV. The measuring apparatus was a Leybold emispherical analyser with a 15 KV X-ray Mg source. The overall resolution was 0.9 eV.

To a careful analysis each spectrum shows a composite structure which changes with . and the surface treatment. A first semi-quantitative analysis of these spectra enables the following conclusions:

- Cu $2p_{3/2}$. As well known this spectrum is formed by a main line and a satellite corresponding to

differently screened complex final states. Limiting ourself to the main line (as the d^9 satellite shows a multiplet structure) it is possible to fit it with the sum of two components that we associate to Cu^{2+} and Cu^{1+} in analogy to what shown for CuO [2]. Their relative weights change with the stoichiometry from about 49% and 51% respectively in samples with $\delta \simeq 1$ to about 83% and 17% for $\delta \simeq 0$. It is worth noting that upon oxygen exposure it is the Cu^{1+} component which increases.

- O 1s. It is well established [1] that even in "good" superconductor two peaks appears in the O 1s spectrum. One at -528.5 eV and the second at -531.5 eV with a weight at least 70% of the main one. We found this second peak about 90% for $\delta \simeq 0$ and about 60% for $\delta \simeq 1$. In both samples upon oxygen exposure the relative intensity of these peaks increases slightly.

- Ba $3d_{5/2}$. In the superconductor samples a clear asymmetry is observed on the low binding energy (B.E.) side of the peak at -779.3. The difference between the spectra corresponding to the two δ values is a small peak at -777.7 eV B.E., with a weight of about 12.5 %. A similar shifted component had been observed in the 4d doublet by Steiner et al.[3].

- Y 3d. This spectrum shows a tail on the high B.E. side and can be fairly well fitted by the sum of two doublets identical in shape with the larger at -156.1 and the smaller shifted by about 2 eV at higher B.E.. Its weight is about 12% for $\delta \simeq 0$ and reduces to about 9% for $\delta \simeq 1$. It also reduces upon oxygen exposure or sputtering.

A more detailed analysis of these data is in progress with particular attention to the role of the screening of O 2p holes.

[1] J.C. Fuggle et al.:Int.J. Mod. Phys. B1, 1185 (1989)
[2] F. Parmiggiani and G. Samoggia: to be published
[3] P. Steiner et al.: Z. Phys. B69, 449 (1988)