

**Experiment title:**High Resolution directional Compton Profiles measurements in single crystal $\text{YBa}_2\text{Cu}_3\text{O}_7$ and $\text{PrBa}_2\text{Cu}_3\text{O}_7$ **Experiment number:**

HE66

Beamline:

ID15B

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30

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Report:

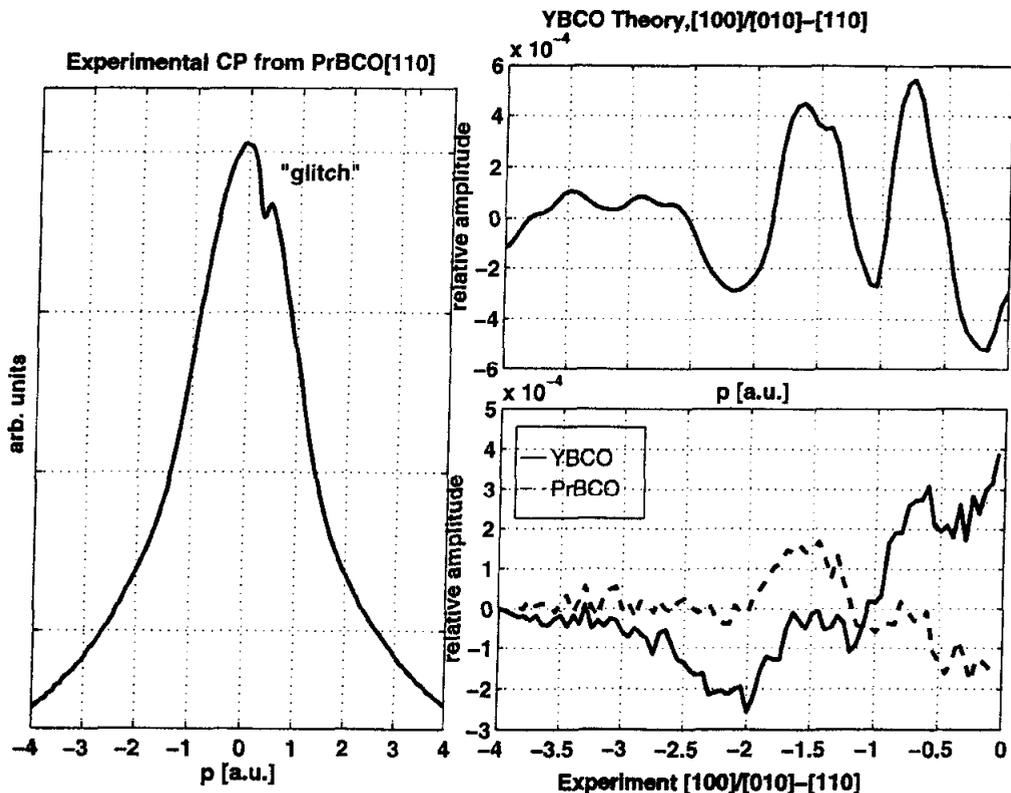
This experiment had several difficult aspects to it, all related to the nature of the samples. Firstly samples are small, typically $1\text{mm} \times 1\text{mm} \times 0.3\text{mm}$. Absorption being high in these samples, full use of the available beam size has to be made to get a respectable count-rate and to do this we mounted three samples in a stack formation. These samples had been **previously** cut to a triangular shape to facilitate the measurement of the two crystallographic directions, $[100]/[010]$ and $[110]$. Another problem was the high background due to Ba fluorescence, which was solved partly by implementing for the **first** time, an energy analysis of the incoming photons seen by the **NaI** scintillator. Apart from increasing the background, fluorescence lines were also detected by the off-equatorial (3,3,1) planes of the Ge 440 analyzer as intense features distorting the Compton profile substantially and the only way to overcome this completely was to change the analyzer crystal.

Accordingly we switched to a Ge 440 crystal with a different axial orientation. A sample spectrum for the $\text{PrBa}_2\text{Cu}_3\text{O}_7$ (**PrBCO**) $[110]$ orientation, after standard corrections is shown in figure 1. It can be seen that near the Compton peak, a 'glitch' appears in the data which is due to the fact that at this particular energy the Bragg condition is fulfilled for an off-equatorial reflection which is not seen by the detector, resulting in a local loss of intensity. Spectra were collected for both samples in the two crystallographic directions proposed. The total number of counts in the peaks of the profiles varied from $4 \cdot 10^5$ to $6 \cdot 10^5$. The countrate obtained at the Compton peak was 800 counts/set.

The data were subjected to the standard treatment for corrections including absorption, analyser reflectivity and analyzer acceptance. The background correction mentioned earlier turned out to be very efficient and only a small additional subtraction, using a polynomial fit was made and it was checked that this correction itself did not introduce any features. The spectra were then folded taking into account the symmetry of the Compton profile. The directional differences obtained are shown in figure 2. The upper figure is a FLAPW calculation for $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO), and the lower figure the experimental difference obtained for YBCO (solid line) and PrBCO (dashed line). The glitch seen in figure 1 is a problem in data analysis since it's proximity to the Compton peak means that in some spectra it extends beyond it, so that the symmetry of the Compton profile cannot be used reliably to compensate. This means that data in the range between 0 and 0.5 a.u. is not reliable.

The following remarks are to be made:

- The amplitude of the experimental anisotropy is about 60% of that predicted by theory. The anisotropy is larger in YBCO than in PrBCO.
- The behaviour of the difference profiles for YBCO and PrBCO is different. This is remarkable because the momentum density as seen by positrons, which sample only the Cu-O chains in these compounds is identical for the two compounds. This indicates that the difference is related to the fundamental difference between the Cu-O layers in PrBCO and YBCO and maybe induced at least in part, by the Fermi surface.
- Though some features correspond there are differences between the theoretical prediction and the experiment for YBCO. These differences are probably due to the fact that the Local Density Approximation used in the band structure calculations is inadequate to describe the electronic structure in the Cu-O planes.



figure(1)

figure(2)