



Experiment title: Measurement of momentum space densities of $\text{Cu}_{1-x}\text{Al}_x$ by means of high resolution Compton scattering	Experiment number: HE 392	
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Report:

Compton profiles $J(p_z)$ are the one-dimensional projections of the electron momentum space density on the direction of the scattering vector \vec{q} . We have performed measurements of Compton profiles for ten different directions of \vec{q} on single crystal $\text{Cu}_{0.9}\text{Al}_{0.1}$. The Rowland spectrometer used consists of a focussing Si(3 11) monochromator, a Ge(440) cylindrically bent analyzer and a NaI detector. An additional Ge solid state detector was used for monitoring. We achieved an average momentum resolution of 0.2 a.u. with an incident energy of 56.18 keV. Each Compton spectrum contains 547 points over an energy range from 39.62 - 56.75 keV. The total number of counts per spectrum is approximately 25×10^6 . The collected data complete a series of measurements on $\text{Cu}_{(1-x)}\text{Al}_x$ with $x = 0, 0.047$ and 0.1 .

The measured Compton spectra have been corrected for absorption, analyzer reflectivity and vertical acceptance of the spectrometer. Furthermore the contributions of multiple scattering, Compton scattering of the core electrons and the scattering background have been subtracted and the resulting valence Compton profiles have been normalized to the mean number of valence electrons per atom.

Differences between Compton profiles for different directions of \vec{q} yield information about the anisotropy of the momentum density. As an example fig. 1 shows the difference between the Compton profiles of $\text{Cu}_{0.9}\text{Al}_{0.1}$ for $\vec{q} \parallel [100]$ and $\vec{q} \parallel [110]$. Differences of corresponding KKR-CPA calculated profiles [1] are in good agreement with our experimental findings.

Furthermore we used the Fourier-Bessel method to reconstruct the full 3-dimensional momentum space density from its ten projections. The procedure leads to an expansion into lattice harmonic functions where the first term in the series describes the isotropic part of the distribution.

Fig.2 (left) shows the anisotropic part for $\text{Cu}_{0.9}\text{Al}_{0.1}$ in the $(\bar{1}10)$ plain. The large positive anisotropy in $[111]$ direction is caused by the $[111]$ high momentum component leading to a continuous momentum distribution across the boundary of the 1st Brillouin zone. The height of this peak seems not to be linearly correlated to the Al-concentration as it increases from Cu to $\text{Cu}_{0.953}\text{Al}_{0.047}$ but decreases from $\text{Cu}_{0.953}\text{Al}_{0.047}$ to $\text{Cu}_{0.9}\text{Al}_{0.1}$.

[1] KKK-CPA calculations by A.Bansil and S.Kaprzyk, unpublished

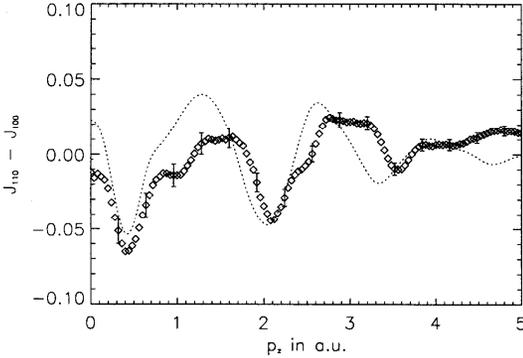


Fig. 1: Compton profile difference $J_{110}(p_z) - J_{100}(p_z)$ of $\text{Cu}_{0.9}\text{Al}_{0.1}$.
solid line: KKK-CPA profiles
data points: experiment

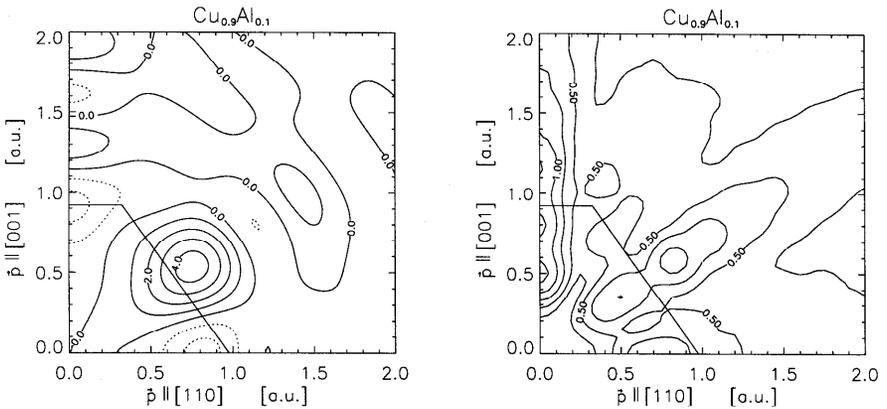


Fig.2: Anisotropy of the momentum density ($\times 100$) of $\text{Cu}_{0.9}\text{Al}_{0.1}$ in the $(\bar{1}10)$ plain (left) and the corresponding error map (right). Positive and negative anisotropies are marked with solid lines and dashed lines respectively. The boundary of the 1st Brillouin zone is marked by solid lines.