ESRF	<b>Experiment title:</b> Measurement of momentum space densities of $Cu_{1-x}Al_x$ by means of high resolution Compton scattering	Experiment number: HE 168
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Names and affiliations of applicants (\*indicates experimentalists):

W. Schtilke, G. Döring\*, A. Kaprolat \*, C. Sternemann\* Universität Dortmund, Institut für Physik, D-44221 Dortmund, Germany

S. Kaprzyk

University of mining and metallurgy, 30-059 Krakow, Poland

F. Maniawski, J. Kwiatkowska Institute of nuclear physics, 31-342 Krakow, Poland

## Report:

Compton profiles  $J(p_z)$  yield information about the one dimensional projection of the electron momentum density on the direction of the scattering vector  $\vec{q}$ . Therefore measurements of  $J(p_z)$  for a sufficient number of directions of {provide the possibility to obtain the full 3-dimensional electron momentum density and the occupation number function.

We have performed Compton profile measurements on  $Cu_{0.053}Al_{0.047}$  for 10 directions of  $\vec{q}$  with about 2 x  $10^7$  counts per spectrum, a primary energy of 55.9 keV and a resolution of approximately 0.2 a.u. in  $p_z$ . Each spectrum contains 561 points over an energy range from 39.6 - 57.4 keV.

Unfortunately the Compton profiles were effected by an unwanted n-beam case reflection within the analyzer resulting in a "glitch" near  $p_z \approx +2.2a.u$ . Therefore this region of the Compton profiles could not be taken into account at the expense of statistics.

After a correction for energy dependent effects (absorption, reflectivity, vertical acceptance) and multiple scattering similar to previous measurements on Cu (see report to HE 65), the electron momentum densities and the occupation number function of Cu and  $Cu_{0.953}Al_{0.047}$  have been reconstructed using the Fourier-Bessel method<sup>1,2</sup>.

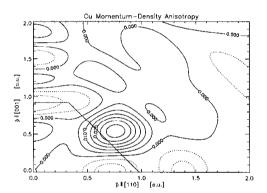
Fig. 1 shows the anisotropic part of the momentum density of Cu and  $Cu_{0.953}Al_{0.047}$  in the  $(\overline{1}10)$  plane. One can see the large anisotropies near the boundary of the  $1^{st}$  Brillouin-Zone in the [ 100] and the [ 11 1] direction and their increase with Al concentration. This increase is beyond statistical errors which was proved by an error map calculation. These features arise from the [ 11 1] high momentum component which causes a continuous momentum density distribution across the boundary of the  $1^{st}$  Brillouin-Zone.

On the other hand band structure calculations show a steep decrease of the mometum density at the Fermi momentum in the [100] direction and therefore a positive anisotropy in the [111] and a negative one in the [100] direction.<sup>3</sup>

Fig. 2 shows the occupation number function of Cu and Cu<sub>0.953</sub>Al<sub>0.047</sub>. The well known neck-structure is visible in the [111] direction and the radius of the necks also increases with Al concentration.

To find out if this effects persist at higher Al concentrations we plan to perform measurements on Cu<sub>0.9</sub>Al<sub>0.1</sub>.

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- [3] P.E. Mijnarends, Physica 63,235 (1973)



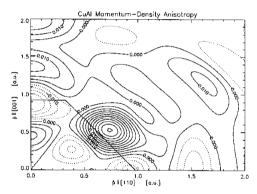
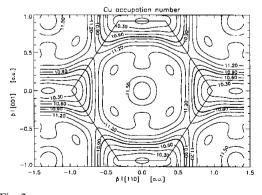


Fig. 1: Cu and  $Cu_{0.953}Al_{0.047}$  electron momentum density anisotopy. Positive and negative anisotropies are marked **with solid** lines and dashed lines respectively.

The boundary of the 1st Brillouin-Zone is marked by the solid line.



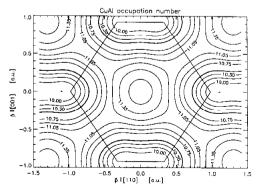


Fig. 2: Cu and  $Cu_{0.953}Al_{0.047}$  occupation number function. The bold line marks the Fermi surface The boundary of the  $1^{\rm st}$  Brillouin-Zone is marked by the solid line.