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A Study of Bonding in Copper by QCBED Measurements

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A new set of high accurate low order structure factors of copper have been measured with quantitative convergent beam electron diffraction (QCBED). Since the charge distribution between atoms depends most on the low order structure factors, the results will be used to investigate bonding in Cu.

The QCBED experiments were done using a LEO 912B electron microscope operating at 120 kV equipped with an in-column Ω-filter and a Gatan MSC CCD camera. The sample, a pure electrolytic polished copper foil, was kept at liquid nitrogen temperature in order to avoid contamination and to reduce phonon scattering. The structure factors are obtained by comparing sensitive line scans of the CBED pattern with Bloch wave simulations [1] of the same intensities. In fig. 1a and 1b the best fit is plotted together with the chosen line scans. Several measurements are done for each spot with different beam directions and sample thicknesses in order to ensure consistency and to get good statistics. The electron structure factors, so obtained, are converted into X-ray structure factors using the Mott formula. They are also converted to zero temperature assuming the adiabatic harmonic approximation for thermal vibrations.

In fig. 2a the obtained structure factors are plotted relative to the neutral atom values [2]. A charge density difference map is calculated in fig. 2b, by Fourier transformation of the difference between the measured structure factors and their corresponding neutral atom values. Even though this map may contain big truncation errors, it shows higher charge concentration between nearest neighbors than second nearest neighbors, which indicates that pure metal bonding is not a sufficient description of copper. To further investigate the bonding a multipole refinement will be done.

In table 1 the measured structure factors are compared to neutral atom values [2], a self-consistent band-structure calculation [3] and density functional theory calculations using the linearized-argumented-plane-wave algorithm of WIEN2K [4]. Both the local density approximation (LDA) and the generalized gradient approximation (GGA) were tested. As a measure of how well these calculations fit the experiment, the residual (R) is listed in the bottom of the table. Best fit is obtained with the GGA calculation. This agree with the results in [5], where GGA was found to give a good description of the valence electrons. [6]

References

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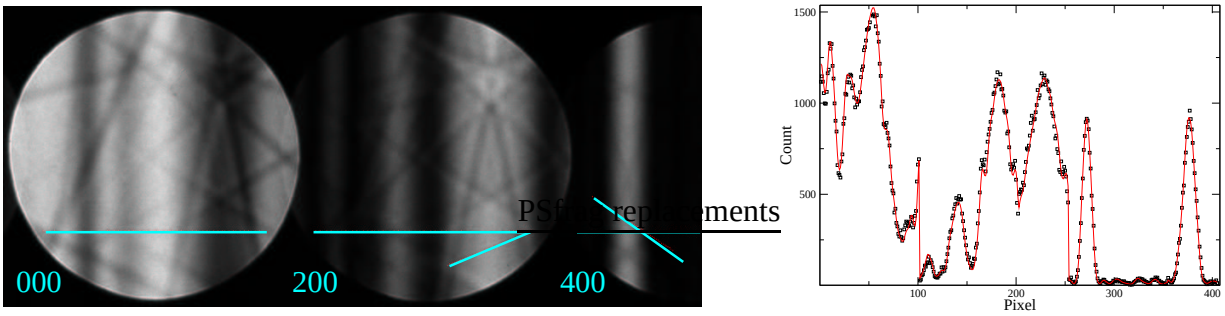
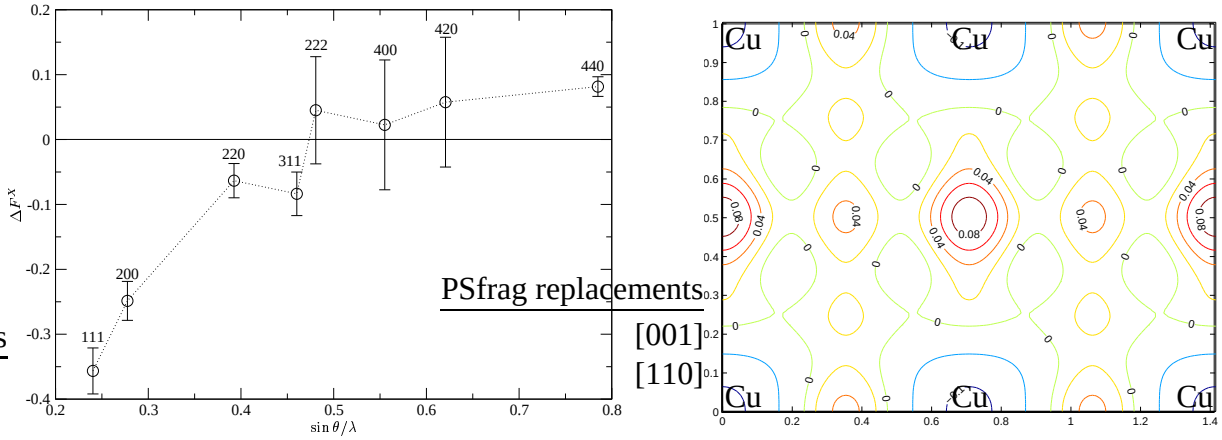


(a) (b)

Figure 1: (a) (200) systematic row in copper with the used line scans drawn on it. (b) The fit between experimental intensities (points) and the corresponding calculated intensities (solid line).



(a) (b)

Figure 2: (a) The difference between the measured structure factors in Cu (converted to X-ray and zero temperature) and neutral atom values [2] versus scattering angle. (b) Charge density difference map in the $(1\bar{1}0)$ plane based on the 6 lowest order structure factors.

Table 1: Theoretical calculated X-ray structure factors for Cu at zero temperature compared with this experiment.

hkl	Neutral atom [2]	Band structure calculation [3]	WIEN2K [4] LDA	WIEN2K [4] GGA(96)	QCBED experiment
111	22.05	21.68	21.70	21.70	21.69(4)
200	20.69	20.35	20.37	20.38	20.44(3)
220	16.74	16.62	16.66	16.67	16.68(3)
311	14.74	14.70	14.75	14.76	14.66(3)
222	14.19	14.17	14.21	14.22	14.24(8)
400	12.42	12.42	12.48	12.48	12.45(10)
420	11.14	11.13	11.19	11.19	11.19(10)
440	8.82		8.88	8.87	8.90(2)
$R(\%)$	0.71	0.34	0.23	0.22	

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