ESRF

Experiment title:
Three beam diffraction in metallic systems

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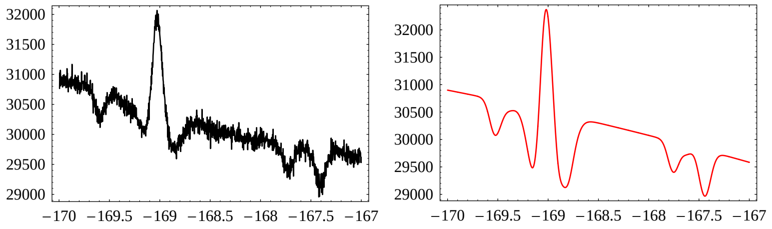
Local contact(s):
Jon Are Beukes

Received at ESRF:

Names and affiliations of applicants (* indicates experimentalists):
Helge B. Larsen*, Gunnar Thorkildsen*, Atle Kverneland*, Aasgeir Vatne*
– Stavanger University College

The orientation matrix for two single crystals of copper were obtained and the samples oriented for three-beam measurements. Crystal thickness: $t \approx 1.0\,\mathrm{mm}$. Wavelength applied: $\lambda = 0.6999\,\text{Å}$. Owing to high absorption only Bragg reflections were available for orientation. Rocking curves of low angle reflections were uniform having FWHM's in the range $0.10 - 0.16°$, depending on the position of the illuminated area on the crystal surface. Owing to instrument constraints, when operated in the horizontal mode, only two reflections were candidates for acting as primary reflections. Figure 1 shows a comparison of measured and calculated power profiles following a scan in ω (the rotation angle about the primary lattice vector).



(a) (b)

Figure 1: First crystal (a) Experiment: Scan in ω: $1500 \times 0.002°$. Measurement time: $T = 0.2\,\mathrm{s}$ per. step. (b) Theory: Independent three-beam contributions – kinematical mode.

Table 1 gives the actual three-beam cases within the measured range. A kinematical analysis, following Chang (ACA 38, 41-48, 1982), seems to account very well for the observed power variation. There may be some dynamical contributions in the quasi four beam case $3\bar{1}\bar{1}/200/1\bar{1}\bar{1}$-$3\bar{1}\bar{1}/\bar{1}\bar{1}\bar{1}/400$ that represents the strongest perturbation.

This question awaits further theoretical investigations.

ω	$\mathbf{h}/\mathbf{g}/\mathbf{h}-\mathbf{g}$	Q	C	M
-169.534	$3\bar{1}\bar{1}/\bar{2}\bar{4}\bar{2}/531$	0.387	LBL	$+-$
-169.511	$3\bar{1}\bar{1}/1\bar{5}\bar{3}/242$	0.386	LBL	$+-$
-168.944	$3\bar{1}\bar{1}/200/1\bar{1}\bar{1}$	3.436	LBB	$-+$
-168.911	$3\bar{1}\bar{1}/\bar{1}\bar{1}\bar{1}/400$	1.578	LBL	$+-$
-167.755	$3\bar{1}\bar{1}/204/1\bar{1}\bar{5}$	0.565	LBL	$+-$
-167.452	$3\bar{1}\bar{1}/3\bar{1}5/00\bar{6}$	0.315	LBB	$-+$
-167.446	$3\bar{1}\bar{1}/004/3\bar{1}\bar{5}$	0.389	LBL	$-+$

Table 1: Actual many-beam interactions - Case a. Q denotes the coupling factor calculated after Weckert and Hümmer (ACA 53, 108-143, 1997), C denotes the actual type of three-beam diffraction. L – Laue diffraction, B – Bragg diffraction. M gives the in/out ($-+$) or out/in ($+-$) movement of the secondary reciprocal lattice point with respect to the Ewald sphere.

The power distribution following larger scans in ω, revealing the true nature of kinematical Bragg scattering, is given in Fig. 2. The observed behaviour is well explained by changes in beam-paths in the crystal as it is being rotated. However, one has to take into account a small precession of the primary reciprocal lattice vector during rotation to explain the skewness of the right section in the figure.

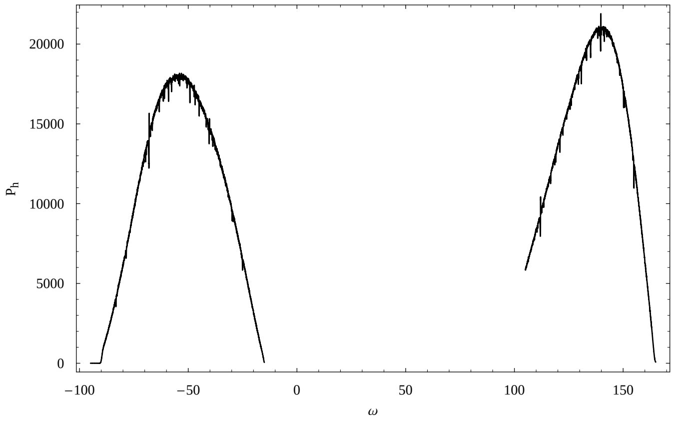


Figure 2: Second Crystal, power of $3\bar{1}1$ as function of ω. The ordinary two beam power level changes rapidly owing to absorption.

The following points must be mentioned:

1. The measurements demands high precision of the diffractometer. There seems to be a small misalignment ($\leq 0.05°$) of the $\hat{\omega}$ axis with respect the laboratory axis $\mathbf{e}_3$ *cf.* Thorkildsen, Mathiesen and Larsen (JAC 32, 943-950, 1999).
2. Comparison with theoretical calculations that involve a matrix formulation of the exchange of energy among the various beams, seems to account for well for all "pure" *Aufhellung*-cases.
3. Further investigations of the measurement procedures should be carried out.