ESRF	**Experiment title:** X-ray topography using the three-beam cases of diffraction	**Experiment number:** HS 401
Beamline: ID 19	**Date of experiment:** from: 15-Oct-97 7:00 to: 21-Oct-97 7:00	**Date of report:** 1-Feb-98
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Report:

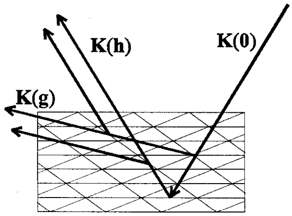

Fig. 1: three-beam case in the direct space (crystal)

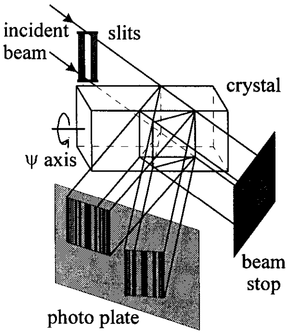

Fig. 2: experimental setup

The purpose of this experiment was the first investigation of the topographic contrast in section topographs using the three-beam case of diffraction. /1,2/ In this case, two Bragg reflections **h** and g are simultaneously excited and three strong wave fields **K(O), K(h), K(g)** exist inside the crystal. The intensity diffracted into the direction of **K(h)** can then be imagined as an interference between the wave diffracted at the lattice planes of **h** (direct wave) and a wave which is diffracted at g and afterwards at **h-g** (Umweg wave). /3/

For the systematical investigation of such a case, a Ψ - rotation (a rotation around one of the primary diffraction vectors e.g. **h)** was used. The distance of G to the Ewald sphere can then be changed independently from H. For this purpose a precise adjustment and an extension of the horizontal diffractometer at ID19 was necessary.

With this experimental setup (see Fig. 2) we could take several series of section topographs in different three-beam interferences. The control parameter was the ψ- position of the crystal. Section topographs were also taken as a reference in the corresponding two-beam cases.

We used a vertical arranged double crystal monochromator and a horizontal diffraction plane for the h-reflection of the sample.

The following four contrast phenomena could be identified in our section topographs from three-beam interferences in the Laue-Laue geometry.

a) A hook shaped contrast is generated in a wide range around the exact excited three-beam position. In generally it is asymmetric with respect to this position. The contrast is caused by a variation of the effective structure factor. (see Fig. **3-I;II;V)**

b) The width and form of the section topographs is changed near the three beam position. This effect is related to the energy transfer between D(g) and **D(h)** (see Fig. 3-VII;III)

c) In addition a highly intense contrast is created in this region. It can be assigned to a strong deformation of the dispersion surfaces. (see the black line on the left side of Fig. 3-1;II)

d) Under the exact excited three-beam conditions the interference between the direct and Umweg wave produce a new interference pattern. (see Fig. 3-1II;IV;VII)

However the individual contrast, shape and expansion of each pattern strongly depends on the geometry and the structure factor of the involved reflections (compare for instance Fig. 3 III and VII). Exact calculations for simulations are in preparation.

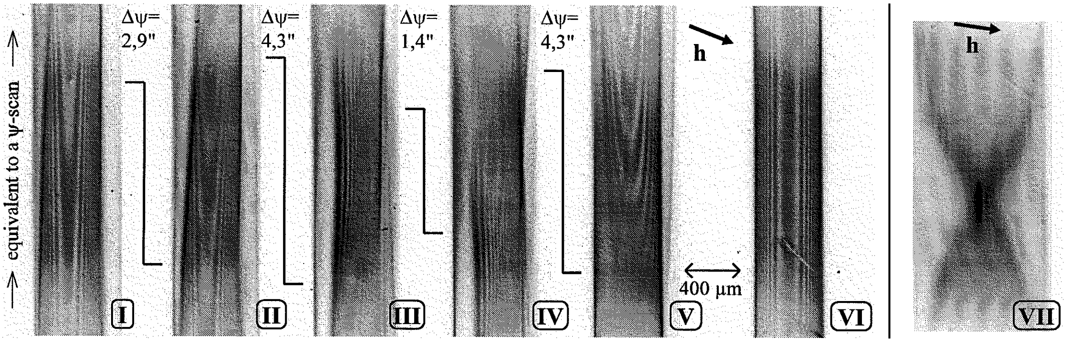

Fig. 3 : Examples for section topographs that show the change in Kato's **pendellösung** fringes, when scanning through a three-beam case. A quasi-monochromatic incident beam ($\lambda \approx 0.71$Å) on a silicon crystal plate with a (111) surface and a 25µm wide slit was used.

I-V topographs from the **h**-reflection of the three-beam case $\mathbf{h} = (3\bar{3}\bar{1}); \mathbf{g} = (4\bar{2}\bar{2}); \mathbf{h} - \mathbf{g} = (\bar{1}\bar{1}1)$ taken at different distances ψ away from the exact excited position. The lines connect equivalent ψ values in the images.

Due to the long distance source to sample of 145 m and the small source size (vertically about 30 pm) the incident white beam can be approximated as a divergent beam coming from a point source. This divergence is transformed by the monochromator in a dispersion convoluted with the rocking curve of the monochromator. Therefore in our diffraction geometry rays with different positions in the incident beam have a slightly different incident angle and wavelength on the crystal. This means that a scan along the height of a section topograph is equivalent to a ψ-scan.

VI corresponding section topograph in the two-beam case for $\mathbf{h} = (3\bar{3}\bar{1})$

VII exact excited three-beam interference $\mathbf{h} = (51\bar{5}); \mathbf{g} = (22\bar{4}); \mathbf{h} - \mathbf{g} = (3\bar{1}\bar{1})$

references

/1/ Höche, H.R.; Heyroth, F. & Eisenschmidt, C. (1997) „X-Ray topography using three-beam interferences" ECM-17 Lisboa.

/2/ Heyroth, F.; Eisenschmidt, C. & Höche, H.R. (1998) „X-ray Topography of Perfect Crystals using the Laue-Laue Three-beam case of Diffraction" accepted for Crystal Research and Technology **33,** No. 3.

/3/ Weckert, E. & Hümmer, K. (1997) „Multiple-Beam X-ray Diffraction for Physical Determination of Reflection Phases and its Applications" Acta Cryst. **A53,** 108-143.