Simulation of multiple diffraction patterns of strong primary reflections with UMWEG-99

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The determination of precise valence and deformation electron density maps from X-ray diffraction requires Bragg intensity data sets of high accuracy. These intensities can be strongly affected, especially by extinction, absorption and multiple diffraction. Whereas for extinction and absorption effects formalism are available in the literature [4], [5] no expressions exist to correct intensity data sets routinely for multiple diffraction.

The program UMWEG-xx, which represents an attempt to solve this problem, was originaly developed for the simulation of Renninger scans of forbidden reflections. The algorithm used, for example in UMWEG-95 for the calculation of the peak positions, peak widths and peak hights of multiple diffraction events in ψ-scans was restricted to the **Umweganregung** effect [1]. In the case of possible primary reflections the additional effects of **Aufhellung** and **interference** between the primary reflection and the beam caused by **Umweganregung** have to be considered [2], [6].

In the actual version of the program [3], these three effects are taken into account together with primary and secondary extinction and absorption. The polarization factors and the peak width formulae are suitable for X-ray tube radiation as well as for synchrotron radiation. Using strong reference reflections for the determination of the intensity of the incident beam the multiple diffraction pattern is calculated by UMWEG-99 on absolute scale.

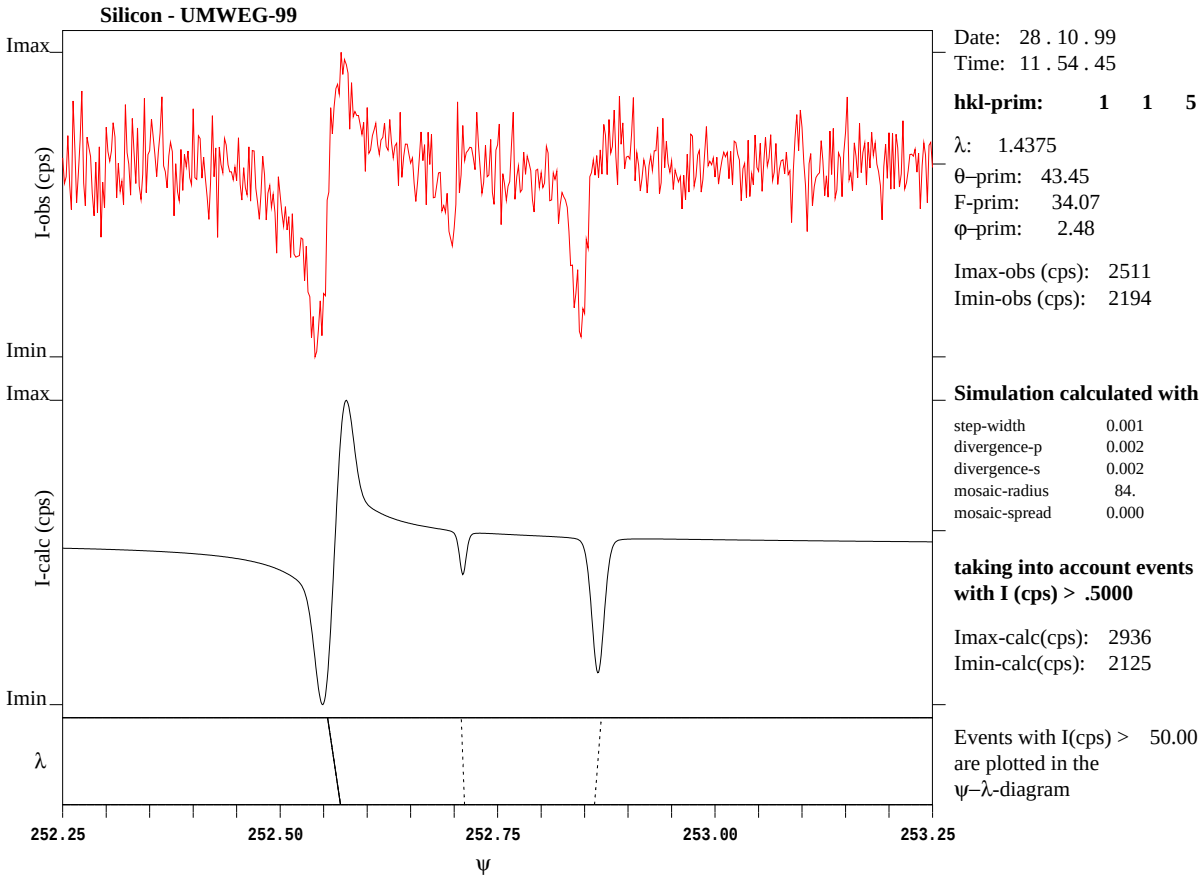

Figure 1: Multiple diffraction pattern of the strong 1 1 5 reflection of a perfect spherical Si-crystal

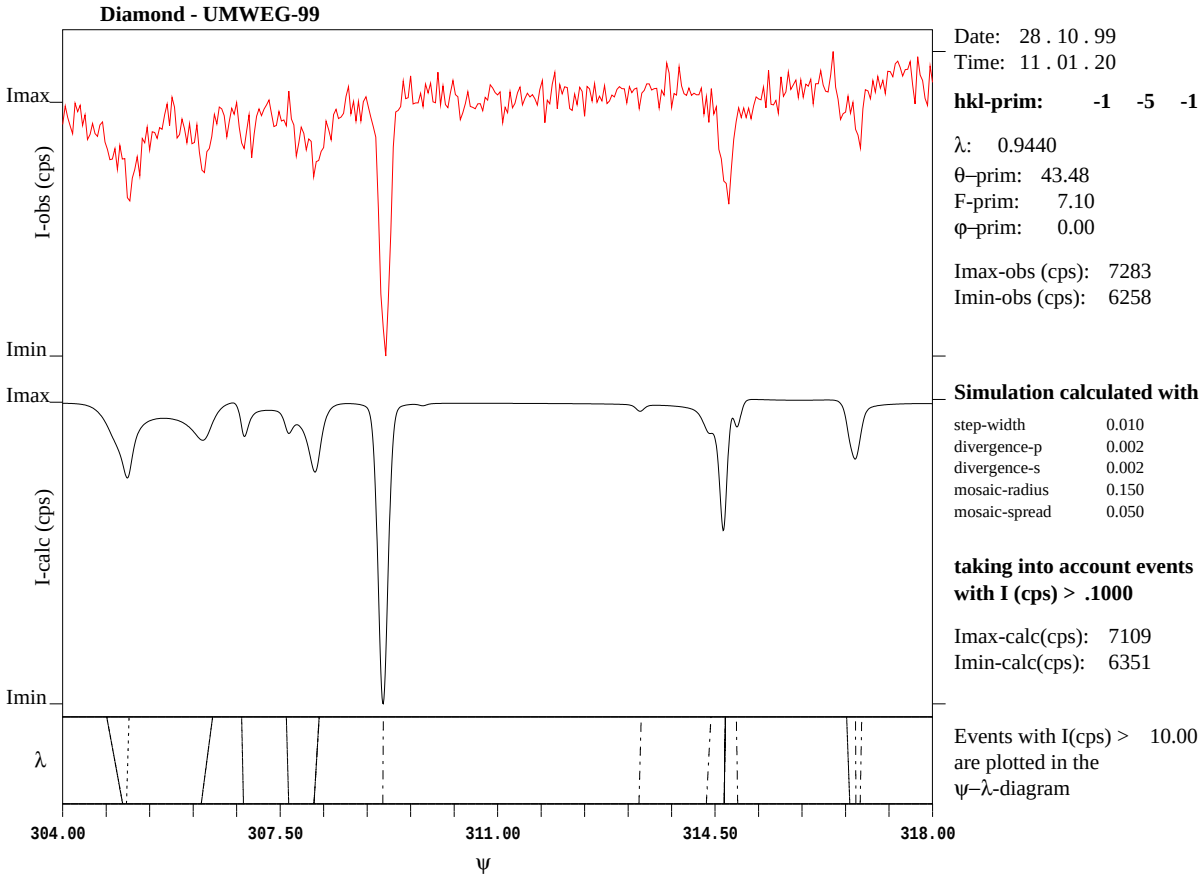

Figure 2: Multiple diffraction pattern of the strong -1 -5 -1 reflection of a mosaic octahedral diamond-crystal

The Figs. 1 and 2 show examples for the graphical output of UMWEG-99. The red (upper) scans, which correspond to the measurements performed in the ω-ψ-scanning technique with the 4-circle-HUBER-diffractometer at beamline D3 at HASYLAB, are compared with the theoretical scans given in the lower parts of the two figures. Details about the experimental conditions and the results for the integrated intensities are given in the legend at the right of the figures.The **interference** effect between the primary reflection and the **Umweganregung** beam is clearly visible only in the case of the perfect Si-crystal. The minimum and maximum at $\psi = 252.55$ in Fig. 1 is solely caused by this effect [6]. In both cases, for the perfect spherical silicon single crystal (Fig. 1) as well as for the ideally imperfect octahedral diamond crystal (Fig. 2), satisfactory agreement between the measured and calculated intensities is obtained on absolute scale.

Further information about the program can be obtained via http://www.rrz.uni-hamburg.de/mpi/rossmanith

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References

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