



ESRF	Experiment title: Study of protein crystal quality by X-ray diffraction topography and other X-ray diffraction methods	Experiment number: LS590
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Report:

Recently, a significant effort has been made to improve the quality of macromolecular crystals for high-resolution structure determination. Usually, the quality of the crystals is inferred from the x-ray diffraction data, but other characterization techniques, such as atomic force microscopy, rocking curve measurements and interferometry have been used recently to access the quality of protein crystals.

For the present experiment we have proposed to use X-ray diffraction topography in conjunction with rocking curve measurements to compare the quality of macromolecular crystals grown by different techniques under different conditions (temperature, purity).

Turkey egg white lysozyme crystals (TEWL) grown by the hanging drop method were used as a test case for these measurements. One set of crystals was doped with 30% hen egg white lysozyme (THEWL). Both TEWL and THEWL belong to the primitive hexagonal space group. This protein was chosen because in previous synchrotron experiments a clear difference was observed between the quality of the pure, TEWL, and the doped, THEWL, crystals. Similar results were observed in this experiment. The pure (TEWL) crystals diffracted to higher resolutions, and presented a better signal to noise. Sharp rocking curves could be recorded (Figure 1). The doped (THEWL) crystals diffracted to lower resolutions, presented a poor signal to noise ratio and the rocking curves of different reflections was broad (Figure 2). Several topographs were taken on different rocking curves on different crystals. The X-ray diffraction topographs and the rocking curve measurements are still under analysis and are being complemented with oscillation diffraction data taken on BM14. The result will allow us to follow the deformation/mosaic structure in the crystals and its effects on structure determination.

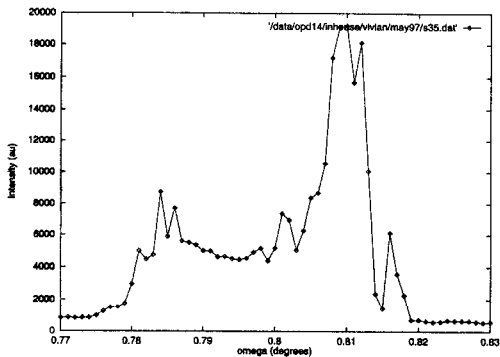


Figure 1: Rocking curve of a TEWL crystal grown by the hanging drop method at constant temperature.

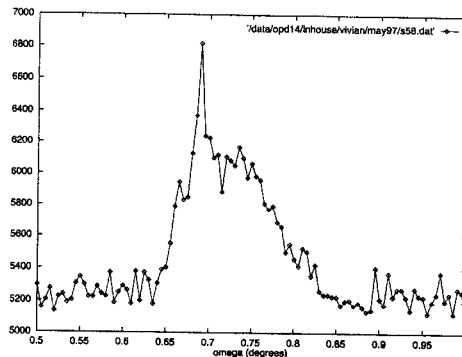


Figure 2: Rocking curve of a THEWL crystal grown by the hanging drop method at constant temperature. The percentage of hen egg white lysozyme in the crystals was 30%.

The success of the experiment was strongly dependent upon the availability of a chi/phi circle, which was borrowed from the previous user. The setup for X-ray diffraction topography as a standard method for protein crystal quality assessment would benefit greatly if this chi/phi circle could be made available upon request. Also the precise and independent movement of the detector axis would make it possible to map the reciprocal space. Of course these kind of measurements would need more than 6 shifts to be accomplished.