ESRF	**Experiment title:** Study of protein crystal quality by X-ray diffraction topography and other X-ray diffraction methods	**Experiment number:** MI240
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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.

In 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 the temperature controlled technique. The main advantages of this method is that it allows for an accurate control of the temperature and since the crystals are grown in capillaries they are not subjected to mechanical damage due to manipulation.

As a benchmark protein for the temperature control system that was setup at the EMBL in the JSBG laboratory we used Hen Egg White Lysozyme (HEWL) for being redly available at low cost. Five crystals grown in different conditions of protein purity, protein concentration, and geometrical environment were studied. For two of the crystals a couple of different reflections were analised. The FWHM of the individual reflections varied between 5 and 20 mdeg. However for all crystals the rocking curve presented at least two main resolved peaks. The interpretation of the topographic images taken at these peaks are currently under investigation. These crystals were then taken to a standard macromolecular crystallography beam line (BM14). Oscillation data was collected for three of the crystals studied.

The results of the analysis lead us to further modify these growth parameters, purity and temperature. Crystals are currently being grown under refined conditions. It is our goal to understand how these parameters affect the quality of the crystals and apply this knowledge to the growth of protein crystals of known, for further refinement of the structure, and latter to protein crystals of unknown structure.

It was essential for the success of this experiment the availability of a triple axis diffractometer that has been build since our previous experiment at ID19. It would be helpful for future experiments to have included in the setup an image plate detector or a CCD detector to align properly the crystal. We have also built a collimator beam-stop assembly to improve the signal to noise ratio.

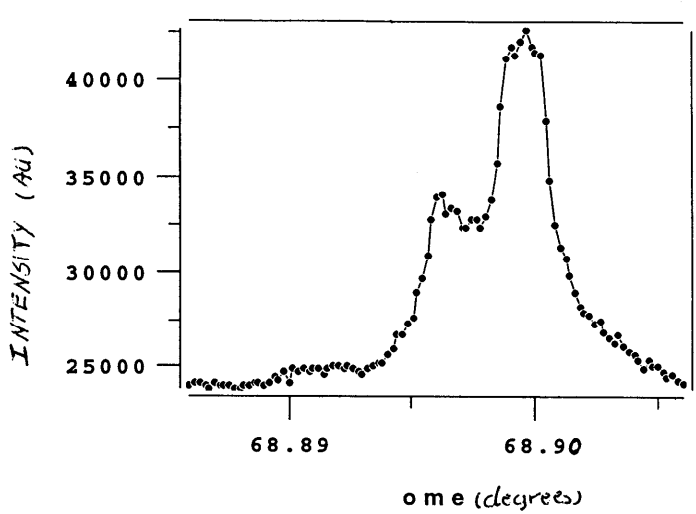

Figure 1: Rocking curve of a HEWL crystal grown by the temperature controlled technique at 11°C in a round capillary from a purified protein stock.

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