

4.2. X-RAYS

conventional diffractometers of that era. For accurate Rietveld modelling or accurate charge-density studies, the theoretical scattered intensity must be known. This is not a problem at synchrotron-radiation sources, where the incident beam is initially almost completely linearly polarized in the plane of the orbit, and is subsequently made more linearly polarized through Bragg reflection in the monochromator systems. Rather,

it is a problem in the laboratory-based systems where the source is in general a source of elliptical polarization. It is essential to determine the polarization for the particular monochromator and the source combined to determine the correct form of the polarization factor to use in the formulae used to calculate scattered intensity (Chapter 6.2).

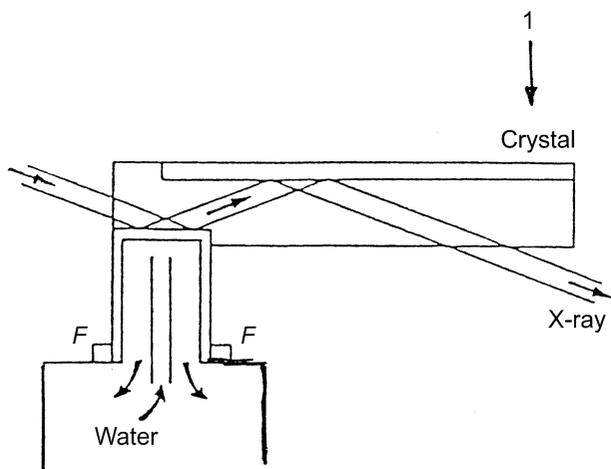


Fig. 4.2.5.6. A schematic diagram of a Hart-type tuneable channel-cut monochromator is shown. The monochromator is cut from a single piece of silicon. The reflecting surfaces lie parallel to the (111) planes. Cuts are made in the crystal block so as to form a lazy hinge, and the second wafer of the monochromator is able to be deflected by a force generated by a current in an electromagnet acting on an iron disc glued to the upper surface of the wafer. Cooling of the primary crystal of the monochromator is by a jet of water falling on the underside of the wafer. This type of system can tolerate incident-beam powers of 500 W mm^{-2} without significant change to the width of the reflectivity curve.

4.2.6. X-ray dispersion corrections (By D. C. Creagh)

The term ‘anomalous dispersion’ is often used in the literature. It has been dropped here because there is nothing ‘anomalous’ about these corrections. In fact, the scattering is totally predictable.

For many years after the theoretical prediction of the dispersion of X-rays by Waller (1928), and the application of this theory to the case of hydrogen-like atoms by Hönl (1933a,b), no real use was made by experimentalists of dispersion-correction effects in X-ray scattering experiments. The suggestion by Bijvoet, Peerdeman & Van Bommel (1951) that dispersion effects might be used to resolve the phase problem in the solution of crystal structures stimulated interest in the practical usefulness of this hitherto neglected aspect of the scattering of photons by atoms. In one of the first texts to discuss the problem, James (1955) collated experimental data and discussed both the classical and the non-relativistic theories of the anomalous scattering of X-rays. James’s text remained the principal reference work until 1974, when an Inter-Congress Conference of the International Union of Crystallography dedicated to the discussion of the topic produced its proceedings (Ramaseshan & Abrahams, 1975).

At that conference, reference was made to a theoretical data set calculated by Cromer & Liberman (1970) using relativistic quantum mechanics. This data set was later used in *IT IV* (1974) and has been used extensively by crystallographers for more than a decade.

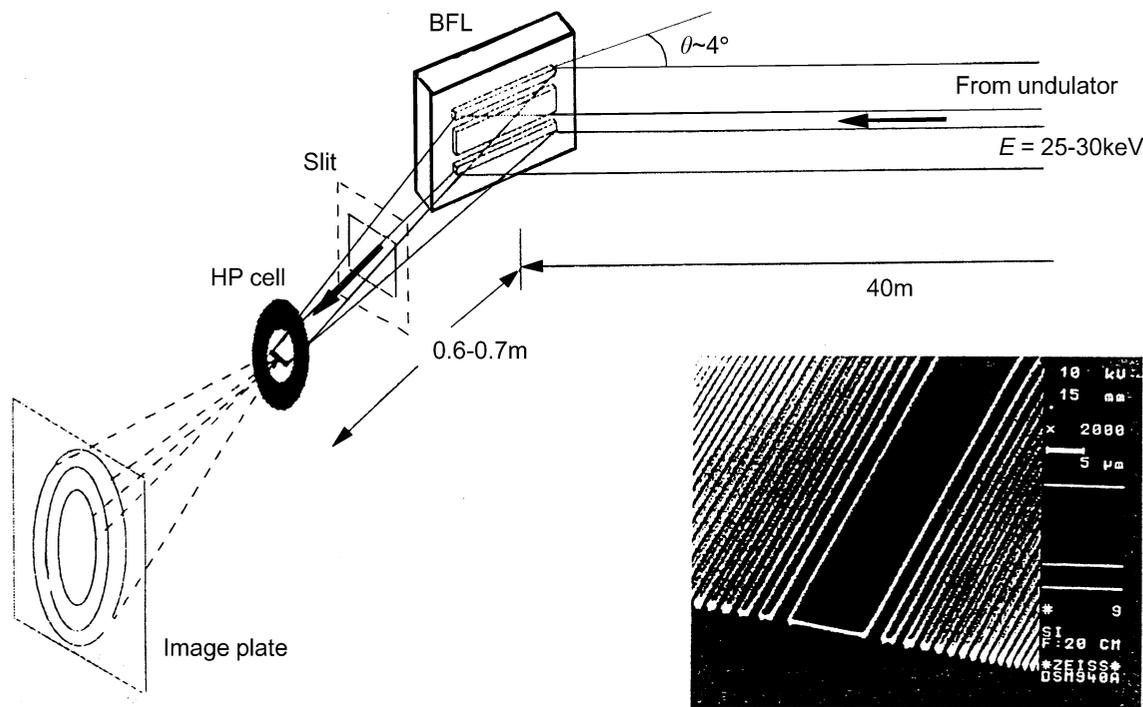


Fig. 4.2.5.7. A schematic diagram of the use of a Bragg-Fresnel lens to focus hard X-rays onto a high-pressure cell. The diameter of the sample in such a cell is typically $10 \mu\text{m}$. The insert shows a scanning electron micrograph of the surface of the Bragg-Fresnel lens.