International Tables for Crystallography (2006). Vol. C, Section 4.2.5.4.4, pp. 240–241.

that is not acceptable, for example, for the study of small-angle scattering (SAXS, Chapter 2.6). The effect of the tails can be reduced significantly through the use of multiple Bragg reflections.

The use of multiple Bragg reflections from a channel cut in a monolithic silicon crystal such that the channel lay parallel to the (111) planes of the crystal was shown by Bonse & Hart (1965) to remove the tails of reflections almost completely. This class of device, referred to as a (symmetrical) channel-cut crystal, is the most frequently used form of monochromator produced for modern X-ray laboratory diffractometers and beamlines at synchrotron-radiation sources (Figs. 4.2.5.2, 4.2.5.5).

The use of symmetrical and asymmetrical Bragg reflections for the production of highly collimated monochromatic beams has been discussed by Beaumont & Hart (1973). This paper contains descriptions of the configurations of channel-cut monochromators and combinations of channel-cut monochromators used in modern laboratory diffractometers produced by Philips, Siemens, and Bede Scientific. In another paper, Hart (1971) discussed the whole gamut of Bragg reflecting X-ray optical devices. Hart & Rodriguez (1978) extended this to include a class of device in which the second wafer of the channel-cut monochromator could be tilted with respect to the first (Fig. 4.2.5.6), thereby providing an offset of the crystal rocking curves with the consequent removal of most of the contaminant harmonic radiation (Fig. 4.2.5.4). The version of monochromator shown here is designed to provide thermal stability for high incident-photon fluxes. Berman & Hart (1991) have also devised a class of adaptive X-ray monochromators to be used at high thermal loads where thermal expansion can cause a significant degradation of the rocking curve, and therefore a significant loss of flux and spectral purity. The cooling of Bragg-geometry monochromators at high photon fluxes presents a difficult problem in design.

Kikuta & Kohra (1970), Matsushita, Kikuta & Kohra (1971) and Kikuta (1971) have discussed in some detail the performance of asymmetrical channel-cut monochromators. These find application under circumstances in which beam widths need to be condensed or expanded in X-ray tomography or for micro X-ray fluorescence spectroscopy. Hashizume (1983) has described the design of asymmetrical monolithic crystal monochromators for the elimination of harmonics from synchrotron-radiation beams.

Many installations use a system designed by the Kohzu Company as their primary monochromator. This is a separated element design in which the reference crystal is set on the axis of the monochromator and the first crystal is set so as to satisfy the Bragg condition in both elements. One element can be tilted slightly to reduce harmonic contamination. When the wavelength is changed (*i.e.* θ is changed), the position of the first wafer is changed either by mechanical linkages or by electronic positioning devices so as to maintain the position of the outgoing beam in the same place as it was initially. This design of a fixed-height, separated-element monochromator was due initially to Matsushita, Ishikawa & Oyanagi (1986). More recent designs incorporate liquid-nitrogen cooling of the first crystal for use with high-power insertion devices at synchrotron-radiation sources. In many installations, the second crystal can be bent into a cylindrical shape to focus the beam in the horizontal plane. The design of such a sagittally focusing monochromator is discussed by Stephens, Eng & Tse (1992). Creagh & Garrett (1965) have descibed the properties of a monochromator based on a primary monchromator (Berman & Hart, 1991) and a sagittally focusing second monochromator at the Australian National Beamline at the Photon Factory.

A recent innovation in X-ray optics has been made at the European Synchrotron Radiation Facility by the group led by Snigirev (1994). This combines Bragg reflection of X-rays from a silicon crystal with Fresnel reflection from a linear zone-plate structure lithographically etched on its surface. Hanfland *et al.* (1994) have reported the use of this class of reflecting optics for the focusing of 25 to 30 keV photon beams for high-pressure crystallography experiments (Fig. 4.2.5.7).

Further discussion on these monochromators is to be found in this volume in Subsection 2.2.7.2, §2.3.5.4.1, Chapter 2.7, and Section 7.4.2.

4.2.5.4.4. *Polarization*

All scattering of X-rays by atoms causes a probable change of polarization in the beam. Jennings (1981) has discussed the effects of monochromators on the polarization state for

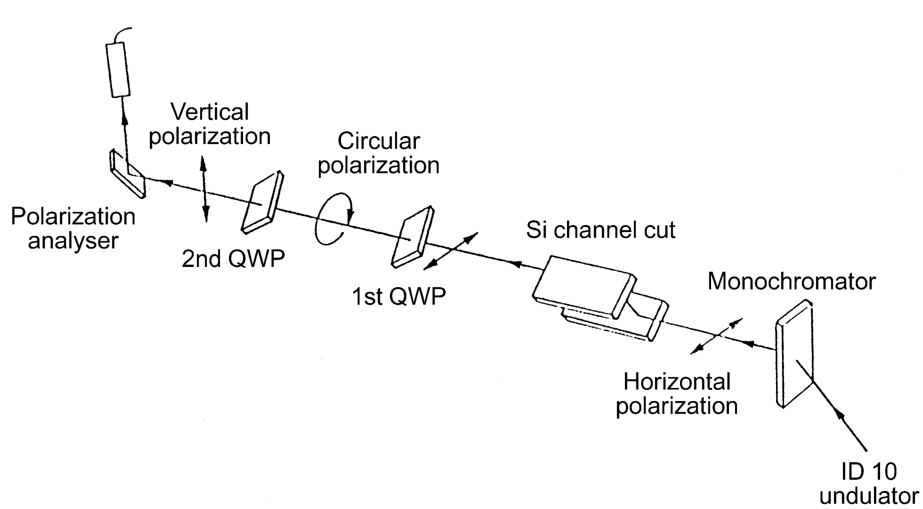

Fig. 4.2.5.5. A schematic diagram of a beamline designed to produce circularly polarized light from initially linearly polarized light using Laue-case reflections. Radiation from an insertion device is initially monochromated by a cooled diamond crystal, operating in Laue geometry. The outgoing radiation has linear polarization in the horizontal plane. It then passes through a silicon channel-cut monochromator and into a silicon crystal of a thickness chosen so as to produce equal amounts of radiation from the σ and π branches of the dispersion surface. These recombine to produce circularly polarized radiation at the exit surface of the crystal.

Copyright © 2006 International Union of Crystallography

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).

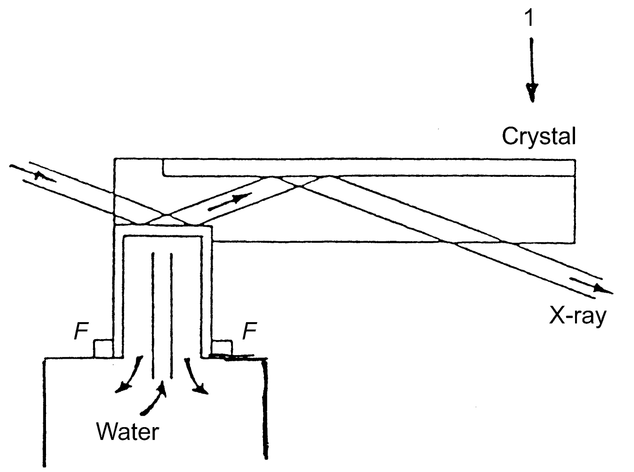

Fig. 4.2.5.6. A schematic diagram of a Hart-type tuneable channel-cut monochromator is shown. The monochromator is cut from a single piece of silicon. The reflecting surfaces lie parallel to the (111) planes. Cuts are made in the crystal block so as to form a lazy hinge, and the second wafer of the monochromator 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 (1933*a*,*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.

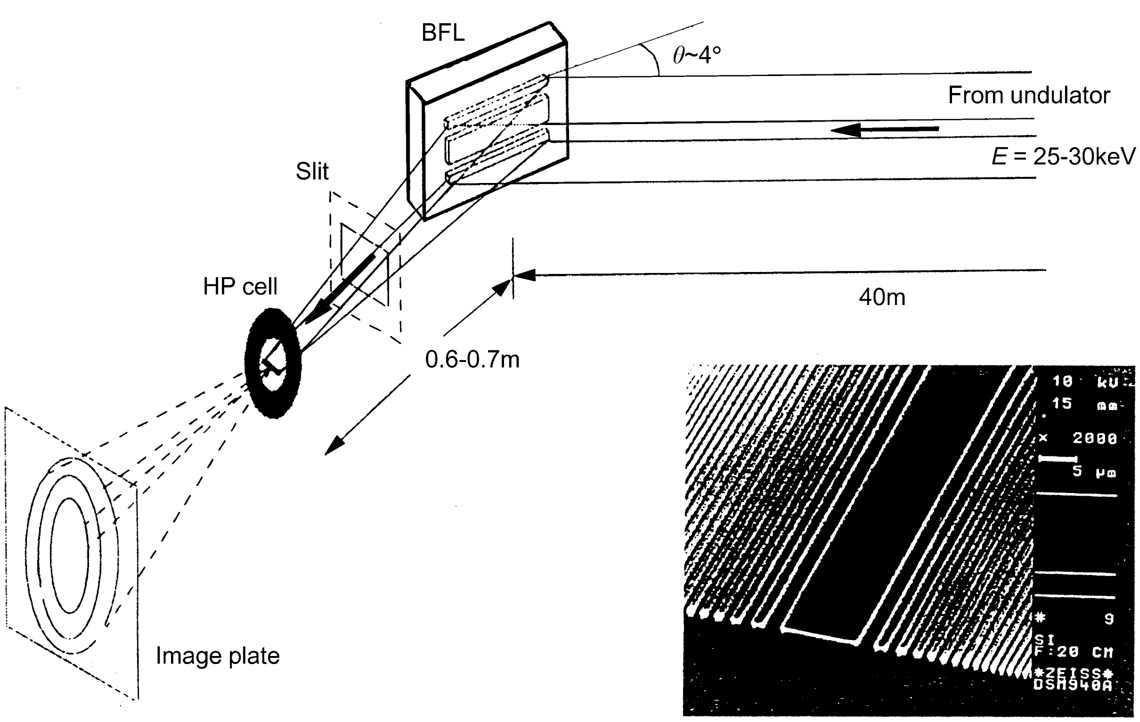

Fig. 4.2.5.7. A schematic diagram of the use of a Bragg–Fresnel lens to focus hard X-rays onto a high-pressure cell. The diameter of the sample in such a cell is typically 10 μm. The insert shows a scanning electron micrograph of the surface of the Bragg–Fresnel lens.

references