narrow pulse-height analyser window (see Section 7.1.2) may be helpful. In any case, a simple powder pattern will show if the unwanted wavelengths are reaching the specimen.

To achieve maximum performance in terms of intensity and resolution, it is essential to design the X-ray optics so that the properties of the monochromator match the characteristics of the source, specimen, and instrument geometry. A flat crystal is used for parallel beams and a curved crystal for focusing geometries. The curved crystal can accept a much larger divergent primary beam and has the property of converting the incident divergent beam to a convergent beam after reflection. The quality of the crystal and its surface preparation by fine lapping and etching are crucial.

The crystal materials most commonly used are silicon, germanium, and quartz, which have small rocking angles, and graphite and LiF which have large mosaic spreads. A large variety of crystals is available with large and small d spacings for use in X-ray fluorescence spectroscopy. The crystal must be chemically stable and not deteriorate with X-ray exposure. Synthetic multilayer microstructures have recently been developed for longer-wavelength X-rays. A lower atomic number element avoids fluorescence from the crystal.

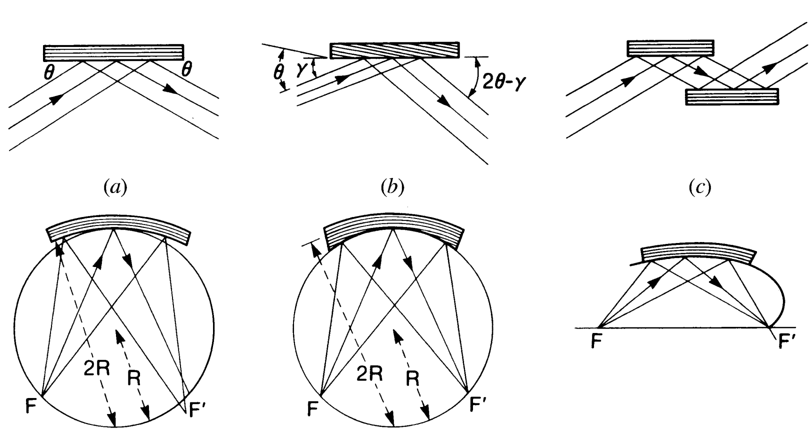
The common types of monochromators are illustrated in Fig. 2.3.5.6. The beam reflected from a flat crystal (*a*) is nearly parallel. If the incident beam is divergent and the crystal is rotated, the reflection will broaden as the rays that make the correct Bragg angle 'walk' across the surface. If the crystal is cut at an angle γ to the reflecting plane, the beam is broadened as shown in (*b*) (or narrowed if reversed) (Fankuchen, 1937; Evans, Hirsch & Kellar, 1948).

A channel-cut monochromator [Fig. 2.3.5.6(*c*)] is cut from a single-crystal ingot and both plates, therefore, have exactly the same orientation (Bonse & Hart, 1965, 1966). They are usually made from a high-quality dislocation-free silicon ingot. They can also be designed to give more than two reflections per channel, and can be cut at an angle to the reflecting plane (Deutsch, 1980). Originally designed for small-angle scattering, they are now also used for parallel-beam diffractometry, interferometry, and spectroscopy. They have the important property that the position and direction of the monochromatic beam remain nearly the same for a wide range of wavelengths. This avoids realignment and recalibration of the diffractometer when changing wavelengths in synchrotron diffractometry. The reflections are narrow with minimal tails. The resolution is determined by the energy spread of the perfect-crystal bandpass [which is 1.33×10^{-4} for Si(111)] and the wavelength dispersion, which is small at small 2θ's and increases with $\tan\theta$ (Beaumont & Hart, 1974; Hart, Rodrigues & Siddons, 1984).

Thin crystals can be bent to form a section of a cylinder for focusing, Fig. 2.3.5.6(*d*) (Johann, 1931). The safe bending radius is of the order of 1000 to 2000 times the thickness of the crystal plate. The bending radius $2R$ forms a surface tangent to the focusing circle of radius R. The cylindrical form allows the line focus of the X-ray tube to be used. Because the lattice planes are not always tangent to the focusing circle, as would be required for perfect focusing, the aberrations broaden the focus, but this may not be a serious problem in powder diffraction. If the crystal is also ground so that its surface radius R matches the focusing circle, the aberrations are removed, Fig. 2.3.5.6(*e*) (DuMond & Kirkpatrick, 1930; Johannson, 1933). The crystal may be initially cut at an angle γ to the surface to change the focal length FL of the incident and reflected beams. Here, $FL_1 = 2R\sin(\theta - \gamma)$ and $FL_2 = 2R\sin(\theta + \gamma)$.

Another type of focusing monochromator requires a plane-parallel thin single-crystal plate bent into a section of a logarithmic spiral, Fig. 2.3.5.6(*f*) (Barraud, 1949). de Wolff (1968*b*) developed a method of applying unequal forces to the ends of the plate in adjusting the curvature to give a sharp focus (Subsection 2.3.1.2). It has the important advantage that the curvature can be changed while set on a reflection to obtain the best results in setting up the diffractometer.

The most widely used monochromator is highly oriented pyrolytic graphite in the form of a cylindrically curved plate. It is generally used in the diffracted beam after the receiving slit. The basal reflection $d(002) = 3.35$ Å. Because of its softness, it cannot be ground or cut at an angle to the plane. It is not a true single crystal and has a broad rocking angle of 0.3 to 0.6°, but this is not a problem when the receiving slit determines the profile. Its greatest advantage is the extraordinarily high reflectivity of about 50% for Cu $K\alpha$, which is far higher than any other crystal (Renninger, 1956). In practice, some graphite plates may have a reflectivity as low as about 25–30%.



(*a*) (*b*) (*c*)

(*d*) (*e*) (*f*)

Fig. 2.3.5.6. Crystal monochromators most frequently used in powder diffraction. (*a*)-(*c*) Non-focusing parallel beam, (*d*)-(*f*) focusing bent crystals. All may be cut parallel to the reflecting lattice plane (symmetric cut) or inclined (asymmetric cut). The latter are used to expand or condense beam depending on the direction of inclination, and to change focal lengths. (*a*) Flat symmetric plate. (*b*) Flat asymmetric plate in orientation to expand beam and increase intensity (Fankuchen, 1937). (*c*) Channel monochromator cut from highly perfect ingot (Bonse & Hart, 1965). (*d*) Focusing crystal bent to radius $2R$ (Johann, 1931). (*e*) Crystal bent to $2R$ and surface ground to R (DuMond & Kirkpatrick, 1930; Johannson, 1933). (*f*) Crystal bent to section of logarthmic spiral (Barraud, 1949; de Wolff, 1968*b*).