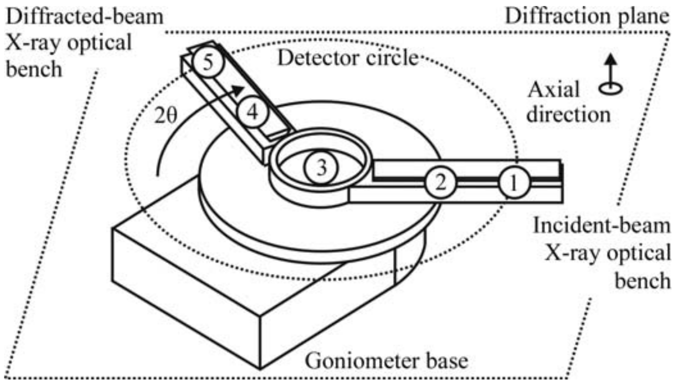

Figure 2.1.2
The basic design principle of modern diffractometers. Currently available instruments are built around a centrally mounted specimen and represent an X-ray optical bench with mounting positions for any (1) X-ray sources, (2) incident-beam optics, (3) specimen stages, (4) diffracted-beam optics and (5) detectors. The 2θ position of the scattered-X-ray optical bench refers to the 2θ angle of the Debye cone shown in bold in Fig. 2.1.1(*b*).

direction. The *detector circle* (also called the 'goniometer circle' or 'diffractometer circle') is defined either by the centre of the active window of a stationary detector, or, in most cases, by a detector moving around the specimen, and is coplanar to the diffraction plane. The 2θ angle of both the diffracted beam in Fig. 2.1.1(*a*) and the Debye cone in Fig. 2.1.1(*b*) (shown in bold) refers to the 2θ position of the diffracted-beam X-ray optical bench in Fig. 2.1.2. It is obvious from Figs. 2.1.1 and 2.1.2 that, in principle, diffraction from single crystals and (ideal) powders can be measured using the same instrument.

An instrument design with a centrally mounted specimen has the important advantage that it implicitly allows the operation of one and the same instrument in both Bragg–Brentano and Debye–Scherrer geometry, depending on the beam divergence chosen. The actual instrument geometry is thus a function of the actual beam propagation angle (divergent, parallel or convergent), making the X-ray optics the most important part of any instrument-geometry conversion. The relationship between the two geometries and their implementation in a single instrument using an incident-beam X-ray optical bench is illustrated in Fig. 2.1.3.

As laboratory X-ray sources invariably produce divergent beams, the 'natural' instrument geometry is self-focusing, 'automatically' leading to the Bragg–Brentano geometry as shown in Fig. 2.1.3(*a*). In this geometry the angle of both the incident and the diffracted beam is θ with respect to the specimen surface. The X-ray-source-to-specimen and the specimen-to-detector distances are equal. The diffraction pattern is collected by varying the incidence angle of the incident beam by θ and the diffracted-beam angle by 2θ. The focusing circle is defined as positioned tangentially to the specimen surface. The focusing condition is fulfilled at the points where the goniometer circle intersects the focusing circle, and thus requires measurements in reflection mode.

The Bragg–Brentano geometry may be extended by an incident- or a diffracted-beam monochromator. In the case of an incident-beam monochromator as shown in Fig. 2.1.3(*b*), the focus of the X-ray source is replaced by the focus of the monochromator crystal. This involves mounting the monochromator crystal (and the X-ray source) a certain distance away along the incident-beam X-ray optical bench, as given by the focusing length of the monochromator crystal (the dotted line in Fig. 2.1.3*b*). For a diffracted-beam monochromator or mirror, the geometry shown in Fig. 2.1.3(*b*) can be thought of as reversed (simply consider the X-ray source and detector switching their positions).

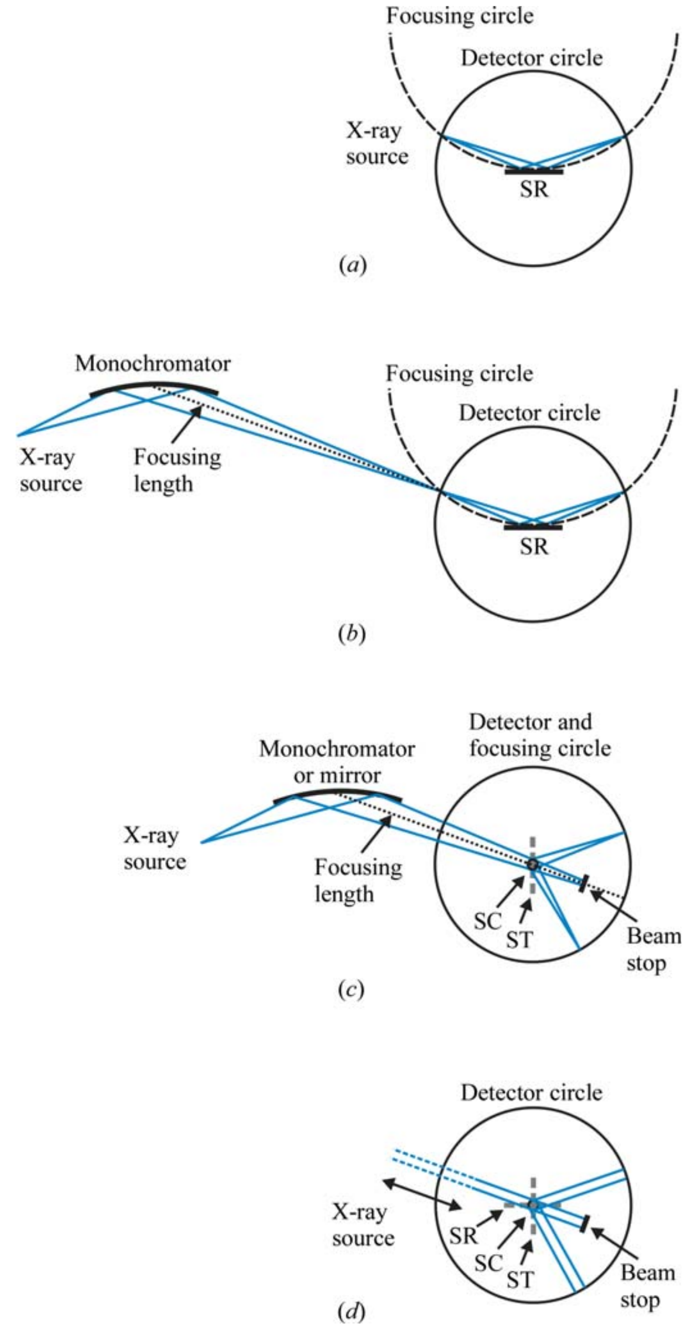

Figure 2.1.3
Transformation between the Bragg–Brentano and Debye–Scherrer geometries using a incident-beam X-ray optical bench. SR: flat specimen, reflection mode; SC: capillary specimen, transmission mode; ST: flat specimen, transmission mode. The actual instrument geometry is a function of the actual beam-propagation angle, making the X-ray optics the most important part of any instrument-geometry conversion. (*a*) Divergent beam: Bragg–Brentano geometry, (*b*) divergent beam: Bragg–Brentano geometry extended by an incident-beam monochromator. (*c*) Convergent beam: focusing Debye–Scherrer geometry, (*d*) parallel beam: Debye–Scherrer geometry. Transformation is achieved by mounting the X-ray tube and pre-aligned optical components at pre-defined positions of the optical bench. None of the figures are to scale.

The conversion from Bragg–Brentano to Debye–Scherrer geometry involves the mounting of some kind of optics designed to convert the divergent beam coming from the X-ray source into a focusing or parallel beam; this is shown in Figs. 2.1.3(*c*) and (*d*), respectively.

Copyright © 2018 International Union of Crystallography