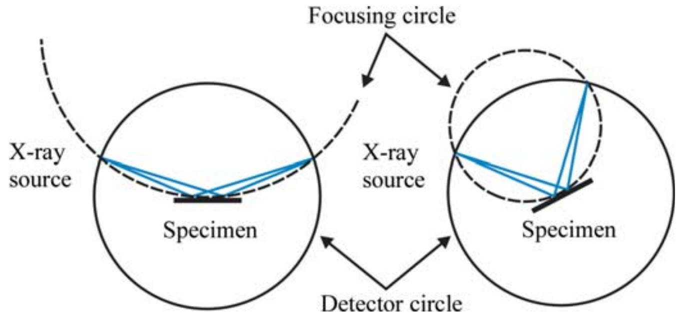

Figure 2.1.4
Bragg–Brentano geometry. The focusing circle, given for two different angles 2θ, is tangential to the specimen surface. Its diameter is given by the intersections between the detector and the focusing circles and is thus 2θ dependent.

In a focusing Debye–Scherrer geometry setup, as shown in Fig. 2.1.3(*c*), the divergent beam coming from the X-ray source is normally focused on the detector circle (for highest resolution) by means of an incident-beam monochromator or a focusing mirror. The focusing circle is identical to the detector circle and the focusing condition requires measurements in transmission mode. When employing an incident-beam monochromator with sufficient focusing length, then conversion between the Bragg–Brentano geometry and the focusing Debye–Scherrer geometry involves a shift of the monochromator crystal (and the X-ray source) along the incident-beam X-ray optical bench (note the identical focusing length of the monochromator shown in Figs. 2.1.3*b* and *c*).

For a parallel-beam setup, as shown in Fig. 2.1.3(*d*), parallelization of the divergent beam coming from the X-ray source may be achieved by different means, such as collimators (classic Debye–Scherrer geometry) or reflective optics such as mirrors or capillaries. In principle, the X-ray source and the detector may be placed at any distance from the specimen, as there are no focusing requirements. As a consequence, measurements can be performed in both reflection and transmission mode.

In a simplified scheme, conversion between the geometries discussed above involves repositioning of the X-ray source, together with mounting of X-ray optics with suitable beam divergence. To make this possible, the incident-beam optical X-ray bench offers the necessary predefined mounting positions including relevant translationary and rotationary degrees of freedom.

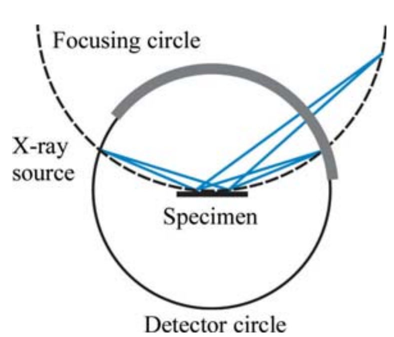

Figure 2.1.5
Bragg–Brentano geometry. While all diffracted beams focus on the (variable-diameter) focusing circle (here shown for two beams), focusing on the detector circle is only achieved at the X-ray source and detector positions (located at the intersections between the detector and the focusing circles). This prevents the use of larger position-sensitive detectors because of defocusing, as indicated by the hypothetical large position-sensitive detector represented by the bold grey line.

An important aspect directly related to the choice of the instrument geometry is the geometric compatibility with position-sensitive detectors. In contrast to Debye–Scherrer geometry, large line and area detectors may not be used in Bragg–Brentano geometry. This is an important limitation of the latter, as the focusing circle does not coincide with the detector circle and has a 2θ-dependent diameter, as illustrated in Fig. 2.1.4. As a consequence, the diffracted beam is only focused on a single point of the goniometer circle, as shown in Fig. 2.1.5. However, small position-sensitive detectors with an angular coverage of not more than about 10° 2θ are used with great success, as defocusing can be ignored at diffraction angles larger than about 20° 2θ if high angular accuracy and resolution are not required. For measurements at smaller 2θ angles, or for highest angular accuracy and resolution, the active window size of a position-sensitive detector may be reduced by means of slits and/or electronically down to a point, allowing the use of this detector as a point detector.

2.1.4.2. *Range of hardware*

An X-ray diffractometer is generally characterized by the relationship between a conditioned beam, the specimen orientation and the subsequent interception of the diffracted beams by a detector of given geometry and imaging properties. There are only a very few instrument configurations that will be ideal for any two application areas, or every conceivable sample within a single application area. It is the user's responsibility to match the instrument to the specimen properties, which can be challenging, particularly in multi-user environments with a large variety of sample types. The platform and the X-ray optical-bench concepts allow the user to choose and mount the most appropriate beam-path components in order to optimize an instrument with respect to a specific application and specimen-property requirements. Table 2.1.1 provides an overview of the currently available types of beam-path components from the X-ray source through to the detector.

The length of available X-ray optical benches varies, and is typically in the range of about 15 cm up to 100 cm. Larger benches allow mounting of bulky components (*e.g.* moving-target X-ray sources or large detectors) as well as mounting of several X-ray optics in a row (*e.g.* combinations of mirrors and channel-cut monochromators). Some diffractometer models allow mounting of two incident- and/or diffracted-beam X-ray optical benches to mount different beam-path components in parallel, *e.g.* X-ray sources with different wavelengths or beam shapes (very popular in single-crystal diffraction), X-ray optics with different beam divergence (*e.g.* to switch between Bragg–Brentano and Debye–Scherrer geometry), and different detector types.

While Table 2.1.1 and the above may imply an enormous combinatorial diversity, in practice this is not entirely the case. In general, beam-path components have to be compatible with the selected instrument geometry, which is dictated by the choice of the X-ray source (point or line), the beam characteristics (wavelength distribution, divergence) and the detector (point, linear or area). This automatically narrows down the range of combinations. As an obvious example, many crystal monochromators and X-ray mirrors are only compatible with a particular wavelength. Also, the size and weight of bulky components, such as moving-target X-ray sources, large specimen stages and large two-dimensional detectors, may impose practical constraints that require consideration. For example, the acces-