Considering this, Liouville's theorem given in equation (2.5.14) should be expressed as

$$S_1\alpha \le S_2\beta. \qquad (2.5.15)$$

This states that the product of the divergence and image size can be equal to or greater than the product of the capture angle and source size. If the X-ray source is a point with zero area, the focus image from focusing optics or the cross section of a parallel beam can be any chosen size. For focusing optics, the source size must be considerably smaller than the output beam size in order to achieve a gain in flux. In this case, the flux gain is from the increased capture angle. For parallel optics, the divergence angle β is infinitely small by definition, so it is necessary to use an X-ray source as small as possible to achieve a parallel beam. Focusing optics have an advantage over parallel optics in terms of beam flux. Using an X-ray beam with a divergence much smaller than the mosaicity of the specimen crystal does not improve the resolution, but does sacrifice diffraction intensity. For many X-ray diffraction applications with polycrystalline materials, a large crossfire is acceptable as long as the diffraction peaks concerned can be resolved. The improved peak profile and counting statistics can most often compensate for the peak broadening due to large crossfire.

2.5.3.1.3. *X-ray source*

A variety of X-ray sources, from sealed X-ray tubes and rotating-anode generators to synchrotron radiation, can be used for 2D powder diffraction. The history and principles of X-ray generation can be found in many references (Klug & Alexander, 1974; Cullity, 1978). The X-ray beam intensity depends on the X-ray optics, the focal-spot brightness and the focal-spot profile. The focal-spot brightness is determined by the maximum target loading per unit area of the focal spot, also referred to as the specific loading. A microfocus sealed tube (Bloomer & Arndt, 1999; Wiesmann *et al.*, 2007), which has a very small focal spot size (10–50 µm), can deliver a brilliance as much as one to two orders of magnitude higher than a conventional fine-focus sealed tube. The tube, which is also called a 'microsource', is typically air cooled because the X-ray generator power is less than 50 W. The X-ray optics for a microsource, either a multilayer mirror or a polycapillary, are typically mounted very close to the focal spot so as to maximize the gain on the capture angle. A microsource is highly suitable for 2D-XRD because of its spot focus and high brilliance.

If the X-rays used for diffraction have a wavelength slightly shorter than the *K* absorption edge of the sample material, a significant amount of fluorescent radiation is produced, which spreads over the diffraction pattern as a high background. In a conventional diffractometer with a point detector, the fluorescent background can be mostly removed by either a receiving monochromator mounted in front of the detector or by using a point detector with sufficient energy resolution. However, it is impossible to add a monochromator in front of a 2D detector and most area detectors have insufficient energy resolution. In order to avoid intense fluorescence, the wavelength of the X-ray-tube $K\alpha$ line should either be longer than the *K* absorption edge of the sample or far away from the *K* absorption edge. For example, Cu $K\alpha$ should not be used for samples containing significant amounts of the elements iron or cobalt. Since the $K\alpha$ line of an element cannot excite fluorescence of the same element, it is safe to use an anode of the same metallic element as the sample if the X-ray tube is available, for instance Co $K\alpha$ for Co samples. In general, intense fluorescence is produced when the atomic number of the anode material is 2, 3, or 4 larger than that of an element in the sample. When the sample contains Co, Fe or Mn (or Ni or Cu), the use of Cu $K\alpha$ radiation should be avoided; similarly, one should avoid using Co $K\alpha$ radiation if the sample contains Mn, Cr or V, and avoid using Cr $K\alpha$ radiation if the sample contains Ti, Sc or Ca. The effect is reduced when the atomic-number difference increases.

2.5.3.1.4. *X-ray optics*

The function of the X-ray optics is to condition the primary X-ray beam into the required wavelength, beam focus size, beam profile and divergence. Since the secondary beam path in a 2D-XRD system is an open space, almost all X-ray optics components are on the primary side. The X-ray optics components commonly used for 2D-XRD systems include a β-filter, a crystal monochromator, a pinhole collimator, cross-coupled multilayer mirrors, a Montel mirror, a polycapillary and a monocapillary. Detailed descriptions of these optic devices can be found in Chapter 2.1. In principle, the cross-sectional shape of the X-ray beam used in a 2D diffraction system should be small and round. In data-analysis algorithms, the beam size is typically considered to be a point. In practice, the beam cross section can be either round, square or another shape with a limited size. Such an X-ray beam is typically collimated or conditioned by the X-ray optics in two perpendicular directions, so that the X-ray optics used for the point beam are often called 'two-dimensional X-ray optics'.

A pinhole collimator is normally used to control the beam size and divergence in addition to other optic devices. The choice of beam size is often a trade-off between intensity and the ability to illuminate small regions or resolve closely spaced sample features. Smaller beam sizes, such as 50 µm and 100 µm, are preferred for microdiffraction and large beam sizes, such as 0.5 mm or 1 mm, are typically used for quantitative analysis, or texture or crystallinity measurements. In the case of quantitative analysis and texture measurements, using too small a collimator can actually be a detriment, causing poor grain-sampling statistics. The smaller the collimator, the longer the data-collection time. The beam divergence is typically determined by both the collimator and the coupling optic device. Lower divergence is typically associated with a long beam path. At the same time, the beam flux is inversely proportional to the square of the distance between the source and the sample. There are two main factors determining the length of the primary beam path: the first is the required distance for collimating the beam into the required divergence, the second is the space required for the primary X-ray optics, the sample stage and the detector. On the condition that the above two factors are satisfied, the primary X-ray beam path should be kept as short as possible.

2.5.3.2. *2D detector*

Two-dimensional (2D) detectors, also referred to as area detectors, are the core of 2D-XRD. The advances in area-detector technologies have inspired applications both in X-ray imaging and X-ray diffraction. A 2D detector contains a two-dimensional array of detection elements which typically have identical shape, size and characteristics. A 2D detector can simultaneously measure both dimensions of the two-dimensional distribution of the diffracted X-rays. Therefore, a 2D detector may also be referred to as an X-ray camera or imager. There are many technologies for area detectors (Arndt, 1986; Krause & Phillips, 1992; Eatough *et al.*, 1997; Giomatartis, 1998; Westbrook,