International Tables for Crystallography (2006). Vol. F, Figure 9.1.6.5, p. 181.

If the crystal is rotated during exposure, the ellipses observed on a still image change their position on the detector. In effect, all reflections diffracting during one exposure will be contained within lunes formed between the two limiting positions of each ellipse at the start and end of the given rotation. The width of the lunes in the direction of the crystal rotation, perpendicular to the rotation axis, is proportional to the rotation range per exposure. In contrast, along the rotation axis the width of the lunes is very small, since the intersection of the reciprocal-lattice plane with the Ewald sphere does not change significantly. For crystals of small molecules, the lunes are not pronounced, owing to the sparse population of reciprocal space, but for crystals with large cell dimensions, the lunes are densely populated by diffraction spots and often exhibit clear and well pronounced edges. At high resolution, the mapping of the reciprocal lattice within each lune is distorted, and rows of reflections form hyperbolas. At low diffraction angles, where the surface of the Ewald sphere is approximately flat, this distortion is minimal, and the lunes look like fragments of precession photographs.

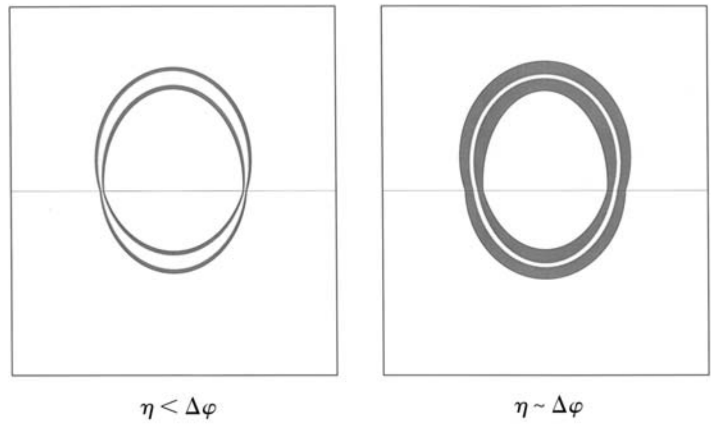

Fig. 9.1.6.5. Appearance of a lune for (*a*) a crystal of low mosaicity and (*b*) a highly mosaic crystal. Characteristically, the width of the lune along the rotation axis is wider if the mosaicity is high.

9.1.6.5. *Partially and fully recorded reflections*

The rotation method gives rise to lunes of data between the ellipses that relate to the start and the end of the rotation range used for the exposure. The data are complete if the Ewald sphere has been crossed by all reflections in the asymmetric part of the reciprocal lattice, which means that the crystal has to be rotated by a substantial angle. However, it is impossible to record all the data in a single exposure with such a wide rotation, owing to overlapping of the diffraction spots.

In practical applications to macromolecules, the total rotation is divided into a series of narrow individual rotations of width $\Delta\varphi$. In each of these, the crystal is exposed for a specified time or X-ray dose per angular unit. Each reflection diffracts over a defined crystal rotation and hence time interval, owing to the finite value of the rocking curve or angular spread, here referred to as ξ, the combined effect of beam divergence (δ) and crystal mosaicity (η). Provided ξ is less than $\Delta\varphi$, some reflections will start and finish crossing the Ewald sphere and hence diffract within one exposure. Their full intensity will be recorded on a single image, and these are referred to as fully recorded reflections, or fullys.

Other reflections will start to diffract during one exposure, but will still be diffracting at the end of the $\Delta\varphi$ rotation range. The remaining intensity of these reflections will be recorded on subsequent images. There will of course be corresponding reflections at the start of the present image. These reflections are termed partially recorded, or partials. Fig. 9.1.6.4 shows schematically how a lune appears on two consecutive exposures, with partials at each edge. The partials at the bottom edge of each lune contain the rest of the intensity of the partials from the previous exposure. The rest of the intensity of the partials at the top of the lune will appear on the next exposure. Superposition of two successive images will reveal some spots common to both: they are the partials shared between the two. If the angular spread ξ is small compared to the rotation range $\Delta\varphi$ then most reflections will be fully recorded. As ξ increases, the proportion of partials will rise, and when it reaches or exceeds $\Delta\varphi$ in magnitude there will be no fully recorded reflections. If the rotation range per image is small compared with the rocking curve, individual reflections can be spread over several images.

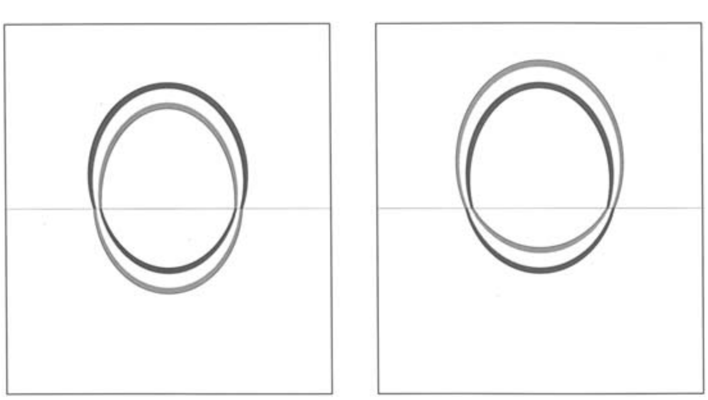

Fig. 9.1.6.4. A single lune on two consecutive exposures. The partial reflections appear on both images and their intensity is distributed over both.

As ξ increases, the lunes become wider (Fig. 9.1.6.5), since there are more partial reflections crossing the Ewald sphere at any one time. The appearance of the lunes can be used to estimate the mosaicity of the crystal. If the edges are sharply defined, then the mosaicity is low. In contrast, if the intensities at the edges gradually fade away, then the mosaicity must be high. Indeed, this phenomenon can be exploited by the integration software to provide accurate definition of the orientation parameters and of the mosaicity.

A key characteristic of high mosaicity is that all lunes are wide in the region along the rotation axis. On still exposures, the width of the rings is proportional to the angular spread. The width of lunes is expected to be very small along the rotation axis. If they are wide in this region, this is especially indicative of high mosaic spread. While highly ordered crystals with low mosaicity are preferable and often lead to data of the highest quality, high mosaic spread is not a prohibitive factor in accurate intensity estimation, provided it is properly taken into account in estimating the data collection and integration parameters, such as individual rotation ranges.

9.1.6.6. *The width of the rotation range per image: fine φ slicing*

An important variable in the rotation method is the width of the rotation ranges per individual exposure. The two basic approaches can be termed wide and fine φ slicing and differ in the relation between the angular spread and the rotation range per exposure. The two methods are applicable under different experimental constraints.

Fine φ slicing requires that the individual intensities are divided over several consecutive images, *i.e.* $\Delta\varphi$ should be substantially less than ξ (Kabsch, 1988). This approach possesses two very positive features. Firstly, it minimizes the background by integrating intensities only over a φ range equivalent to the rocking

references