symmetry; there is some misalignment which results in spots of a triangular ‘shape’ (i.e. made up of a group of little sub-spots) rather than the clear and distinct single spots of Fig. 11.7. Other, more complicated five-fold patterns of spots may also arise. It is not surprising that the first reported occurrences of quasiperiodic crystals were greeted with considerable scepticism throughout much of the crystallographic community.

11.5 Kikuchi and electron backscattered diffraction (EBSD) patterns

11.5.1 Kikuchi patterns in the TEM

We first consider the trajectories, or paths, of the inelastically scattered electrons within the specimen (Section 11.1). These occur over a range of angles, the scattering being most intense at small angles to the incident beam and decreasing at larger angles, giving in effect a ‘pear-shaped’ distribution of intensity as shown schematically in the upper part of Fig. 11.8. This distribution of intensity around the incident electron beam (the centre spot) is shown in the lower part of Fig. 11.8. Such a distribution is only observed in practice in ‘thicker’ specimens (in the range 200 nm upwards) and in which the amount of inelastic scattering is significant. It is almost entirely absent in the thin foil specimens from which the electron diffraction patterns shown in Figs 11.5(a), 11.17, 11.18 and 11.19 were obtained.

Now we describe the elastic scattering, or Bragg reflection, of the weakly inelastically scattered electrons that have suffered negligible changes in wavelength. Consider a specimen in which a set of \( hkl \) planes is at an angle to the incident beam slightly smaller
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Incident beam

Distribution of inelastic scattered intensity within specimen

Intensity distribution around incident beam

Fig. 11.8. The distribution of inelastic scattered intensity within a specimen and (below) the distribution intensity around the incident (unscattered) electron beam.

than the Bragg angle (Fig. 11.9(a)). No reflection of the incident beam, or given the extension of the reciprocal lattice point (Section 11.2), only a weak reflection of the incident beam occurs. However, those inelastically scattered beams which are incident to the planes at the Bragg angle are reflected. Figure 11.9(a) shows two such beams, AB and AC, AB being more intense than AC since the inelastic scattering angle is smaller. Beam AB is reflected to D (solid line), giving an increase in intensity; at the same time it is attenuated in the direction to E (dotted line) giving a reduction in intensity. A similar reflection (solid line) and attenuation (dotted line) occurs for AC. However, because beam AC is weaker the overall effect will still be an increase in intensity at D and a decrease in intensity at E. Now these peaks are not spots but are sections through cones of intensity which intersect the reflecting sphere to give nearly straight lines running parallel to the reflecting planes, i.e. perpendicular to the plane of the paper. These—the 'light' and 'dark' Kikuchi lines—are shown in the plane of the diffraction pattern in Fig. 11.9(b). Also shown is the (weak) $hkl$ diffraction spot and the downwards projected trace of the planes which lies half-way in between the Kikuchi lines (dashed line). The angle between the Kikuchi lines is $2\theta$ and thus they have the same separation $R$ as the distance between the centre spot and $hkl$ diffraction spot.

From Fig. 11.9(a) two angles are of interest: $\phi$, the deviation of the planes from the exact Bragg angle, and $\rho$, the deviation of the planes from exact parallelism with the incident beam. There angles may be determined by measuring the distance $a_K$ (from the dark Kikuchi line to the centre spot) and $a_t$ (from the trace of the planes and the centre spot). Given the camera length $L$ (Fig. 11.4), then $\phi = a_K/L$ and $\rho = a_t/L$.

The geometry may also be represented in terms of the Ewald reflecting sphere construction, Fig. 11.10. $k$ and $k_0$ are the vectors representing the directions of the diffracted
Fig. 11.9. (a) A crystal with a set of planes at an angle to the incident beam slightly smaller than the Bragg angle. AB and AC show two inelastically scattered beams (see Fig. 11.8) which are incident to the planes at the Bragg angle and which are partly reflected (solid lines) and partly attenuated (dotted lines) resulting in light (electron excess) and dark (electron deficient) Kikuchi lines, shown in plan in (b) together with the diffraction and centre spots and the projected trace of the reflecting planes.

and direct beams and $\mathbf{g}_{hkl} (\equiv d_{hkl})$ is the reciprocal lattice vector for the reflecting planes (see footnote, page 198, Section 8.3). The $hkl$ reciprocal lattice point lies outside the sphere and the vector $\mathbf{s}$ (closely parallel to $\mathbf{k}$ and $\mathbf{k}_0$) represents the deviation of $\mathbf{g}_{hkl}$ from the exact Bragg condition, the modulus of which is given by $|s| = \phi \left| \mathbf{g}_{hkl} \right|$. Now we see the value of Kikuchi lines in establishing the precise orientation of the reflecting planes: as we (say) rotate the crystal clockwise, the pair of Kikuchi lines move to the left and at the exact Bragg angle ($\phi = 0$), the dark Kikuchi line passes through the centre spot and the bright Kikuchi line passes through the diffraction spot. Similarly, when the crystal is
rotated such that the planes are exactly parallel to the incident beam, the Kikuchi lines will be at equal distances each side of the centre spot.\footnote{In this situation the (simplified) explanation of Kikuchi line contrast given above breaks down. A more detailed analysis shows that the lines are still observed.}

In practice we may see many Kikuchi lines—as many pairs as there are diffraction spots (Fig. 11.11). However, just two pairs of lines, and two diffraction spots, are sufficient to determine the orientation of the crystal with respect to the incident electron beam direction. Figure 11.12 shows a pattern with two spots, $h_1k_1l_1$ and $h_2k_2l_2$ and their associated Kikuchi lines; half way in between which are drawn the downwards projected traces of the planes (dashed lines). The downwards direction of the zone axis $\overline{uvw}$ lies at the intersection of the traces as shown; the upwards direction $[uvw]$ (i.e. anti-parallel to the electron beam) lies on the opposite side of the centre spot and is found by cross-multiplication of the indices as described in the footnote on p. 281. The angle $\eta$ between $[uvw]$ and the centre spot, 000, is simply found by measuring the distance $P$, again using the relationship $\eta = P/L$.

The pattern of Kikuchi lines also reflects the symmetry of planes in a crystal and ‘maps’ may be created showing the patterns of lines for different crystal orientations. Figure 11.13 shows one such map for an fcc crystal centered on [001], the four-fold symmetry of which is clearly evident. Note that the spacings of the pairs of lines correspond to the reciprocal lattice spacings; 200 and 020 passing through the centre being the narrowest, then 220, 220, and so on. The value of such maps is that they provide a means of tilting the specimen into any desired orientation: one simply ‘moves along’ a pair of lines (like railway lines!) to bring the desired zone axis to the centre of the projection.
11.5 Kikuchi and electron backscattered diffraction patterns

11.5.2 Electron backscattered diffraction (EBSD) patterns in the SEM

The geometry of the formation of EBSD patterns is analogous to that of Kikuchi patterns except that the incident electron beam is at a small angle, typically $\sim 20^\circ$, to the specimen surface. Only those electrons inelastically-elastically scattered from depths some 10–20 nm below the specimen surface (depending on the specimen, incident beam energy and angle) emerge from the specimen to be recorded on a phosphor screen and a CCD camera. Hence EBSD is essentially a surface technique and any surface damage or distortion must be removed by careful preparation techniques. An example of an EBSD pattern is shown in Fig. 11.14. The orientation analysis is of course carried out by computer software. The great value of EBSD is that it can be used to determine the orientations of crystals in a specimen and therefore the misorientations and nature of the boundaries between them. The beam is scanned across the specimen surface and the crystal orientation is measured at each point—the resulting map reveals the constituent crystal morphology, orientations and boundaries. The resolution depends of course on the diameter of the incident beam and interaction volume—at present, under favourable conditions, resolutions of 10–20 nm are obtainable. The crystal orientations may also be presented in the form of a pole figure in an analogous way to the X-ray pole figures described in Section 12.5.3. They are in fact complementary techniques: X-rays record
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Fig. 11.12. Determination of the exact orientation of a crystal from a spot-Kikuchi line electron diffraction pattern. The downwards zone axis, $\bar{uvw}$, lies at the intersection of the projected traces of the reflecting planes $h_1k_1l_1$ and $h_2k_2l_2$. The angle $\eta$ of the zone axis $uvw$ to the incident beam direction is given by $\eta = P/L$.

the reflections non-sequentially from one set of planes in a larger volume (area and depth) of the specimen.

EBSD is also complementary to the Laue X-ray diffraction technique (Section 9.4); again in the X-ray technique the X-rays penetrate into a much greater depth in the specimen (typically 5–20 $\mu$m) compared to the 10–20 nm of EBSD.

11.6 Image formation and resolution in the TEM

The Abbe criterion for image formation, discussed in Section 7.5, applies equally to light and electron microscopy. Electron wavelengths are very much smaller (4 pm for 100 kV instruments) than atomic dimensions, but atomic resolution (perhaps the ultimate goal in microscopy) is limited by the severe spherical aberration of electron (electromagnetic) lenses which limits numerical aperture (NA) values to the order of 0.01. Using the equation $a = 0.5\lambda/NA$ gives a limit of resolution of 2Å—a dimension of the same order as atomic dimensions and interatomic spacings. The development of higher kV instruments (smaller $\lambda$) and improvements to the corrections (for spherical aberration and