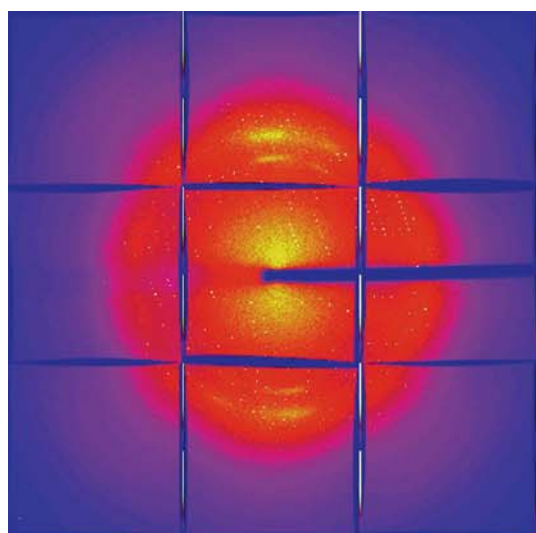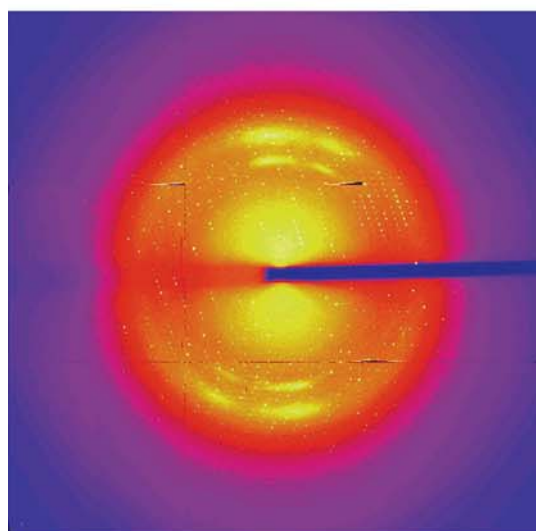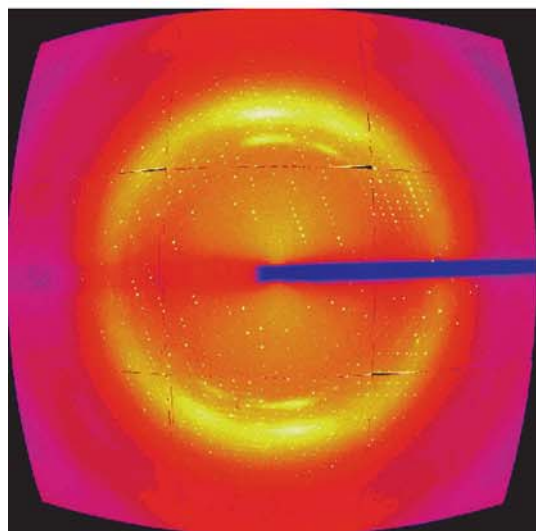11.4. *DENZO* AND *SCALEPACK*



*(a)*



*(b)*



*(c)*

Fig. 11.4.5.1. The transformations in *DENZO* applied to APS-1 detector data. (*a*) Raw data are affected by geometrical distortion introduced by nine fibre-optic tapers; (*b*) the same image converted to planar Cartesian space; (*c*) the same data converted to a virtual spherical detector.

the X-ray beam completes the definition of the detector goniostat in *HKL*.

### 11.4.5.11. *Crystal goniostat*

The physical goniostat is defined by six angles. Two angles define the direction of the main axis ($\omega$) in the *DENZO* coordinate system. The third angle defines the zero position of the $\omega$ axis. The fourth is the angle between $\omega$ and the second axis ($\kappa$ or $\chi$). The fifth defines the zero position of the second axis. The sixth is the angle between the second and the third axes. This type of goniostat definition allows for the specification of any three-axis goniostat (*EEC Cooperative Workshop on Position-Sensitive Detector Software*, 1986). Each type of goniostat is represented by six angles. Misalignment of the goniostat is represented as an adjustment to these angles, which can be refined by the *HKL* system.

### 11.4.5.12. *Crystal orthogonalization convention*

Crystal orientation specified by the three angles needs a definition of a zero point. Any crystal axis, or its equivalent reciprocal-space zone perpendicular to it, can be used as a reference. The definition of zero point aligns the crystal axis with the beam direction and one of the reciprocal axes with the $x$ direction. The user can specify both axes.

### 11.4.5.13. *Refinement and calibration*

Both the refinement and calibration procedures determine the properties of the instrument. The principal difference between refinement and calibration is that calibration is performed with data obtained outside the current diffraction experiment, and refinement uses data obtained during the current diffraction experiment. *DENZO* performs both refinement and calibration, and in some cases the difference between calibration and refinement is a question of semantics, as the refined data from one experiment can be used as a reference for another experiment, or even as a reference for a subsequent refinement cycle or for another part of the same experiment.

### 11.4.6. Prediction of the diffraction pattern

The autoindexing procedure assigns Miller indices only to strong spots, ones that can be found through a peak search. The target of the experiment is to estimate structure factors for all reflections captured by the detector. Therefore, positions of all spots need to be predicted by applying the following equations to all possible triplets **h**. Using

$$\mathbf{S} = [A]^{-1}\mathbf{h}, \qquad (11.4.6.1)$$

we have to find the matrix $[A]$ that generates the vector **S**, which satisfies the diffraction condition [equation (11.4.2.1)], knowing that the matrix $[A]$ is a function of the crystal orientation [equation (11.4.2.6)]. The rotation of the crystal during the experiment creates a straightforward algebraic problem that results in a complex equation defining the angle at which the reflection occurs. This angle also defines the image at which the reflection appears. Knowing this angle, the vector **S** can be calculated, and, from equation (11.4.2.5), the direction of the vector **X** can be found:

$$\mathbf{X}/|\mathbf{X}| = \lambda(\mathbf{S} - \mathbf{S}_0). \qquad (11.4.6.2)$$

Calculation of the length of vector **X** requires knowledge of the detector orientation, which, for flat detectors, is described here by vector **G**, perpendicular to the detector and with length equal to the crystal-to-detector distance:

**references**