determine the stress-free d-spacing d_o, the instrument should be first calibrated with a stress-free standard of a similar material.

2.5.4.3.4. *Data-collection strategy*

The practice of stress analysis with 2D-XRD involves the selection of the diffraction-system configuration and the data-collection strategy, frame correction and integration, and stress calculation from the processed data points. Most concepts and strategies developed for a conventional diffractometer are still valid for 2D-XRD. We will focus on the new concepts and practices due to the nature of the 2D detectors.

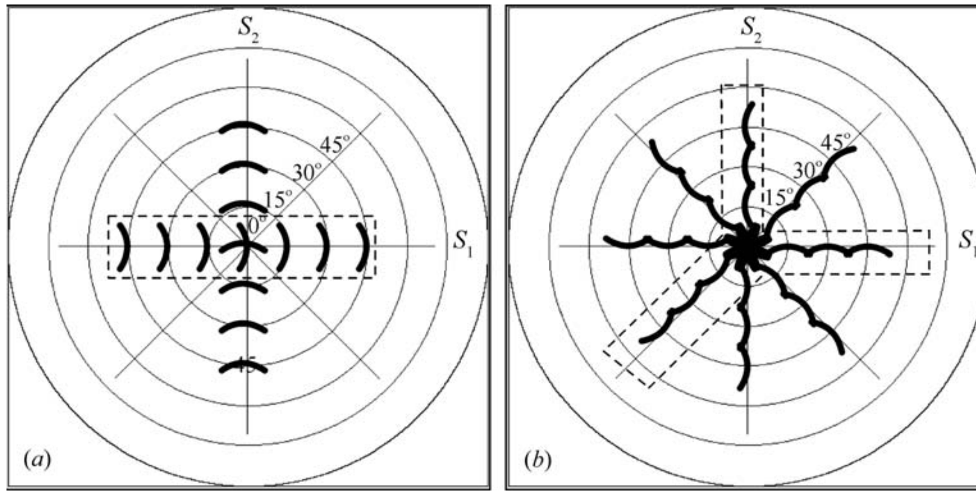

Figure 2.5.25
Data-collection strategy schemes: (a) $\omega + \varphi$ scan; (b) $\psi + \varphi$ scan.

The diffraction vector is in the normal direction to the measured crystalline planes. It is not always possible to have the diffraction vector in the desired measurement direction. In reflection mode, it is easy to have the diffraction vector normal to the sample surface, or tilted away from the normal, but impossible to have the vector on the surface plane. The stress on the surface plane, or biaxial stress, is calculated by elasticity theory from the measured strain in other directions. The final stress-measurement results can be considered as an extrapolation from the measured values. In the conventional $\sin^2\psi$ method, several ψ-tilt angles are required, typically at 15° steps from −45° to +45°. The same is true with a 2D-XRD system. The diffraction vectors corresponding to the data scan can be projected onto a 2D plot in the same way as the pole-density distribution in a pole figure. The 2D plot is called a data-collection strategy scheme.

By evaluating the scheme, one can generate a data-collection strategy suitable for the measurement of the intended stress components. Fig. 2.5.25 illustrates two schemes for data collection. In the bisecting condition ($\omega = \theta$ or $\theta_1 = \theta$ and $\psi = 0°$), the trace of the diffraction vector falls in the vicinity of the scheme centre. Either an ω tilt or a ψ tilt can move the vectors away from the centre. The circles on the scheme are labelled with the tilt angle of 15°, 30° and 45°. Scheme (a) is for an ω tilt of 0°, ±15°, ±30° and ±45° with the φ angle at 0° and 90°. It is obvious that this set of data would be suitable for calculating the biaxial-stress tensor. The data set with $\varphi = 0°$, as shown within the box enclosed by the dashed lines, would be sufficient on its own to calculate σ_{11}. Since the diffraction-ring distortion at $\varphi = 0°$ or $\varphi = 90°$ is not sensitive to the stress component σ_{12}, strategy (a) is suitable for the equibiaxial stress state, but is not able to determine σ_{12} accurately. In scheme (b), the ψ scan covers 0° to 45° with 15° steps at eight φ angles with 45° intervals. This scheme produces comprehensive coverage on the scheme chart in a symmetric distribution. The data set collected with this strategy can be used to calculate the complete biaxial-stress tensor components and shear stress (σ_{11}, σ_{12}, σ_{22}, σ_{13}, σ_{23}). The scheme indicated by the boxes enclosed by the dashed lines is a time-saving alternative to scheme (b). The rings on two φ angles are aligned to S_1 and S_2 and the rings on the third φ angle make 135° angles to the other two arrays of rings. This is analogous to the configuration of a stress-gauge rosette. The three φ angles can also be separated equally by 120° steps. Suitable schemes for a particular experiment should be determined by considering the stress components of interest, the goniometer, the sample size, the detector size and resolution, the desired measurement accuracy and the data-collection time.

2.5.4.3.5. *Data integration and peak evaluation*

The purpose of data integration and peak evaluation is to generate a set of data points along distorted diffraction rings. Data integration for stress analysis is γ integration over several defined segments so as to generate diffraction profiles representing the corresponding segments. The peak position can be determined by fitting the diffraction profile to a given analytic function. Fig. 2.5.26 illustrates data integration over a diffraction frame. The total integration region is defined by $2\theta_1$, $2\theta_2$, γ_1 and γ_2. The integration region is divided into segments given by $\Delta\gamma$. One data point on the distorted diffraction ring is generated from each segment. The γ value in the centre (denoted by the dot-dashed line) of each segment is taken as the γ value of the data point. γ integration of the segment produces a diffraction profile and the 2θ value is determined from the profile. The number of segments and the segment size ($\Delta\gamma$) are selected based on the quality of the data frame. The larger the segment size $\Delta\gamma$ is, the better the integrated diffraction profile as more counts are being integrated. γ integration also produces a smearing effect on the diffraction-ring distortion because the counts collected within the segment size $\Delta\gamma$ are considered as a single γ value at the segment

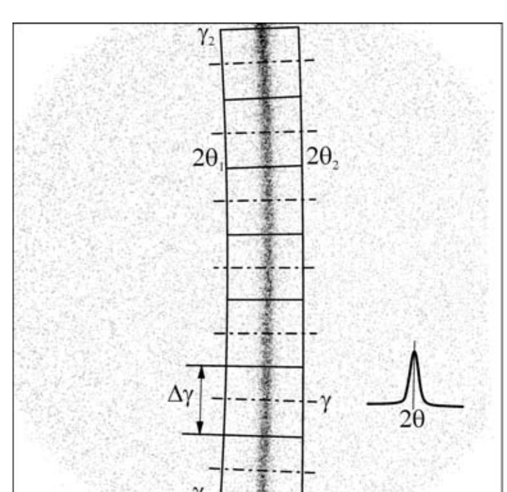

Figure 2.5.26
Data integration for stress measurement.