International Tables for Crystallography (2006). Vol. C, Section 7.3.7, p. 652.

7.3.7. Corrections to the intensity measurements depending on the detection system

A good diffractometer on a reactor is supposed to give point by point for each solid-angle element $d\Omega$ an exact image of the scattered intensity. This is never perfectly achieved in practice and necessitates some corrections. In all cases, it is very important to be aware that additional background might be created when part of the shielding or of the collimator intersect the monochromatic neutron beam. We suppose for the following discussion that this effect has been corrected or avoided. The wavelength dependence of the detector response (which is needed for inelasticity corrections or TOF measurements) is generally computed from the theoretical detector law [see equation (7.3.2.1)]. At each measuring point, the collected intensity is renormalized by the integrated incident neutron flux, which is measured by the monitoring device.

In the case of TOF measurements on a spallation source, the measured intensity must also be renormalized by the wavelength spectrum of the source, obtained from the measurement of an isotropic scatterer such as vanadium.

7.3.7.1. *Single detector*

For up to 10% of dead time in the counting rate, the correction for the dead-time loss is generally considered as linear. If Δt is the electronic dead time for one neutron (1–10 µs for the gas detectors) and n the number of counts per second, the dead-time correction factor is $1/(1 - n\Delta t)$.

7.3.7.2. *Banks of detectors*

In the case of a bank of detectors used for a powder diffractometer in a reactor, one has to calibrate the relative positions of the detectors and their response to the neutron intensity by scanning the detectors through a Bragg pattern.

In the case of TOF measurements, the detector banks are installed at fixed angles. For each detector, the measured intensity depends on the detector type, size, and distance to the sample. The neutron and γ background depends moreover on the detection angle. After background corrections, the intensities measured by each detector bank are calibrated and matched using the overlaps between spectra.

7.3.7.3. *Position-sensitive detectors*

(*a*) *Calibration of the position*. For multi-electrode PSDs, the relative position of the electrodes is fixed and verified at the time of construction. In the case of other PSDs with analogue encoding, an angular calibration is made periodically with the help of a Bragg pattern, a thin neutron beam, or a cadmium mask moved across a diffuse beam incident on the PSD (Berliner, Mildner, Sudol & Taub, 1983).

(*b*) *Calibration of the PSD homogeneity*. The response function might be dependent on the position within the PSD and possibly on the intensities collected at other parts of the PSD. The homogeneity of response of a PSD, which is normally better than 5%, can be calibrated to a much higher accuracy, since the stability of the PSDs is generally very good (*e.g.* 0.1% or better for gas PSDs). In the case of a reactor, the classical method of calibration is the use of an isotropic scatterer such as vanadium. The calibration is made at angles that avoid the very small vanadium Bragg peaks (or with displacement of the PSD to several positions) and that keep a low and isotropic background. Calibration factors, sometimes called cell-efficiency coefficients α_i, are then obtained. Considering the lack of isotropy of the vanadium pattern, this method is limited to about 1% accuracy. For small PSDs, a precision of 0.1% or better is obtainable by scanning the whole PSD with a step equal to the cell spacing through any nearly isotropic pattern.

(*c*) *Particular effects due to high intensities*. The dead time of a PSD is complex. It depends on multiple parameters (the independent amplifiers and the encoding–decoding procedure). However, if there is a unique decoding logic for the whole PSD, and if this gives the highest contribution to the dead time, the ratios of the peak intensities are then conserved. In the case of strong Bragg peaks, the parasitic effect of scattering by the PSD entrance window (*e.g.* 10 mm aluminium for high-pressure gas PSDs) is detectable and can be corrected after calibration (using an intense and well localized thin beam).

references