2. DIFFRACTION GEOMETRY AND ITS PRACTICAL REALIZATION

drum. The wavelength resolution $\Delta\lambda/\lambda$ of velocity selectors is usually between 5 and 40% (full width at half-maximum, FWHM); 10 and 20% are frequently used values.

Alternatively, time-of-flight (TOF) SANS cameras have been developed on pulsed neutron sources (*e.g.* Hjelm, 1988). These use short bunches (about $100\,\mu s$ long) of neutrons with a 'white' wavelength spectrum produced by a pulsed high-energy proton beam impinging on a target with a repetition rate of the order of $10\,ms$. The wavelength and, consequently, the Q value of a scattered neutron is determined by its flight time, if the scattering is assumed to be quasi-elastic. The dynamic Q range of TOF SANS instruments is rather large, especially in the high-Q limit, owing to the large number of rapid neutrons in the pulse. The low-Q limit is determined by the pulse-repetition rate of the source because of frame overlap with the following pulse. It can be decreased, if necessary with choppers turning in phase with the pulse production and selecting only every nth pulse. This disadvantage does not exist for reactor-based TOF SANS cameras, where the pulse-repetition rate can be optimally adapted to the chosen maximal and minimal wavelength. A principal problem for TOF SANS exists in the 'upscattering' of cold neutrons, *i.e.* their gain in energy, by ^{1}H-rich samples: The background scattering may not arrive simultaneously with the elastic signal, and may thus not be attributed to the correct Q value (Hjelm, 1988).

2.6.2.1.2. *Geometry*

With typical neutron wavelengths, low Q need not necessarily mean small angles: The interesting Q range for an inhomogeneity of dimension D can be estimated as $1/D < Q < 10/D$. The scattering angle corresponding to the upper Q limit for $D = 10\,nm$ is $1.4°$ for $CuK\alpha$ radiation, but amounts to $9.1°$ for neutrons of $10\,nm$ wavelength. Consequently, it is preferable to speak of low-Q rather than of small-angle neutron scattering.

'Pin-hole'-type cameras are the most frequently used SANS instruments; an example is the SANS camera D11 at the Institut Max von Laue–Paul Langevin in Grenoble, France (Ibel, 1976; Lindner, May & Timmins, 1992), from which some of the numbers below are quoted. Since the cross section of the primary beam is usually chosen to be rather large (*e.g.* $3 \times 5\,cm$) for intensity reasons, pin-hole instruments tend to be large. The smallest Q value that can be measured at a given distance is just outside the image of the direct beam on the detector (which either has to be attenuated or is hidden behind a beamstop, a neutron-absorbing plate of several $10\,cm^2$, *e.g.* of cadmium). Very small Q values thus require long sample-to-detector distances. The area detector of D11, with a surface of $64 \times 64\,cm$ and resolution elements of $1\,cm^2$, moves within an evacuated tube of $1.6\,m$ diameter and a length of $40\,m$. Thus, a Q range of 5×10^{-3} to $5\,nm^{-1}$ is covered. The geometrical resolution is determined by the length of the free neutron flight path in front of the sample, moving sections of neutron guide into or out of the beam ('collimation'). In general, the collimation length is chosen roughly equal to the sample-to-detector distance. Thus, the geometrical and wavelength contributions to the Q resolution match at a certain distance of the scattered beam from the direct-beam position in the detector plane. In order to resolve scattering patterns with very detailed features, *e.g.* of particles with high symmetry, longer collimation lengths are sometimes required at the expense of intensity.

Much more compact double-crystal neutron diffractometers [described for X-rays by Bonse & Hart (1966)] are being used to reach the very small Q values of some $10^{-4}\,nm^{-1}$ typical of static light scattering. The sample is placed between two crystals. The first crystal defines the wavelength and the direction of the incoming beam. The other crystal scans the scattered intensity. The resolution of such an instrument is mainly determined by the Darwin widths of the ideal crystals. This fact is reflected in the low neutron yield. Slit geometry can be used, but not 2D detectors.

A recent development is the ellipsoidal-mirror SANS camera. The mirror, which needs to be of very high surface quality, focuses the divergent beam from a small (several mm^2) source through the sample onto a detector with a resolution of the order of $1 \times 1\,mm$. Owing to the more compact beam image, all other dimensions of the SANS camera can be reduced drastically (Alefeld, Schwahn & Springer, 1989). Whether or not there is a gain in intensity as compared with pin-hole geometry is strongly determined by the maximal sample dimensions. Long mirror with cameras (*e.g.* $20\,m$) are always superior to double-crystal instruments in this respect (Alefeld, Schwahn & Springer, 1989), and can also reach the light-scattering Q domain (Q_{min} of some $10^{-4}\,nm^{-1}$, corresponding to particles of several μm dimension).

2.6.2.1.3. *Correction of wavelength, slit, and detector-element effects*

Resolution errors affect SANS data in the same way as X-ray scattering data, for which one may find a detailed treatment in an article by Glatter (1982*b*); there is one exception to this; namely, gravity, which of course only concerns neutron scattering, and only in rare cases (Boothroyd, 1989). Since SANS cameras usually work with pin-hole geometry, the influences of the slit sizes, *i.e.* the effective source dimensions, on the scattering pattern are small; even less important is, in general, the pixel size of 2D detectors. The preponderant contribution to the resolution of the neutron-scattering pattern is the wavelength-distribution function after the monochromatizing device, especially at larger angles. The situation is more complicated for TOF SANS (Hjelm, 1988).

As has been shown in an analytical treatment of the resolution function by Pedersen, Posselt & Mortensen (1990), who also quote some relevant references, resolution effects have a small influence on the results of the data analysis for scattering patterns with a smooth intensity variation and without sharp features. Therefore, one may assume that a majority of SANS patterns are not subjected to desmearing procedures.

Resolution has to be considered for scattering patterns with distinct features, as from spherical latex particles (Wignall, Christen & Ramakrishnan, 1988) or from viruses (Cusack, 1984). Size-distribution and wavelength-smearing effects are similar; it is evident that wavelength effects have to be corrected for if the size distribution is to be obtained.

Since measured scattering curves contain errors and have to be smoothed before they can be desmeared, iterative indirect methods are, in general, superior: A guessed solution of the scattering curve is convoluted with known smearing parameters and iteratively fitted to the data by a least-squares procedure. The guessed solution can be a simply parameterized scattering curve, without knowledge of the sample (Schelten & Hossfeld, 1971), but it is of more interest to fit the smeared Fourier transform of the distance-distribution function (Glatter, 1979) or the radial density distribution (*e.g.* Cusack, Mellema, Krijgsman & Miller, 1981) of a real-space model to the data.

2.6.2.2. *Isotopic composition of the sample*

Unlike X-rays, which 'see' the electron clouds of atoms within a sample, neutrons interact with the point-like nuclei. Since their

references