

5. DYNAMICAL THEORY AND ITS APPLICATIONS

defined as the ratio of the observed reflectivity to the ideal one, which is the kinematical reflectivity in this context.

In conventional work, the crystal structure factors of different reflections and the parameters of the mosaic model are fitted together to the experimental data, which are the integrated reflectivities and the angular widths of the rocking curves. In many cases, only the weakest reflections will be free, or nearly free, from extinction. The extinction corrections thus obtained can be considered as satisfactory in cases of moderate extinction. Nevertheless, extinction remains a real problem in cases of strong extinction and in any case if a very precise determination of the crystal structure factors is required.

There exist several forms of the mosaic model of extinction. For instance, in the model developed by Kulda (1988*a,b*, 1991), the mosaic blocks are not considered just as simple perfect blocks but may be deformed perfect blocks. This has the advantage of including the case of macroscopically deformed crystals, such as bent crystals.

A basically different approach, free from the distinction between primary and secondary extinction, has been proposed by Kato (1980*a,b*). This is a wave-optical approach starting from the dynamical equations for diffraction by deformed crystals. These so-called Takagi-Taupin equations (Takagi, 1962; Taupin, 1964) contain a position-dependent phase factor related to the displacement field of the deformed crystal lattice. Kato proposed considering this phase factor as a random function with suitably defined statistical characteristics. The wave amplitudes are then also random functions, the average of which represent the coherent wavefields while their statistical fluctuations represent the incoherent intensity fields.

Modifications to the Kato formulation have been introduced by Al Haddad & Becker (1988), by Becker & Al Haddad (1990, 1992), by Guigay (1989) and by Guigay & Chukhovskii (1992, 1995). Presently, it is not easy to apply this 'statistical dynamical theory' to real experiments. The widely used methods for extinction corrections are still based on the former mosaic model, according to the formulation of Zachariasen (1967), later improved by Becker & Coppens (1974*a,b*, 1975).

As in the X-ray case, acoustic waves produced by ultrasonic excitation can artificially induce a transition from perfect to ideally imperfect crystal behaviour. The effect of ultrasound on the scattering behaviour of distorted crystals is quite complex. A good discussion with reference to neutron-scattering experiments is given by Zolotoyabko & Sander (1995).

The situation of crystals with a simple distortion field is less difficult than the statistical problem of extinction. Klar & Rustichelli (1973) confirmed that the Takagi-Taupin equations, originally devised for X-rays, can be used for neutron diffraction with due account of the very small absorption, and used them for computing the effect of crystal curvature.

5.3.5. Effect of external fields on neutron scattering by perfect crystals

The possibility of acting on neutrons through externally applied fields during their propagation in perfect crystals provides possibilities that are totally unknown in the X-ray case. The theory has been given by Werner (1980) using the approaches (migration of tie points, and Takagi-Taupin equations) that are customary in the treatment of imperfect crystals (see above). Zeilinger *et al.* (1986) pointed out that the effective-mass concept, familiar in describing electrons in solid-state physics, can shed new light on this behaviour: because of the curvature of the dispersion surface at a near-exact Bragg setting, effective masses five orders of

magnitude smaller than the rest mass of the neutron in a vacuum can be obtained. Related experiments are discussed below.

An interesting proposal was put forward by Horne *et al.* (1988) on the coupling between the Larmor precession in a homogeneous magnetic field and the spin-orbit interaction of the neutron with non-magnetic atoms, a term which was dismissed in Section 5.3.2 because its contribution to the scattering length is two orders of magnitude smaller than that of the nuclear term. A resonance is expected to show up as highly enhanced diffracted intensity when a perfect sample is set for Bragg scattering and the magnetic field is adjusted so that the Larmor precession period is equal to the *Pendellösung* period.

5.3.6. Experimental tests of the dynamical theory of neutron scattering

These experiments are less extensive for neutron scattering than for X-rays. The two most striking effects of dynamical theory for non-magnetic nearly perfect crystals, *Pendellösung* behaviour and anomalous absorption, have been demonstrated in the neutron case too. *Pendellösung* measurement is described below (Section 5.3.7.2) because it is useful in the determination of scattering lengths. The anomalous transmission effect occurring when a perfect absorbing crystal is exactly at Bragg setting, *i.e.* the Borrmann effect, is often referred to in the neutron case as the suppression of the inelastic channel in resonance scattering, after Kagan & Afanas'ev (1966), who worked out the theory. A small decrease in absorption was detected in pioneering experiments on calcite by Knowles (1956) using the corresponding decrease in the emission of γ -rays and by Sippel *et al.* (1962), Shil'shtein *et al.* (1971), and Hastings *et al.* (1990) directly. Rocking curves of perfect crystals were measured by Sippel *et al.* (1964) in transmission, and by Kikuta *et al.* (1975). Integrated intensities were measured by Lambert & Malgrange (1982). The large angular amplification associated with the curvature of the dispersion surfaces near the exact Bragg setting was demonstrated by Kikuta *et al.* (1975) and by Zeilinger & Shull (1979).

In magnetic crystals, the investigations have been restricted to the simpler geometry where the scattering vector is perpendicular to the magnetization, and to few materials. *Pendellösung* behaviour was evidenced through the variation with wavelength of the flipping ratio for polarized neutrons by Baruchel *et al.* (1982) on an yttrium iron garnet sample, with the geometry selected so that the defects would not affect the Bragg reflection used. The inclination method was used successfully by Zelepukhin *et al.* (1989), Kvardakov & Somenkov (1990), and Kvardakov *et al.* (1990*a*) for the weak ferromagnet FeBO₃, and in the room-temperature weak-ferromagnetic phase of hematite, α -Fe₂O₃, by Kvardakov *et al.* (1990*b*), and Kvardakov & Somenkov (1992).

Experiments on the influence of defects in nearly perfect crystals have been performed by several groups. The effect on the rocking curve was investigated by Eichhorn *et al.* (1967), the intensities were measured by Lambert & Malgrange (1982) and by Albertini, Boeuf, Cesini *et al.* (1976), and the influence on the *Pendellösung* behaviour was discussed by Kvardakov & Somenkov (1992). Boeuf & Rustichelli (1974) and Albertini *et al.* (1977) investigated silicon crystals curved by a thin surface silicon nitride layer.

Many experiments have been performed on vibrating crystals; reviews are given by Michalec *et al.* (1988) and by Kulda *et al.* (1988). Because the velocity of neutrons is of the same order of magnitude as the velocity of acoustic phonons in crystals, the effect of ultrasonic excitation on dynamical diffraction takes on some original features compared to the X-ray case (Iolin & Entin, 1983); they could to some extent be evidenced experimentally (Iolin *et al.*, 1986; Chalupa *et al.*, 1986). References to experimental work on