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$$F_+ = F_N + F_M \text{ and } F_- = F_N - F_M. \qquad (5.3.3.11)$$

F_N and F_M are related to the scattering lengths of the ions in the unit cell of volume V_c:

$$F_N = V_c u_{\mathbf{h}} = \sum_i b_i \exp(-i\mathbf{h}\cdot\mathbf{r}_i);$$
$$F_M = V_c|\mathbf{Q_h}| = -\frac{\mu_0 m}{2h^2}\mu_n \boldsymbol{\sigma}\cdot\sum_i \boldsymbol{\mu}_{i\perp}(\mathbf{h})f_i\left(\frac{\sin\theta}{\lambda}\right)\exp(-i\mathbf{h}\cdot\mathbf{r}_i).$$

The dispersion surface of order 4 degenerates into two hyperbolic dispersion surfaces, each of them corresponding to one of the polarization states (±). The asymptotes are different; this is related to different values of the refractive indices for neutron polarization parallel or antiparallel to $\mathbf{Q_0}$.

In some special cases the magnitudes of F_N and F_M happen to be equal. Only one polarization state is then reflected. Magnetic crystals with such a property (reflections 111 of the Heusler alloy Cu_2MnAl, or 200 of the alloy Co–8% Fe) are very useful as polarizing monochromators and as analysers of polarization.

If the scattering vector **h** is in the same direction as the magnetization, this reflection is a purely nuclear one (with no magnetic contribution), since F_M is then equal to 0. Purely magnetic reflections (without nuclear contribution) also exist if the magnetic structure involves several sublattices.

If **h** is neither perpendicular to the average magnetization nor in the same direction, the presence of nondiagonal matrices in the dynamical equations cannot be avoided. The dynamical theory of diffraction by perfect magnetic crystals then takes the complicated form already mentioned.

Theoretical discussions of this complicated case of dynamical diffraction have been given by Stassis & Oberteuffer (1974), Mendiratta & Blume (1976), Sivardière (1975), Belyakov & Bokun (1975, 1976), Schmidt *et al.* (1975), Bokun (1979), Guigay & Schlenker (1979*a*,*b*) and Schmidt (1983). However, to our knowledge, only limited experimental work has been carried out on this subject. Successful experiments could only be performed for the simpler cases mentioned above.

5.3.3.4. *The dynamical theory in the case of perfect collinear antiferromagnetic crystals*

In this case, there is no average magnetization ($\mathbf{Q_0} = 0$). It is then convenient to choose the quantization axis in the direction of $\mathbf{Q_h}$ and $\mathbf{Q_{-h}}$. The dispersion surface degenerates into two hyperbolic surfaces corresponding to each polarization state along this direction for any orientation of the diffraction vector relative to the direction of the magnetic moments of the sublattices. These two hyperbolic dispersion surfaces have the same asymptotes. Furthermore, in the case of a purely magnetic reflection, they are identical.

The possibility of observing a precession of the neutron polarization in the presence of diffraction, in spite of the fact that there is no average magnetization, has been pointed out by Baryshevskii (1976).

5.3.3.5. *The flipping ratio*

In polarized neutron diffraction by a magnetically saturated magnetic sample, it is usual to measure the ratio of the reflected intensities I_+ and I_- measured when the incident beam is polarized parallel or antiparallel to the magnetization in the sample. This ratio is called the flipping ratio,

$$R = I_+/I_-, \qquad (5.3.3.12)$$

because its measurement involves flipping the incident-beam polarization to the opposite direction. This is an experimentally well defined quantity, because it is independent of a number of parameters such as the intensity of the incident beam, the temperature factor or the coefficient of absorption. In the case of an ideally imperfect crystal, we obtain from the kinematical expressions of the integrated reflectivities

$$R_{\rm kin}(\mathbf{h}) = (I_+/I_-)_{\rm kin} = \left(\frac{|F_N + F_M|}{|F_N - F_M|}\right)^2. \qquad (5.3.3.13)$$

In the case of an ideally perfect thick crystal, we obtain from the dynamical expressions of the integrated reflectivities

$$R_{\rm dyn}(\mathbf{h}) = (I_+/I_-)_{\rm dyn} = \frac{|F_N + F_M|}{|F_N - F_M|}. \qquad (5.3.3.14)$$

In general, $R_{\rm dyn}$ depends on the wavelength and on the crystal thickness; these dependences disappear, as seen from (5.3.3.14), if the path length in the crystal is much larger than the extinction distances for the two polarization states. It is clear that the determination of $R_{\rm kin}$ or $R_{\rm dyn}$ allows the determination of the ratio F_M/F_N, hence of F_M if F_N is known. In fact, because real crystals are neither ideally imperfect nor ideally perfect, one usually introduces an extinction factor y (extinction is discussed below, in Section 5.3.4) in order to distinguish the real crystal reflectivity from the reflectivity of the ideally imperfect crystal. Different extinction coefficients y_+ and y_- are actually expected for the two polarization states. This obviously complicates the task of the determination of F_M/F_N.

In the kinematical approximation, the flipping ratio does not depend on the wavelength, in contrast to dynamical calculations for hypothetically perfect crystals (especially for the Laue case of diffraction). Therefore, an experimental investigation of the wavelength dependence of the flipping ratio is a convenient test for the presence of extinction. Measurements of the flipping ratio have been used by Bonnet *et al.* (1976) and by Kulda *et al.* (1991) in order to test extinction models. Baruchel *et al.* (1986) have compared nuclear and magnetic extinction in a crystal of MnP.

Instead of considering only the ratio of the integrated reflectivities, it is also possible to record the flipping ratio as a function of the angular position of the crystal as it is rotated across the Bragg position. Extinction is expected to be maximum at the peak and the ratio measured on the tails of the rocking curve may approach the kinematical value. It has been found experimentally that this expectation is not of general validity, as discussed by Chakravarthy & Madhav Rao (1980). It would be valid in the case of a perfect crystal, hence in the case of pure primary extinction. It would also be valid in the case of secondary extinction of type I, but not in the case of secondary extinction of type II [following Zachariasen (1967), type II corresponds to mosaic crystals such that the diffraction pattern from each block is wider than the mosaic statistical distribution].

5.3.4. Extinction in neutron diffraction (nonmagnetic case)

The kinematical approximation, which corresponds to the first Born approximation in scattering theory, supposes that each incident neutron can be scattered only once and therefore neglects the possibility that the neutrons may be scattered several times. Because this is a simple approximation which overestimates the crystal reflectivity, the actual reduction of reflectivity, as compared to its kinematical value, is termed *extinction.* This is actually a typical dynamical effect, since it is a multiple-scattering effect.

Extinction effects can be safely neglected in the case of scattering by very small crystals; more precisely, this is possible when the path length of the neutron beam in the crystal is much smaller than $\Delta = V_c/\lambda F$, where λ is the neutron wavelength and F/V_c is the scattering length per unit volume for the reflection considered. Δ is sometimes called the 'extinction distance'.

A very important fact is that extinction effects also vanish if the crystal is imperfect enough, because each plane-wave component of the incident beam can then be Bragg-reflected in only a small volume of the sample. This is the extinction-free case of 'ideally imperfect crystals'. Conversely, extinction is maximum (smallest value of y) in the case of ideally perfect non-absorbing crystals.

Clearly, no significant extinction effects are expected if the crystal is thick but strongly absorbing, more precisely if the linear absorption coefficient μ is such that $\mu\Delta \gg 1$. Neutron diffraction usually corresponds to the opposite case ($\mu\Delta \ll 1$), in which extinction effects in nearly perfect crystals dominate absorption effects.

Extinction effects are usually described in the frame of the mosaic model, in which the crystal is considered as a juxtaposition of perfect blocks with different orientations. The relevance of this model to the case of neutron diffraction was first considered by Bacon & Lowde (1948). If the mosaic blocks are big enough there is extinction within each block; this is called *primary extinction.* Multiple scattering can also occur in different blocks if their misorientation is small enough. In this case, which is called *secondary extinction*, there is no phase coherence between the scattering events in the different blocks. The fact that empirical intensity-coupling equations are used in this case is based on this phase incoherence.

In the general case, primary and secondary extinction effects coexist. Pure secondary extinction occurs in the case of a mosaic crystal made of very small blocks. Pure primary extinction is observed in diffraction by perfect crystals.

The parameters of the mosaic model are the average size of the perfect blocks and the angular width of their misorientation distribution. The extinction theory of the mosaic model provides a relation between these parameters and the extinction coefficient, 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 nonmagnetic 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 nonmagnetic 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