

5. DYNAMICAL THEORY AND ITS APPLICATIONS

$$\mathbf{K}_h = \mathbf{K}_o - \mathbf{h}. \quad (5.1.2.16) \quad \text{part,}$$

Expression (5.1.2.15) shows that the solution of the propagation equation can be interpreted as an infinite sum of plane waves with amplitudes \mathbf{D}_h and wavevectors \mathbf{K}_h . This sum is a *wavefield*, or *Ewald wave*. The same expression is used to describe the propagation of any wave in a periodic medium, such as phonons or electrons in a solid. Expression (5.1.2.14) was later called a *Bloch wave* by solid-state physicists.

The wavevectors in a wavefield are deduced from one another by translations of the reciprocal lattice [expression (5.1.2.16)]. They can be represented geometrically as shown in Fig. 5.1.2.1(b). The wavevectors $\mathbf{K}_o = \mathbf{OP}$; $\mathbf{K}_h = \mathbf{HP}$ are drawn *away* from reciprocal-lattice points. Their common extremity, P , called the *tie point* by Ewald, characterizes the wavefield.

In an absorbing crystal, wavevectors have an imaginary part,

$$\mathbf{K}_o = \mathbf{K}_{or} + i\mathbf{K}_{oi}; \quad \mathbf{K}_h = \mathbf{K}_{hr} + i\mathbf{K}_{hi},$$

and (5.1.2.16) shows that all wavevectors have the same imaginary part,

$$\mathbf{K}_{oi} = \mathbf{K}_{hi}, \quad (5.1.2.17)$$

and therefore undergo the same absorption. This is one of the most important properties of wavefields.

5.1.2.3. Boundary conditions at the entrance surface

The choice of the 'o' component of expansion (5.1.2.15) is arbitrary in an infinite medium. In a semi-infinite medium where the waves are created at the interface with a vacuum or air by an incident plane wave with wavevector $\mathbf{K}_o^{(a)}$ (using von Laue's notation), the choice of \mathbf{K}_o is determined by the boundary conditions.

This condition for wavevectors at an interface demands that their tangential components should be continuous across the boundary, in agreement with Descartes–Snell's law. This condition is satisfied when the difference between the wavevectors on each side of the interface is parallel to the normal to the interface. This is shown geometrically in Fig. 5.1.2.2 and formally in (5.1.2.18):

$$\mathbf{K}_o - \mathbf{K}_o^{(a)} = \mathbf{OP} - \mathbf{OM} = \overline{MP} \cdot \mathbf{n}, \quad (5.1.2.18)$$

where \mathbf{n} is a unit vector normal to the crystal surface, oriented towards the inside of the crystal.

There is no absorption in a vacuum and the incident wavevector $\mathbf{K}_o^{(a)}$ is real. Equation (5.1.2.18) shows that it is the component normal to the interface of wavevector \mathbf{K}_o which has an imaginary

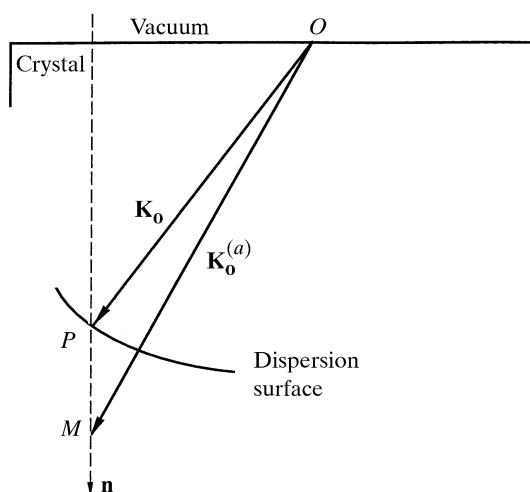


Fig. 5.1.2.2. Boundary condition for wavevectors at the entrance surface of the crystal.

$$\mathbf{K}_{oi} = \mathcal{I}(\overline{MP}) \cdot \mathbf{n} = -\mu\mathbf{n}/(4\pi\gamma_o), \quad (5.1.2.19)$$

where $\mathcal{I}(f)$ is the imaginary part of f , $\gamma_o = \cos(\mathbf{n} \cdot \mathbf{s}_o)$ and \mathbf{s}_o is a unit vector in the incident direction. When there is more than one wave in the wavefield, the effective absorption coefficient μ can differ significantly from the normal value, μ_o , given by (5.1.2.13) – see Section 5.1.5.

5.1.2.4. Fundamental equations of dynamical theory

In order to obtain the solution of dynamical theory, one inserts expansions (5.1.2.15) and (5.1.2.4) into the propagation equation (5.1.2.2). This leads to an equation with an infinite sum of terms. It is shown to be equivalent to an infinite system of linear equations which are the *fundamental equations* of dynamical theory. Only those terms in (5.1.2.15) whose wavevector magnitudes K_h are very close to the vacuum value, k , have a non-negligible amplitude. These wavevectors are associated with reciprocal-lattice points that lie very close to the Ewald sphere. Far from any Bragg reflection, their number is equal to 1 and a single plane wave propagates through the medium. In general, for X-rays, there are only two reciprocal-lattice points on the Ewald sphere. This is the so-called *two-beam* case to which this treatment is limited. There are, however, many instances where several reciprocal-lattice points lie simultaneously on the Ewald sphere. This corresponds to the *many-beam* case which has interesting applications for the determination of phases of reflections [see, for instance, Chang (1987) and Hümmel & Weckert (1995)]. On the other hand, for electrons, there are in general many reciprocal-lattice points close to the Ewald sphere and many wavefields are excited simultaneously (see Chapter 5.2).

In the two-beam case, for reflections that are not highly asymmetric and for Bragg angles that are not close to $\pi/2$, the fundamental equations of dynamical theory reduce to

$$\begin{aligned} 2X_o D_o - kC\chi_h D_h &= 0 \\ -kC\chi_h D_o + 2X_h D_h &= 0, \end{aligned} \quad (5.1.2.20)$$

where $C = 1$ if \mathbf{D}_h is normal to the $\mathbf{K}_o, \mathbf{K}_h$ plane and $C = \cos 2\theta$ if \mathbf{D}_h lies in the plane; this is due to the fact that the amplitude with which electromagnetic radiation is scattered is proportional to the sine of the angle between the direction of the electric vector of the incident radiation and the direction of scattering (see, for instance, *ITC*, Section 6.2.2). The polarization of an electromagnetic wave is classically related to the orientation of the electric vector; in dynamical theory it is that of the electric displacement which is considered (see Section A5.1.1.3 of the Appendix).

The system (5.1.2.20) is therefore a system of four equations which admits four solutions, two for each direction of polarization. In the *non-absorbing* case, to a very good approximation,

$$\begin{aligned} X_o &= K_o - nk, \\ X_h &= K_h - nk. \end{aligned} \quad (5.1.2.21)$$

In the case of an *absorbing crystal*, X_o and K_h are complex. Equation (5.1.5.2) gives the full expression for X_o .

5.1.2.5. Dispersion surface

The fundamental equations (5.1.2.20) of dynamical theory are a set of linear homogeneous equations whose unknowns are the amplitudes of the various waves which make up a wavefield. For the solution to be non-trivial, the determinant of the set must be set equal to zero. This provides a secular equation relating the magnitudes of the wavevectors of a given wavefield. This equation is that of the locus of the tie points of all the wavefields that may