

## 5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

medium by Maxwell's equations:

$$\begin{aligned} \text{curl } \mathbf{E} &= -\partial\mathbf{B}/\partial t \\ \text{curl } \mathbf{H} &= \partial\mathbf{D}/\partial t + \mathbf{j} \\ \text{div } \mathbf{D} &= \rho \\ \text{div } \mathbf{B} &= 0, \end{aligned} \quad (\text{A5.1.1.3})$$

where  $\rho$  is the electric charge density.

The electric field and the electric displacement on the one hand, and the magnetic field and the magnetic induction on the other hand, are related by the so-called *material relations*, which describe the reaction of the medium to the electromagnetic field:

$$\begin{aligned} \mathbf{D} &= \varepsilon\mathbf{E} \\ \mathbf{B} &= \mu\mathbf{H}, \end{aligned}$$

where  $\varepsilon$  and  $\mu$  are the dielectric constant and the magnetic permeability, respectively.

These equations are complemented by the following boundary conditions at the surface between two neighbouring media:

$$\begin{aligned} \mathbf{E}_{T1} - \mathbf{E}_{T2} &= 0 & \mathbf{D}_{N1} - \mathbf{D}_{N2} &= 0 \\ \mathbf{H}_{T1} - \mathbf{H}_{T2} &= 0 & \mathbf{B}_{N1} - \mathbf{B}_{N2} &= 0. \end{aligned} \quad (\text{A5.1.1.4})$$

From the second and the third equations of (A5.1.1.3), and using the identity

$$\text{div}(\text{curl } \mathbf{y}) = 0,$$

it follows that

$$\text{div } \mathbf{j} + \partial\rho/\partial t = 0. \quad (\text{A5.1.1.5})$$

#### A5.1.1.3. Propagation equation

In a vacuum,  $\rho$  and  $\mathbf{j}$  are equal to zero, and the first two equations of (A5.1.1.3) can be written

$$\begin{aligned} \text{curl } \mathbf{E} &= -\mu_0\partial\mathbf{E}/\partial t \\ \text{curl } \mathbf{H} &= \varepsilon_0\partial\mathbf{H}/\partial t, \end{aligned}$$

where  $\varepsilon_0$  and  $\mu_0$  are the dielectric constant and the magnetic permeability of a vacuum, respectively.

By taking the curl of both sides of the second equation, it follows that

$$\text{curl curl } \mathbf{E} = -\varepsilon_0\mu_0\partial^2\mathbf{E}/\partial t^2.$$

Using the identity  $\text{curl curl } \mathbf{E} = \text{grad div } \mathbf{E} - \Delta\mathbf{E}$ , the relation  $\varepsilon_0\mu_0 = 1/c^2$ , where  $c$  is the velocity of light, and noting that  $\text{div } \mathbf{E} = \text{div } \mathbf{D} = 0$ , one finally obtains the equation of propagation of an electromagnetic wave in a vacuum:

$$\Delta\mathbf{E} = \frac{1}{c^2} \frac{\partial^2\mathbf{E}}{\partial t^2}. \quad (\text{A5.1.1.6})$$

Its simplest solution is a plane wave:

$$\mathbf{E} = \mathbf{E}_0 \exp 2\pi i(\nu t - \mathbf{k} \cdot \mathbf{r}),$$

of which the wavenumber  $k = 1/\lambda$  and the frequency  $\nu$  are related by

$$k = \nu/c.$$

The basic properties of the electromagnetic field are described, for instance, in Born & Wolf (1983).

The propagation equation of X-rays in a crystalline medium is derived following von Laue (1960). The interaction of X-rays with charged particles is inversely proportional to the mass of the particle and the interaction with the nuclei can be neglected. As a first approximation, it is also assumed that the magnetic interaction of X-rays with matter is neglected, and that the magnetic permeability  $\mu$  can be taken as equal to the magnetic permeability of a vacuum,  $\mu_0$ . It is further assumed that the negative and positive charges are both continuously distributed and compensate each other in such a way that there is neutrality and no current everywhere:  $\rho$  and  $\mathbf{j}$  are equal to zero and  $\text{div } \mathbf{D}$  is therefore also equal to zero. The electric displacement is related to the electric field by (A5.1.1.1) and the electric part of the interaction of X-rays with matter is expressed through the dielectric susceptibility  $\chi$ , which is given by (A5.1.1.2). This quantity is proportional to the electron density and varies with the space coordinates. It is therefore concluded that  $\text{div } \mathbf{E}$  is different from zero, as opposed to what happens in a vacuum. For this reason, the propagation equation of X-rays in a crystalline medium is expressed in terms of the electric displacement rather than in terms of the electric field. It is obtained by eliminating  $\mathbf{H}$ ,  $\mathbf{B}$  and  $\mathbf{E}$  in Maxwell's equations and taking into account the above assumptions:

$$\Delta\mathbf{D} + \text{curl curl } \chi\mathbf{D} = \frac{1}{c^2} \frac{\partial^2\mathbf{E}}{\partial t^2}. \quad (\text{A5.1.1.7})$$

Only coherent scattering is taken into account here, that is, scattering without frequency change. The solution is therefore a wave of the form

$$\mathbf{D}(\mathbf{r}) \exp 2\pi i\nu t.$$

By replacing  $\mathbf{D}$  with this expression in equation (A5.1.1.7), one finally obtains the propagation equation (5.1.2.2) (Section 5.1.2.1).

In a crystalline medium,  $\chi$  is a triply periodic function of the space coordinates and the solutions of this equation are given in terms of Fourier series which can be interpreted as sums of electromagnetic plane waves. Each of these waves is characterized by its wavevector,  $\mathbf{K}_h$ , its electric displacement,  $\mathbf{D}_h$ , its electric field,  $\mathbf{E}_h$ , and its magnetic field,  $\mathbf{H}_h$ . It can be shown that, as a consequence of the fact that  $\text{div } \mathbf{D} = 0$  and  $\text{div } \mathbf{E} \neq 0$ ,  $\mathbf{D}_h$  is a transverse wave ( $\mathbf{D}_h$ ,  $\mathbf{H}_h$  and  $\mathbf{K}_h$  and are mutually orthogonal) while  $\mathbf{E}_h$  is not. The electric displacement is therefore a more suitable vector for describing the state of the field inside the crystal than the electric field.

#### A5.1.1.4. Poynting vector

The propagation direction of the energy of an electromagnetic wave is given by that of the Poynting vector defined by (see Born & Wolf, 1983)

$$\mathbf{S} = \mathcal{R}(\mathbf{E} \wedge \mathbf{H}^*), \quad (\text{A5.1.1.8})$$

where  $\mathcal{R}()$  means real part of  $()$ .

The intensity  $I$  of the radiation is equal to the energy crossing unit area per second in the direction normal to that area. It is given by the value of the Poynting vector averaged over a period of time long compared with  $1/\nu$ :

$$\mathbf{I} = |\mathbf{S}| = c\varepsilon|\mathbf{E}|^2 = c|\mathbf{D}|^2/\varepsilon.$$