Chapter 7
Kinematical Theory of Diffraction

The **kinematical theory of diffraction** describes the intensity or angle distribution of the X-ray diffraction generated by a mosaic crystal. A mosaic crystal refers to a crystal containing numerous lattice defects such as grain boundaries and dislocations and disordered three-dimensional periodicity. Due to these disorders, the incident X-ray beam can be assumed to scatter only once in the crystal. This is the concept of the kinematical theory of diffraction.

The size of a crystal grain determines whether we select the dynamical theory (discussed in Chapter 6) or kinematical theory of diffraction. If the size of the crystal grain is several micrometers or less, the kinematical theory of diffraction is generally regarded to hold. If the crystal grain is greater, the dynamical theory of diffraction is regarded to hold. The dynamical theory of diffraction holds only in a limited number of materials such as semiconductors (including Si and Ge) and compound semiconductors (including GaAs and AlGaP). The kinematical theory of diffraction discussed in this chapter applies to most inorganic and organic crystals.

7.1 General Description of X-Ray Scattering by Materials

This section discusses the amplitude of the **Thomson scattering** of X-rays by a material of arbitrary form—i.e., not necessarily a crystal.

We assume that X-rays are scattered only once in the material. We also assume that the incident beam in the material contributes only to diffraction and is not weakened by absorption.

7.1.1 Description of Scattered X-Rays

We define $\mathbf{k}_0$ and $\mathbf{k}$ as the wave vectors of the incident and scattered waves when an X-ray beam enters a material and is scattered. (A wave vector is a vector whose length is $1/\lambda$ (the inverse of the wavelength, λ) and whose direction is the same as the direction of the X-ray propagation.) The vector, $\mathbf{k}$-$\mathbf{k}_0$, is called the scattering vector and expressed as $\mathbf{K}$.

$$\mathbf{K} = \mathbf{k} - \mathbf{k}_0 \qquad \textit{Formula 7.1.1}$$

The magnitude of $\mathbf{K}$ is given by the following formula:

$$K = \frac{2}{\lambda}\sin\frac{\Theta}{2} \qquad \textit{Formula 7.1.2}$$

Here, Θ is the angle between $\mathbf{k}_0$ and $\mathbf{k}$, and is called the scattering angle. Fig. 7.1.1 shows the relationship between $\mathbf{k}_0$, $\mathbf{k}$, $\mathbf{K}$, and Θ.

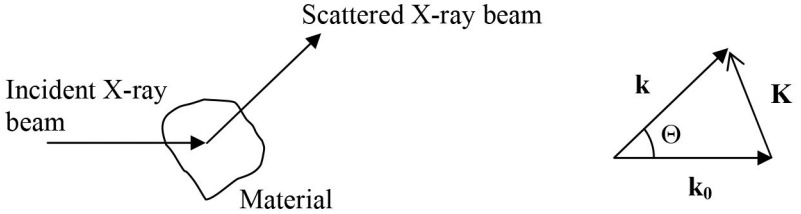

Fig. 7.1.1 Wave vectors of the incident and scattered waves and the scattering vector.

7.1.2 X-Ray Scattering from Entire Material

X-rays in a material are scattered by electrons. In general, the distribution of electrons is not uniform, with electron density varying depending on the position within the material. For this reason, the amplitude of the scattered wave moving from the entire body of the material is the sum of the amplitudes of the scattered waves from different positions in the material with the phase shift considered.

Assume an arbitrary position in the material to be the origin of the coordinates and denote the electron density at the point A separated from the origin by $\mathbf{r}$ as $\rho(\mathbf{r})$. The scattered wave moving from point A has phase difference $\mathrm{K} \cdot \mathbf{r}$ compared to the scattered wave moving from the origin (we calculate phase difference by multiplying $2\pi/\lambda$ and the optical path difference). When $\rho(\mathbf{r})\, d\mathbf{r}$ denotes the probability of existence of an electron in the infinitesimal volume element $d\mathbf{r}$ at point A, the amplitude of the wave scattered at point A is proportional to $\rho(\mathbf{r})e^{-i\mathbf{K}\cdot\mathbf{r}}d\mathbf{r}$, taking into account the phase shift depending on the position. Thus, the amplitude of the scattered wave from a scattering element is obtained by solving the following formula below which integrates $\rho(\mathbf{r})e^{-i\mathbf{K}\cdot\mathbf{r}}d\mathbf{r}$ over the entire scattering element by the scattering amplitude, -$\mathbf{r}$e, for a single electron:

$$\int_{\text{scattering body}} \rho(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}}\, d\mathbf{r} \equiv A(\mathbf{K}) \qquad \textit{Formula 7.1.3}$$

$A(\mathbf{K})$ is the Fourier transformation of the electron density of the scattering element and is called the **structure factor.** The structure factor is related to the structure of the scattering element and is a fundamental quantity in structure analysis.

The amplitude of the electric field of the X-rays undergoing such a scattering process is expressed as follows at position r of the scattering element:

$$\boldsymbol{E}(\mathbf{r}) = \boldsymbol{\varepsilon}_0 e^{i\mathbf{k}_0\cdot\mathbf{r}} + \left\{-r_e \boldsymbol{\varepsilon}_0 \cdot \boldsymbol{\varepsilon}_S A(\mathbf{K})\right\}\frac{\boldsymbol{\varepsilon}_S e^{i\mathbf{k}\cdot\mathbf{r}}}{\mathbf{r}} \qquad \textit{Formula 7.1.4}$$

Here, ε_0 is the permittivity of vacuum and ε_s the permittivity of the material. The second term expresses the scattered wave, which propagates as a spherical wave moving from the scattering element. The intensity of the scattered wave is given by the square of this term, as follows:

$$I = I_0 \frac{P r_e^{\,2}}{\mathbf{r}^2} \left|A(\mathbf{K})\right|^2 \qquad \textit{Formula 7.1.5}$$

This is proportional to the square of the Fourier transform $A(\mathbf{K})$ of the electron density of the scattering element.

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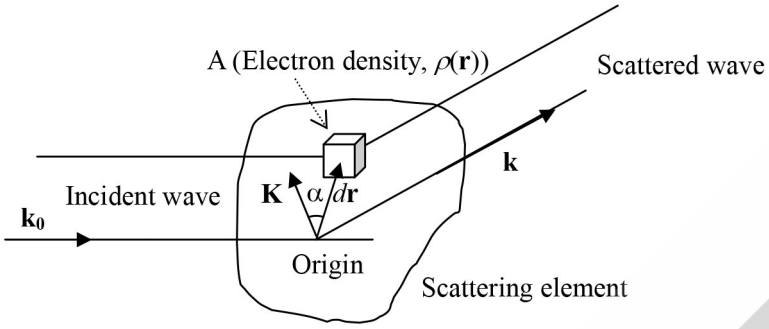

Fig. 7.1.2 X-ray scattering by scattering element

Here, I_0 denotes the intensity of the incident wave. When Ie denotes the scattering intensity for a single electron, intensity can be rewritten, as follows:

$$I = I_e \left| A(\boldsymbol{K}) \right|^2 = I_e \left| \int_{\text{scatterer}} \rho(\boldsymbol{r}) e^{-i\boldsymbol{K}\cdot\boldsymbol{r}} d\boldsymbol{r} \right|^2 \qquad \textit{Formula 7.1.6}$$

This formula is a generic formula that applies whether the scattering element is a solid, liquid, or gas. It constitutes the foundation of the kinematical theory of diffraction.