1
Diffraction Phenomena in Optics

The term *diffraction* in optics is usually used to explain the deviations of light propagation from the trajectories dictated by geometrical (ray) optics. One of the most famous examples is the so-called Fraunhofer diffraction, which explains the transmission of an initially parallel beam of light through a circular hole of radius D fabricated in a nontransparent screen. Within the framework of geometrical optics, behind the screen, the nonzero transmitted intensity will be detected just in front of the hole (see Figure 1.1). It means that, after passing through the screen, the direction of light propagation does not change; the only effect is a reduction in the total light intensity in a proportion dictated by the area of the hole $S = \pi D^2$ with respect to the cross section of the incident beam. However, light scattering by the border of the hole can substantially modify this result and provide additional transmitted intensity in spatial directions that differ by angle Θ from the initial direction of light propagation before the screen (see Figure 1.2, upper panel). In other words, after passing through the screen, light propagates not only in one direction, which is defined by the initial wave vector $\boldsymbol{k}_\mathrm{i}$, but also in many other directions defined by the vectors $\boldsymbol{k}_\mathrm{s} = \boldsymbol{k}_\mathrm{i} + \boldsymbol{q}$. Here, $\boldsymbol{q}$ is a variable wave vector transfer to the screen during scattering events (see Figure 1.3). Note that, for elastic scattering processes

$$|\boldsymbol{k}_\mathrm{s}| = |\boldsymbol{k}_\mathrm{i}| = \frac{2\pi}{\lambda} \tag{1.1}$$

where λ is the wavelength of light. Taking into account Eq. (1.1) and the axial symmetry of the particular scattering problem (at a fixed scattering angle Θ, see Figure 1.3), we find that

$$|\boldsymbol{q}| = q \approx \frac{2\pi}{\lambda}\Theta \tag{1.2}$$

For each $\boldsymbol{q}$-value, the light scattering amplitude is given by the Fourier component $u_\mathbf{q}$ of the wave field $u(\boldsymbol{r})$ just after the screen [1]:

$$u_\mathbf{q} = \iint u(\boldsymbol{r})e^{-i\mathbf{qr}}\,dx\,dy \tag{1.3}$$

However, in the first approximation, we can set $u = u_0$, that is, equal the amplitude of the homogeneous wave field before the screen, and then express the scattering

Basic Concepts of X-Ray Diffraction, First Edition. Emil Zolotoyabko.

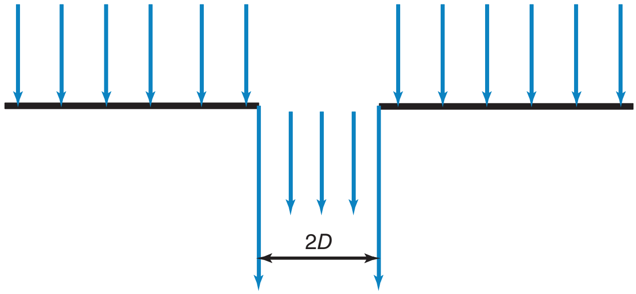

Figure 1.1 Light transmission through a circular hole of radius D in the limit of geometrical optics.

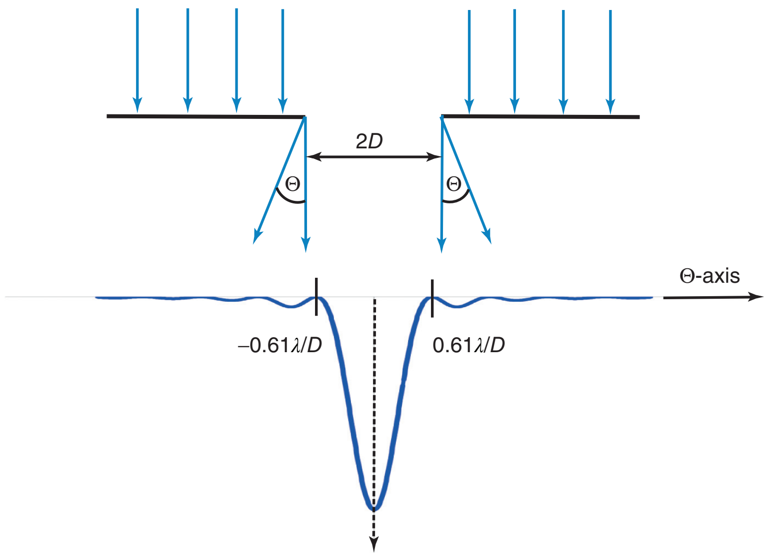

Figure 1.2 Light transmission (upper panel) through a circular hole of radius D, taking into account diffraction phenomenon (Fraunhofer diffraction). Bottom panel: transmitted intensity as a function of angular deviation Θ.

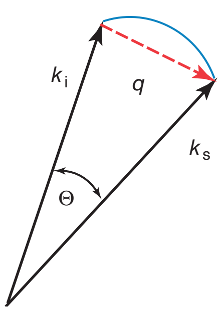

Figure 1.3 Wave vector change $\boldsymbol{q}$ in the course of elastic scattering of propagating light.

amplitude $u_{\mathbf{q}}$ as

$$u_{\mathbf{q}} = \iint u_0 e^{-i\mathbf{qr}} dx dy \tag{1.4}$$

where the integration proceeds over the entire area S of the hole. The diffraction intensity (relative to that in the incident beam) for a given $\boldsymbol{q}$-value within an element of solid angle Ω is expressed as follows [1]:

$$dI_{\text{rel}} = \lambda^{-2} \left| \frac{u_{\mathbf{q}}}{u_o} \right|^2 d\Omega \tag{1.5}$$

In order to find $u_{\mathbf{q}}$, let us introduce the polar coordinates r and φ within the circular hole. In this coordinate system, Eq. (1.4) transforms into

$$u_{\mathbf{q}} = u_0 \int_0^D \int_0^{2\pi} e^{-iqr\cos\varphi}\, r\, d\varphi\, dr = 2\pi u_0 \int_0^D J_0(qr) r\, dr \tag{1.6}$$

where J_0 is the Bessel function of zero order. Note that, in deriving Eq. (1.6), we used the fact that, for small scattering angles Θ, the vector $\boldsymbol{q}$ is nearly situated in the plane of the hole. One can express the integral in (1.6) via a Bessel function of first order J_1, as

$$\int_0^D J_0\,(qr) r\, dr = \frac{D}{q} J_1(Dq) \tag{1.7}$$

and, finally

$$u_{\mathbf{q}} = \frac{2\pi u_0 D}{q} J_1(Dq) \tag{1.8}$$

Substituting Eq. (1.8) into Eq. (1.5) and using Eq. (1.2), we obtain

$$dI_{\text{rel}} = \frac{D^2}{\Theta^2} J_1^2 \left(\frac{2\pi D}{\lambda} \Theta \right) d\Omega \tag{1.9}$$

The distribution of the transmitted intensity (Eq. (1.9)) as a function of the scattering angle Θ is shown in Figure 1.2 (bottom panel). With an increase in the absolute value of the angle Θ, the light intensity shows a fast overall reduction, on which the pronounced oscillating behavior is superimposed. The intensity oscillations are revealed as lateral maxima of diminishing height, separated by the zero-intensity points. The latter are determined by the zeros of the J_1 function. Most of the diffraction intensity (about 84%) is confined within the angular interval $-\Theta_0 \leq \Theta \leq \Theta_0$, which is defined by the first zero of the Bessel function J_1:

$$\frac{2\pi}{\lambda} D\,\Theta_0 = 3.832 \tag{1.10}$$

That is,

$$\Theta_0 = 0.61\, \frac{\lambda}{D} \tag{1.11}$$

It follows from Eq. (1.11) that diffraction is important when the wavelength λ is a significant part of the D-value. If $\lambda / D \ll 1$, the angular deviations are subtle, which implies that diffraction effects (deviations from geometrical optics) are weak. For visible light with $\lambda \approx 0.5\ \mu m$, the diffraction phenomena are regularly observed for objects with the characteristic size D ranging from few micrometers and up to $\sim 10^3\ \mu m$.

Diffraction of light imposes the main limitation on the resolving power of optical instruments. For a telescope, the resolution is defined on an angular scale and is given by the so-called Rayleigh criterion. It states that two objects (stars) can be separately resolved if an angular distance $\Delta\Theta_c$ between the maxima of their intensity distributions (Eq. (1.9)) exceeds the Θ_0 value defined by Eq. (1.11). It implies that the angular resolution of a telescope is given by Eq. (1.11).

For a microscope, length limitations are most useful, helping us to evaluate the size of the smallest objects still visible with the aid of a particular optical device. In order to "translate" the Rayleigh criterion into the length-scale language, let us consider the simplified equivalent scheme of a microscope. The latter is represented by a circular lens of radius D and focal length f, and transforms an object of size Y into its image of size Y' (see Figure 1.4). For high magnification, an object is placed close to the focus (left side of the lens in Figure 1.4). Then

$$\theta \approx \frac{Y}{f} \tag{1.12}$$

Applying the Rayleigh criterion means that $\Theta > \Theta_0$ and hence

$$Y > \Delta = f\theta_0 = 0.61\frac{\lambda}{D}f \tag{1.13}$$

For focusing effect (see Figure 1.5), we illuminate our lens with a wide parallel beam and obtain a small spot Y' in the focal plane (right side of the lens in Figure 1.5). Now

$$\theta = \frac{Y'}{f} \tag{1.14}$$

Applying again the Rayleigh criterion and Eq. (1.11), we find that the spot size Y' cannot be smaller than parameter Δ given by Eq. (1.13), that is,

$$Y' > \Delta = f\theta_0 = 0.61\frac{\lambda}{D}f \tag{1.15}$$

Therefore, the spatial resolution Δ, when using the circular focusing element, is completely defined by its radius D, focal length f, and radiation wavelength λ. We will use the obtained results in Chapter 23 when describing the focusing elements for X-ray optics. More information on diffraction optics of visible light and, in particular, on the Fraunhofer and Fresnel diffraction can be found in [2, 3].

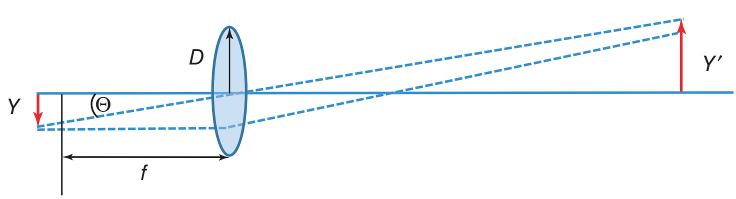

Figure 1.4 Illustration of the diffraction-limited spatial resolution of a microscope.

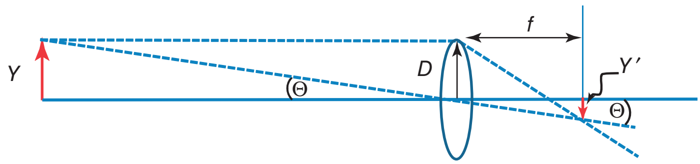

Figure 1.5 Illustration of the diffraction-limited focal spot size that is achievable by using a lens.

When considering potential diffraction effects for X-rays, we stress that they have wavelengths of about 0.1 nm = 1 Å: that is, 5000 times shorter than for visible light. If so, what kind of objects could potentially cause the diffraction of X-rays? Clearly, characteristic sizes in these objects should be very small. It was the great idea of Max von Laue, who had proposed in 1912 the diffraction experiment of X-rays in crystals, bearing in mind that crystals are built of periodic three-dimensional atomic networks; that is, they reveal translational symmetry. Fortunately, the characteristic distances between adjacent atomic unit cells (translation lengths) are comparable with X-ray wavelengths. Today, we can say that mainly translational symmetry together with appropriate lengths of the translation vectors is the origin of X-ray diffraction in crystals. This subject is comprehensively treated in Chapter 2.