

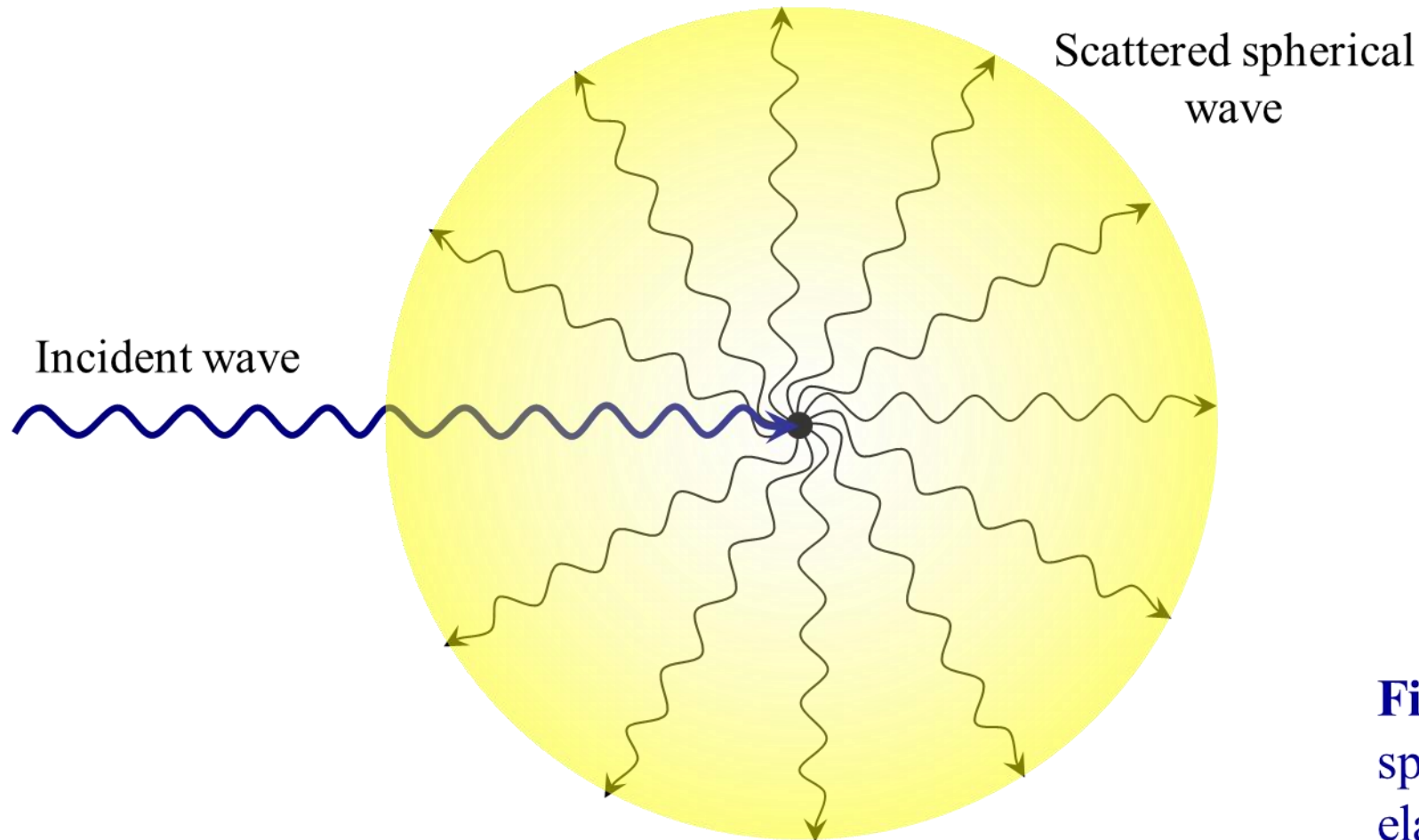
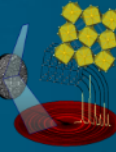


Figure 7.1. The illustration depicts a spherical wave generated from the elastic scattering of an incident wave by a point object (represented as a filled dot *at the center*).

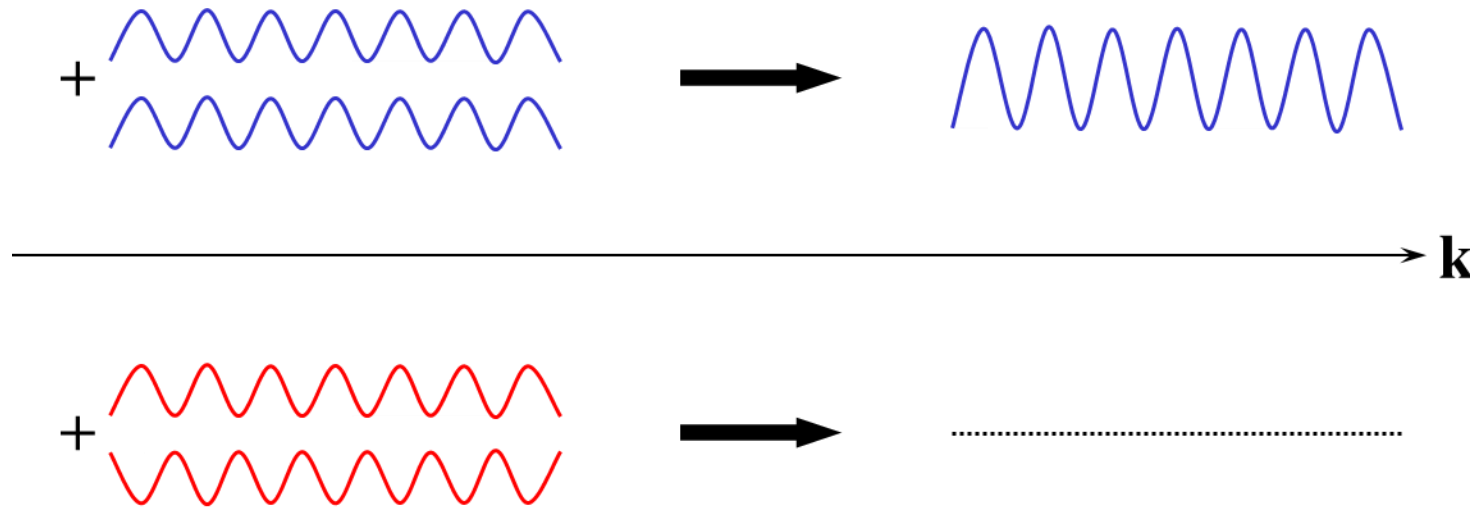
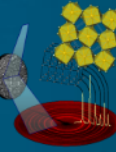
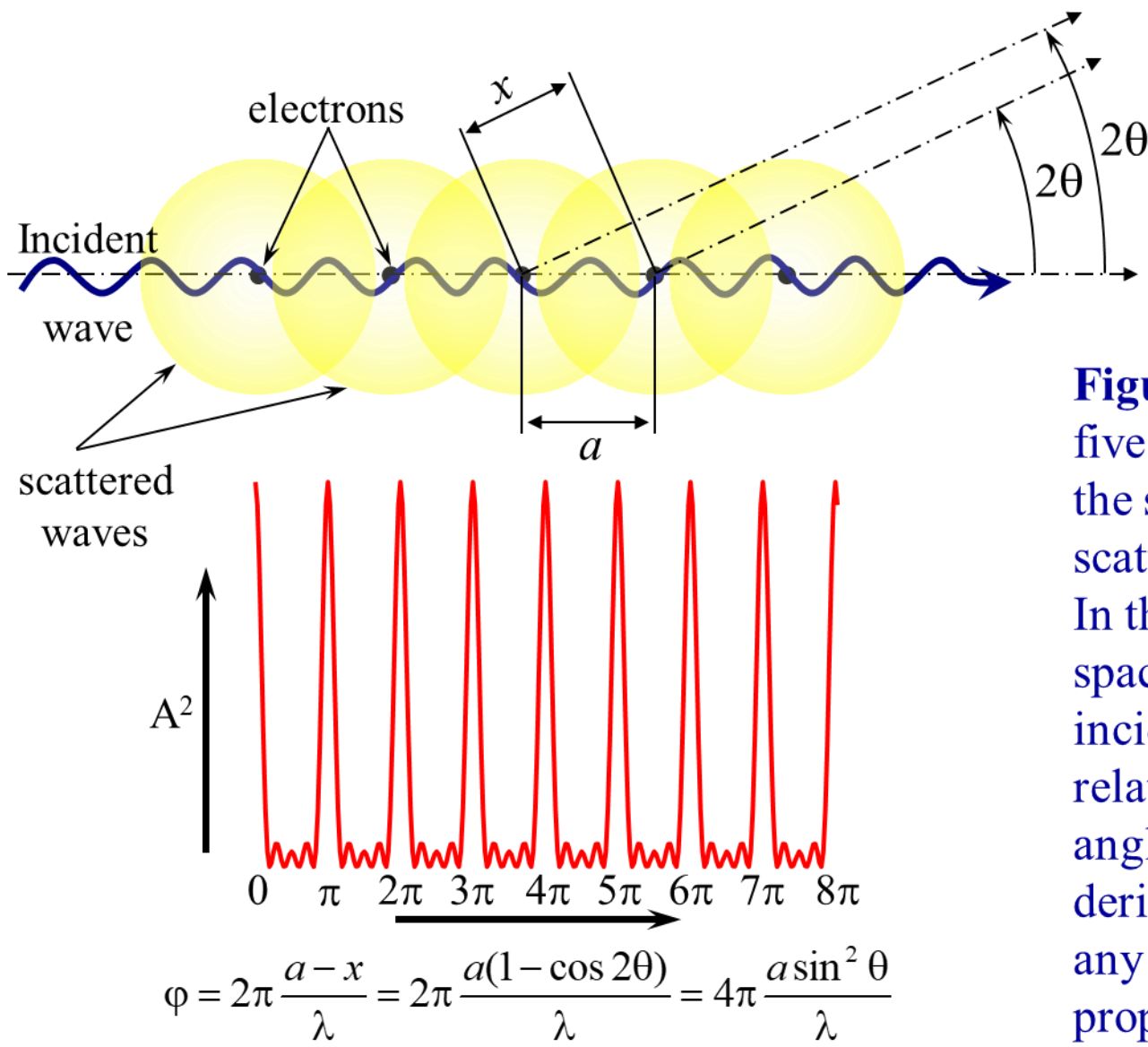


Figure 7.2. The interaction between two waves with parallel propagation vectors ($\mathbf{k}$) manifests in two limiting cases: constructive interference, where two in-phase waves combine to form a new wave with double the amplitude (*top*), and destructive interference, where two completely out-of-phase waves cancel each other out, resulting in zero amplitude for the resultant wave (*bottom*).



$$I(\phi) \propto \frac{\sin^2 N \phi}{\sin^2 \phi}$$

Eq. 7.1

Figure 7.3. Top – five equally spaced points producing five spherical waves as a result of elastic scattering of the single incident wave. Bottom – the resultant scattered amplitude as a function of the phase angle, ϕ . In this geometry, the phase angle is a function of the spacing between the points, a , the wavelength of the incident beam, λ , and the scattering angle, 2θ . The relationship between the phase (ϕ) and scattering (θ) angles for the arrangement shown on *top* is easily derived by considering path difference ($a-x$) between any pair of neighboring waves, which have parallel propagation vectors.

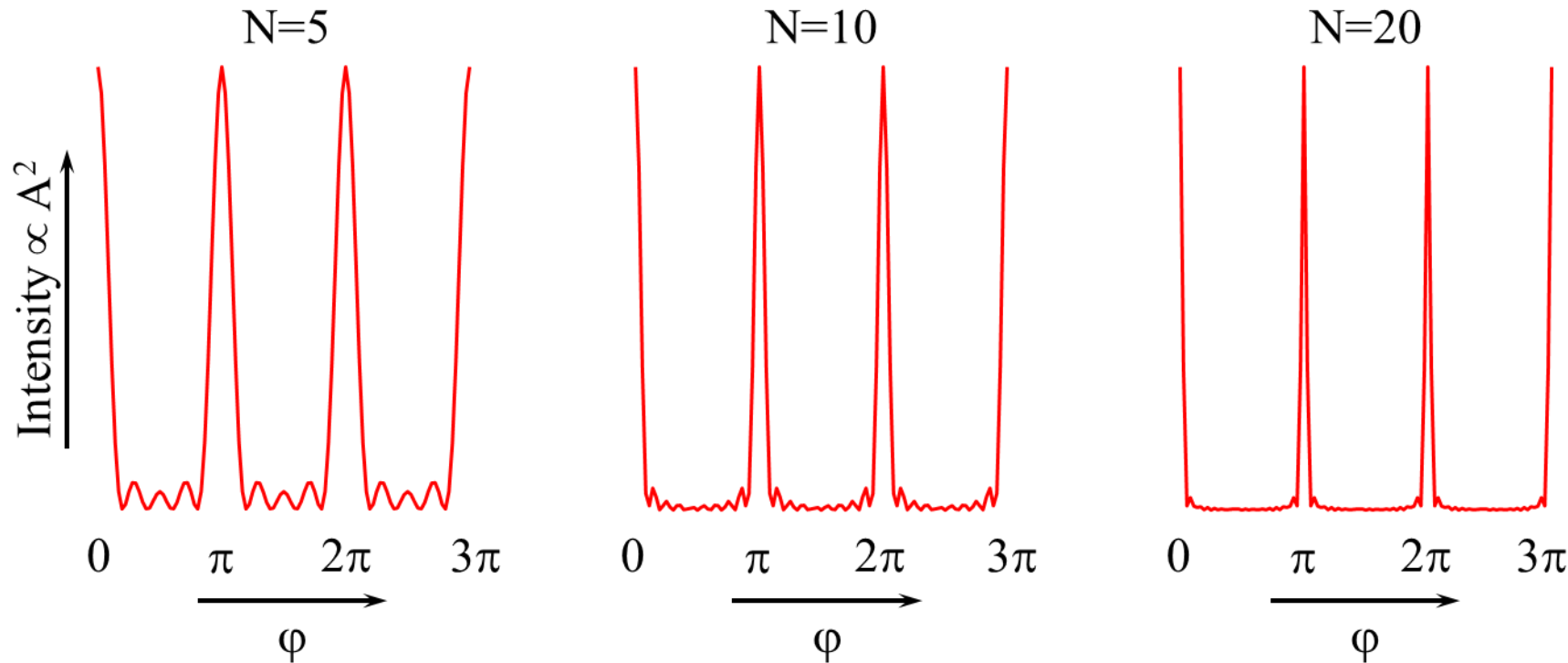
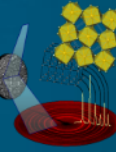


Figure 7.4. The illustration of the changes in the diffraction pattern from a one-dimensional periodic arrangement of scattering points when the number of points (N) increases from 5 to 20. The horizontal scales are identical, but the vertical scales are normalized for the three plots.

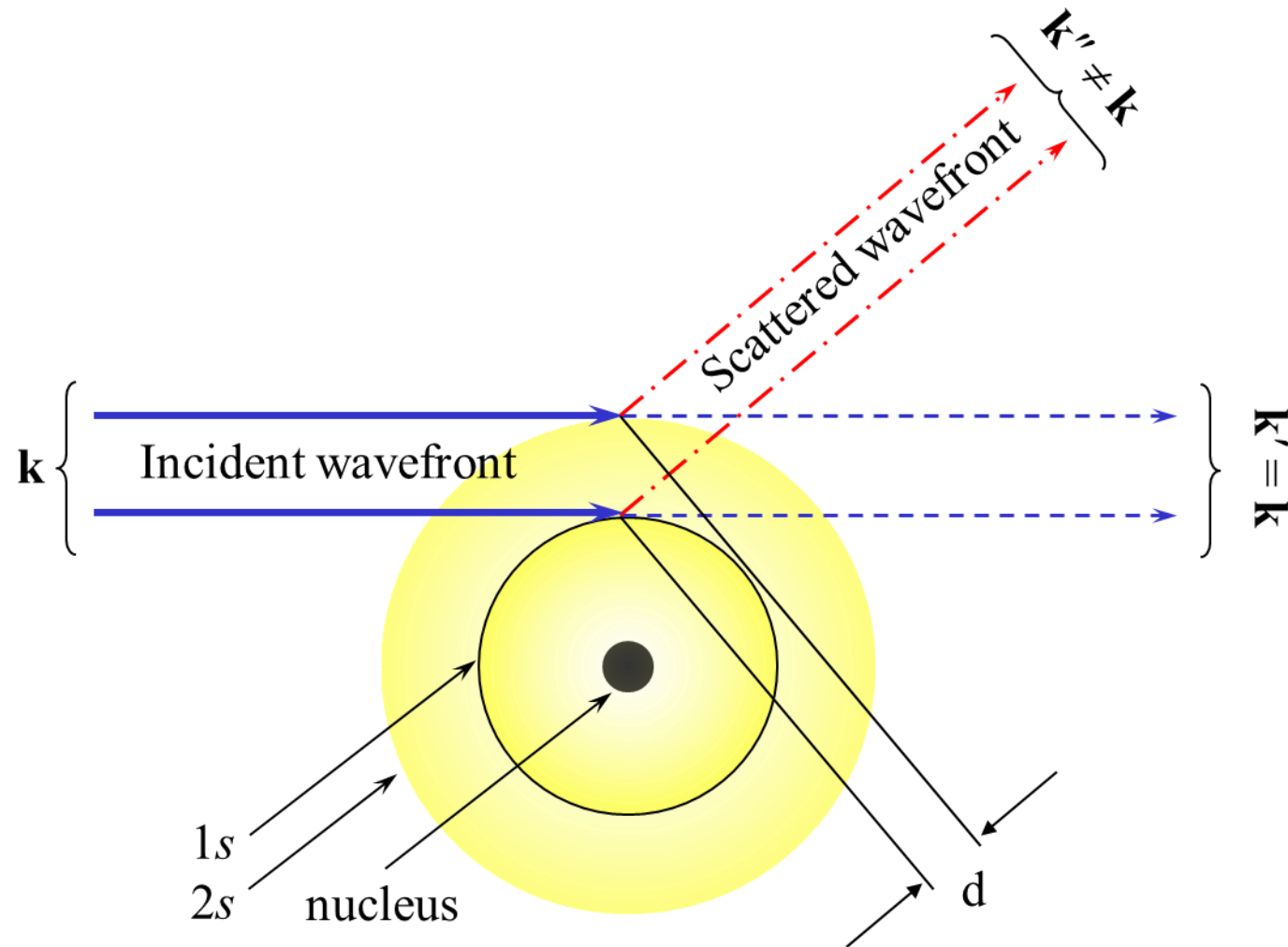
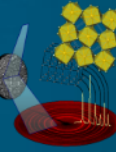


Figure 7.5. The schematic of the elastic scattering of X-rays by s electrons illustrating the introduction of a path difference, δ , into the wavefront with a propagation vector $\mathbf{k}''$, when it is different from the propagation vector, $\mathbf{k}$, of the incident beam. The distribution of electrons in two s -orbitals is determined from the corresponding wave functions.

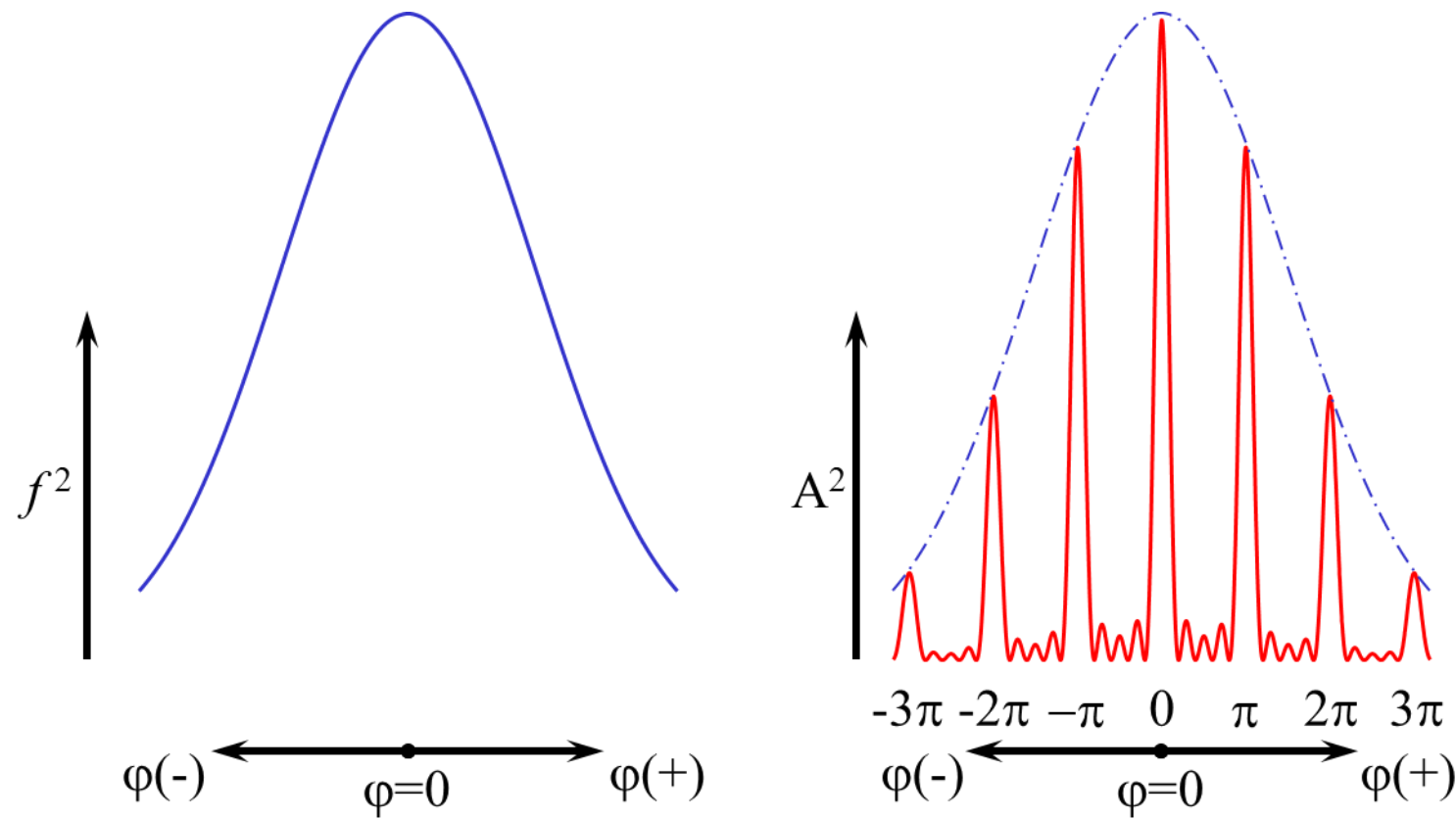
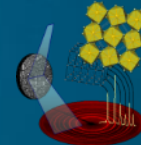


Figure 7.6. The schematic showing the dependence of the intensity scattered by an atom, i.e., the atomic scattering factor, $f^2 \propto A^2$, as a function of the phase angle (*left*), and the resultant decrease of the intensity of the diffraction pattern from the row of five regularly spaced atoms, also as a function of the phase angle (*right*).

$$I(\varphi) \propto f^2(\varphi) \frac{\sin^2 N \varphi}{\sin^2 \varphi} \qquad \text{Eq. 7.2}$$

$$I(\varphi) \propto f^2(\varphi) \frac{\sin^2 N_1 h \pi}{\sin^2 h \pi} \frac{\sin^2 N_2 k \pi}{\sin^2 k \pi} \frac{\sin^2 N_3 l \pi}{\sin^2 l \pi} \qquad \text{Eq. 7.4}$$

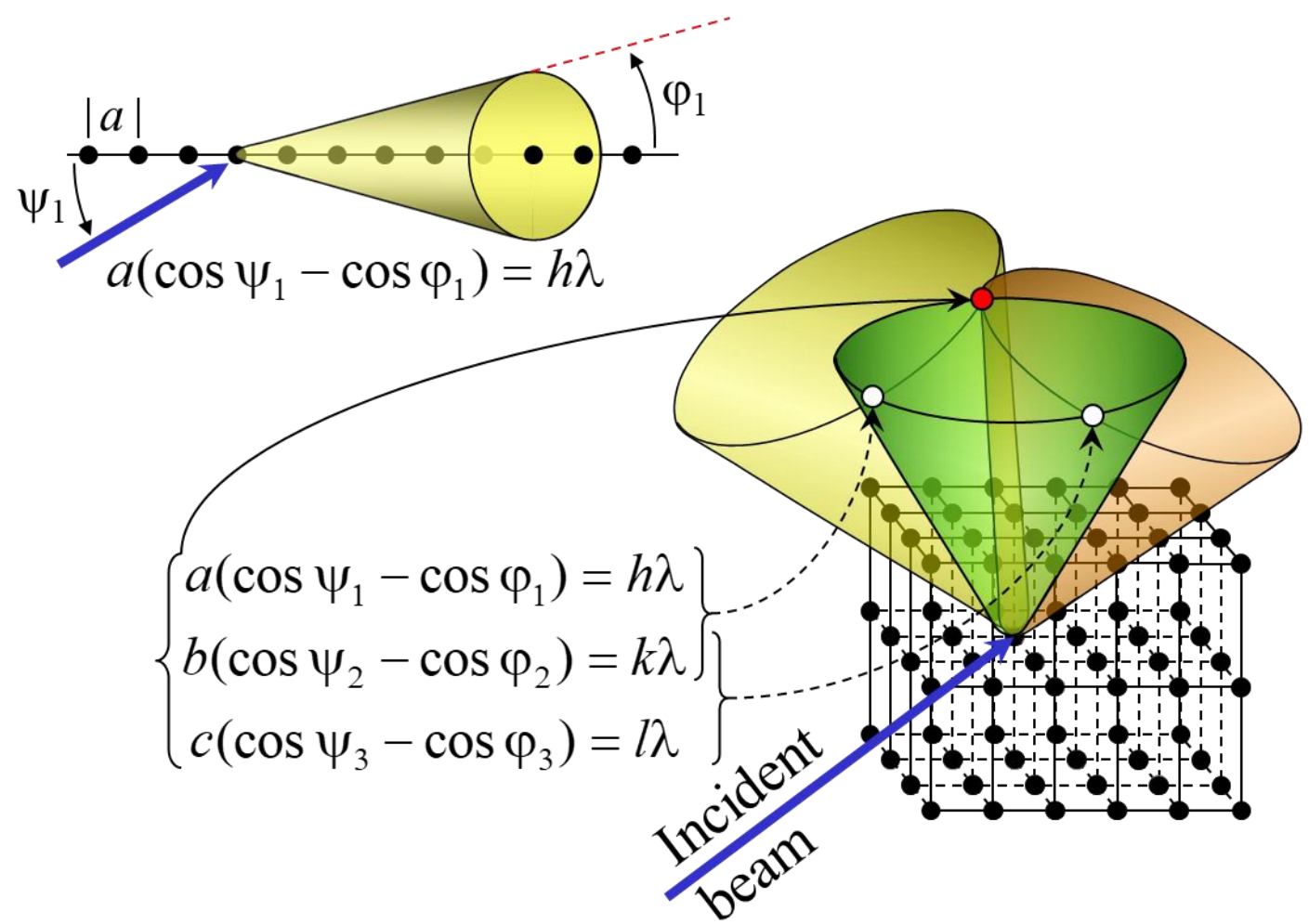


Figure 7.7. Graphical illustration of Laue equations. A cone of diffracted beams, all forming the same angle φ_1 with a row of atoms, satisfying one Laue equation is shown on top left. Each of the three cones shown on bottom right also satisfies one of the three equations, while the intersecting cones satisfy either two, or all three equations simultaneously as shown by arrows. A sharp diffraction peak is only observed in the direction of a point where three Laue equations are simultaneously satisfied.

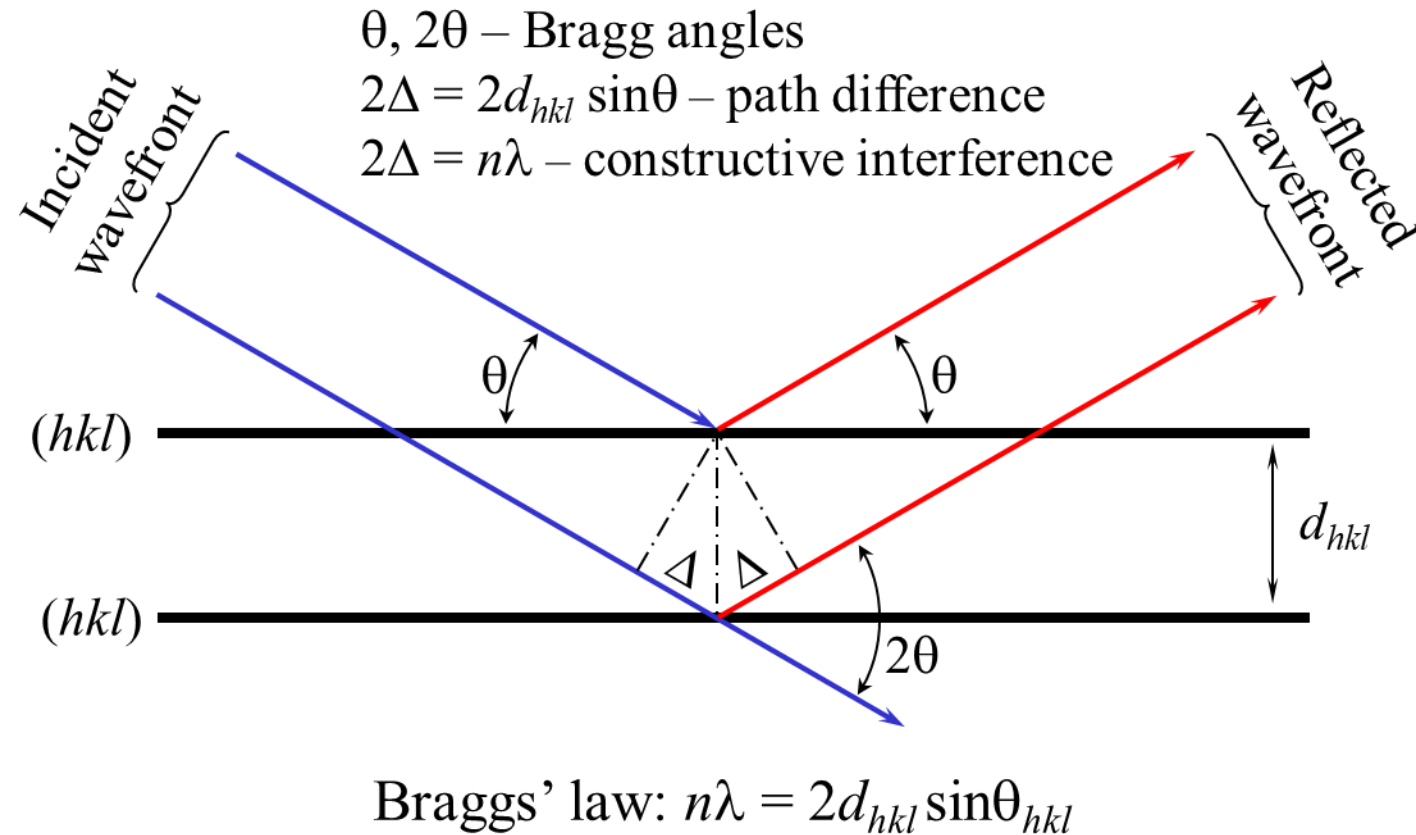
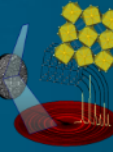


Figure 7.8. Geometrical illustration of the Braggs' law.

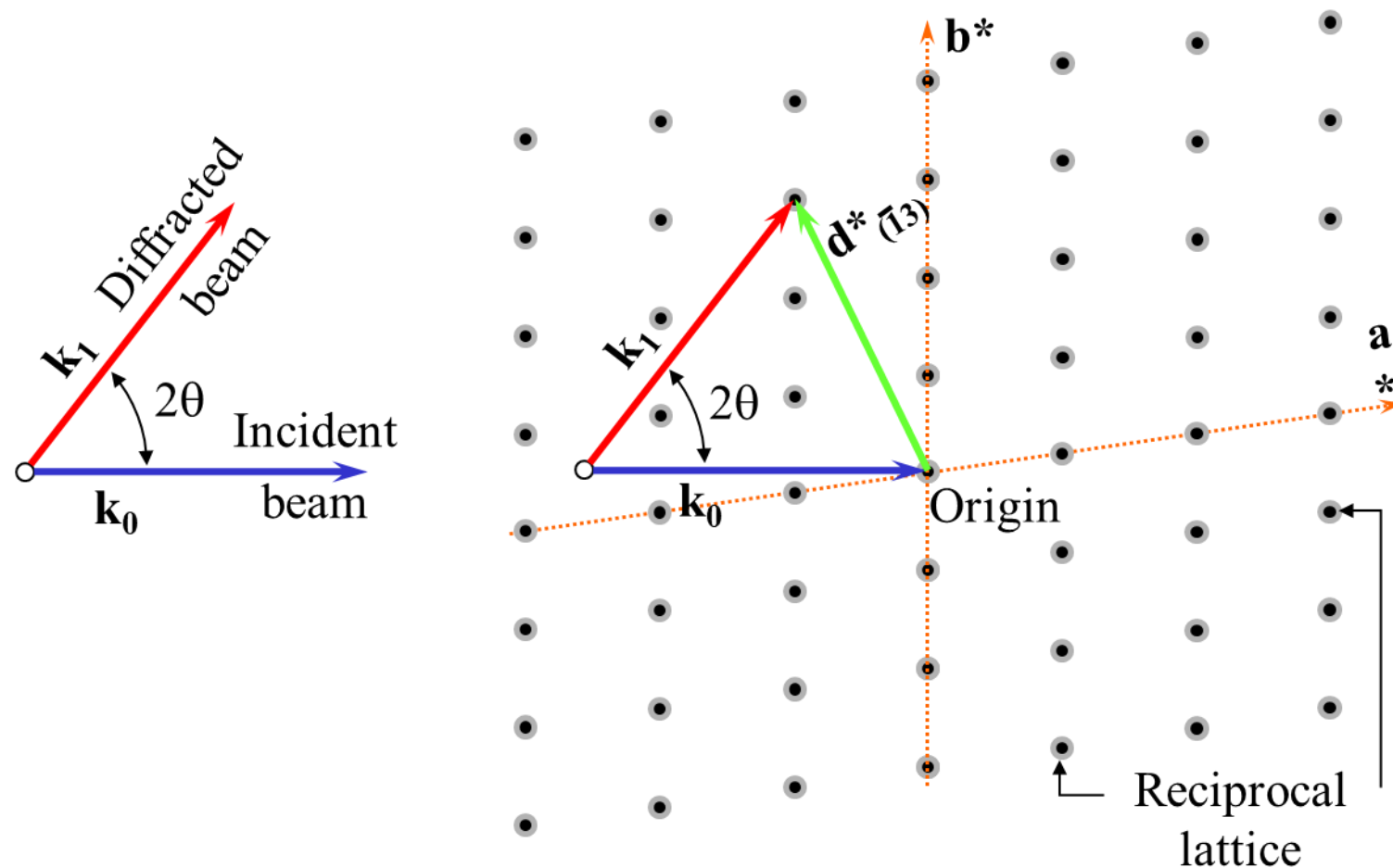
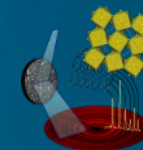


Figure 7.9. The incident ($\mathbf{k}_0$) and diffracted ($\mathbf{k}_1$) wavevectors originating from a common point (*left*) and the same two vectors overlapped with the two-dimensional reciprocal lattice, which is based on the unit vectors $\mathbf{a}^*$ and $\mathbf{b}^*$ (*right*). The origin of the reciprocal lattice is chosen at the end of $\mathbf{k}_0$. When diffraction occurs from a point in the reciprocal lattice, e.g., the point $(\bar{1}3)$, the corresponding reciprocal lattice vector $\mathbf{d}_{(hkl)}^*$ [e.g., $\mathbf{d}_{(\bar{1}3)}^*$] extends between the ends of $\mathbf{k}_0$ and $\mathbf{k}_1$.

$$|\mathbf{k}_1| = |\mathbf{k}_0| = 1/\lambda$$

$$\text{Eq. 7.13}$$

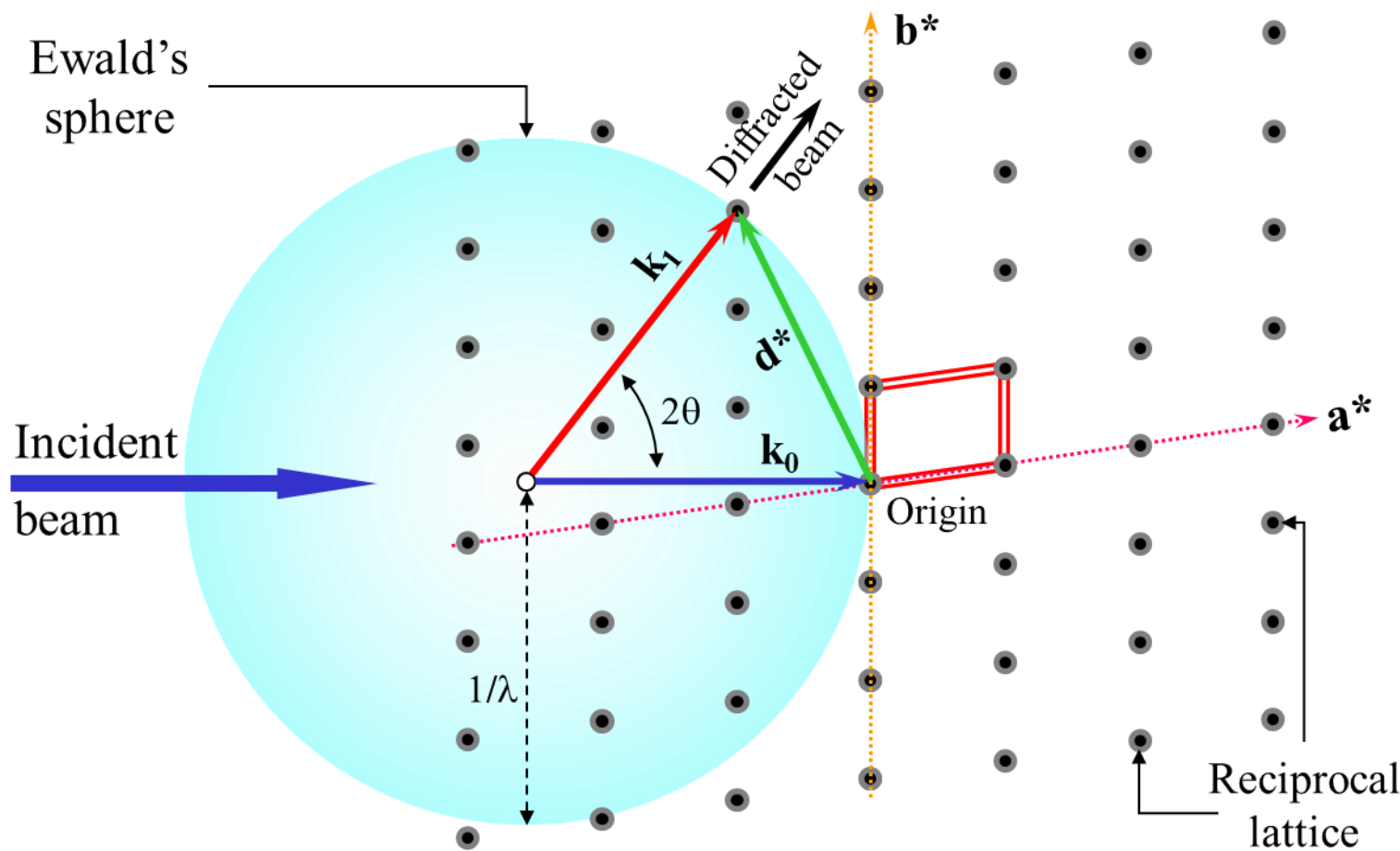
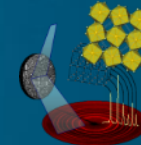


Figure 7.10. The visualization of diffraction using the Ewald's sphere with radius $1/\lambda$ and the two-dimensional reciprocal lattice with unit vectors $\mathbf{a}^*$ and $\mathbf{b}^*$. The origin of the reciprocal lattice is located on the surface of the sphere at the end of $\mathbf{k}_0$. Diffraction can only be observed when a reciprocal lattice point, other than the origin, intersects with the surface of the Ewald's sphere [e.g., the point $(\bar{1}3)$]. The incident and the diffracted beam wavevectors, $\mathbf{k}_0$ and $\mathbf{k}_1$, respectively, have common origin in the center of the Ewald's sphere. The two wavevectors are identical in length, which is the radius of the sphere. The unit cell of the reciprocal lattice is shown using double lines.

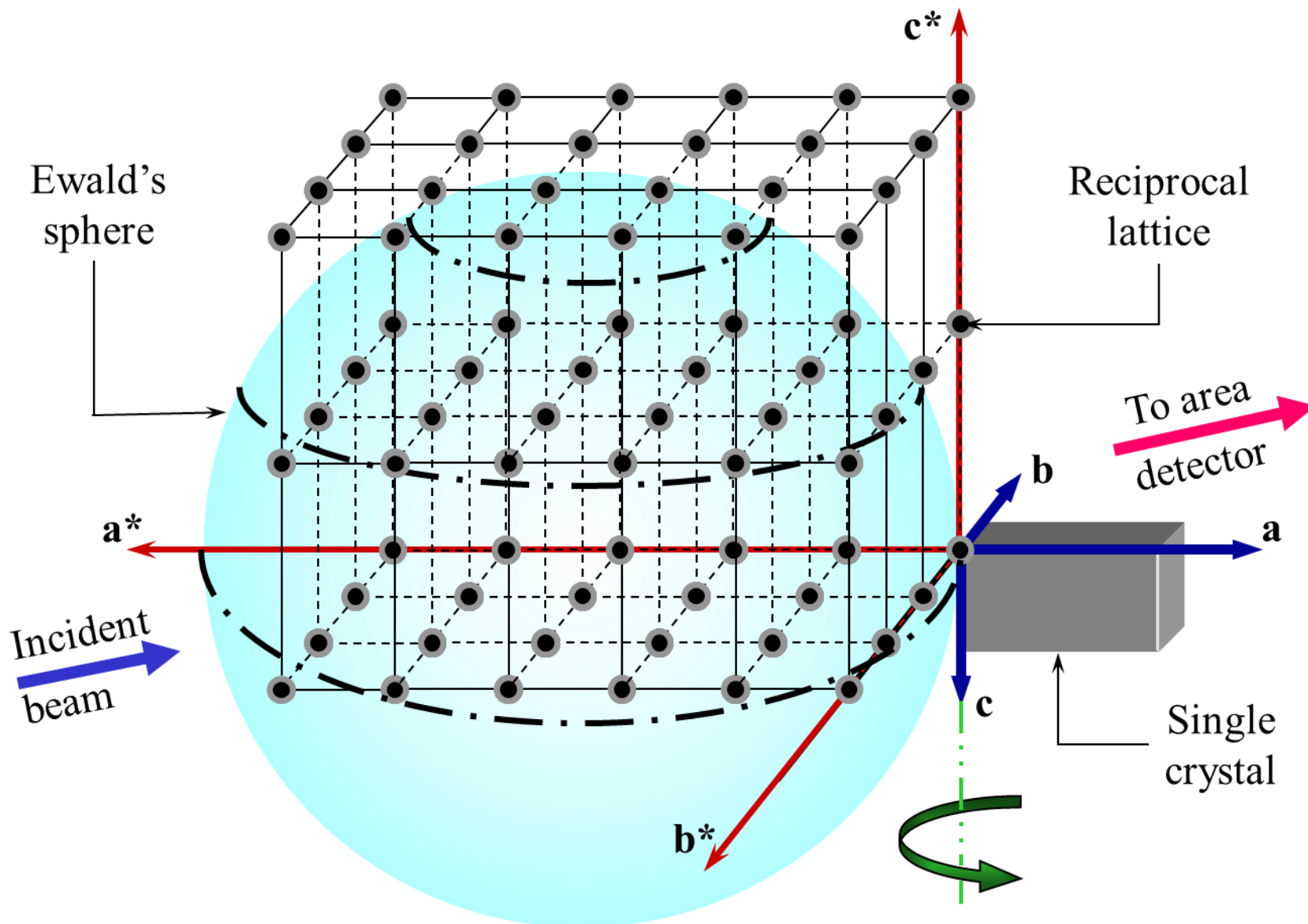
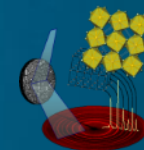


Figure 7.11. The illustration of a single crystal showing the orientations of the basis vectors corresponding to both the direct ($\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$) and reciprocal ($\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$) lattices and the Ewald's sphere. The reciprocal lattice is infinite in all directions but only one octant (where $h > 0$, $k > 0$ and $l > 0$) is shown for clarity.

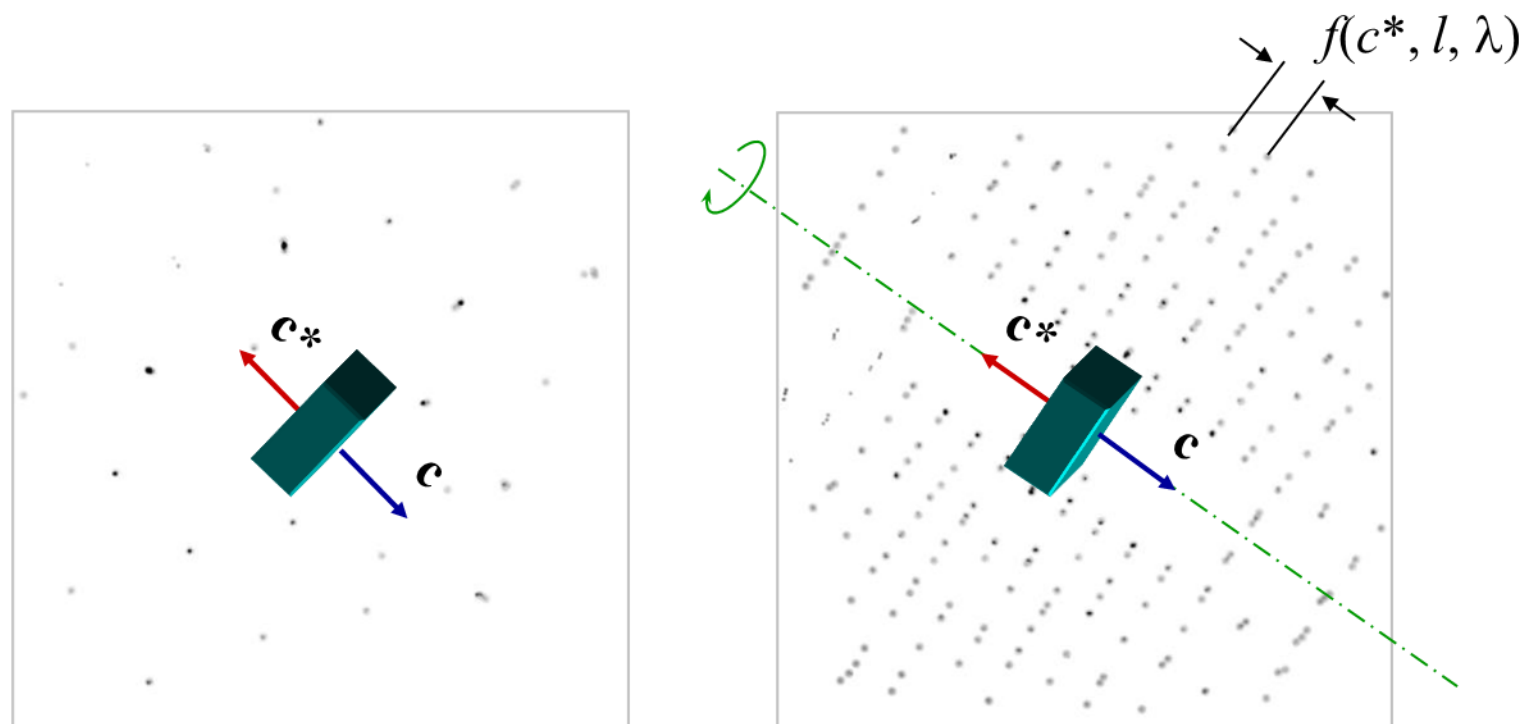
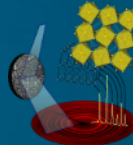


Figure 7.12. The two-dimensional diffraction patterns from stationary (*left*)^[1] and rotating (*right*)^[2] single crystals recorded using a CCD detector. The incident wavevector is perpendicular to both the detector and the plane of the figure. The *dash-dotted* line on the *right* shows the rotation axis, which is collinear with $\mathbf{c}^*$.

- [1] The single crystal is triclinic $\text{Pb}_3\text{F}_5(\text{NO}_3)$: space group $\text{P}\bar{1}$, $a = 7.3796(6)$, $b = 12.1470(9)$, $c = 16.855(1)$ Å, $\alpha = 100.460(2)$, $\beta = 90.076(1)$, $\gamma = 95.517(1)^\circ$. [D.T. Tran, P.Y. Zavalij and S.R.J. Oliver, A cationic layered material for anion-exchange, *J. Am. Chem. Soc.* **124**, 3966 (2002)]
- [2] The single crystal is orthorhombic, $\text{FePO}_4 \cdot 2\text{H}_2\text{O}$: space group Pbca , $a = 9.867(1)$, $b = 10.097(1)$, $c = 8.705(1)$ Å. [Y. Song, P.Y. Zavalij, M. Suzuki, and M.S. Whittingham, New iron(III) phosphate phases: Crystal structure, electrochemical and magnetic properties, *Inorg. Chem.* **41**, 5778 (2002)].