

# Theory of Semiconductor Devices (반도체 소자 이론)

## Lecture 4

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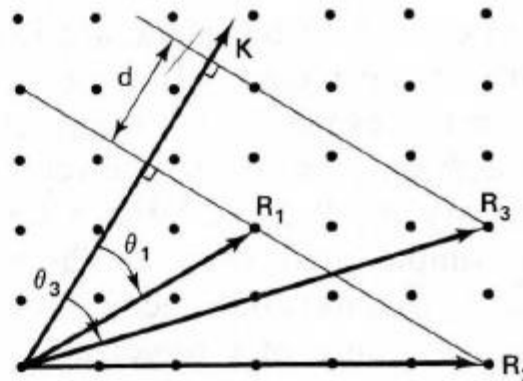
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# Miller Indices

- An **important relationship** exists between the **reciprocal lattice vectors**,  $\mathbf{K}$ , given by (1.17) and the **planes** of the corresponding direct lattice.
- A **lattice plane** is determined by **three noncollinear** lattice sites. Because of the **translational symmetry** of the Bravais lattice, however, each plane contains an **infinite** number of sites (Fig. 1.18).
- The relationship is that **each  $\mathbf{K}$**  of the reciprocal lattice is **normal** to some set of planes in the direct lattice and the **length of  $\mathbf{K}$**  is **inversely** proportional to the spacing between planes of this set.
- Consider the reciprocal lattice vector  $\mathbf{K}$  in (1.17) with **integral components  $h, k, l$**  which have no common factor, and a direct lattice point,

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \quad (1.25)$$

$$\mathbf{K} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$



**Figure 1.18** Two-dimensional direct lattice showing relationship between lattice planes and reciprocal lattice vectors.

# Miller Indices

- From (1.13) we have

$$\mathbf{K} \cdot \mathbf{R} = 2\pi(hn_1 + kn_2 + ln_3) = 2\pi N \quad (1.26)$$

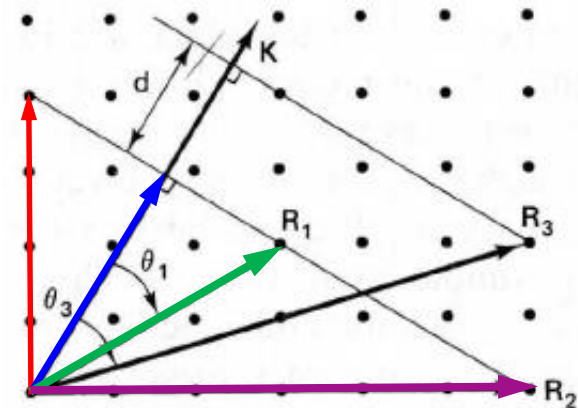
- Equation (1.26) tells us that the **projection** of the vector  $\mathbf{R}_1$  along the direction of the vector  $\mathbf{K}$  is

$$|\mathbf{R}_1| \cos \theta_1 = \frac{2\pi N}{|\mathbf{K}|} \quad (1.27)$$

- Since the Bravais lattice is **infinite**, we can find an *additional* point with this **same projection**. For example, the vector  $\mathbf{R}_2$  defined by

$$\mathbf{R}_2 = (n_1 - pl)\mathbf{a}_1 + (n_2 - pl)\mathbf{a}_2 + [n_3 + p(h + k)]\mathbf{a}_3 \quad (1.28)$$

where  $p$  is an **integer**, is such a point. If we then let  $p$  range through all integer values, we construct an infinite set of points on the same plane (while keeping  $N$  **constant**). This plane is, of course, **orthogonal** to  $\mathbf{K}$  because of the projection.



# Miller Indices

- In a similar manner, we can define the *next adjacent* plane by

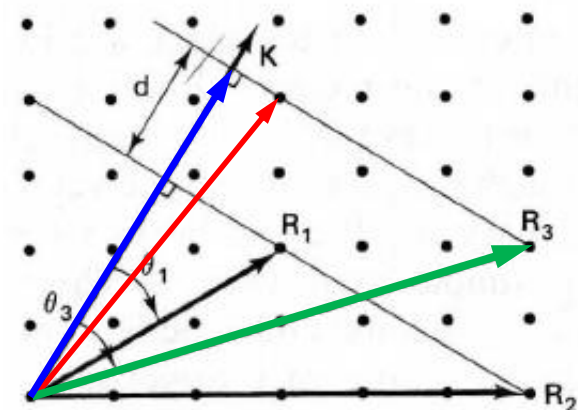
$$|\mathbf{R}_3| \cos \theta_3 = \frac{2\pi(N + 1)}{|\mathbf{K}|} \quad (1.29)$$

so that the *spacing* between adjacent lattice planes *perpendicular* to  $\mathbf{K}$  is

$$d = \frac{2\pi}{|\mathbf{K}|} \quad (1.30)$$

- Therefore, it is easy to see that sets of planes in a direct lattice can *conveniently* be *characterized* by reciprocal lattice vectors or points in the corresponding reciprocal lattice.

- For this to be a *unique* prescription, the integers  $h, k, l$  in (1.26) must have *no common factors*.



# Miller Indices

- The use of **reciprocal lattice vectors** to designate planes in direct space is *entirely equivalent to* the **Miller indices of crystallography**. This can be seen by taking a given  $\mathbf{K}$  and choosing the  $n_i$  of (1.25) so that one plane of the set defined by (1.26) intersects the  $\mathbf{a}_i$  axes at  $n_i \mathbf{a}_i$ ,  $i = 1, 2, 3$ .

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \quad (1.25)$$

- From (1.26) we then have

$$\mathbf{K} \cdot \mathbf{R} = 2\pi(hn_1 + kn_2 + ln_3) = 2\pi N \quad (1.26)$$

$$\mathbf{K} \cdot n_1 \mathbf{a}_1 = 2\pi hn_1 = 2\pi N \quad (1.31)$$

and so on, or

$$n_1 = \frac{N}{h}, \quad n_2 = \frac{N}{k}, \quad n_3 = \frac{N}{l} \quad (1.32)$$

- Thus the **intercepts** of the plane are **inversely proportional to the integral components of the reciprocal lattice vector**. This result can also be demonstrated for planes that do not intersect the  $\mathbf{a}_i$  axes at **discrete** lattice sites.

- Although the primitive lattice vectors,  $\mathbf{a}_i$ , are in general **not orthogonal**, it is **customary** in all cubic lattices for the Miller indices to refer to the **orthogonal simple cubic vectors**.

- The **notation** used for **specific reciprocal lattice vectors** (points) and **specific sets of direct lattice planes** is  $(hkl)$ .

# Miller Indices

- If a plane does **not intercept** a direct lattice vector (intercept at infinity), the corresponding **Miller index is zero**.
  - If a plane **intercepts in a negative direction**, the Miller index has a line drawn over it.
- Figure 1.19 shows several examples of this notation for lattice planes in cubic lattices.

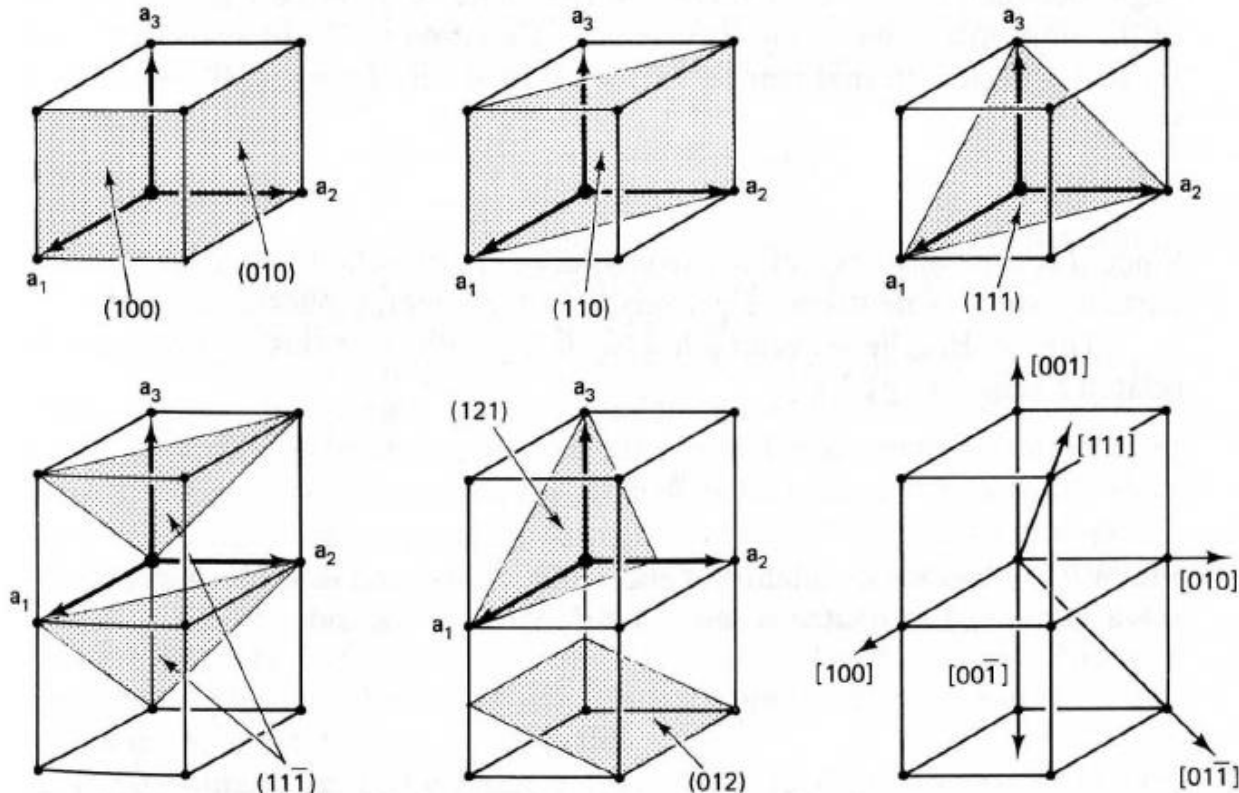


Figure 1.19 Examples of Miller indices for various planes and directions in a cubic lattice.

# Miller Indices

- Referring to Figs. 1.15 and 1.17, the corresponding notation for reciprocal lattice vectors is  $k_x = (100)$ ,  $k_y = (010)$ ,  $k_z = (001)$ . The origin or  $\Gamma$ -point is also referred to as  $(000)$ .

-To avoid confusion with *planes in the direct lattice* and *directions in the reciprocal lattice*, square brackets are used for directions in the direct lattice and planes in the reciprocal lattice. That is,  $\mathbf{a}_1 = [100]$ ,  $\mathbf{a}_2 = [010]$ , and so on, and the point

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

lies in the direction  $[n_1n_2n_3]$  from the origin.

-There is also a specific notation to indicate families of planes or reciprocal lattice vectors which are equivalent because of the lattice symmetry.

-For example,  $\{100\}$  is taken to indicate all the planes  $(100)$ ,  $(010)$ , and  $(001)$ .

- The equivalent notation for directions is  $\langle 100 \rangle$ , which is taken to mean all the directions  $[100]$ ,  $[010]$ ,  $[001]$  and their reciprocals  $[\bar{1}00]$ ,  $[0\bar{1}0]$ ,  $[00\bar{1}]$ .

# Miller Indices

**Table 1** Miller Indices and Their Represented Plane or Direction of a Crystal Surface

Miller Indices	Description of plane or direction
$(hkl)$	For a plane that intercepts $1/h$ , $1/k$ , $1/l$ on the $x$ -, $y$ -, and $z$ -axis, respectively.
$(\bar{h}kl)$	For a plane that intercepts the negative $x$ -axis.
$\{hkl\}$	For a full set of planes of equivalent symmetry, such as $\{100\}$ for $(100)$ , $(010)$ , $(001)$ , $(\bar{1}00)$ , $(0\bar{1}0)$ , and $(00\bar{1})$ in cubic symmetry.
$[hkl]$	For a direction of a crystal such as $[100]$ for the $x$ -axis.
$\langle hkl \rangle$	For a full set of equivalent directions.
$[hk\bar{l}m]$	For a plane in a hexagonal lattice (such as wurtzite) that intercepts $1/h$ , $1/k$ , $1/l$ , $1/m$ on the $a_1$ -, $a_2$ -, $a_3$ -, and $z$ -axis, respectively (Fig. 1g).



# Miller Indices

- **Four** Miller indices are used for **hexagonal** lattices: one for each of **three coplanar vectors**, which are spaced at  $120^\circ$ , and **one** in the direction **normal** to this plane.
- Thus **planes** and **reciprocal vectors** are  $(hk\ell m)$ , while **directions** in the direct lattice are  $[hk\ell m]$ . Otherwise, the notation is the same as for cubic lattices.
- Several examples are shown in Fig. 1.20.

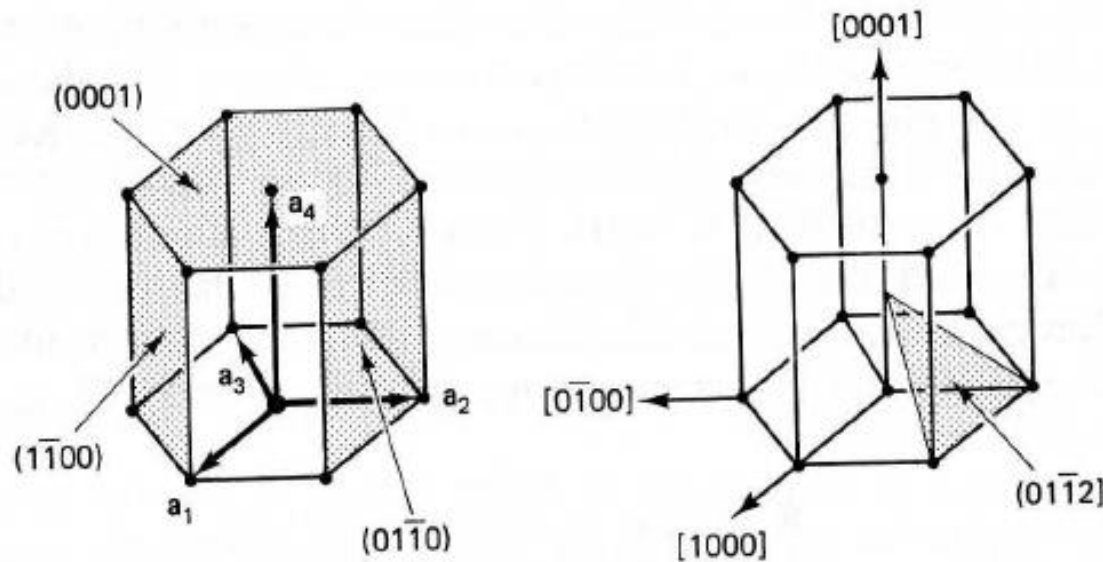
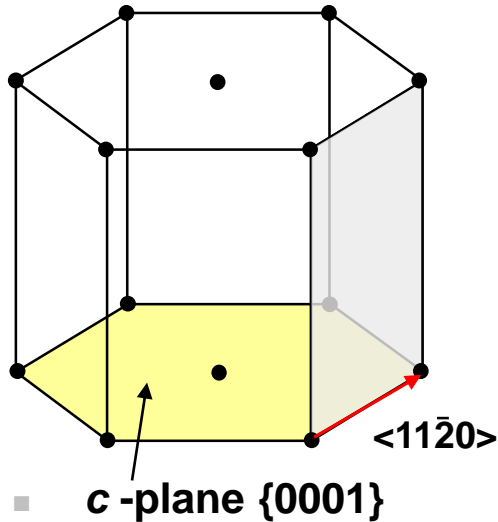


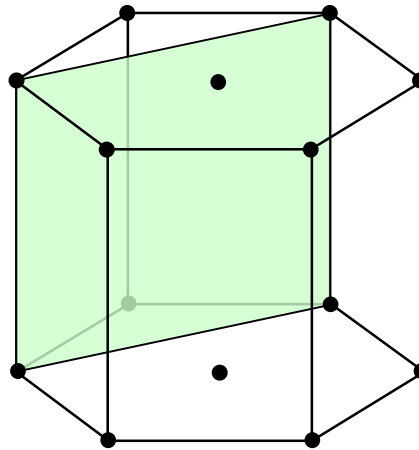
Figure 1.20 Examples of Miller indices for hexagonal lattices.

# Hexagonal GaN Planes

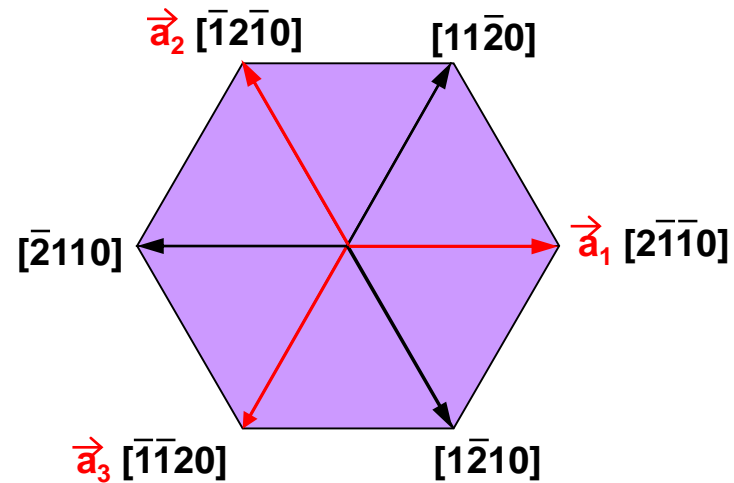
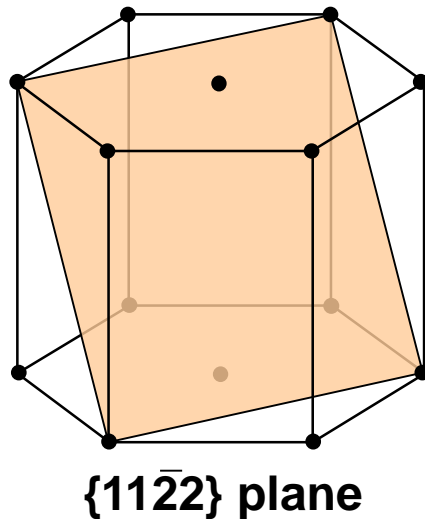
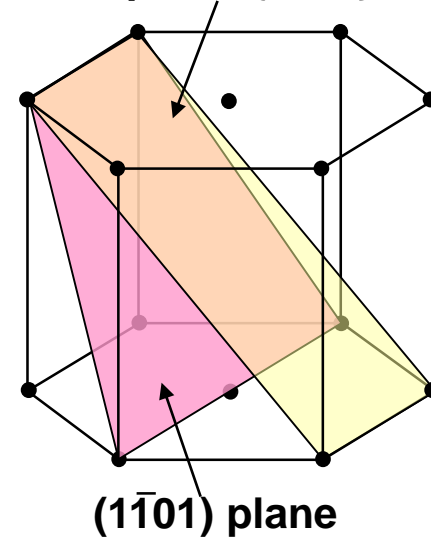
*m* -plane  $\{1\bar{1}00\}$



*a* -plane  $\{11\bar{2}0\}$



*r* -plane  $\{1\bar{1}02\}$



# Diffraction

An important application for the concepts discussed in this chapter is the analysis of wave diffraction by a crystal. As we will show, diffraction is governed by the Bragg condition,

$$2d \sin \theta = n\lambda \quad (1.33)$$

where  $d$  is the spacing between adjacent  $\{hkl\}$  planes given by (1.30),  $\theta$  the angle between the incident wave and the plane,  $n$  an integer indicating the diffraction order, and  $\lambda$  the wavelength. Equation (1.33) indicates that the longest wavelength that can be diffracted by a set of planes with spacing  $d$  is

$$\lambda_{\max} = 2d \quad (1.34)$$

Since  $d$  is typically several angstroms, crystal diffraction is limited to wave particles such as neutrons, electrons, and high-energy photons (x-rays).

$$d = \frac{2\pi}{|\mathbf{K}|} \quad (1.30)$$

# Diffraction

The de Broglie wavelength associated with neutrons or electrons is related to the energy by

$$\mathcal{E} = \frac{h^2}{2m\lambda^2} \quad (1.35)$$

where  $h$  is Planck's constant ( $6.6262 \times 10^{-34}$  J·s) and  $m$  is the mass of the wave particle. For neutrons,  $m = 1.675 \times 10^{-27}$  kg and

$$\lambda(\text{\AA}) = \frac{0.28601}{[\mathcal{E}(\text{eV})]^{1/2}} \quad (1.36)$$

where an electron-volt (eV) is equal to  $1.60219 \times 10^{-19}$  J. Thus very low energy neutrons can be diffracted by a crystal. For electrons,  $m = 9.10956 \times 10^{-31}$  kg and

$$\lambda(\text{\AA}) = \frac{12.2643}{[\mathcal{E}(\text{eV})]^{1/2}} \quad (1.37)$$

# Diffraction

For x-rays and other photons the wavelength is related to energy by

$$\mathcal{E} = \frac{hc}{\lambda} \quad (1.38)$$

where  $c$  is the velocity of light ( $2.9979 \times 10^8$  m/s). From (1.38),

$$\lambda(\text{\AA}) = \frac{1.23986 \times 10^4}{\mathcal{E}(\text{eV})} \quad (1.39)$$

and x-rays with energies of order  $10^4$  eV will be diffracted.

# Lattice Structure Factor

To analyze the conditions under which diffraction occurs, consider an x-ray plane wave with electric field,

$$E = E_0 \exp [i(\mathbf{k} \cdot \mathbf{r} - \omega t)] \quad (1.40)$$

incident on a multielectron atom. In (1.40)  $\mathbf{k}$  is the wavevector, which is related to the wavelength  $\lambda$  by  $|\mathbf{k}| = 2\pi/\lambda$  and  $\omega$  is the angular frequency. The incident electric field accelerates the electrons to higher energy, during which time they emit x-rays in all directions with the electric field,

$$E = \frac{E_0 f_d}{r} \exp [i(\mathbf{k}' \cdot \mathbf{r} - \omega t)] \quad (1.41)$$

The electric field in (1.41) is a solution of the radial wave equation where  $\mathbf{k}'$  indicates a change in wavevector and phase and  $f_d$  is the *atomic scattering factor* of an atom indexed by a basis vector  $\mathbf{d}$ .



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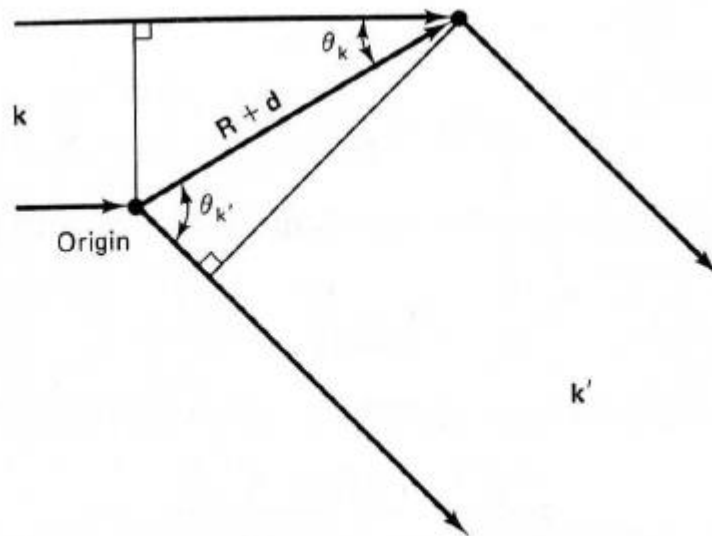
$$E = \frac{E_0 f_d}{r} \exp [i(\mathbf{k}' \cdot \mathbf{r} - \omega t)] \quad (1.41)$$

The atomic scattering factors depend on the number of electrons per atom, the scattering angle, and the incident wavelength and are defined as the ratio of the amplitude scattered by the actual electron distribution in an atom to the amplitude scattered by one isolated electron. When all the electrons in an atom scatter in phase ( $\theta$ ) with respect to the observation point,  $f_d$  is equal to the atomic number.

# Lattice Structure Factor

To examine these interference effects, consider the difference in phase between the radiation scattered by two atoms separated by a lattice vector  $\mathbf{R}$  and basis vector  $\mathbf{d}$ . As indicated in Fig. 1.21, the path difference between the incident and scattered waves for the two atoms is

$$|\mathbf{R} + \mathbf{d}| \cos \theta_k - |\mathbf{R} + \mathbf{d}| \cos \theta_{k'} = \frac{(\mathbf{R} + \mathbf{d}) \cdot \mathbf{k}}{|\mathbf{k}|} - \frac{(\mathbf{R} + \mathbf{d}) \cdot \mathbf{k}'}{|\mathbf{k}'|} \quad (1.42)$$



**Figure 1.21** Schematic of phase difference between radiation scattered from an atom at the origin and an atom at  $\mathbf{R} + \mathbf{d}$ .



# Lattice Structure Factor

For elastic scattering (no energy loss) the magnitudes of the incident and scattered wavevectors are equal,

$$|\mathbf{k}| = |\mathbf{k}'| \quad (1.43)$$

and the phase difference is

$$(\mathbf{k} - \mathbf{k}') \cdot (\mathbf{R} + \mathbf{d}) = \Delta \mathbf{k} \cdot (\mathbf{R} + \mathbf{d}) \quad (1.44)$$

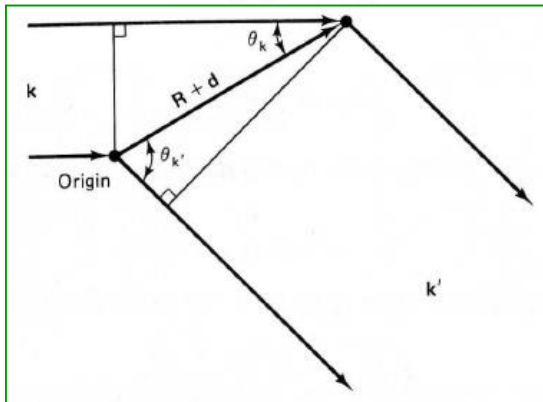
where  $\Delta \mathbf{k}$  is the scattering vector.

If we use the phase of the wave scattered from the atom at the origin as our phase reference, the associated phase factor for this atom is

$$\exp(0) = 1 \quad (1.45)$$

The phase factor for the atom at  $\mathbf{R} + \mathbf{d}$  is then

$$\exp[i \Delta \mathbf{k} \cdot (\mathbf{R} + \mathbf{d})] \quad (1.46)$$



# Lattice Structure Factor

Summing the phase factors for all  $N$  unit cells indexed by the lattice vectors  $\mathbf{R}$  and all atoms in the unit cell indexed by the basis vectors  $\mathbf{d}$ , we define a lattice structure factor,

$$F_R \equiv \sum_R \sum_d f_d \exp [i \Delta \mathbf{k} \cdot (\mathbf{R} + \mathbf{d})] \quad (1.47)$$

which from (1.41) has the phase of and is proportional to the electric field of the resultant scattered radiation. It is also useful to define a basis structure factor,

$$F_d \equiv \sum_d f_d \exp (i \Delta \mathbf{k} \cdot \mathbf{d}) \quad (1.48)$$

in which case (1.47) for the lattice structure factor becomes

$$F_R \equiv F_d \sum_R \exp (i \Delta \mathbf{k} \cdot \mathbf{R}) \quad (1.49)$$

where  $\mathbf{R}$  is given by (1.1).

# Lattice Structure Factor

Since the intensity of the scattered radiation depends on the square of the resultant electric field, we will examine the variation of  $F_R^* F_R$  with  $\Delta \mathbf{k} \cdot \mathbf{R}$ . For simplicity, assume a one-dimensional lattice with  $N$  unit cells, so that

$$\mathbf{R} = n\mathbf{a} \quad (1.50)$$

for

$$n = 0, 1, 2, \dots, N - 1$$

Equation (1.49) is then

$$\frac{F_R}{F_d} = \sum_{n=0}^{N-1} \exp(in \Delta \mathbf{k} \cdot \mathbf{a}) \quad (1.51)$$

for

$$x \equiv \Delta \mathbf{k} \cdot \mathbf{a} \quad (1.52)$$

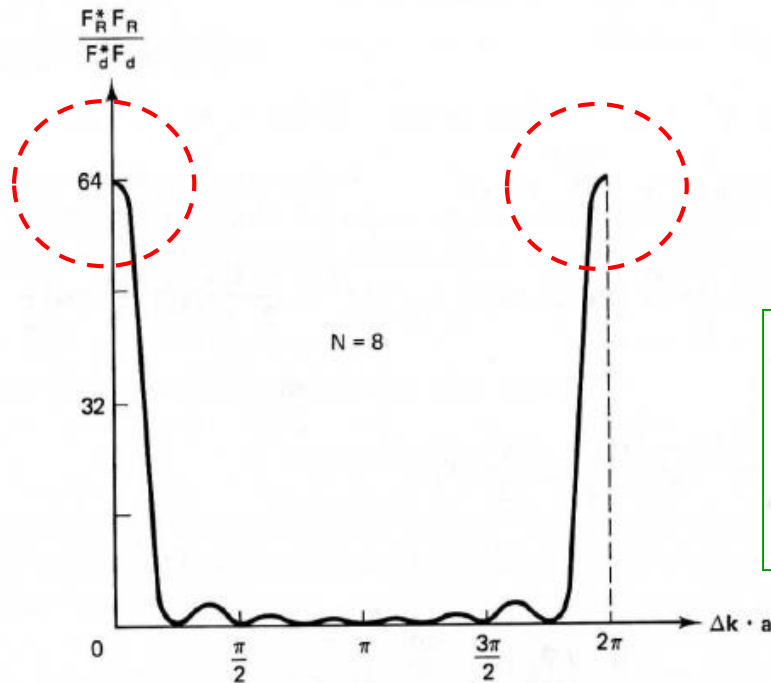
$$\frac{F_R^* F_R}{F_d^* F_d} = \frac{\sin^2 \frac{N \Delta \mathbf{k} \cdot \mathbf{a}}{2}}{\sin^2 \frac{\Delta \mathbf{k} \cdot \mathbf{a}}{2}} \quad (1.56)$$

# Diffraction Conditions

Equation (1.56) for the relative intensity of the scattered radiation as a function of  $\Delta \mathbf{k} \cdot \mathbf{a}$  is plotted in Fig. 1.22 for  $N = 8$ . As can be seen, the scattered radiation has significant value only when

$$\Delta \mathbf{k} \cdot \mathbf{a} = 2\pi n \quad (1.57)$$

where  $n$  has integer values (including zero).



$$\frac{F_R^* F_R}{F_d^* F_d} = \frac{\sin^2 \frac{N \Delta \mathbf{k} \cdot \mathbf{a}}{2}}{\sin^2 \frac{\Delta \mathbf{k} \cdot \mathbf{a}}{2}} \quad (1.56)$$

**Figure 1.22** Variation of scattered intensity with  $\Delta \mathbf{k} \cdot \mathbf{a}$  for a one-dimensional lattice with eight unit cells.

# Diffraction Conditions

In fact, for large values of  $N$ ,

(1.56) becomes approximately

$$\frac{F_R^* F_R}{F_d^* F_d} \simeq N^2 \delta(\Delta \mathbf{k} \cdot \mathbf{a} - 2\pi n) \quad (1.58)$$

where  $\delta(\Delta \mathbf{k} \cdot \mathbf{a} - 2\pi n)$  is the Dirac delta function. (The secondary maxima in Fig. 1.22 persist, however, even as  $N$  approaches infinity.) Thus (1.57) is the condition for constructive interference or diffraction maxima for a one-dimensional crystal. In three dimensions (1.57) is

$$\Delta \mathbf{k} \cdot \mathbf{R} = 2\pi(\text{integer}) \quad (1.59)$$

which from (1.19) defines a reciprocal lattice vector,  $\mathbf{K}$ . Thus the condition for diffraction is that the scattering vector  $\Delta \mathbf{k}$  be a reciprocal lattice vector  $\mathbf{K}$ , or

$$\mathbf{k} - \mathbf{k}' \equiv \Delta \mathbf{k} = \mathbf{K} \quad (1.60)$$

$$\mathbf{K} \cdot \mathbf{R} = 2\pi(hn_1 + kn_2 + ln_3) = 2\pi(\text{integer}) \quad (1.19)$$

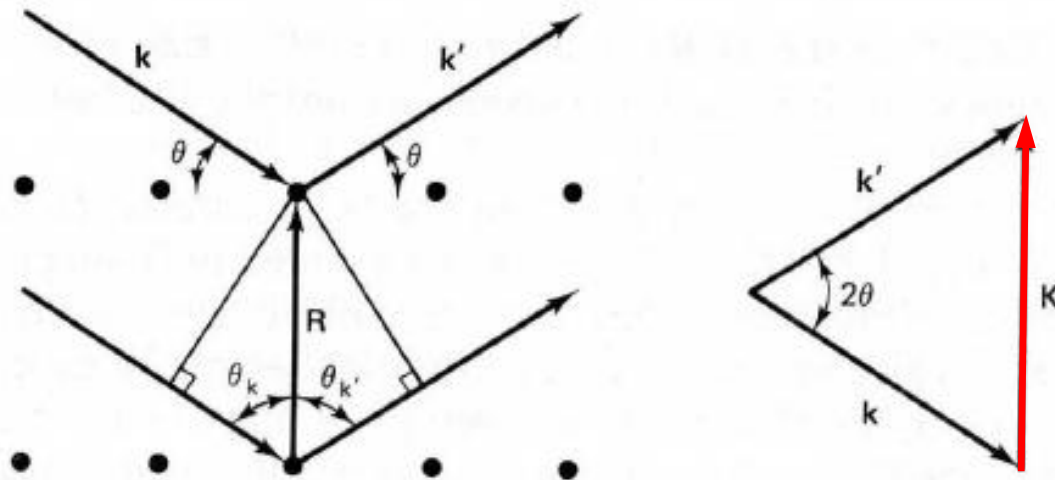
# Diffraction Conditions

To derive the Bragg condition, notice from Fig. 1.23 that

$$| \mathbf{K} | = | \mathbf{k}' | \sin \theta + | \mathbf{k} | \sin \theta \quad (1.61)$$

For  $| \mathbf{k} | = | \mathbf{k}' | = 2\pi/\lambda$ , (1.61) is

$$| \mathbf{K} | = \frac{2\pi}{\lambda} (2 \sin \theta) \quad (1.62)$$



**Figure 1.23** Diagram indicating the Bragg diffraction condition.



# Diffraction Conditions

From (1.30),

$$|\mathbf{K}| = \frac{2\pi}{d} \quad (1.63)$$

where  $d$  is the spacing between adjacent  $\{hkl\}$  planes. Allowing for higher-order diffraction, (1.62) and (1.63) give

$$2d \sin \theta = n\lambda \quad (1.33)$$

where  $n$  is an integer denoting the order of diffraction.

The spacing between adjacent  $\{hkl\}$  planes can be calculated from (1.63), (1.17), and the reciprocal lattice unit cell vectors. For a simple cubic unit cell, (1.17) and (1.21) result in

$$\mathbf{K} = \frac{2\pi}{a} (h\hat{x} + k\hat{y} + l\hat{z}) \quad (1.64)$$

where  $a$  is the lattice constant or length of the side of the cube.

# Diffraction Conditions

From (1.30),

$$d = \frac{2\pi}{|\mathbf{K}|} \quad (1.30)$$

where  $d$  is the spacing between adjacent  $\{hkl\}$  planes. Allowing for higher-order diffraction, (1.62) and (1.63) give

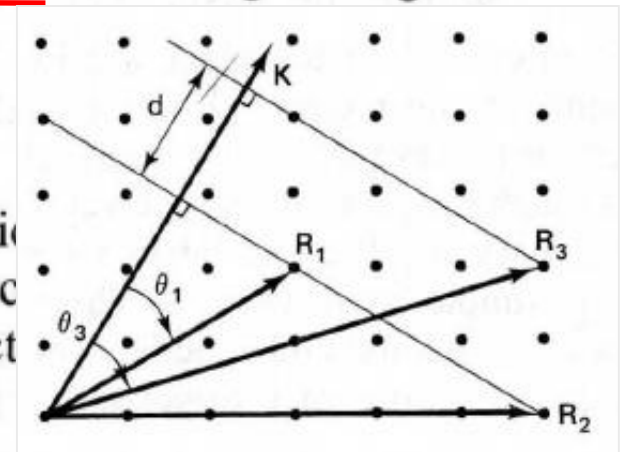
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The spacing between adjacent  $\{hkl\}$  planes can be found from (1.63), (1.17), and the reciprocal lattice unit cell vector unit cell, (1.17) and (1.21) result in

$$\mathbf{K} = \frac{2\pi}{a} (h\hat{x} + k\hat{y} + l\hat{z}) \quad (1.64)$$

where  $a$  is the lattice constant or length of the side of the cube.





# Diffraction Conditions

Using (1.63) and (1.64) gives us

$$d = \frac{a}{(h^2 + k^2 + l^2)^{1/2}} \quad (1.65)$$

The diffraction maxima corresponding to this spacing and indicated by the reciprocal lattice points or vectors in (1.64) are referred to as  $hkl$  maxima.

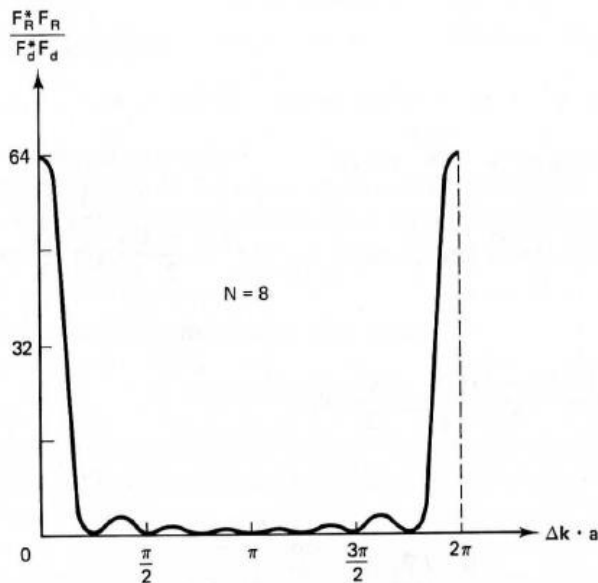


Figure 1.22 Variation of scattered intensity with  $\Delta \mathbf{k} \cdot \mathbf{a}$  for a one-dimensional lattice with eight unit cells.

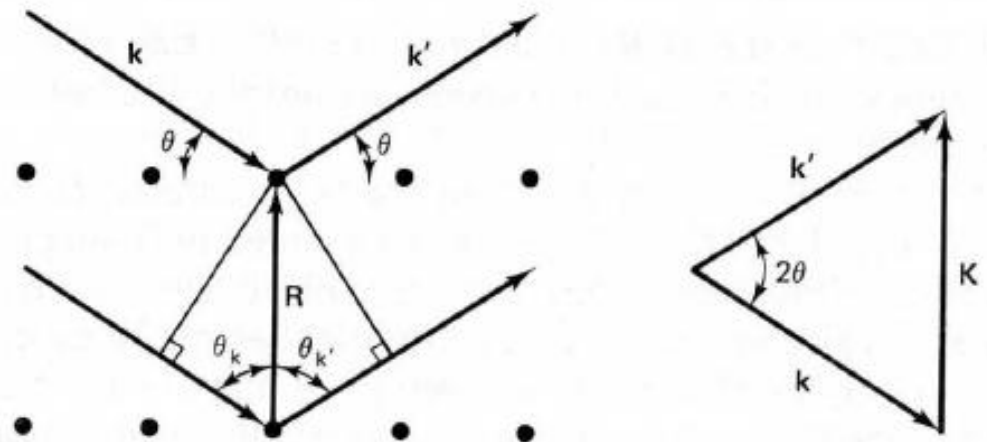


Figure 1.23 Diagram indicating the Bragg diffraction condition.

# Basis Structure Factor

In the discussion above we ignored the contents of the unit cell and examined the phase differences in the radiation scattered from  $N$  unit cells to establish the conditions under which diffraction occurs. In a real crystal with a basis, however, many of the maxima allowed by

$$\Delta \mathbf{k} \cdot \mathbf{R} = 2\pi(\text{integer}) \quad (1.59)$$

are not observed because of phase cancellation within the unit cell. For this reason we will now examine the basis structure factor,

$$F_d \equiv \sum_d f_d \exp(i \Delta \mathbf{k} \cdot \mathbf{d}) \quad (1.48)$$

where the basis vector  $\mathbf{d}$  indexes the atoms in the unit cell.

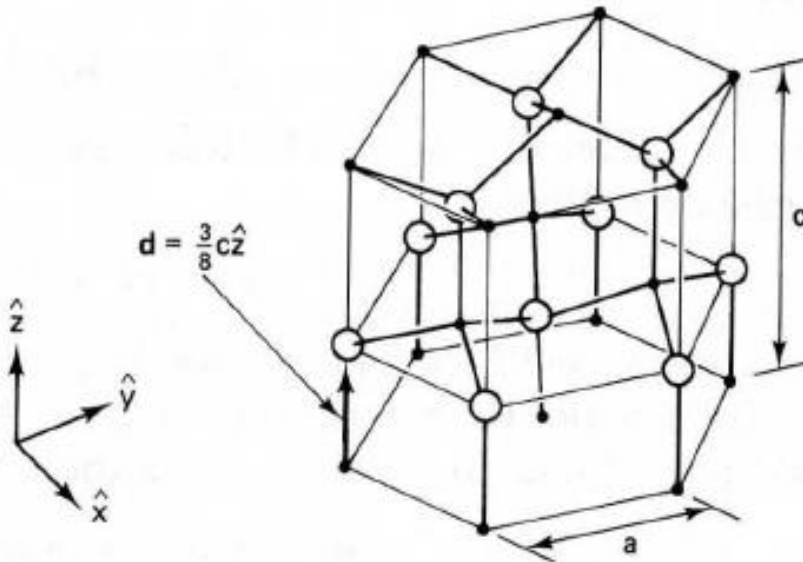
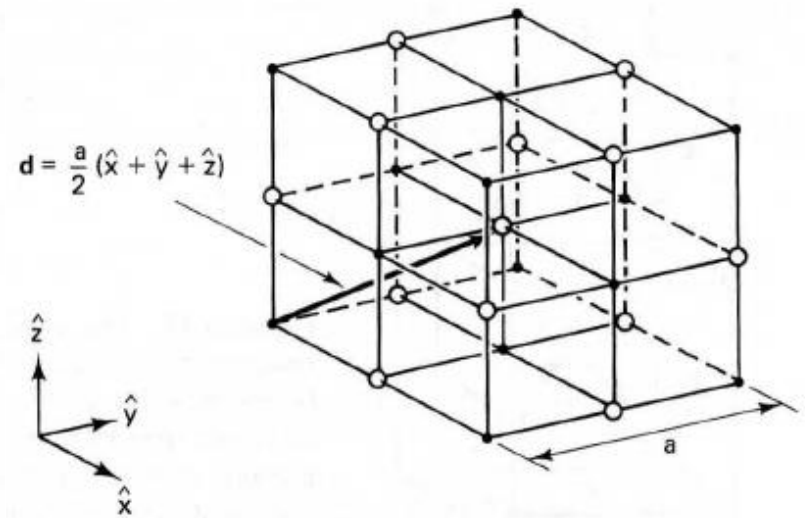
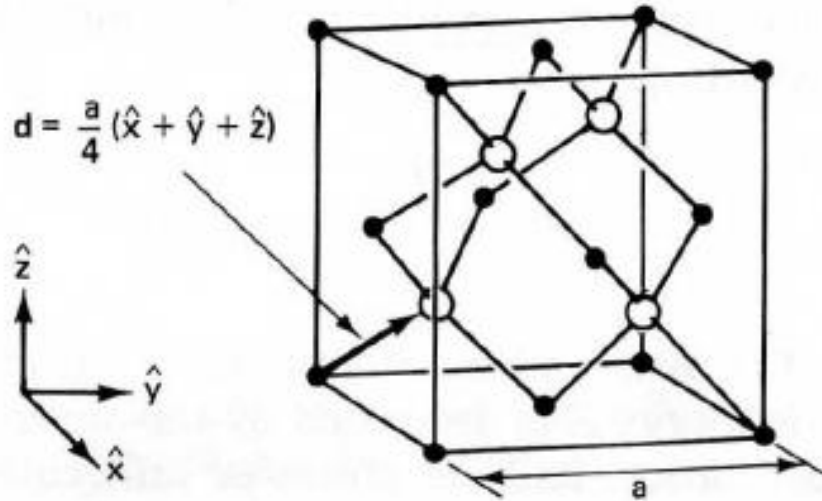
The basis vectors for the various crystal structures are shown in Figs. 1.10, 1.11, and 1.12 and, in general, are given by

$$\mathbf{d} = x_d \mathbf{a}_1 + y_d \mathbf{a}_2 + z_d \mathbf{a}_3 \quad (1.66)$$

where  $x_d$ ,  $y_d$ , and  $z_d$  indicate the position of atom  $d$  with respect to the primitive vectors of the unit cell. The scattering vector  $\Delta \mathbf{k}$  is a reciprocal lattice vector given, in general, by

$$\Delta \mathbf{k} = h \mathbf{b}_1 + k \mathbf{b}_2 + l \mathbf{b}_3 \quad (1.67)$$

# Basis Structure Factor



# Basis Structure Factor

For a simple cubic unit cell (1.2) and (1.66) result in

$$\mathbf{d} = a(x_d\hat{x} + y_d\hat{y} + z_d\hat{z}) \quad (1.68)$$

and (1.21) and (1.67) produce

$$\Delta \mathbf{k} = \frac{2\pi}{a} (h\hat{x} + k\hat{y} + l\hat{z}) \quad (1.69)$$

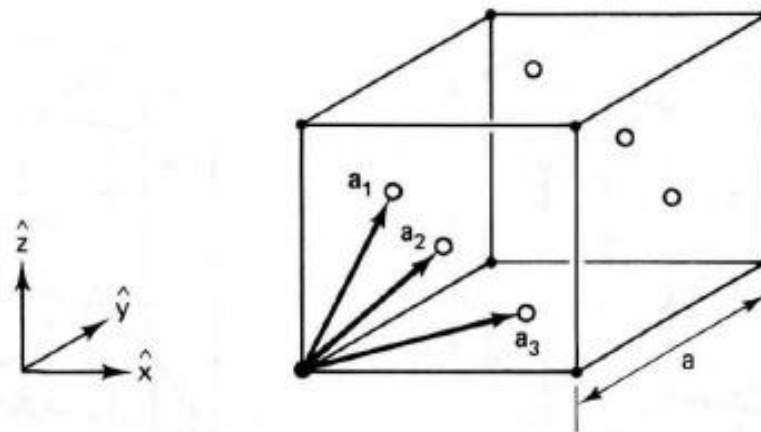
Using (1.68) and (1.69) in (1.48), the basis structure factor is

$$F_d = \sum_d f_d \exp [2\pi i(hx_d + ky_d + lz_d)] \quad (1.70)$$

where  $h$ ,  $k$ , and  $l$  are the Miller indices of the diffracting planes. Equation (1.70) determines which diffraction maxima are not allowed because of phase cancellation within the unit cell.

# Basis Structure Factor

As an example, consider atoms in the face-centered cubic (fcc) unit cell shown in Fig. 1.5. This cell can be represented as a simple cubic unit cell with a basis of four atoms: one at the origin and one at each of the three primitive vectors given by (1.5). That is, the eight atoms in the cube corners are each shared by eight cells for an average of one atom per cell; the six atoms on the cube faces are each shared by two cells for an average of three atoms per cell.



**Figure 1.5** Face-centered cubic Bravais lattice with symmetrical primitive vectors.



# Basis Structure Factor

The basis vectors for these four atoms are

$$\mathbf{d} = 0, \quad \frac{a}{2}(\hat{x} + \hat{y}), \quad \frac{a}{2}(\hat{y} + \hat{z}), \quad \text{and} \quad \frac{a}{2}(\hat{z} + \hat{x}) \quad (1.71)$$

Assuming that all four atoms are the same, (1.70) is

$$\frac{F_d}{f_d} = 1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)} \quad (1.72)$$

Thus, for planes such that  $h$ ,  $k$ , and  $l$  are either all even or all odd,

$$F_d = 4f_d \quad (1.73)$$

and diffraction occurs. For planes such that one of the  $h$ ,  $k$ , or  $l$  is even or one is odd,

$$F_d = 0 \quad (1.74)$$

and no diffraction occurs.