CHAPTER 5

Energy Bands in Crystals

5.1. One-Dimensional Zone Schemes

$$\alpha = \sqrt{\frac{2m}{\hbar^2}} E^{1/2},$$

for free electron

$$\alpha = k_x$$

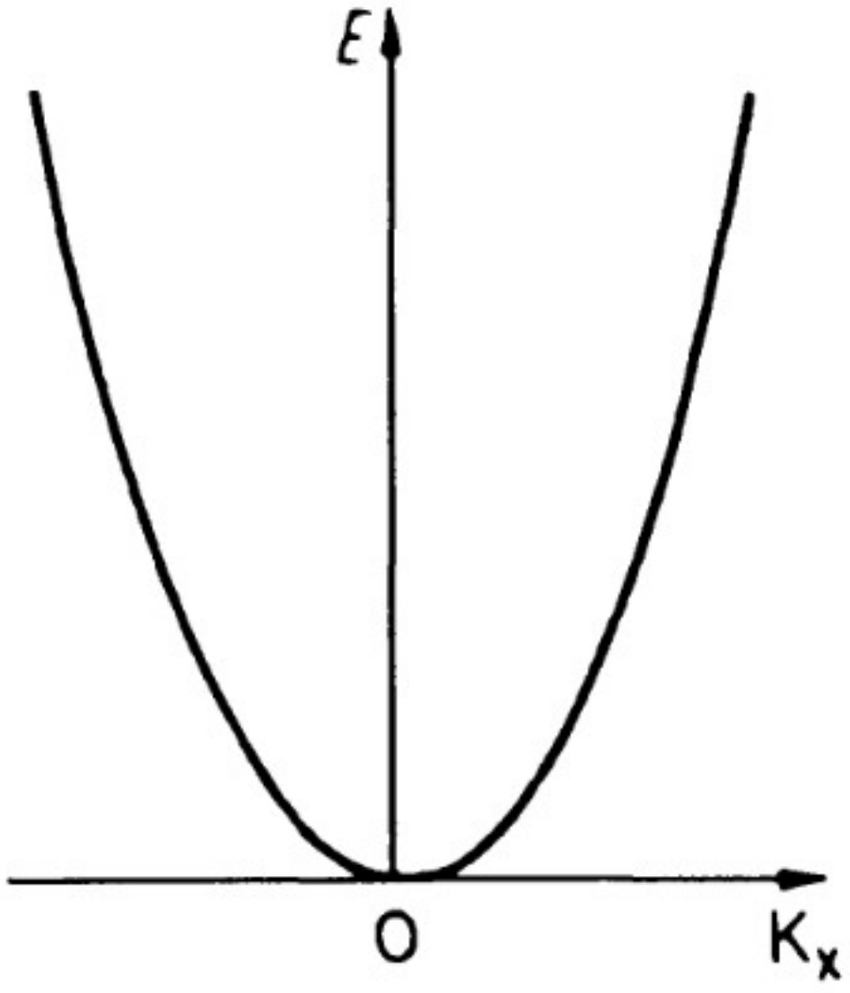
for periodic potential

$$\alpha a = k_x a + n2\pi.$$

$$\alpha = k_x + 2n\pi/a$$

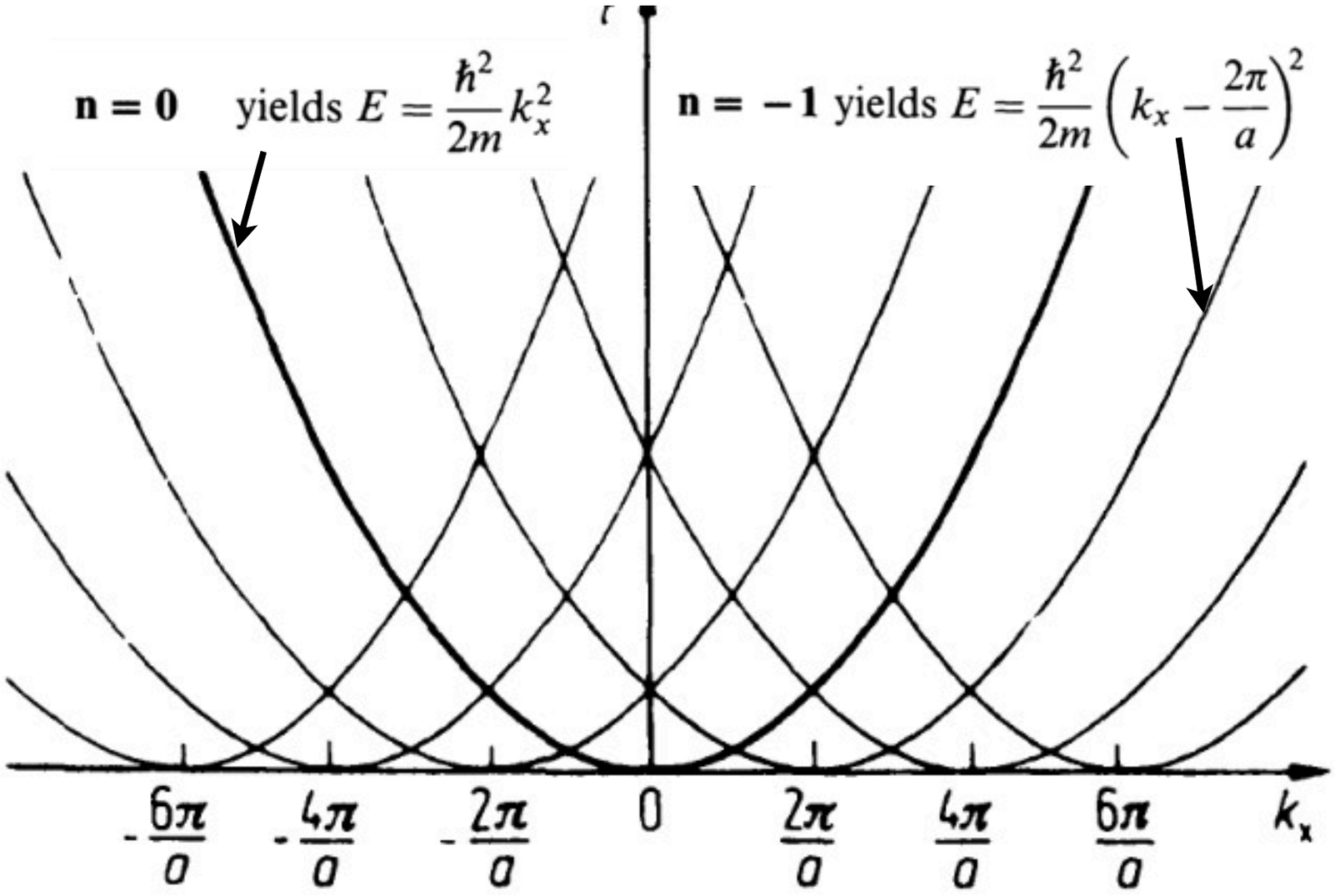
$$k_x + n\frac{2\pi}{a} = \sqrt{\frac{2m}{\hbar^2}} E^{1/2}.$$

$$E = \frac{\hbar^2}{2m}\left(k_x + n\frac{2\pi}{a}\right)^2, \quad n = 0, \pm 1, \pm 2, \ldots .$$



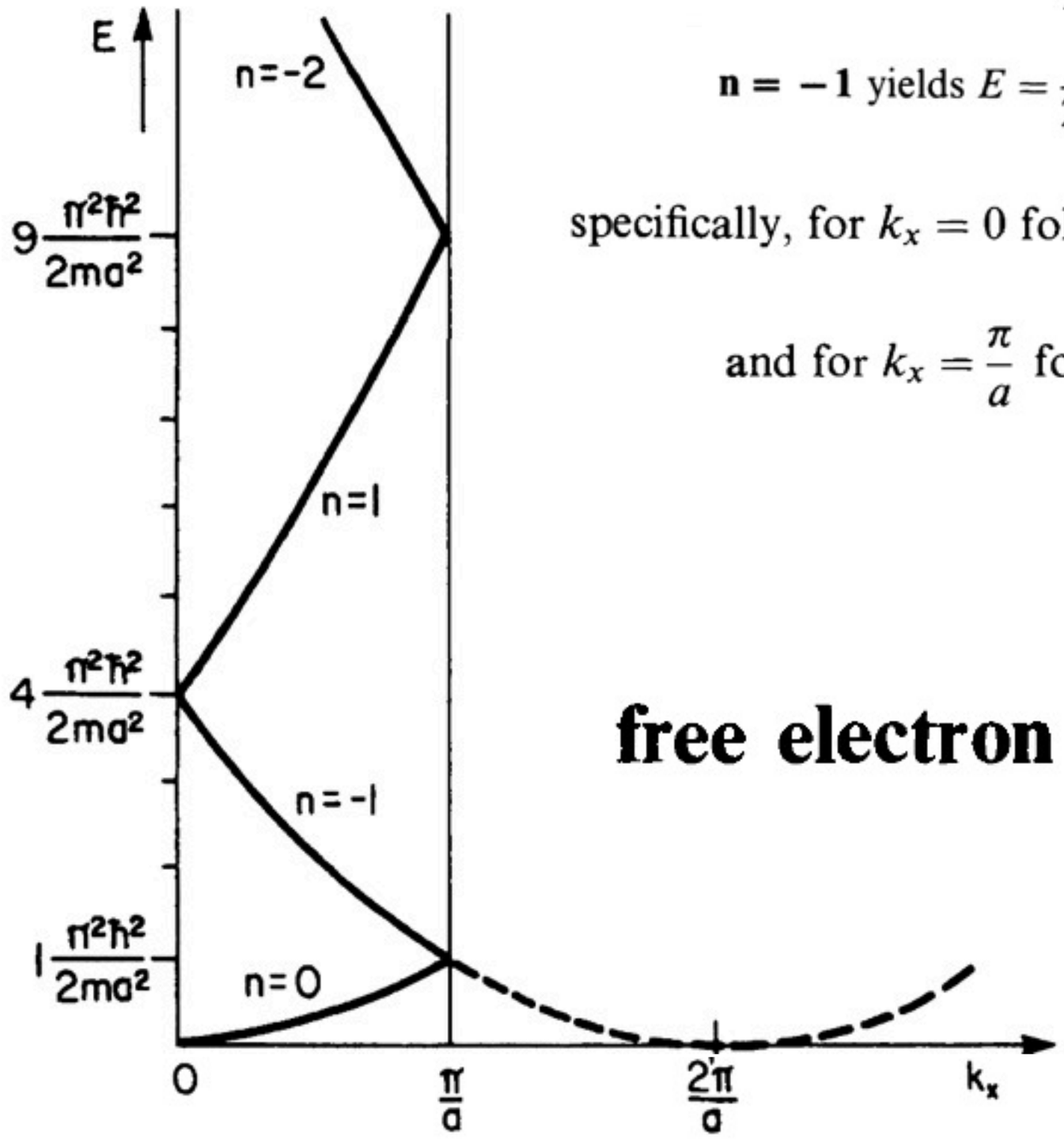
dispersion relationship
for free electron

"extended zone scheme"



dispersion relationship
for electron in periodic
potential

Reduced zone scheme.



free electron bands

$\mathbf{n = 0}$ yields $E = \dfrac{\hbar^2}{2m} k_x^2$

$\mathbf{n = -1}$ yields $E = \dfrac{\hbar^2}{2m}\left(k_x - \dfrac{2\pi}{a}\right)^2$

specifically, for $k_x = 0$ follows $E = 4\dfrac{\pi^2\hbar^2}{2ma^2}$;

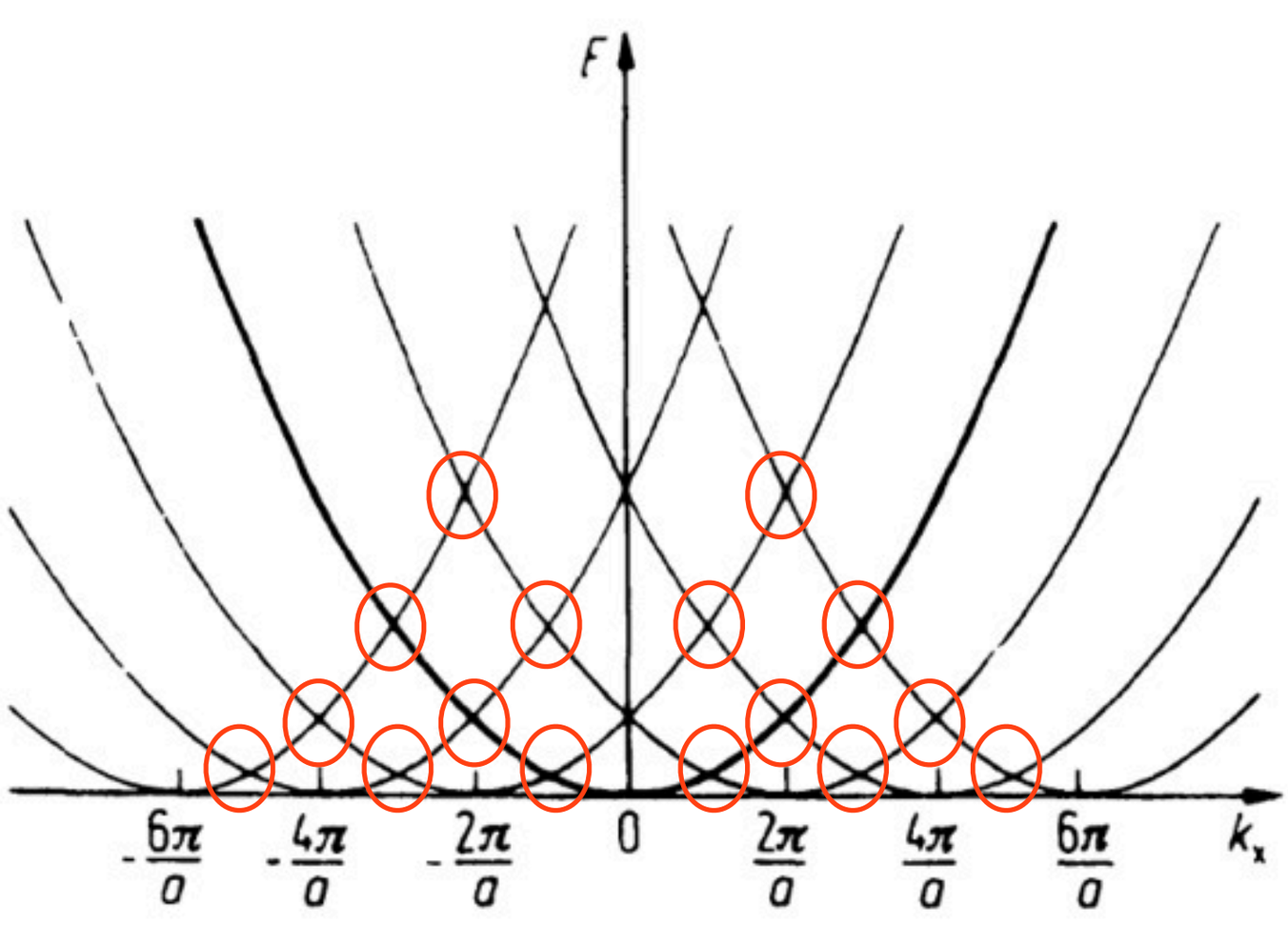
and for $k_x = \dfrac{\pi}{a}$ follows $E = 1\dfrac{\pi^2\hbar^2}{2ma^2}$.

if an electron propagates in a periodic potential
we always observe discontinuities of the energies when
$\cos k_x a$ has a maximum or a minimum, i.e., when $\cos k_x a = \pm 1$

$$k_x a = n\pi, \quad n = \pm 1, \pm 2, \pm 3, \ldots,$$

or

$$k_x = n \cdot \frac{\pi}{a}.$$



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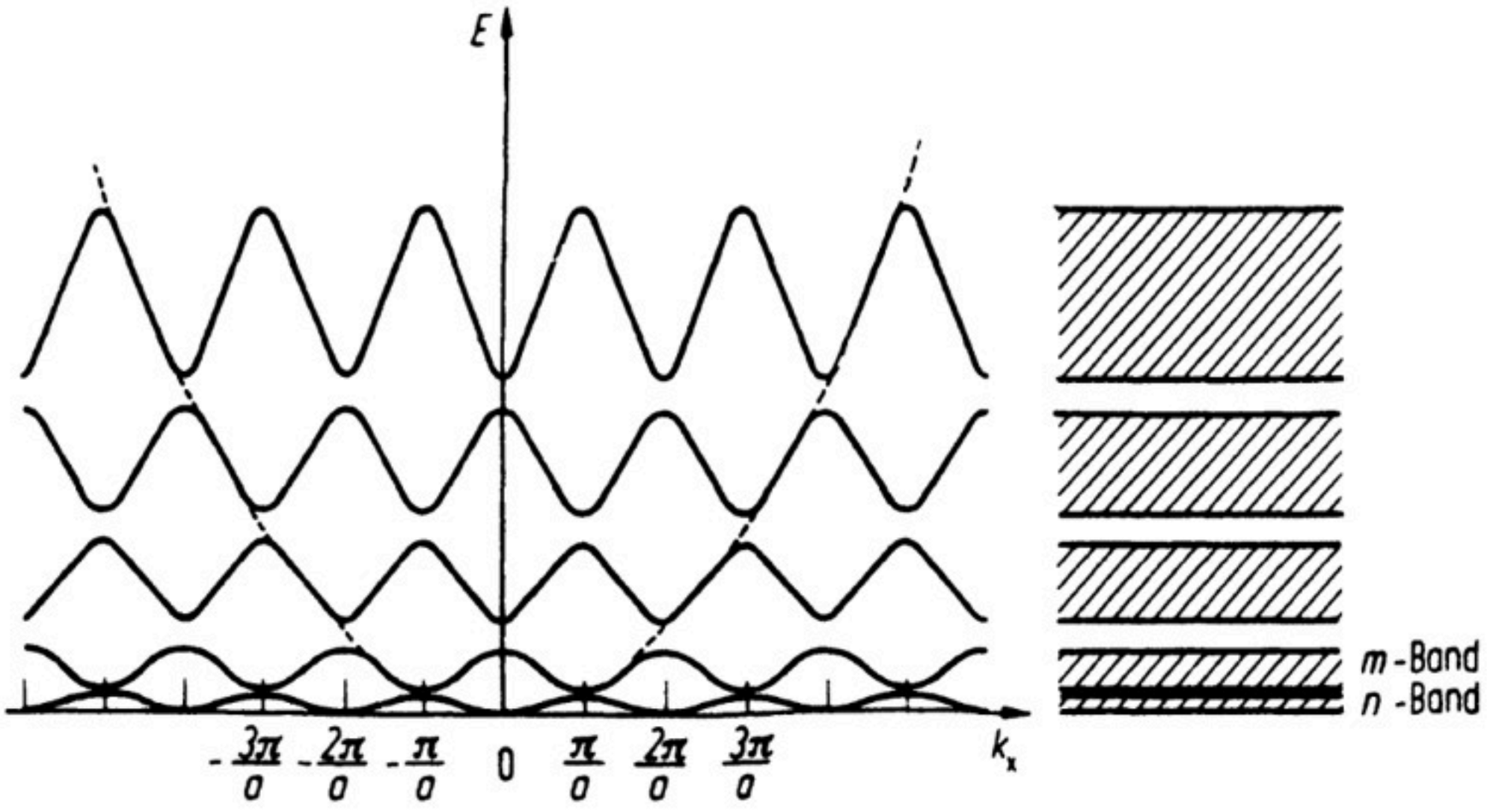
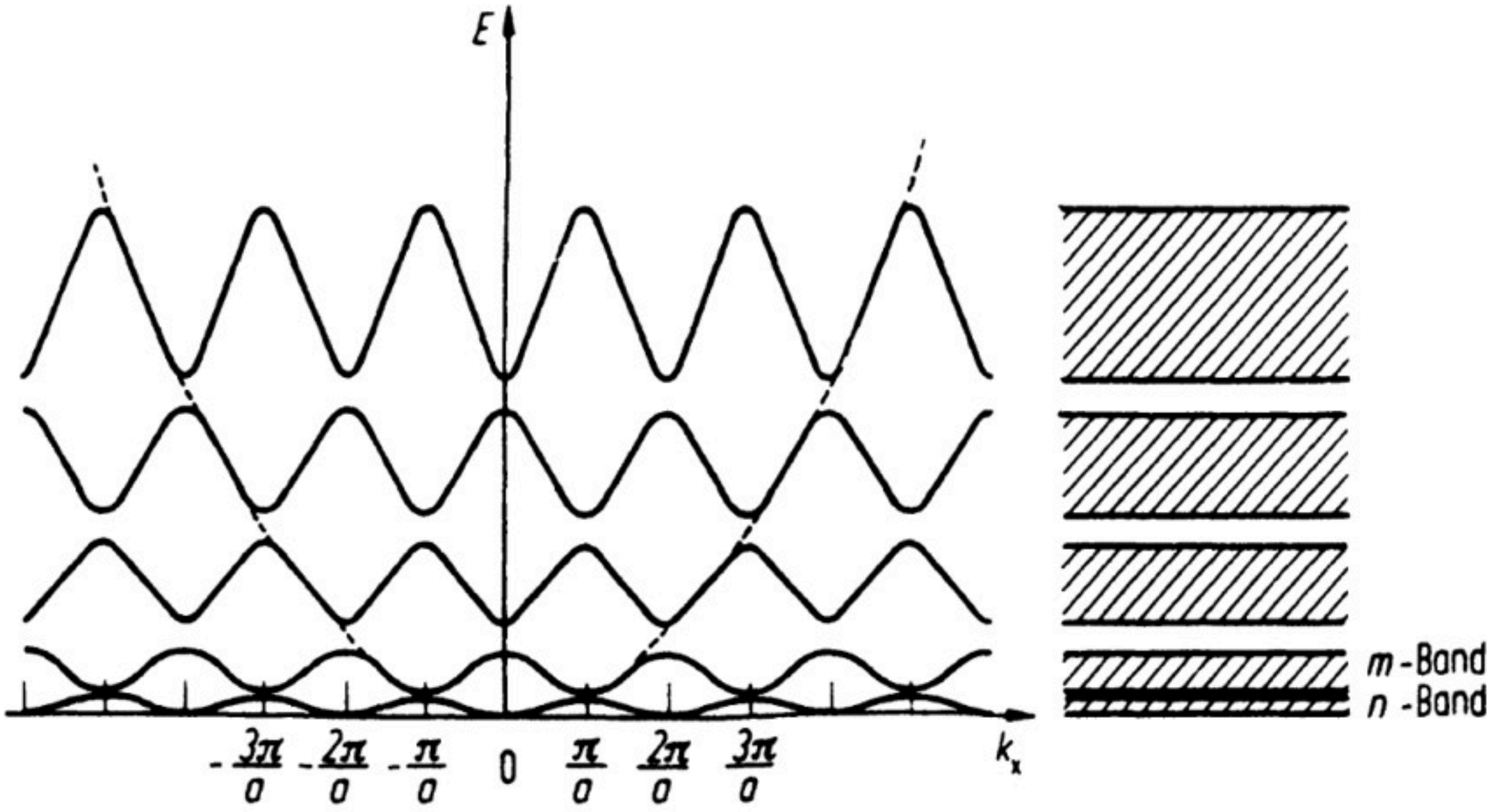
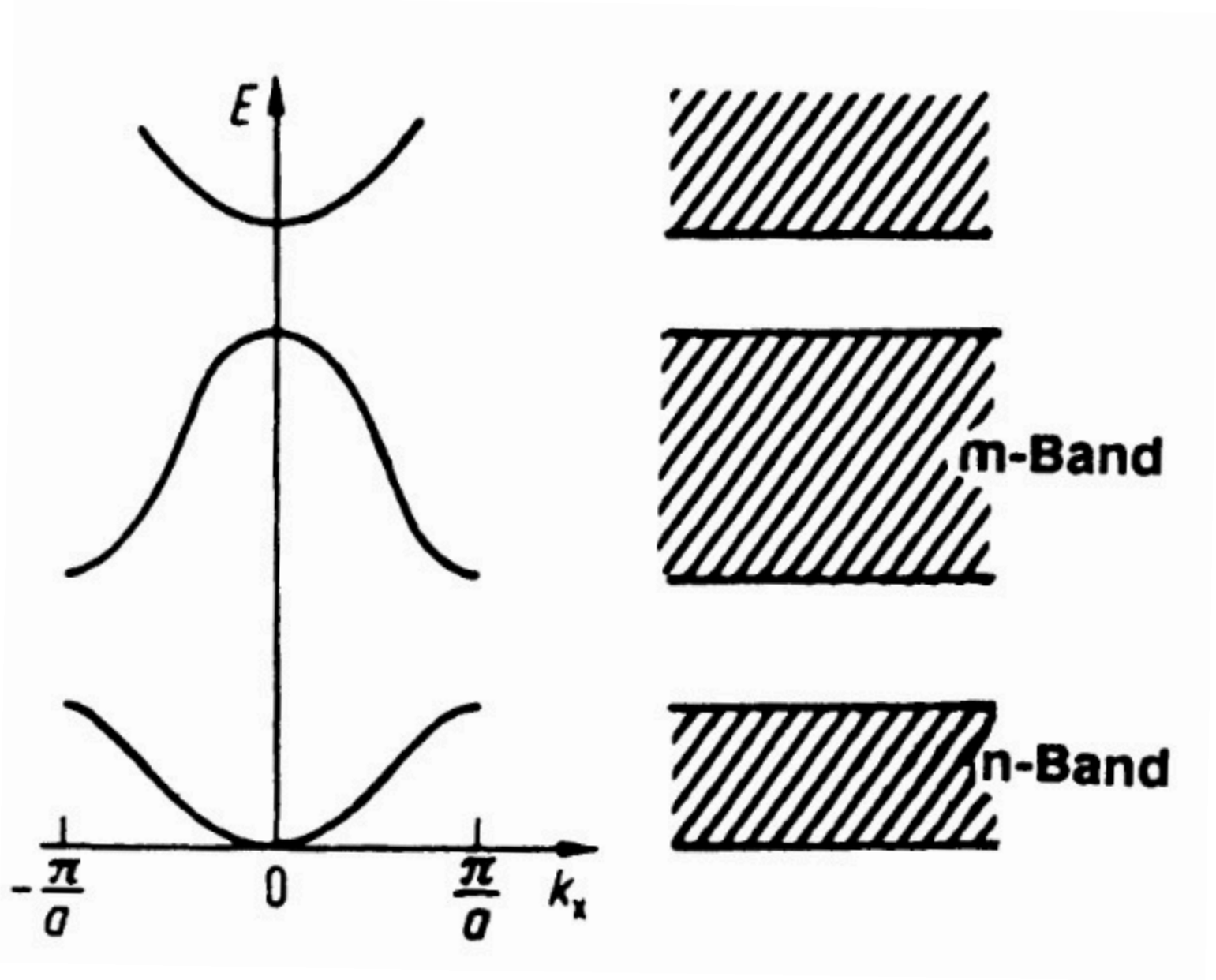


Periodic Zone Scheme

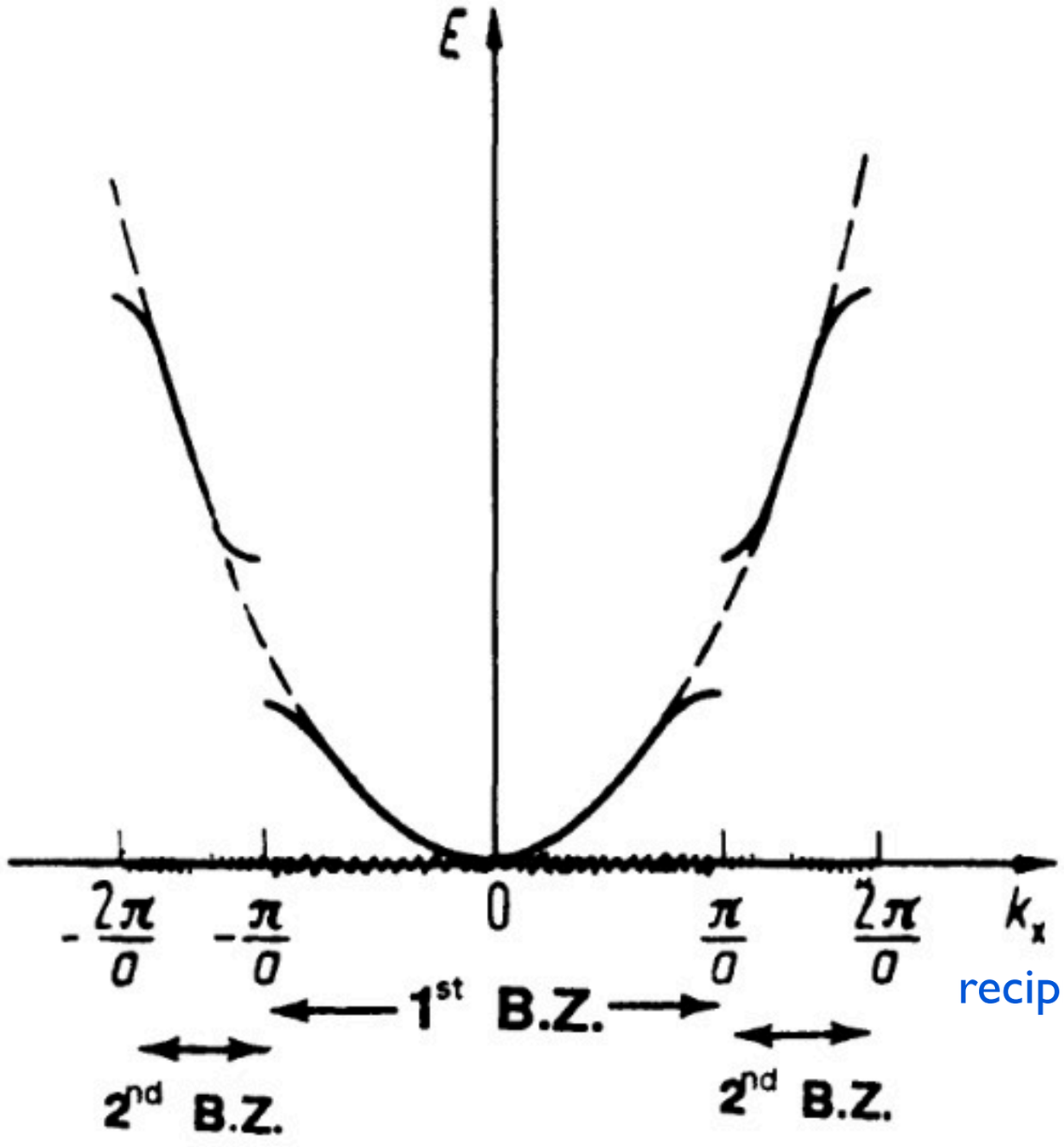
Periodic Zone Scheme



Reduced zone scheme.



$v_g = \partial E / \partial k$: group velociety



conduction band

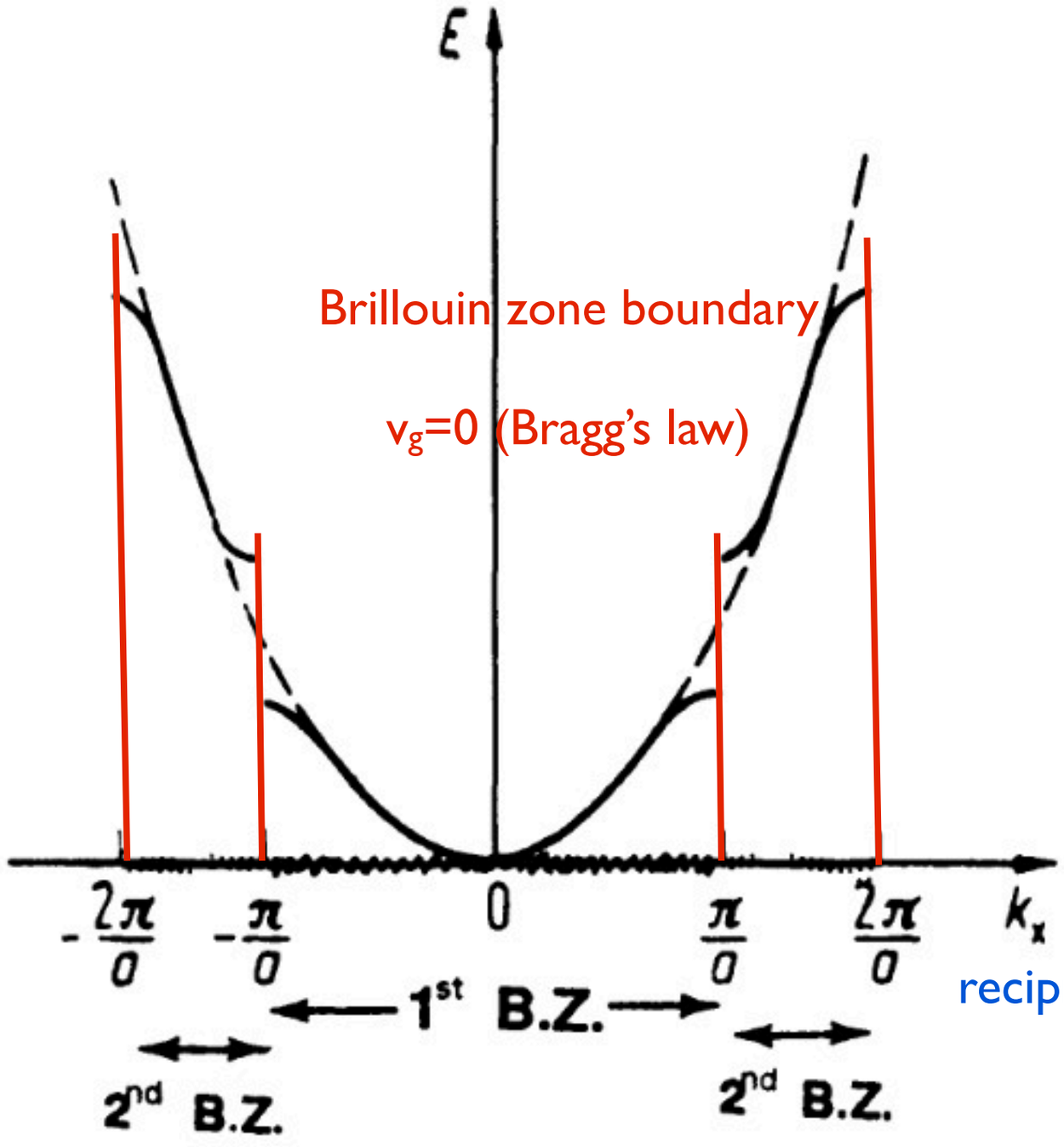
valance band

reciprocal space

Extended zone scheme.

electrons in a crystal behave, for most k_x values, like free electrons, except when k_x approaches the value $n \cdot \pi/a$.

$v_g = \partial E / \partial k$: group velociety



Extended zone scheme.

conduction band

valance band

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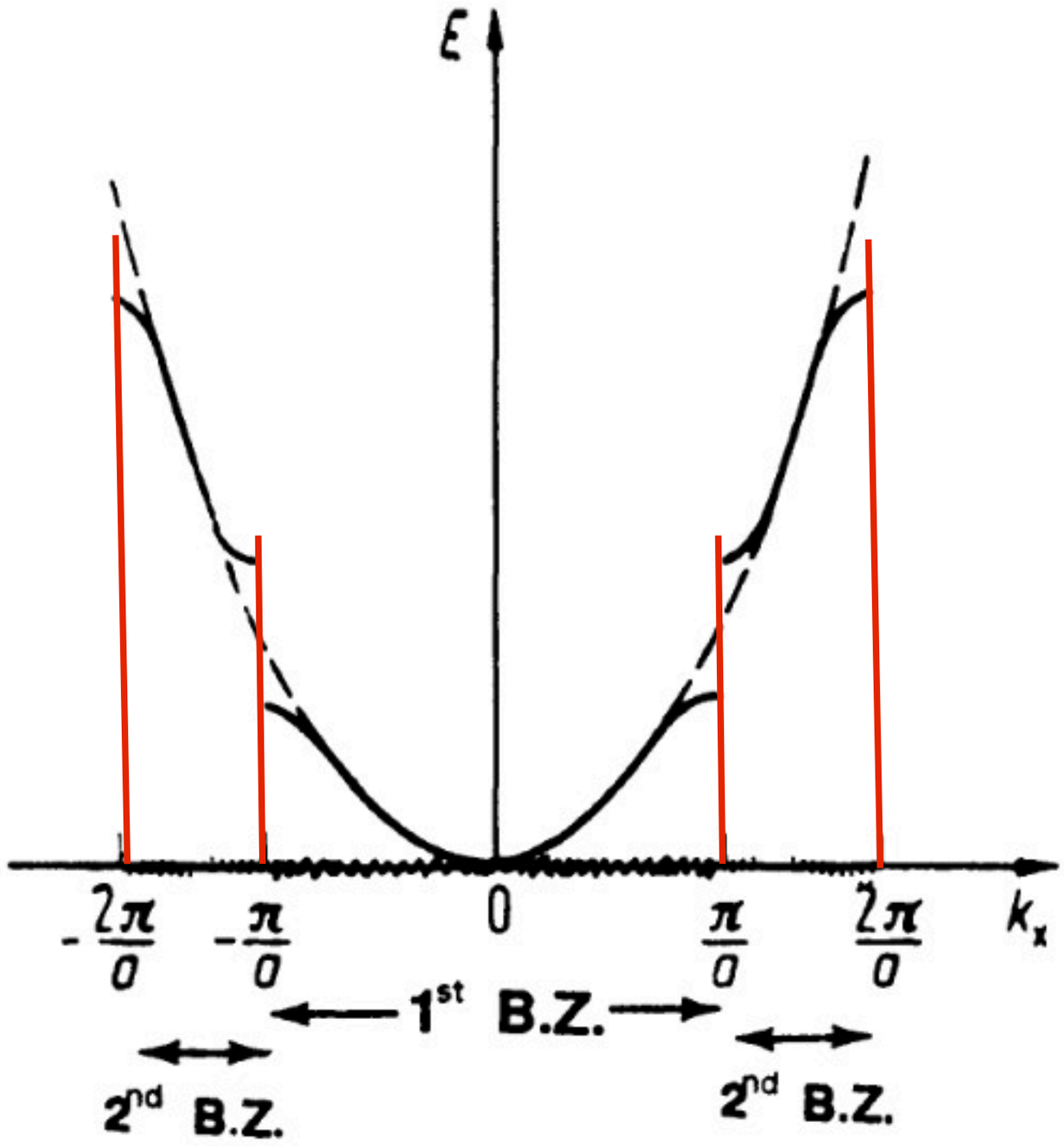
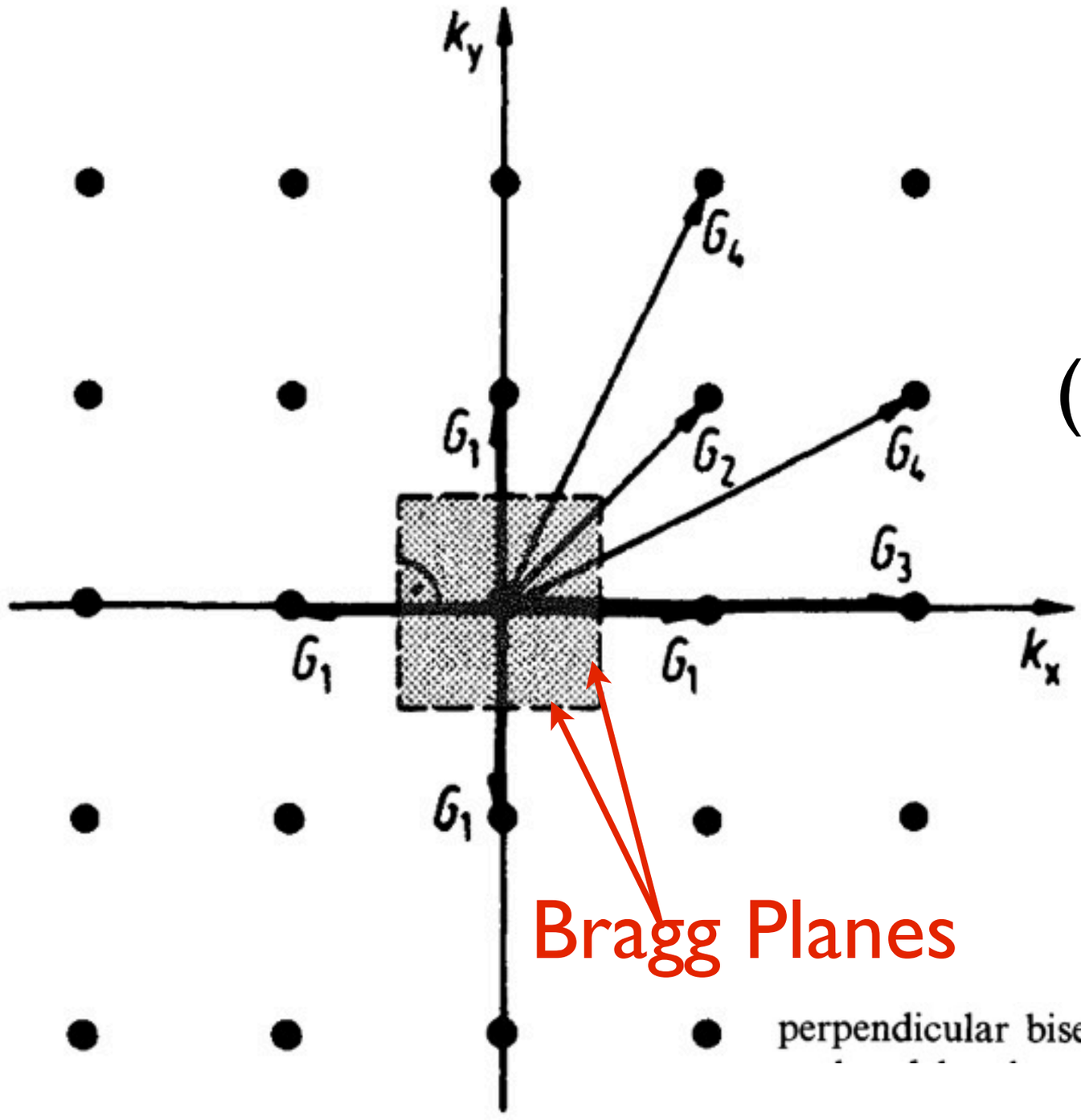
5.2. One- and Two-Dimensional Brillouin Zones



2nd Brillouin zone

1st Brillouin zone

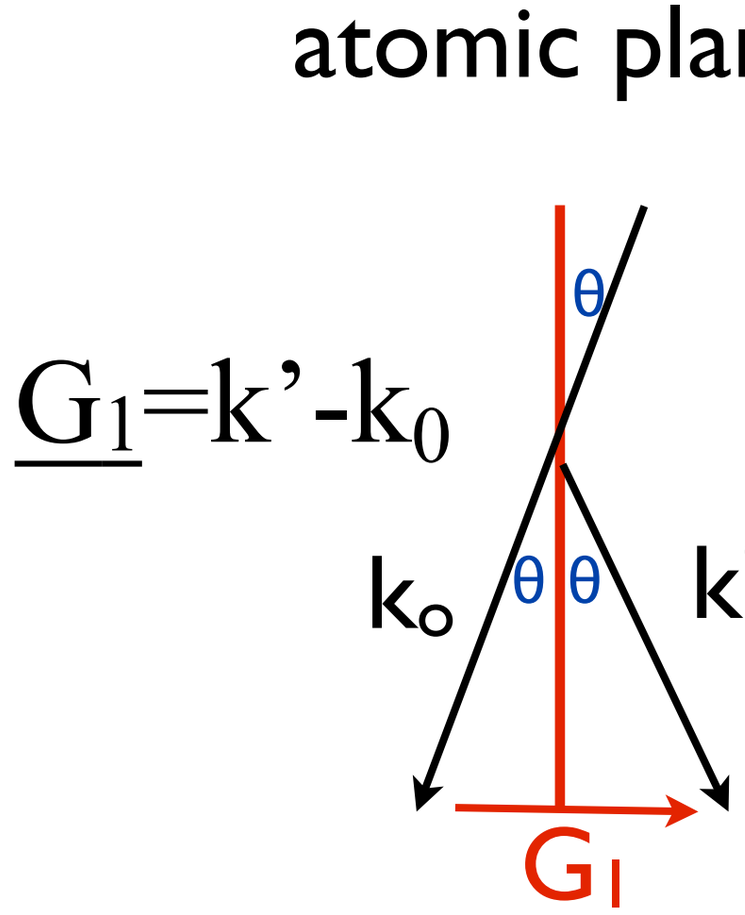
5.2. One- and Two-Dimensional Brillouin Zones



reciprocal space
(momentum space)

Bragg Planes

perpendicular bisectors on the shortest lattice vectors, G_1.



$\underline{G_1}\perp$ 原子平面跡 (plane trace)

原子平面跡是k_0及k'的分角線

$1/2\,|G|=|k_0|\sin\theta_B$, $|k_0|=1/\lambda$

$\lambda=2/|G|\sin\theta_B$ ， 與 $\lambda=2d\sin\theta_B$ 比較

$|G|=1/d$, 且$\underline{G}$ //原子平面之法向量（有建設性干涉的原子平面）

$\perp$原子平面跡

{G}代表晶體可產生“建設性”干涉的平面組,其方向為平行平面之法向量且長度為對應的平面間距

實空間與倒空間

(晶體結構與繞射花樣 (Band Gap)

為何需要另一個空間?

- 倒空間能使我們方便描述及處理晶體繞射的問題
- 事實上,“倒”晶格空間和“實”晶格空間一樣的“真實”
- 我們可以把晶體想成有兩個“晶格”一個“實”晶格,一個“倒”晶格

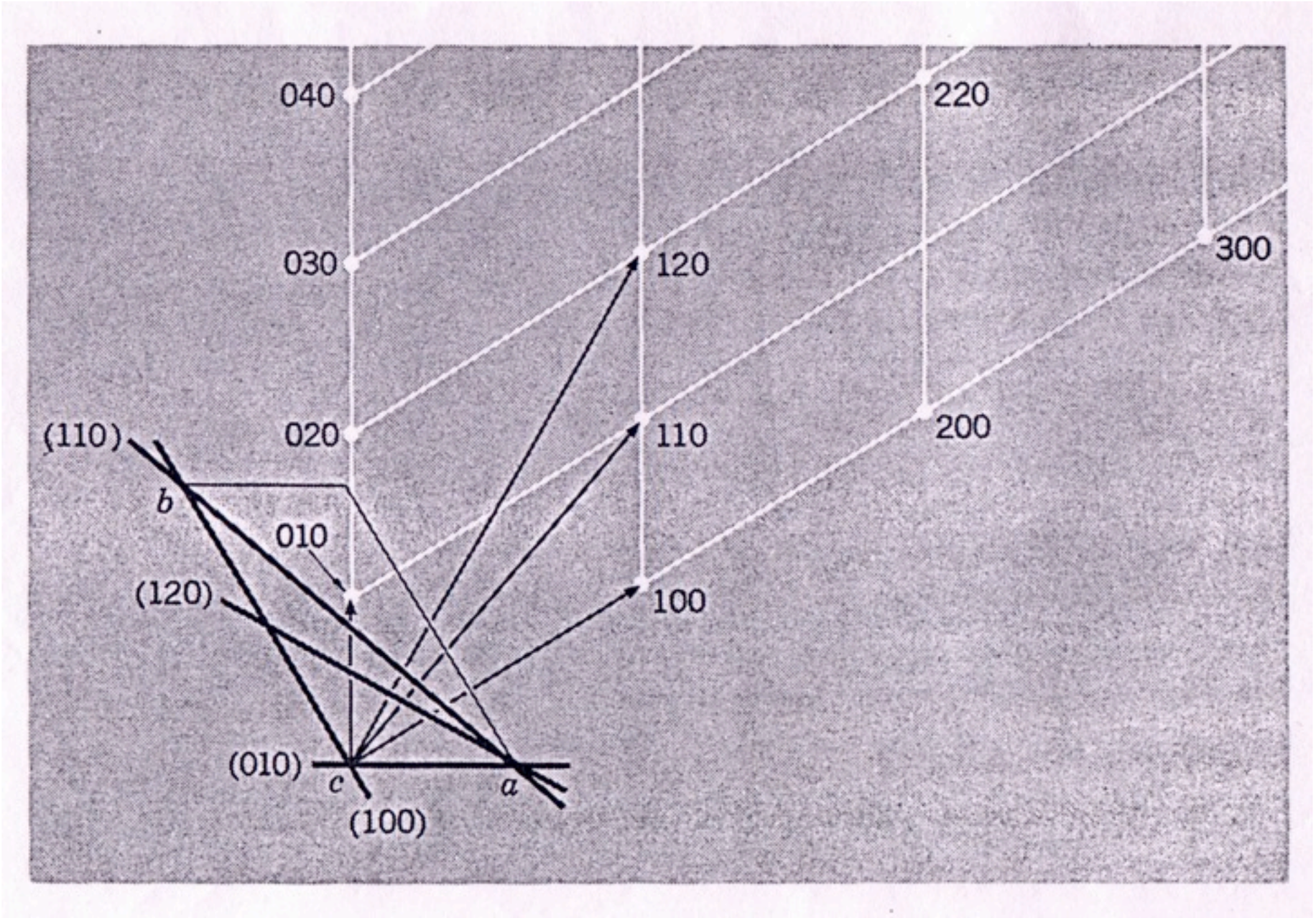
實晶格是晶體本身,倒晶格則是繞射空間的點陣

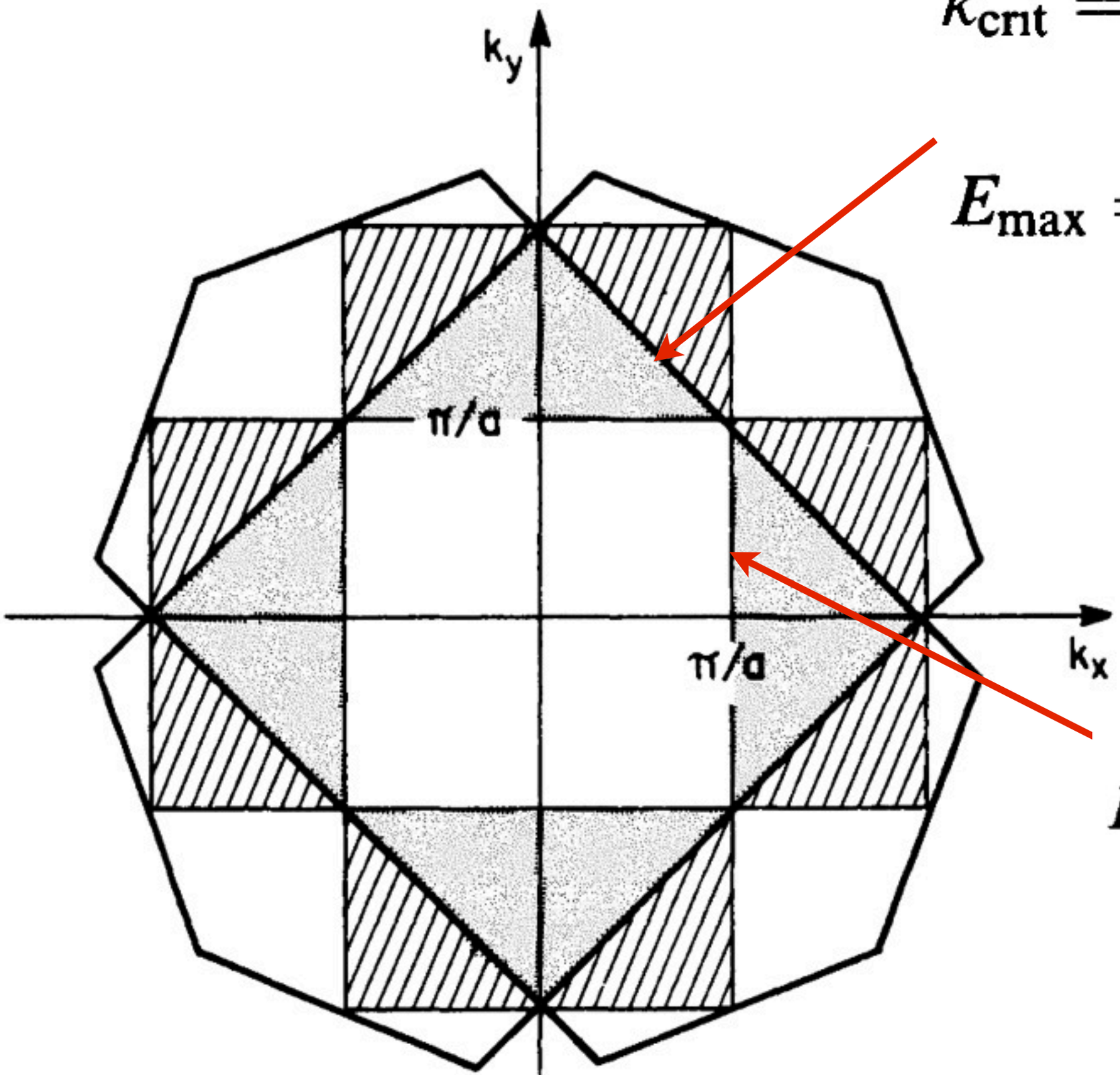
倒空間

1) 倒空間: 與實空間一樣真實

2) 倒空間的一點相對於實空間的一平面

3)倒空間的一點至原點的距離等於平面間距的倒數





$$k_{\text{crit}} = \frac{\pi}{a}\sqrt{2}$$

$$E_{\max} = \frac{\hbar^2}{2m}k_{\text{crit}}^2 = \frac{\pi^2\hbar^2}{a^2 m}$$

$$k_{\text{crit}} = \frac{\pi}{a}$$

$$E_{\max} = \frac{1}{2}\left(\frac{\pi^2\hbar^2}{a^2 m}\right)$$

Bragg relation

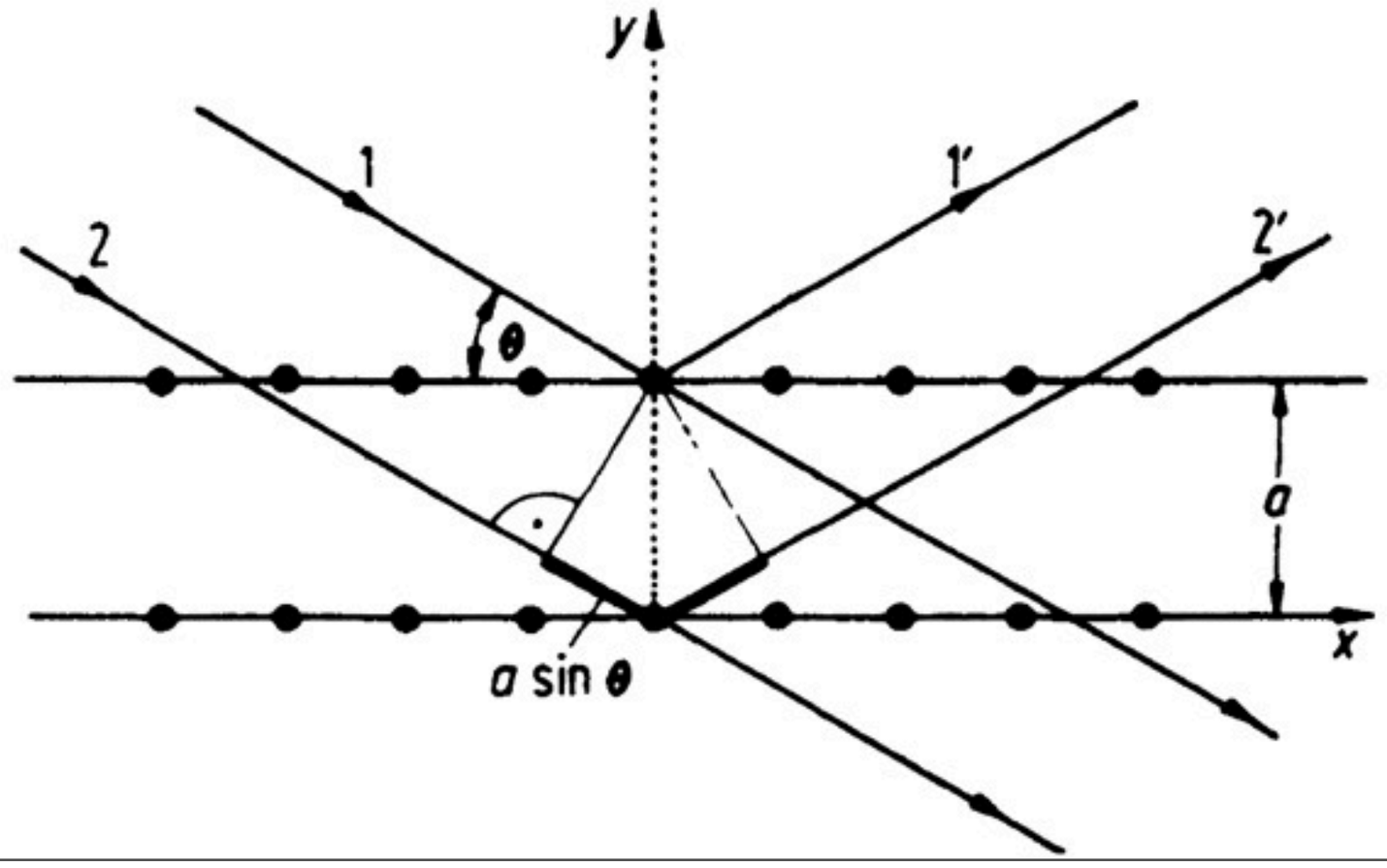
$$2a \sin\theta = n\lambda, \qquad n = 1, 2, 3, \ldots$$

$$2a \sin\theta = n\frac{2\pi}{k}$$

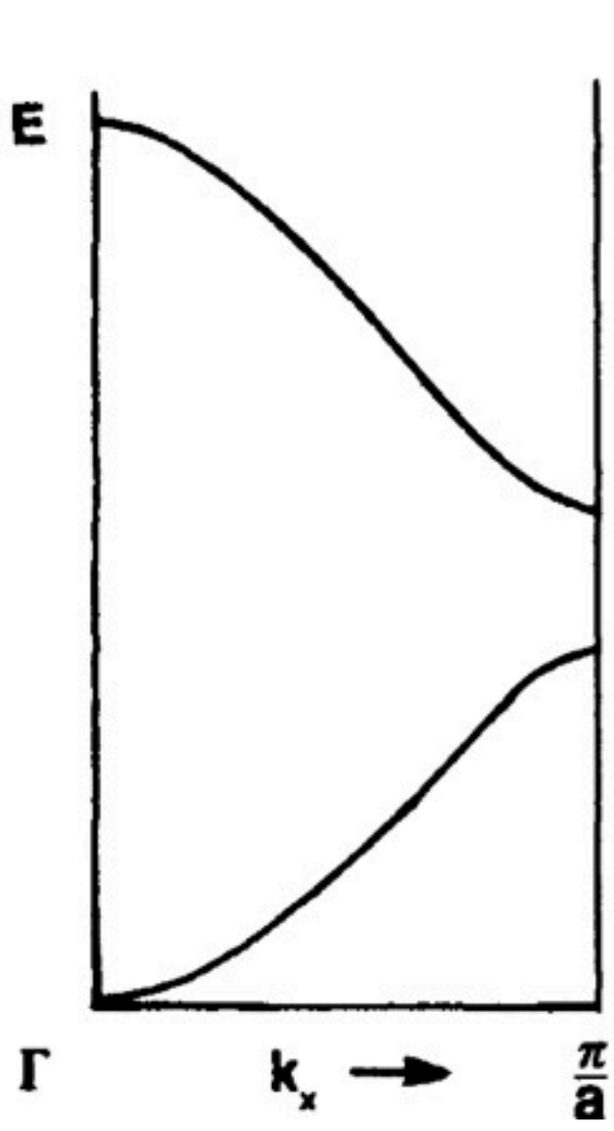
$$k_{\text{crit}} = n\frac{\pi}{a \sin\theta}$$

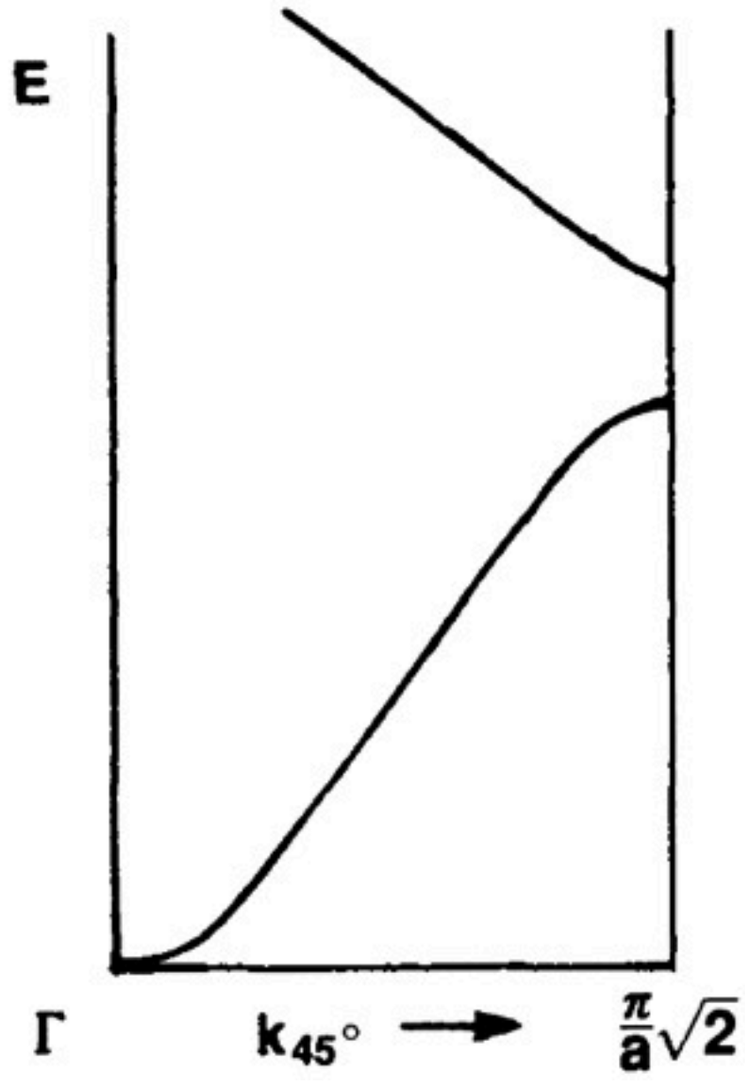
(a) $\theta = 0°$ $\quad k_{\text{crit}} = \frac{\pi}{a}$

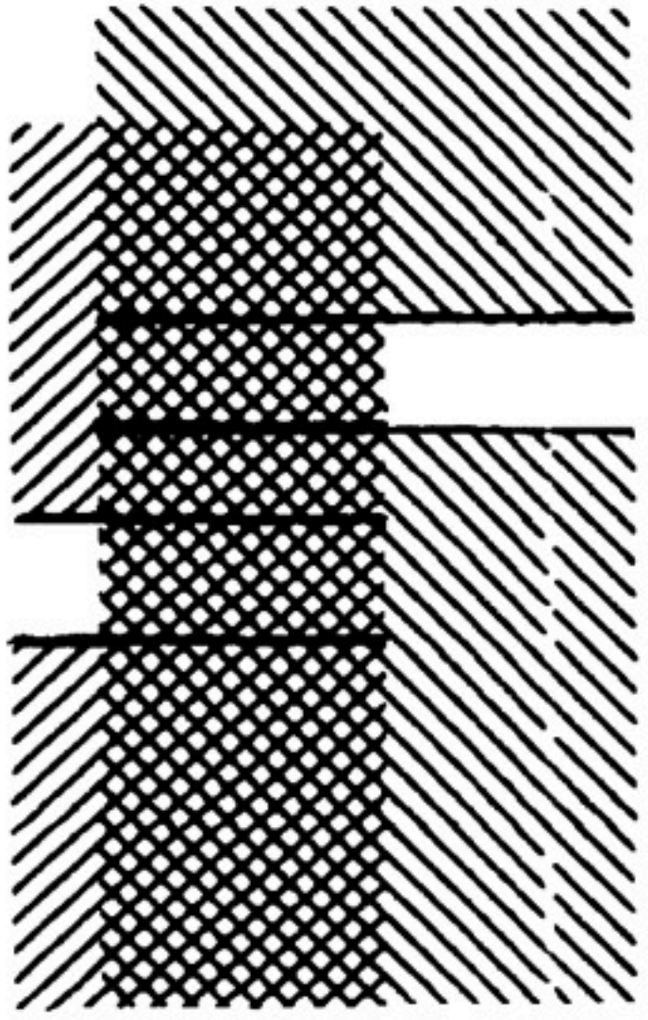
(b) $\theta = 45°$ $\quad k_{\text{crit}} = \frac{\pi}{a}\sqrt{2}$



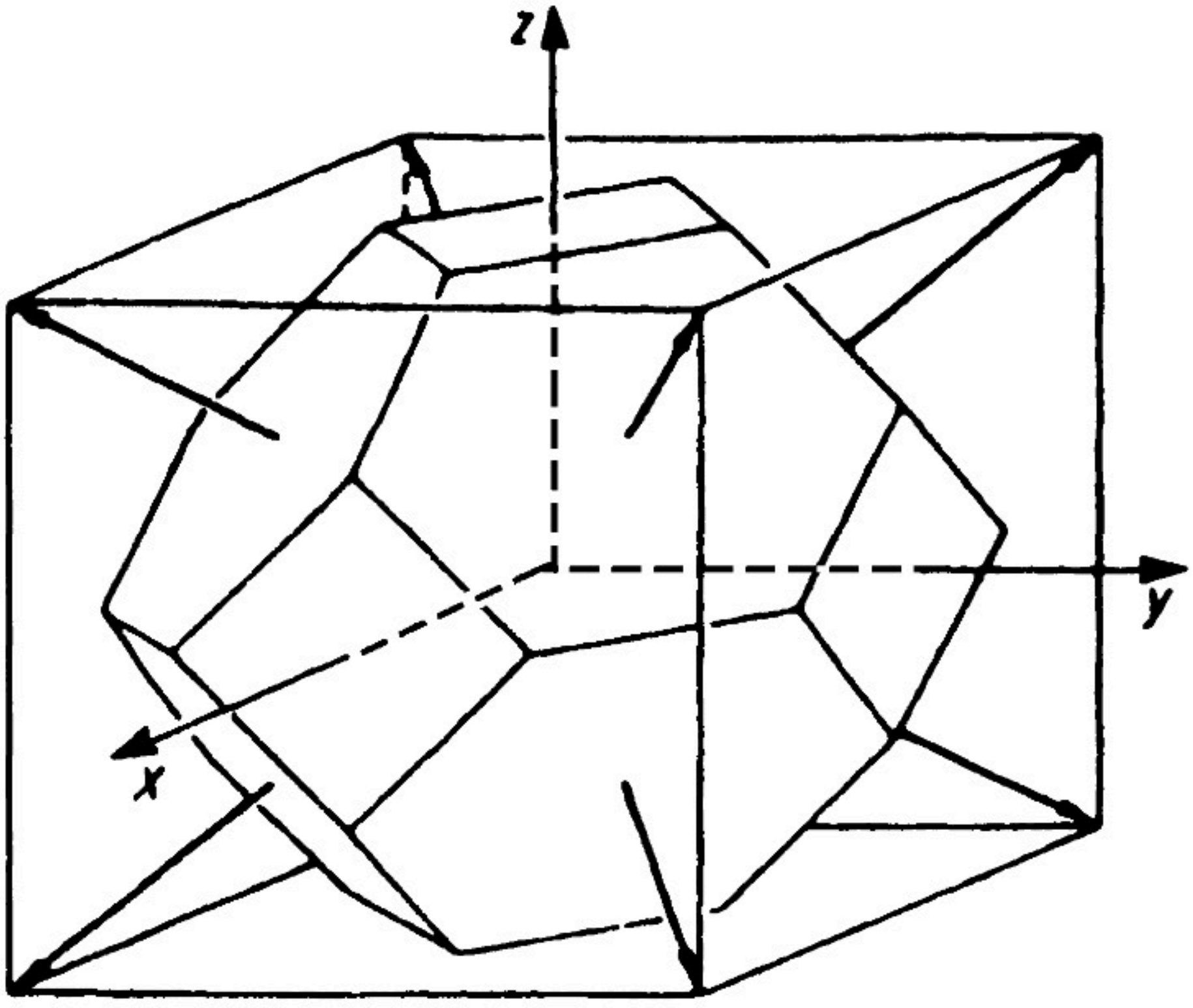
Overlapping of allowed energy bands.





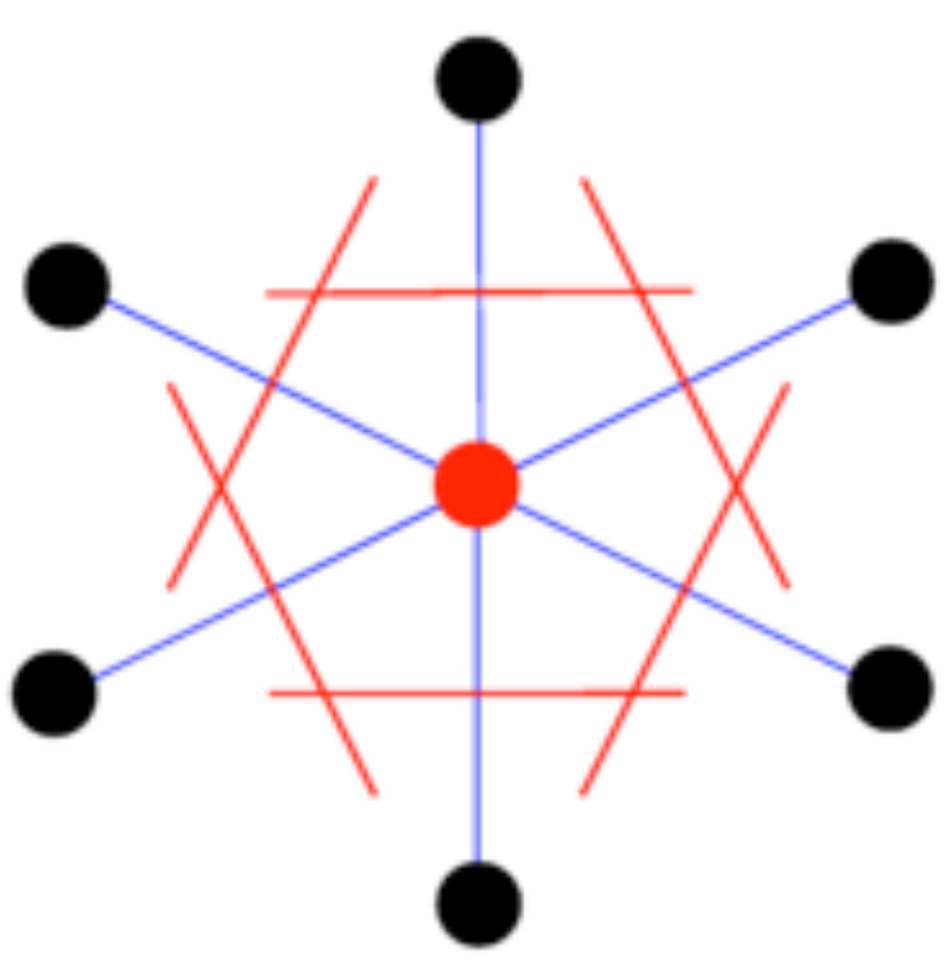


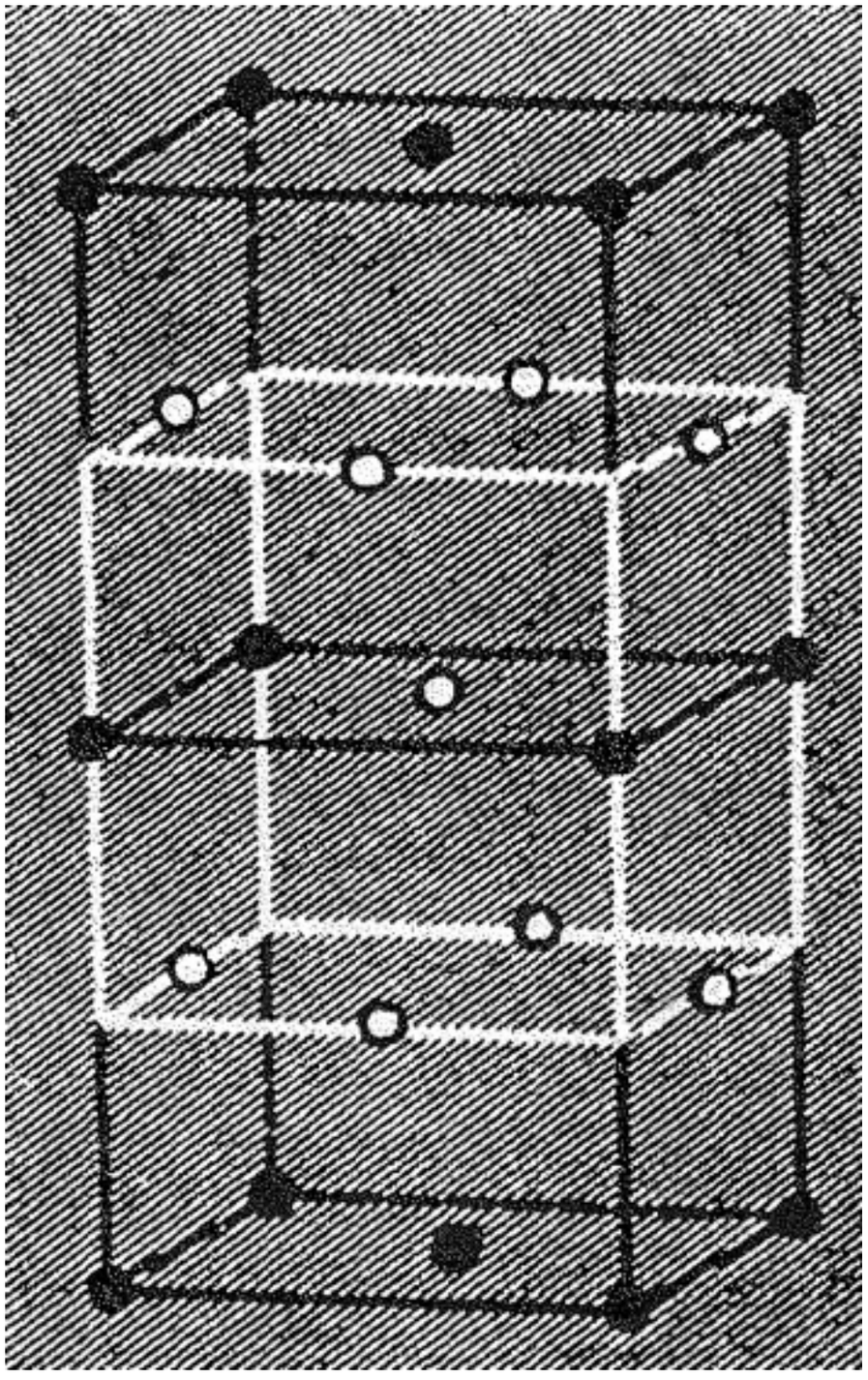
*5.3. Three-Dimensional Brillouin Zones



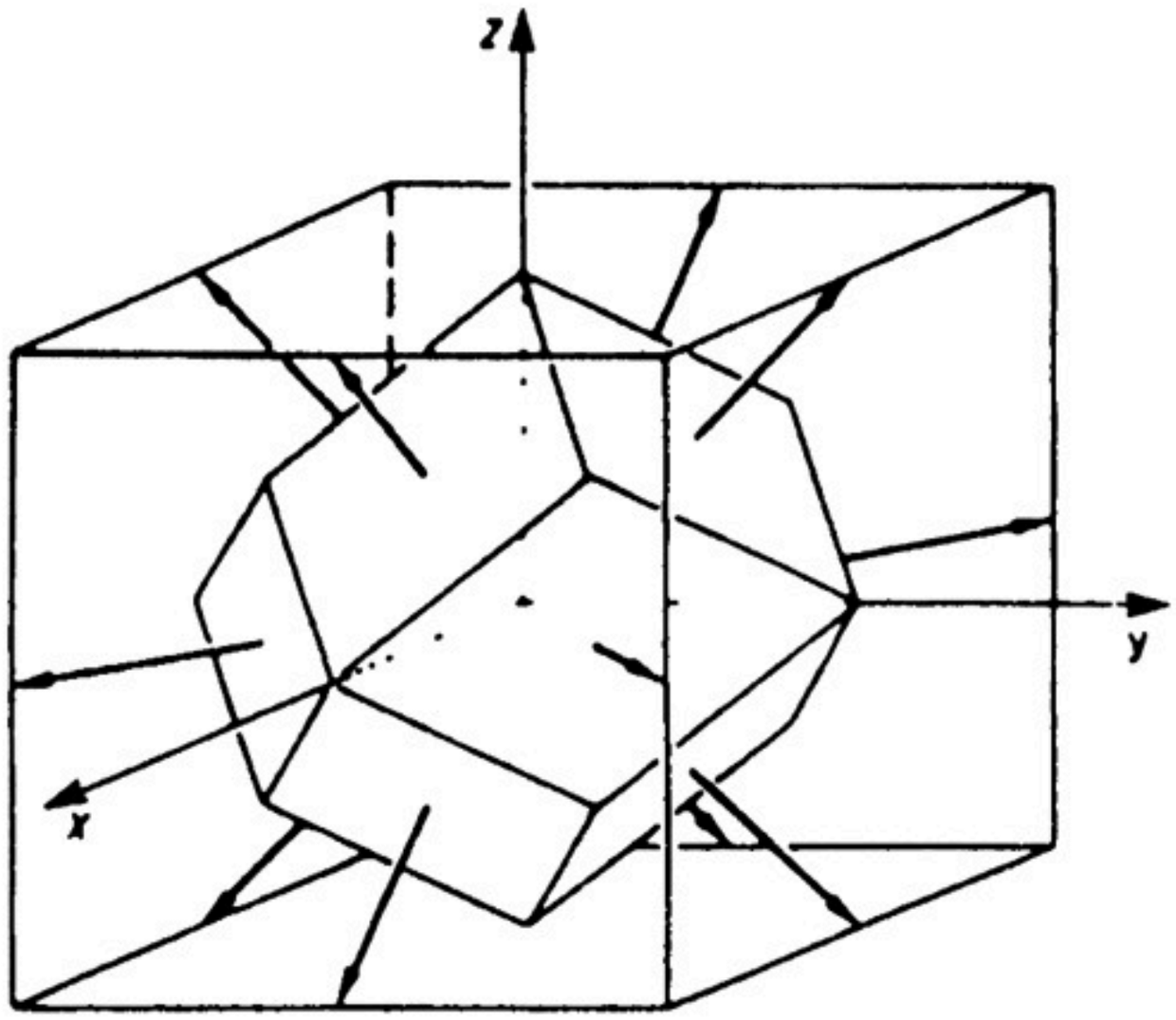
*5.4. Wigner–Seitz Cells

The Wigner–Seitz cell is a special type of primitive unit cell that shows the cubic symmetry of the cubic cells. For its construction, one bisects the vectors from a given atom to its nearest neighbors and places a plane perpendicular to these vectors at the bisecting points.





Conventional unit cell of the fcc structure



Wigner–Seitz cell for the fcc structure

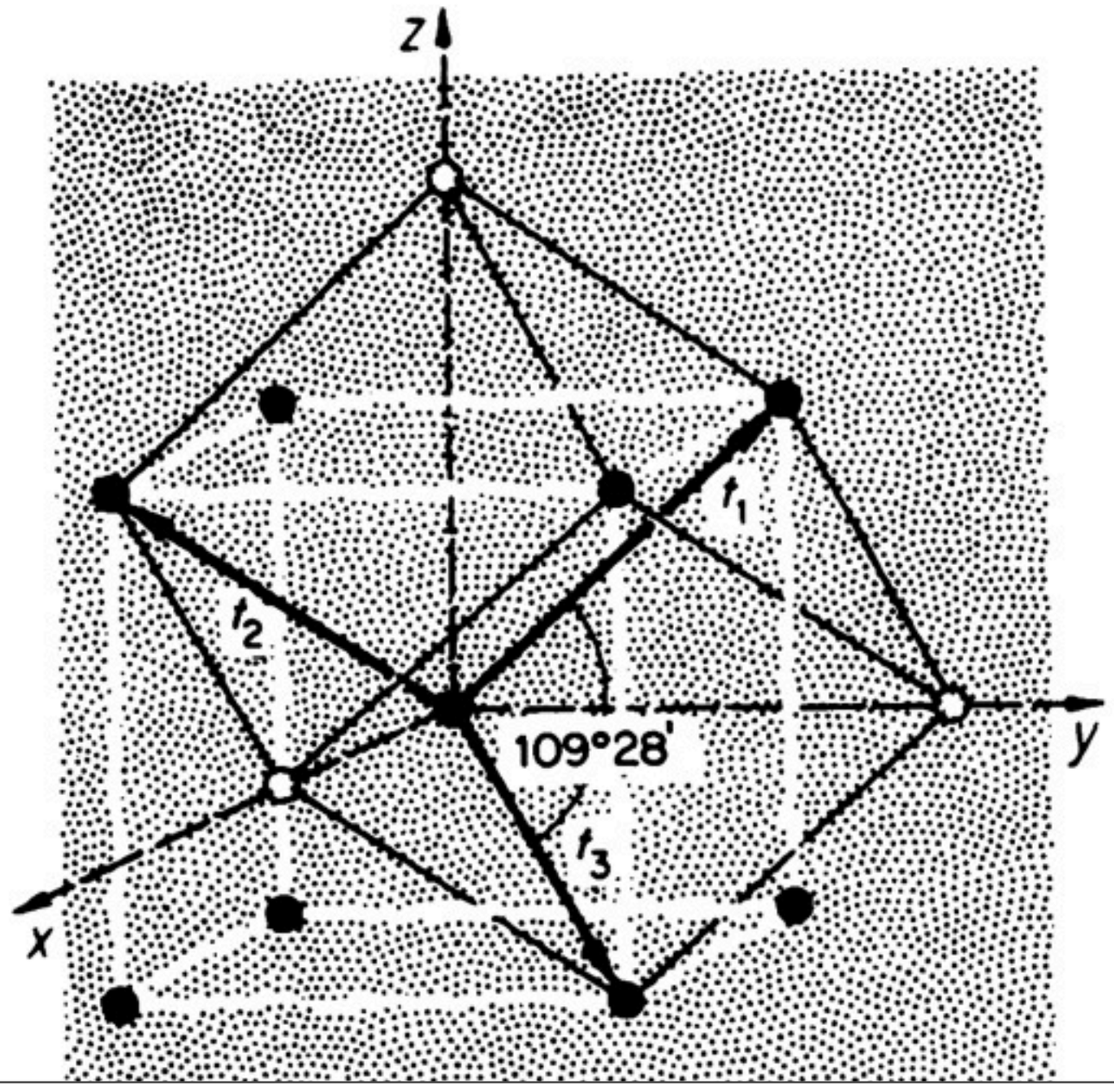
5.5. Translation Vectors and the Reciprocal Lattice

t1, t2, and t3 are basis vector of a primitive unit cell.

By combination of these "primitive vectors" a translation vector,

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

can be defined.



the fundamental vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ of the reciprocal lattice in terms of real lattice vectors.

$$\mathbf{b}_1 = \frac{\mathbf{t}_2 \times \mathbf{t}_3}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}.$$

$$\mathbf{b}_2 = \frac{\mathbf{t}_3 \times \mathbf{t}_1}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3},$$

$$\mathbf{b}_3 = \frac{\mathbf{t}_1 \times \mathbf{t}_2}{\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3}.$$

For BCC structure

$$\mathbf{t}_1 = \frac{a}{2}(\bar{1}11)$$

$$\mathbf{t}_2 = \frac{a}{2}(1\bar{1}1),$$

$$\mathbf{t}_3 = \frac{a}{2}(11\bar{1}).$$

Kronecker-Delta symbol,

$$\mathbf{b}_n \cdot \mathbf{t}_m = \delta_{nm},$$

$$\mathbf{t}_2 \times \mathbf{t}_3 = \frac{a^2}{4}\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{l} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \frac{a^2}{4}(\mathbf{i}+\mathbf{j}+\mathbf{l}+\mathbf{l}-\mathbf{i}+\mathbf{j}) = \frac{a^2}{4}(2\mathbf{j}+2\mathbf{l})$$

$$= \frac{a^2}{2}(\mathbf{j}+\mathbf{l}) \qquad (\text{面心})$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 \times \mathbf{t}_3 = \frac{a^3}{4}(-\mathbf{i}+\mathbf{j}+\mathbf{l}) \cdot (0+\mathbf{j}+\mathbf{l}) = \frac{a^3}{4}(0+1+1) = \frac{a^3}{2}.$$

$$\mathbf{b}_1 = \frac{\frac{a^2}{2}(\mathbf{j}+\mathbf{l})}{\frac{a^3}{2}} = \frac{1}{a}(\mathbf{j}+\mathbf{l}),$$

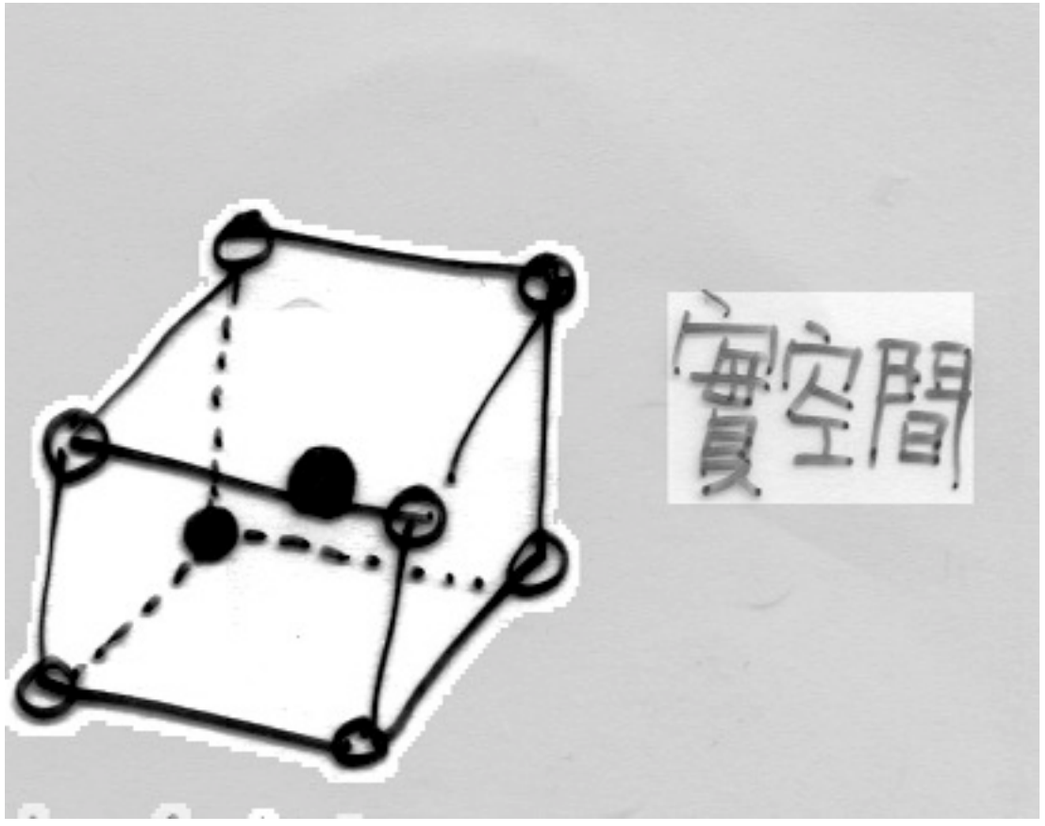
$$\mathbf{b}_2 = \frac{1}{a}(101),$$

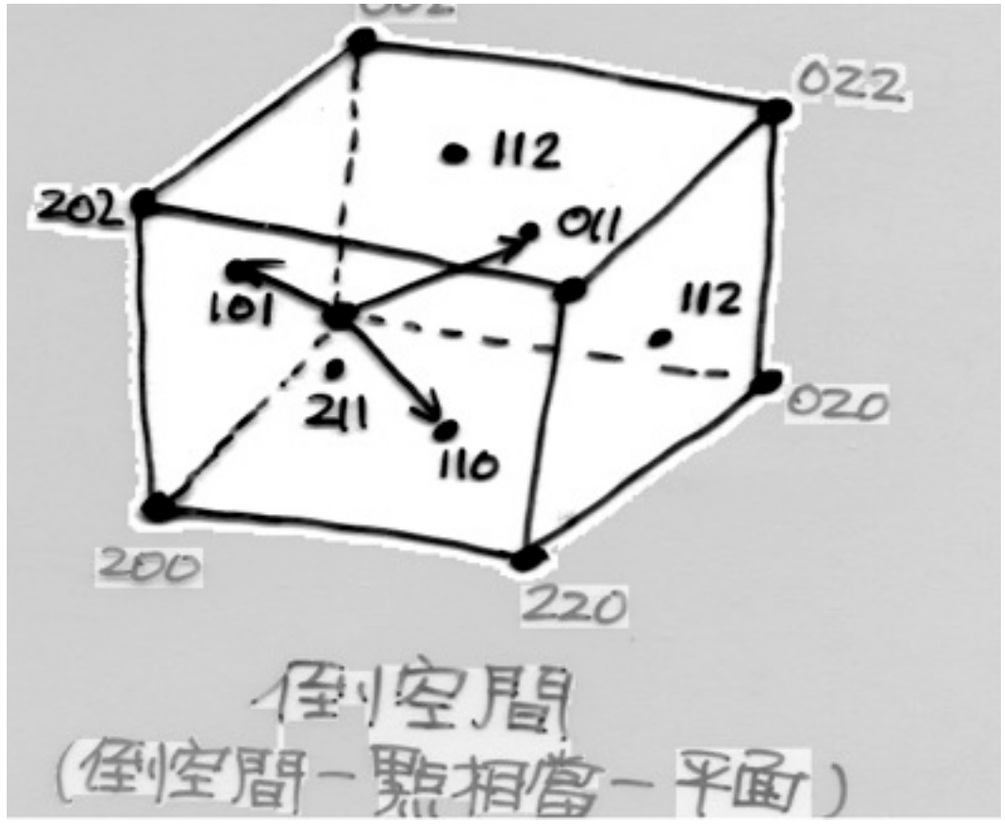
~面心立方向量

$$\mathbf{b}_1 = \frac{1}{a}(011).$$

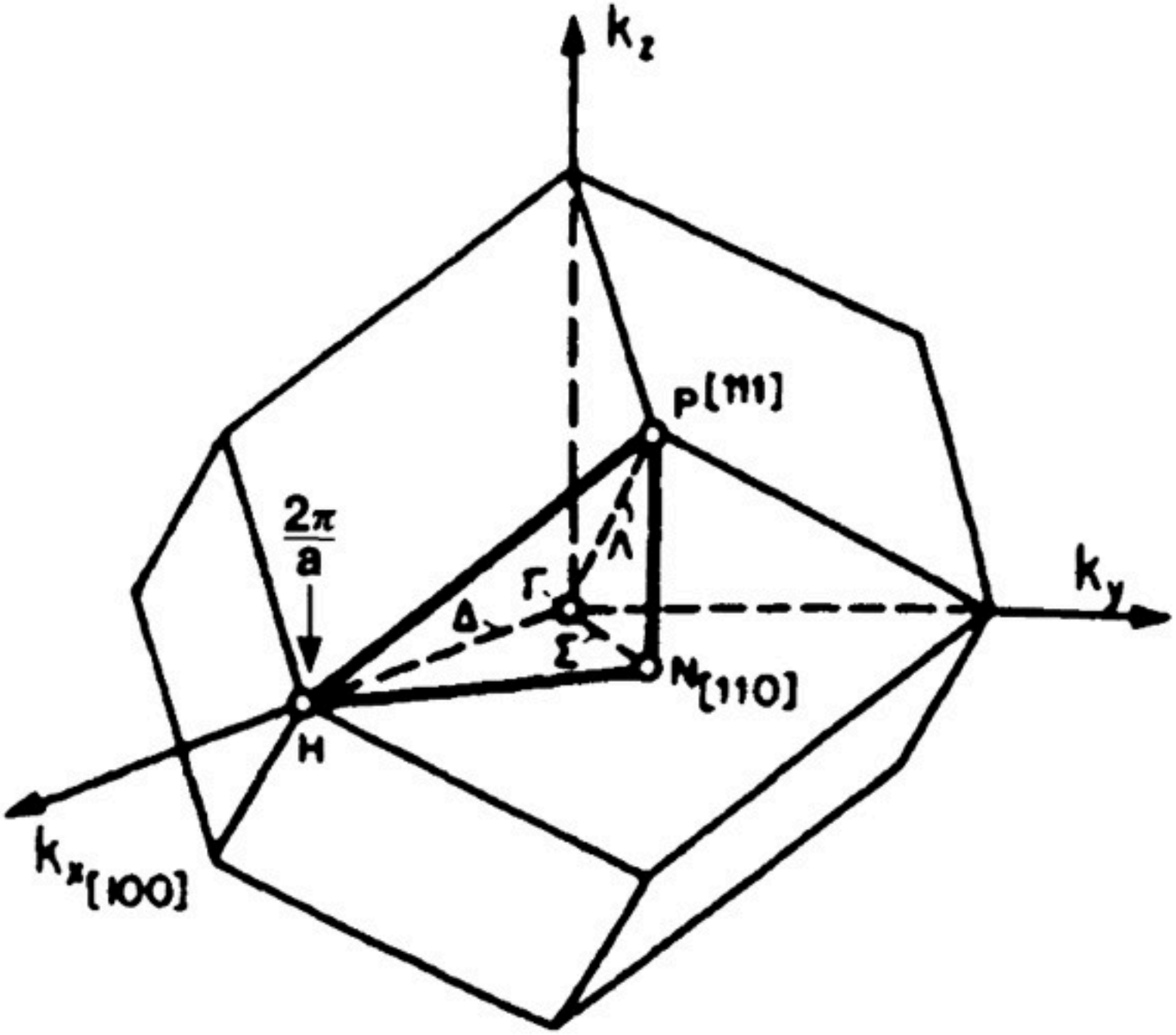
$$\mathbf{b}_3 = \frac{1}{a}(110).$$

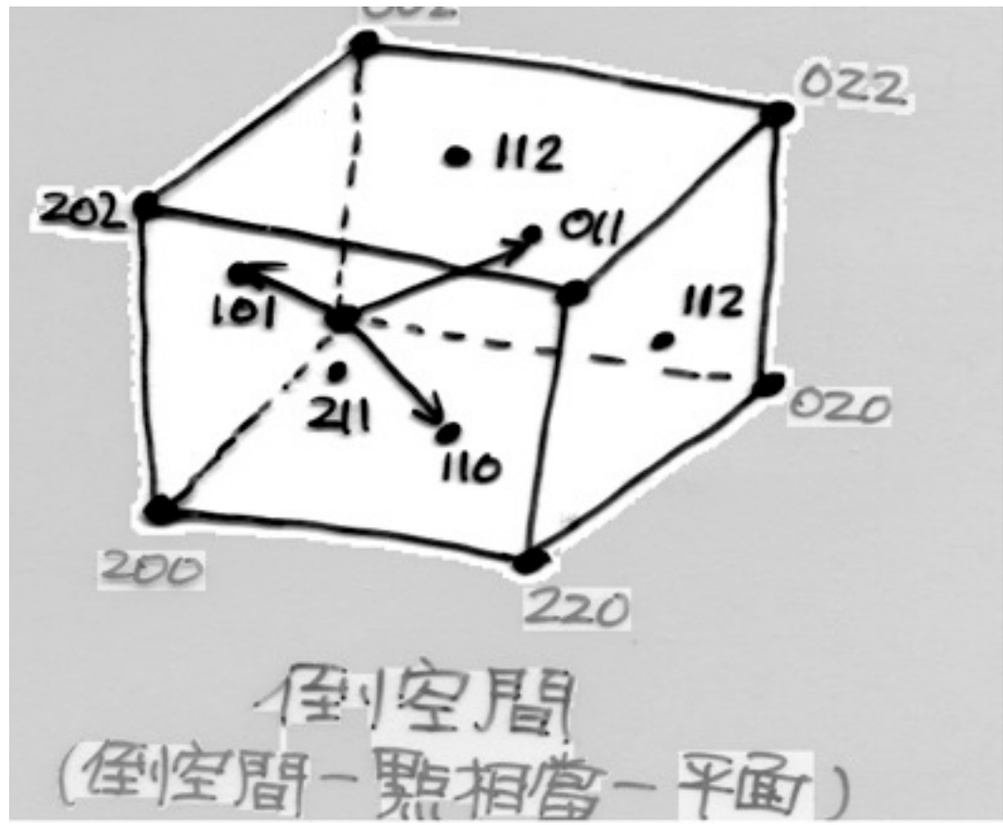
the reciprocal lattice points of the fcc structure and the real lattice points of the bcc structure are identical.





First Brillouin zone of the bcc crystal structure.





5.6. Free Electron Bands

because of the $E(\mathbf{k})$ periodicity

the energy $E_{\mathbf{k}'}$ for $\mathbf{k}'$ outside the first zone is identical to the energy $E_{\mathbf{k}}$ within the first zone if a suitable translation vector $\mathbf{G}$ can be found so that a wave vector $\mathbf{k}'$ becomes

$$\mathbf{k}' = \mathbf{k} + \mathbf{G}$$

$$E_{\mathbf{k}'} = \frac{\hbar^2}{2m}(\mathbf{k} + \mathbf{G})^2$$

Energy bands of the free electrons for the bcc structure.

$\Gamma - H$ direction

vector $\mathbf{k}_{\Gamma H} \equiv \mathbf{k}_x$ between 0 and $2\pi/a$

$$E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}x\mathbf{i} + \mathbf{G}\right)^2$$

x may take values between 0 and 1

let $\mathbf{G}$ be $0 \longrightarrow (000)$

$$E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 (x\mathbf{i})^2 \equiv Cx^2 \qquad C = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = \frac{2\hbar^2\pi^2}{ma^2}$$

$$\mathbf{G} = 2\pi(h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3)$$

let $h_1 = 0$, $h_2 = -1$, and $h_3 = 0$.

$$\mathbf{G} = -\frac{2\pi}{a}(\mathbf{i} + \mathbf{l})$$

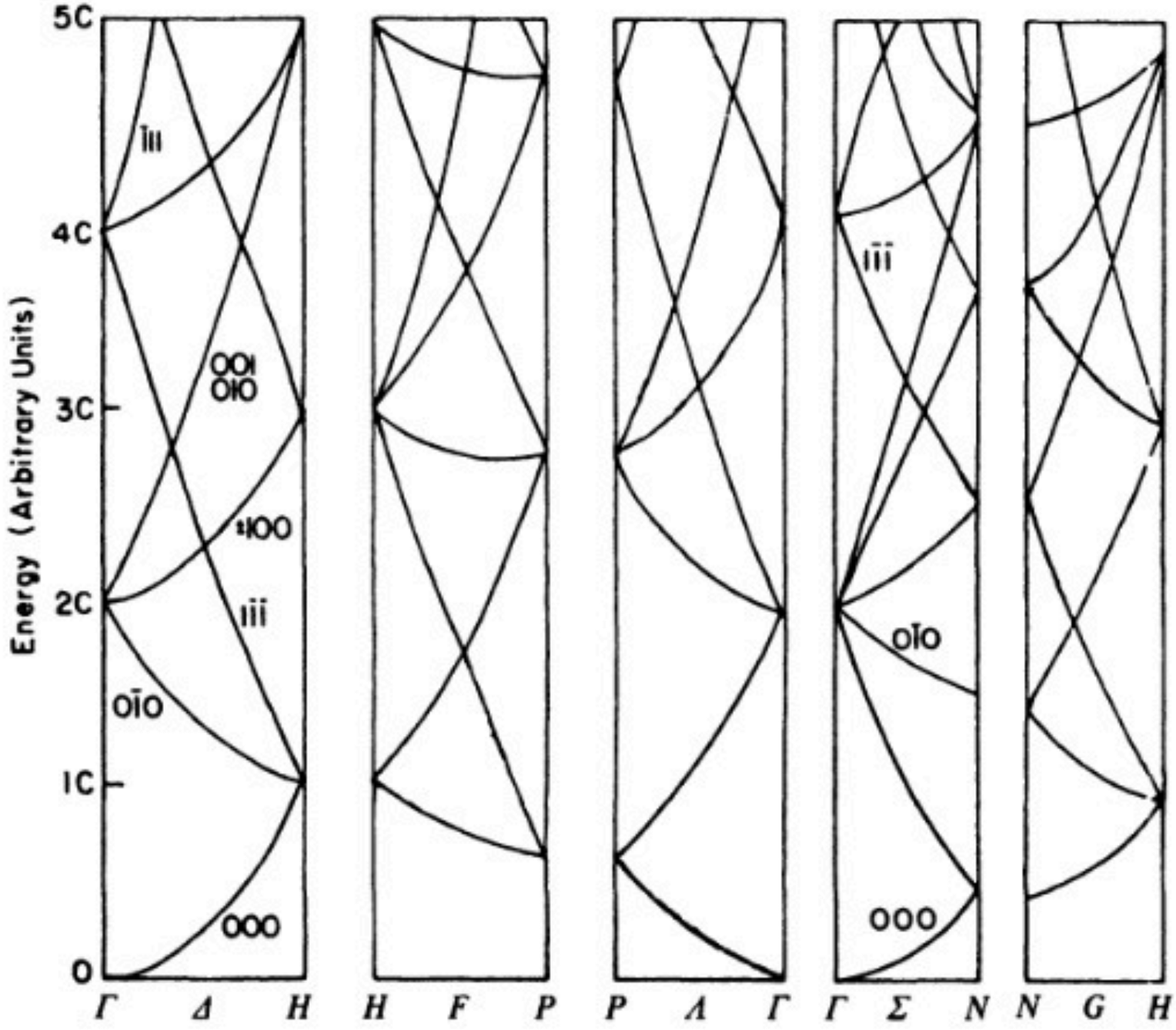
$$E = \frac{\hbar^2}{2m}\left[\frac{2\pi x}{a}\mathbf{i} - \frac{2\pi}{a}(\mathbf{i} + \mathbf{l})\right]^2 = C[\mathbf{i}(x-1) - \mathbf{l}]^2$$

$$= C[(x-1)^2 + 1] = C(x^2 - 2x + 2)$$

$$x = 0 \rightarrow E = 2C$$

$$x = 1 \rightarrow E = 1C$$

Energy bands of the free electrons for the bcc structure.



$$C = \hbar^2 2\pi^2 / ma^2$$

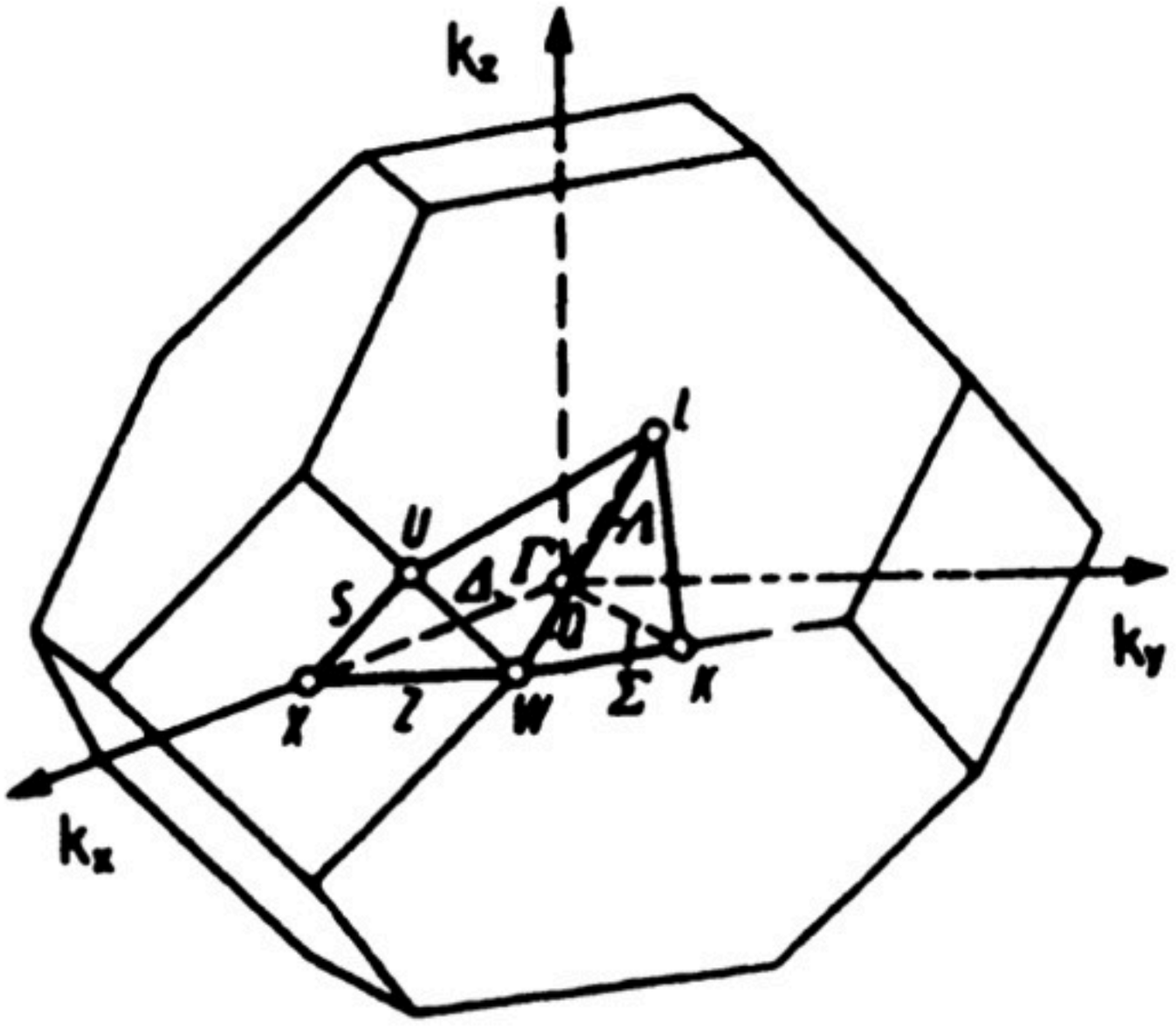
[100] [111] [110]

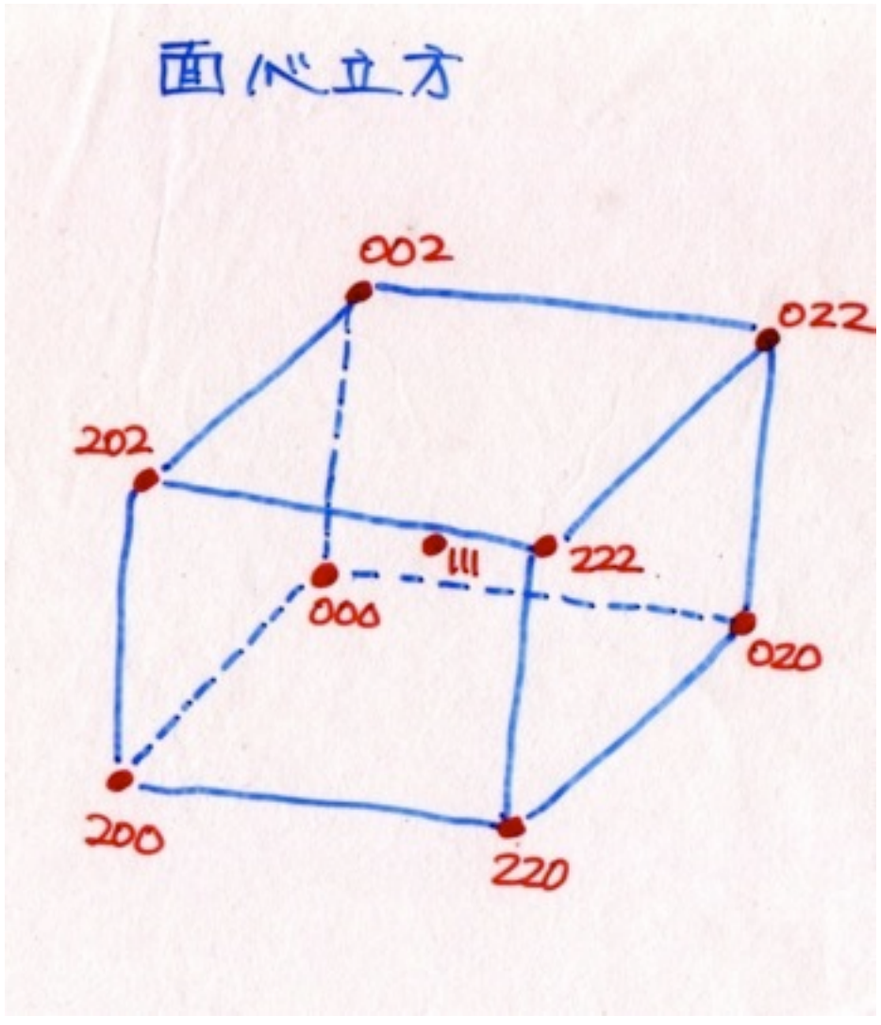
all bands

$$E_{\mathbf{k}'} = \frac{\hbar^2}{2m}(\mathbf{k} + \mathbf{G})^2$$

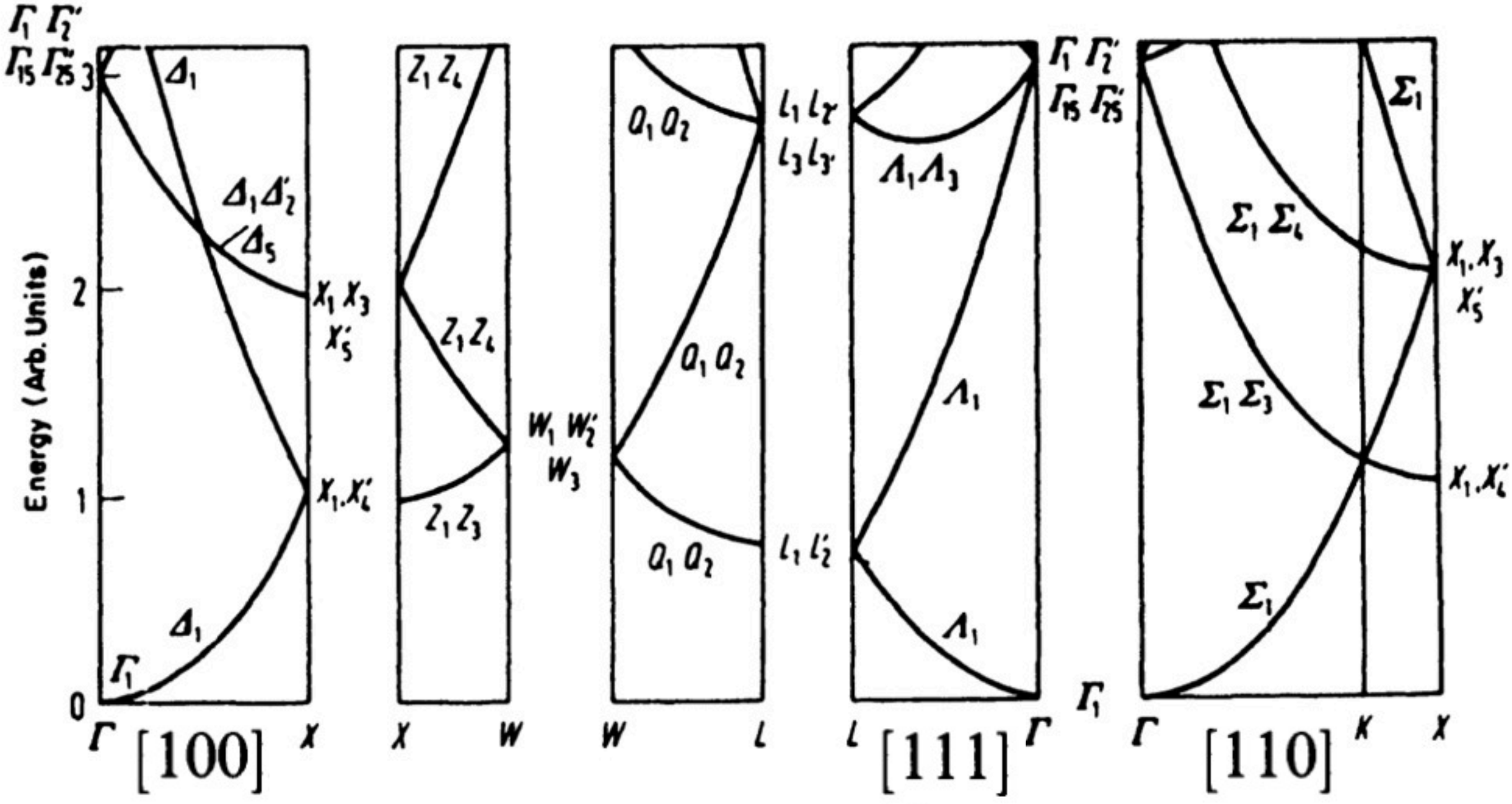
can be calculated by variation of the h values and $\mathbf{k}$-directions

The free electron bands are very useful for the following reason: by comparing them with the band structures of actual materials, an assessment is possible if and to what degree the electrons in that material can be considered to be free.





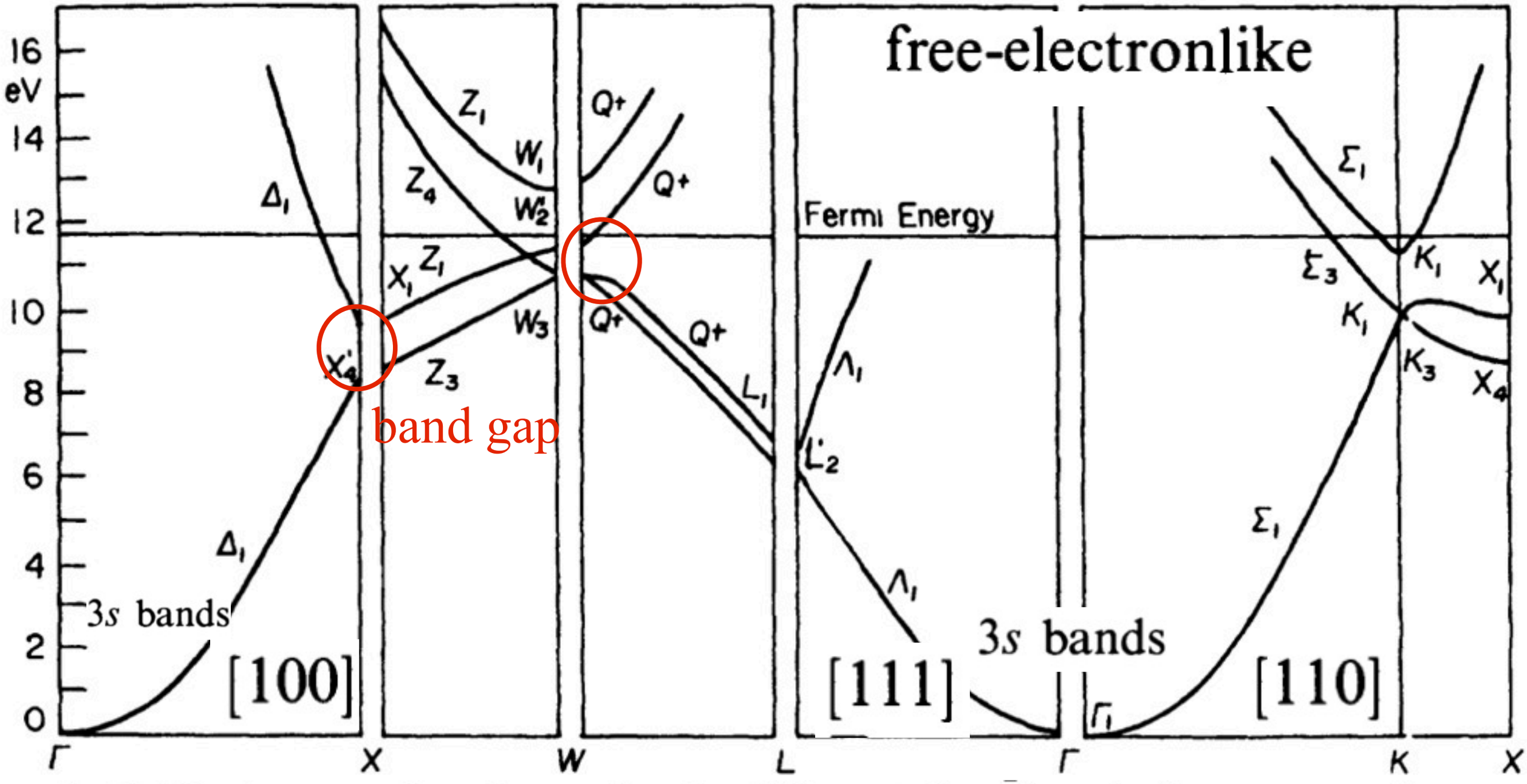
First Brillouin zone of the fcc structure



Free electron bands of the fcc structure

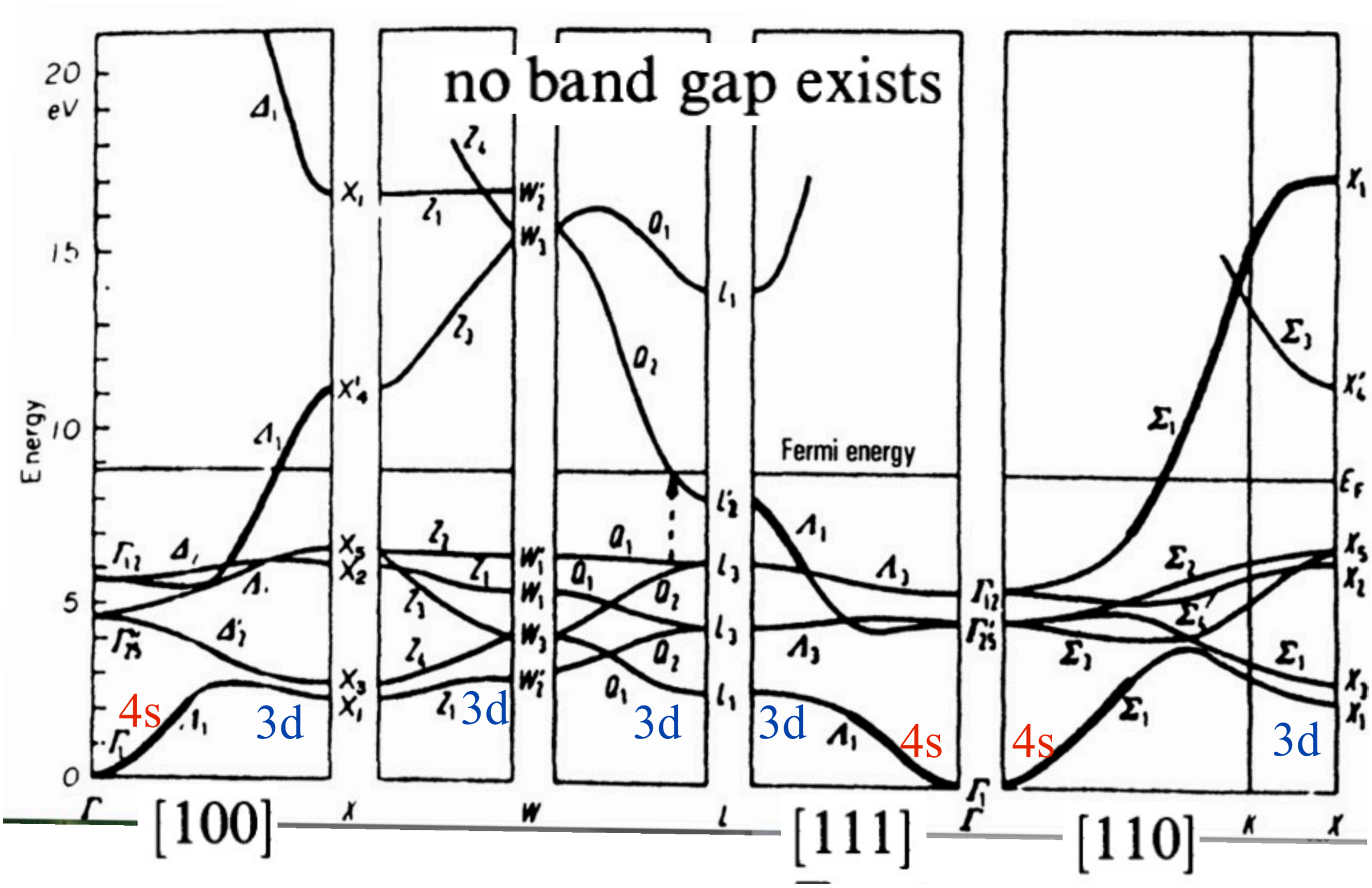
5.7. Band Structures for Some Metals and Semiconductors

Energy bands for aluminum.

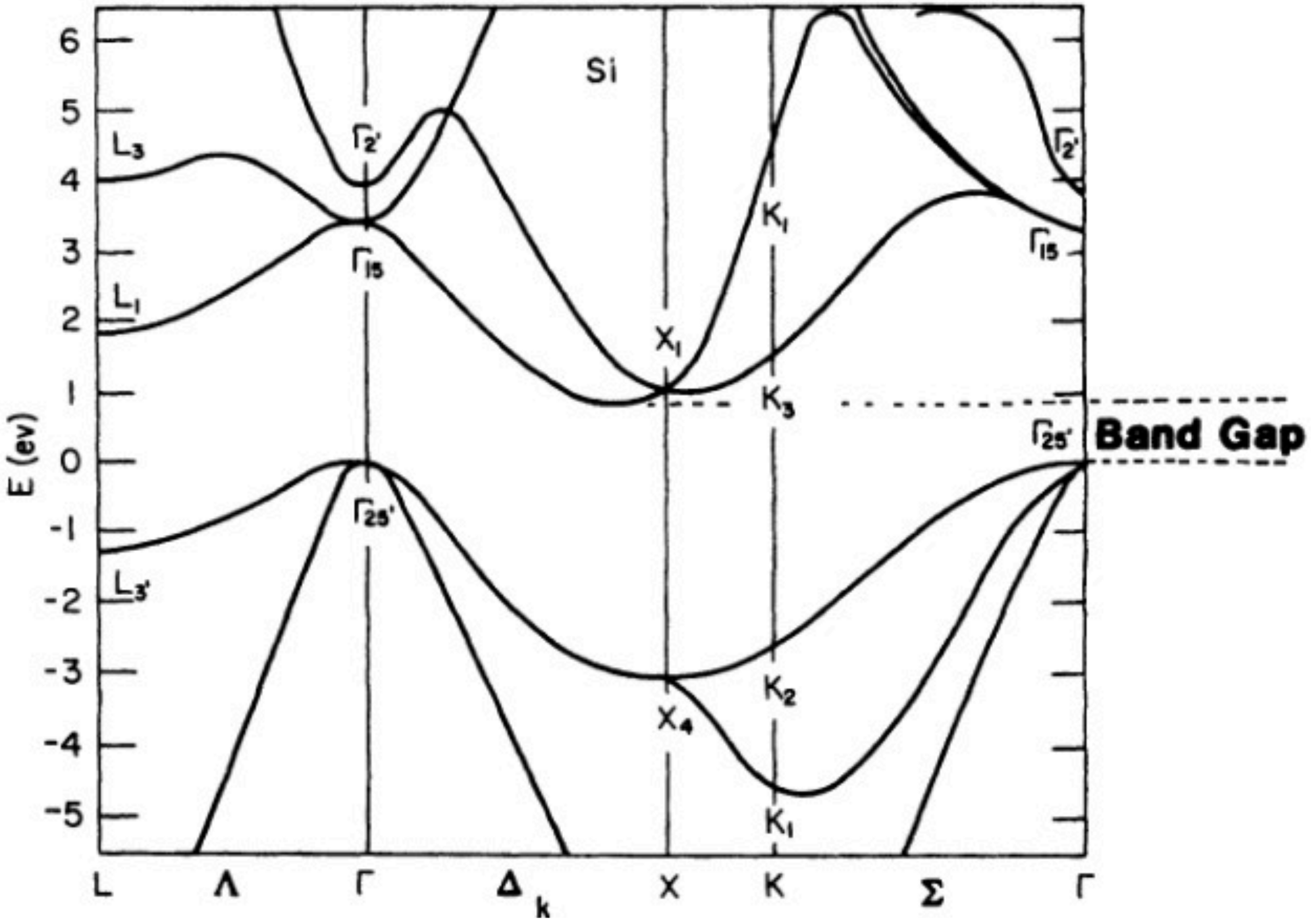


individual energy bands overlap in different directions in *k*-space, so that as a whole no band gap exists.

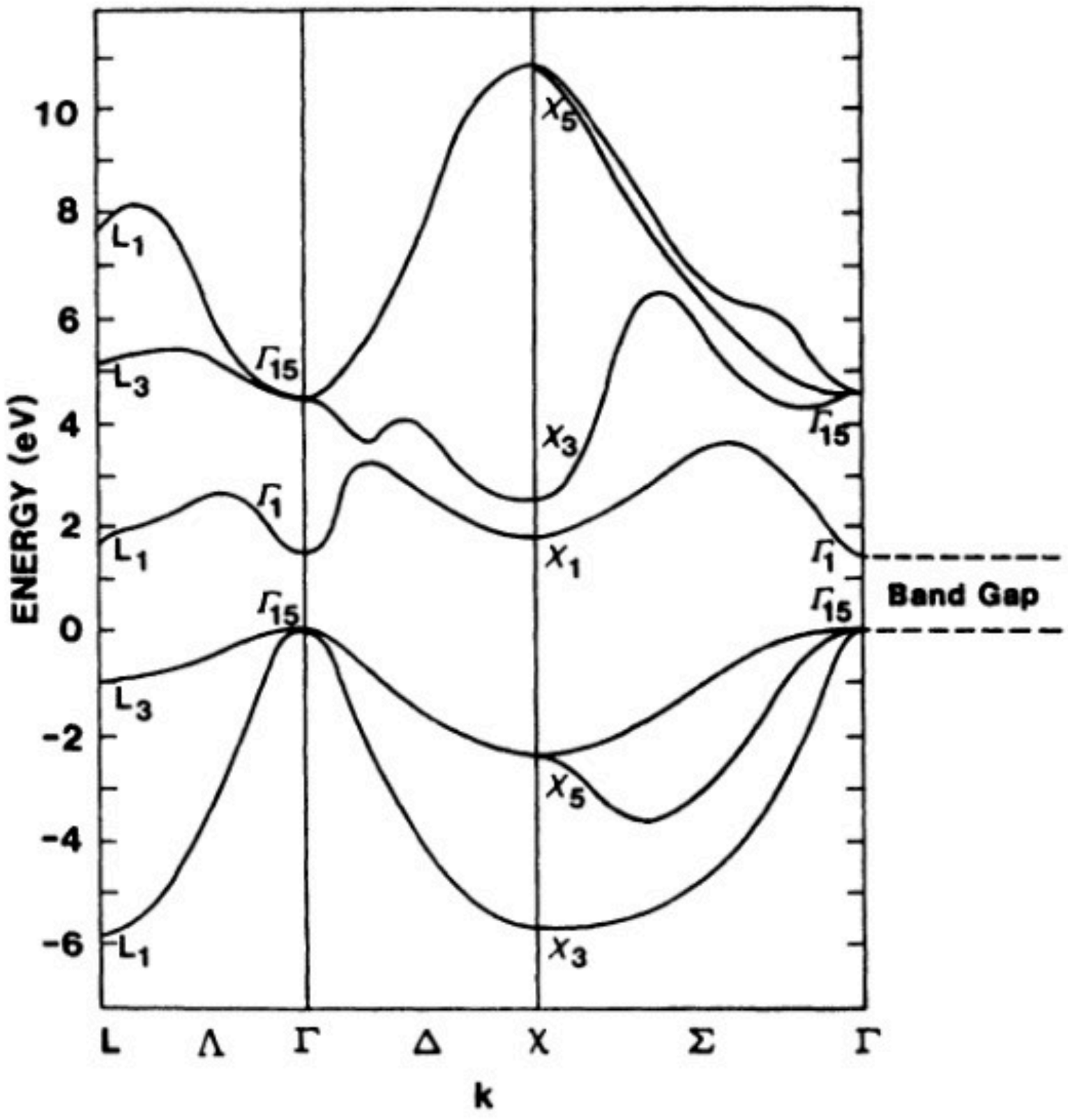
band structure for **copper**



Calculated energy band structure of silicon



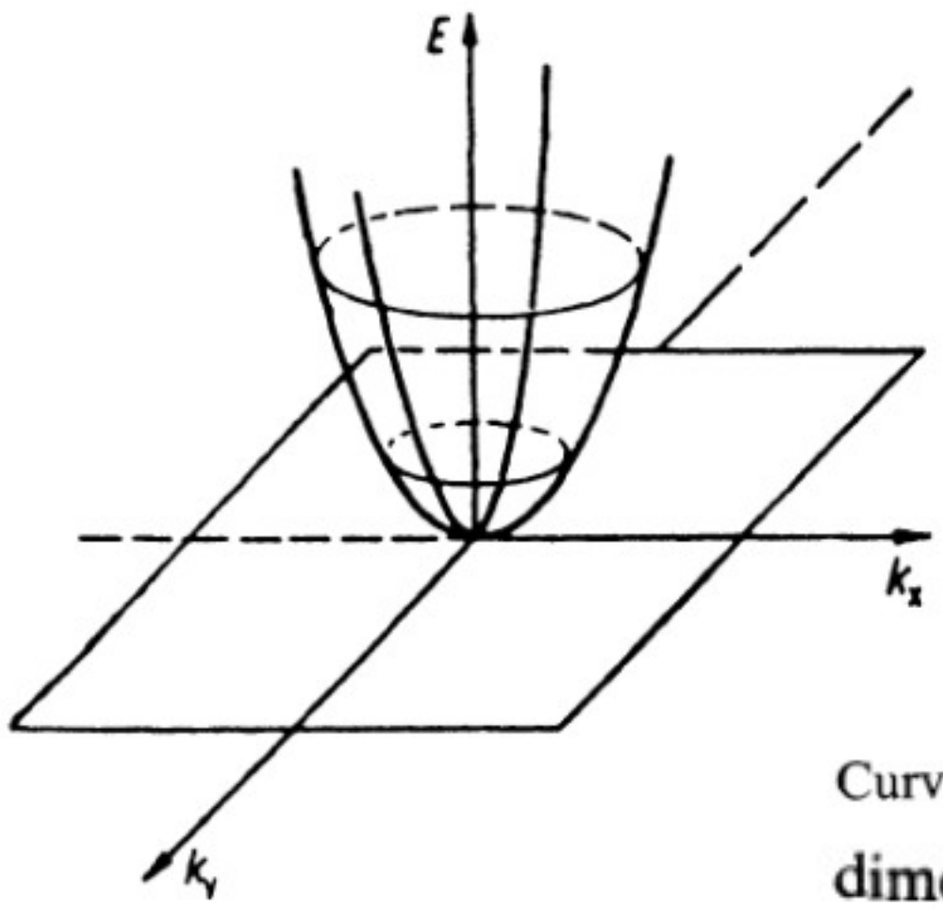
Calculated energy band structure of GaAs.

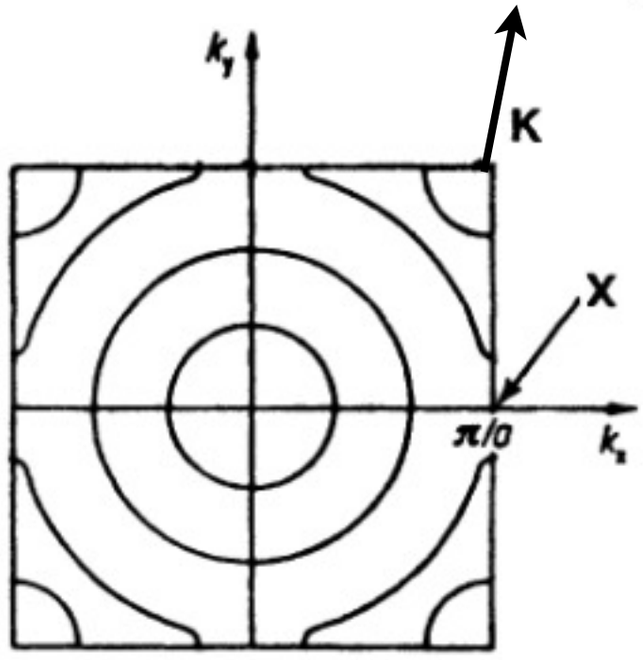


5.8. Curves and Planes of Equal Energy

$$E_{\max} = \frac{\hbar^2}{2m} k_{\text{crit}}^2 = \frac{\pi^2 \hbar^2}{a^2 m}$$

$$k_{\text{crit}} = \frac{\pi}{a}\sqrt{2}$$



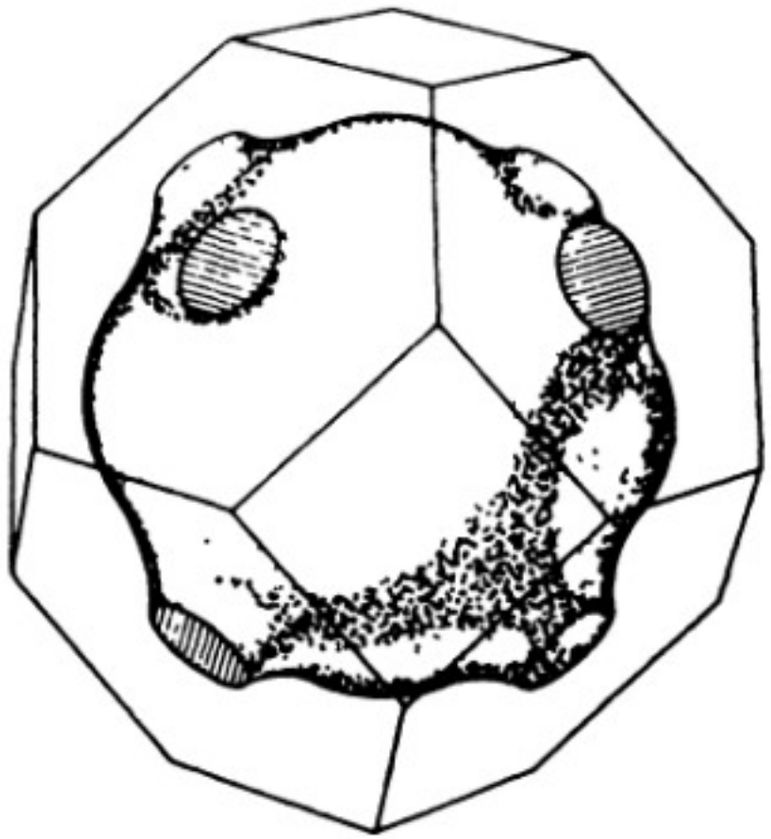


$$k_{\text{crit}} = \frac{\pi}{a}$$

$$E_{\max} = \frac{1}{2}\left(\frac{\pi^2 \hbar^2}{a^2 m}\right)$$

Curves of equal energy inserted into the first Brillouin zone for a two-dimensional square lattice.

Conclusions



A particular surface of equal energy
the first Brillouin zone for copper.

For copper and aluminum the band overlapping leads to quasi-continuous allowed energies (in different directions of **k**-space).

For semiconductors the band overlapping is not complete, which results in the already-mentioned energy gap