



Chapter 13 Diffraction

Reading Assignment:

1. D. Sherwood, Crystals, X-rays, and Proteins—chapter 9





Contents



- 1 Scattering of X-ray by electron**
- 2 Electron Density Function**
- 3 Atomic Scattering Factor**
- 4 Structure Factor**
- 5 Systematic Absences**





Contents of the Unit Cell



- diffraction pattern of a crystal- in terms of reciprocal lattice

$$Tf(\text{crystal}) = Tf(\text{motif}) \cdot [Tf(\text{infinite lattice}) * Tf(\text{shape function})]$$

- motif (contents of the unit cell)

envelop that of the finite crystal lattice

intensity determined by the diffraction pattern of motif

- intensities of all the diffraction maxima

→ inverse Fourier transform

→ parameters pertaining molecules within unit cell

→ scattering of the incident X-rays by electrons

→ distribution of electron within the unit cell





Scattering of X-ray by a Single Electron



- interaction of X-rays with an electron

Thomson scattering vs. Compton scattering

- Thomson scattering (coherent scattering)

assumption- free electron, passive response

incident X-ray with electric field \vec{E}_{in}

→ accelerate electron of charge e and mass m

$$\vec{a} = \frac{e}{m} \vec{E}_{in}$$

→ act as a source of radiation, scattered wave \vec{E}_{scat}

$$\frac{\vec{E}_{scat}}{\vec{E}_{in}} = \frac{e^2}{4\pi\epsilon_0 r m c^2} \frac{1 + \cos^2 2\theta}{2}, \text{ well defined phase relationship}$$





Scattering of X-ray by a Single Electron



- Compton scattering

a definite set of waves with wavelength rather longer
than that of the incident wave

collision between an electron and a photon

particle-particle collision

no well defined phase relationship

incoherent scattering

No discrete diffraction effects result from Compton Scattering

(overall background scattering)





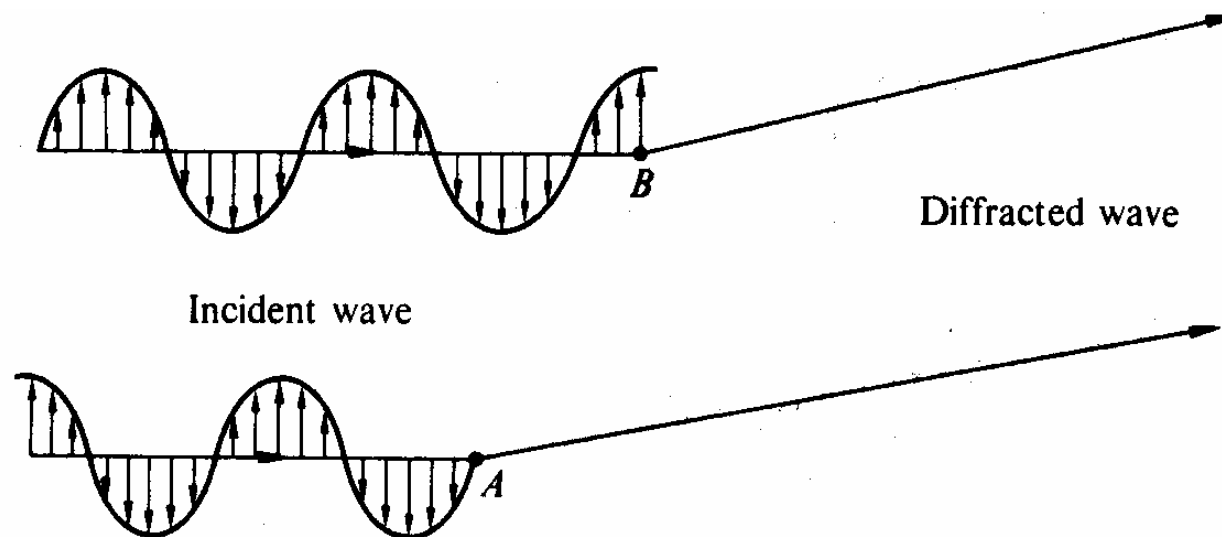
Scattering of X-ray by a Distribution of Electrons



- X-ray diffraction by Thomson scattering

$$\frac{\vec{E}_{scat}}{\vec{E}_{in}} = \frac{e^2}{4\pi\epsilon_0 r m c^2} \frac{1 + \cos^2 2\theta}{2} = f_e p(2\theta)$$

f_e : electronic scattering factor, $p(2\theta)$: polarization factor





Scattering of X-ray by a Distribution of Electrons



- $(E_{scat})_A = f_e E_{in}$

$$(E_{scat})_B = f_e E_{in} e^{i\phi}$$

- principle of superposition

$$(E_{scat})_{total} = (E_{scat})_A + (E_{scat})_B$$

$$\frac{(E_{scat})_{total}}{E_{in}} = f_e + f_e e^{i\phi}$$

- from an array of electrons

$$\frac{(E_{scat})_{total}}{E_{in}} = \sum_n f_e e^{i\phi_n} \quad \Leftrightarrow \quad F(\Delta\vec{k}) = \int_{all \vec{r}} f(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r}$$





Scattering of X-ray by a Distribution of Electrons



- electron density function $\rho(\vec{r})$

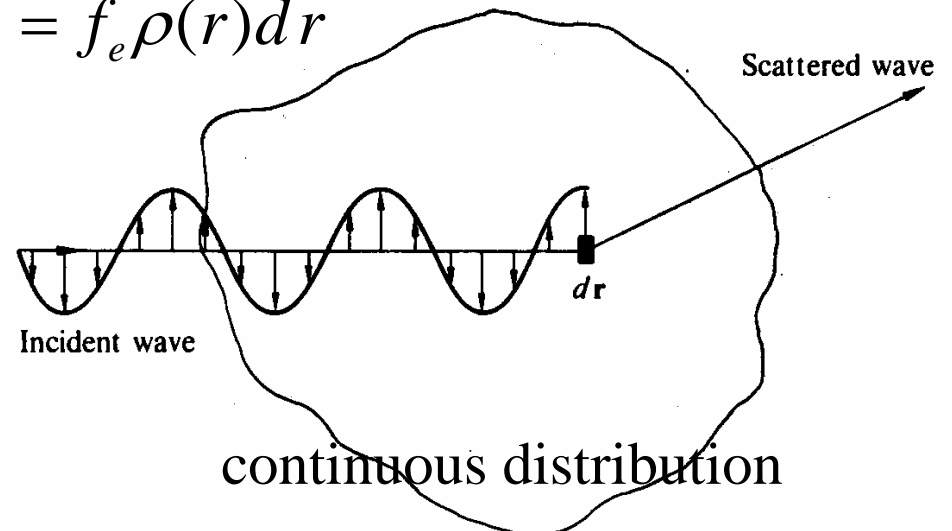
any element of volume, centered on the point \vec{r} , which
represented by $d\vec{r}$

average number of electrons within the volume $d\vec{r}$ is

given by $\rho(\vec{r})d\vec{r}$

scattered wave amplitude $dE_{scat} = f_e \rho(\vec{r})d\vec{r}$

-
$$F(\Delta\vec{k}) = \int_{all \vec{r}} f_e \rho(\vec{r}) e^{i\Delta\vec{k} \cdot \vec{r}} d\vec{r}$$





Diffraction Pattern of the Motif

- within a single unit cell

electron density function $\rho(\vec{r}) \rightarrow$ position of atoms from the
electron density maxima \rightarrow bond lengths, bond angles

$$- F(\Delta\vec{k}) = \int_{\text{all } \vec{r}} f_e \rho(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r} \Rightarrow F(\Delta\vec{k}) = f_e \int_{\text{unit cell}} \rho(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r}$$

- $F(\Delta\vec{k}) / f_e$: relative scattering ability of the contents of the unit cell compared to a single electron

$$- F_{rel}(\Delta\vec{k}) = \int_{\text{unit cell}} \rho(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r}$$





Diffraction Pattern of the Motif



- triclinic system, $\vec{a} = a\hat{a}$, $\vec{b} = b\hat{b}$, $\vec{c} = c\hat{c}$

$$- F_{rel}(\Delta\vec{k}) = \int_{unit\ cell} \rho(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r}$$

- any point within the unit cell

$$\vec{r} = X\hat{a} + Y\hat{b} + Z\hat{c} \quad 0 \leq X \leq a, 0 \leq Y \leq b, 0 \leq Z \leq c$$

$$x = X/a, \quad y = Y/b, \quad z = Z/c$$

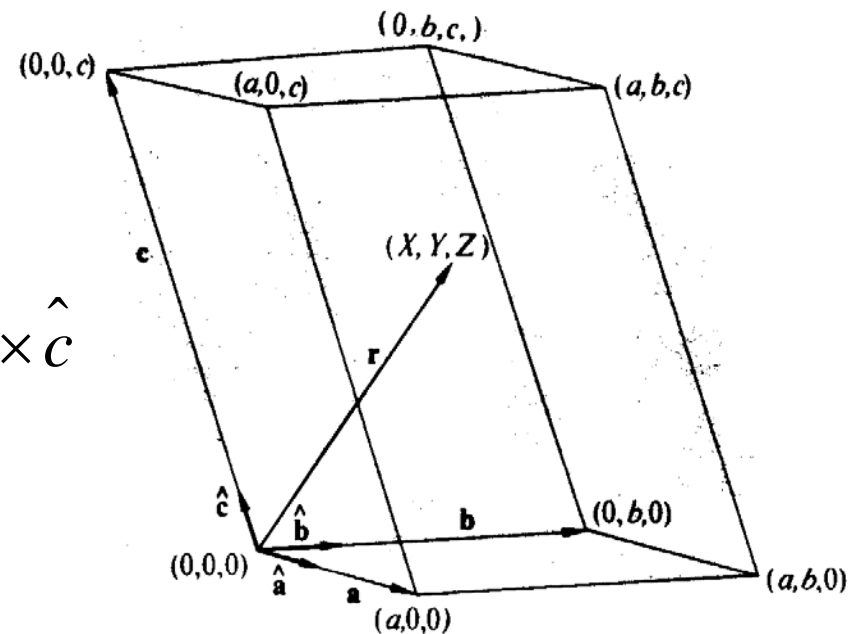
$$0 \leq x \leq 1, \quad 0 \leq y \leq 1, \quad 0 \leq z \leq 1$$

$$\Rightarrow \vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$$

- volume element $d\vec{r} = dXdYdZ\hat{a}\cdot\hat{b}\times\hat{c}$

$$= dx dy dz \vec{a}\cdot\vec{b}\times\vec{c}$$

$$= V dx dy dz$$





Diffraction Pattern of the Motif



- amplitude of the diffraction pattern of the contents of the unit cell

$$F_{rel}(\Delta\vec{k}) = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x, y, z) e^{i\Delta\vec{k} \cdot (x\vec{a} + y\vec{b} + z\vec{c})} dx dy dz$$

⇒ envelop the diffraction pattern of the crystal lattice

⇒ restrict the values of the scattering vector $\Delta\vec{k}$ to those which correspond crystal lattice diffraction maxima

- $\Delta\vec{k} = 2\pi\vec{G}_{hkl}$

$$\begin{aligned} \Delta\vec{k} \cdot \vec{r} &= 2\pi(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot (x\vec{a} + y\vec{b} + z\vec{c}) \\ &= 2\pi(hx + ky + lz) \end{aligned}$$





Diffraction Pattern of the Motif



- for a single particular maximum corresponding to the reciprocal lattice point hkl

$$[F_{rel}(\Delta\vec{k})]_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x, y, z) e^{2\pi i(hx+ky+lz)} dx dy dz$$

amplitude of the diffraction pattern at the point indexed as hkl

- structure factor

$$F_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x, y, z) e^{2\pi i(hx+ky+lz)} dx dy dz$$

- in general , complex quantity

$$F_{hkl} = |F_{hkl}| e^{i\alpha_{hkl}}$$

- $I_{hkl} = |F_{hkl}|^2$





Calculation of the Electron Density Function



$$- F_{rel}(\Delta\vec{k}) = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x, y, z) e^{2\pi i(hx+ky+lz)} dx dy dz$$

$$- \rho(x, y, z) = \frac{1}{V} \int_{all \Delta\vec{k}} F_{rel}(\Delta\vec{k}) e^{-i\Delta\vec{k} \cdot (x\vec{a} + y\vec{b} + z\vec{c})} d(\Delta\vec{k})$$

$$- \rho(x, y, z) = \frac{1}{V} \int_{all \Delta\vec{k}} F_{hkl} e^{-2\pi i(hx+ky+lz)} d(\Delta\vec{k})$$

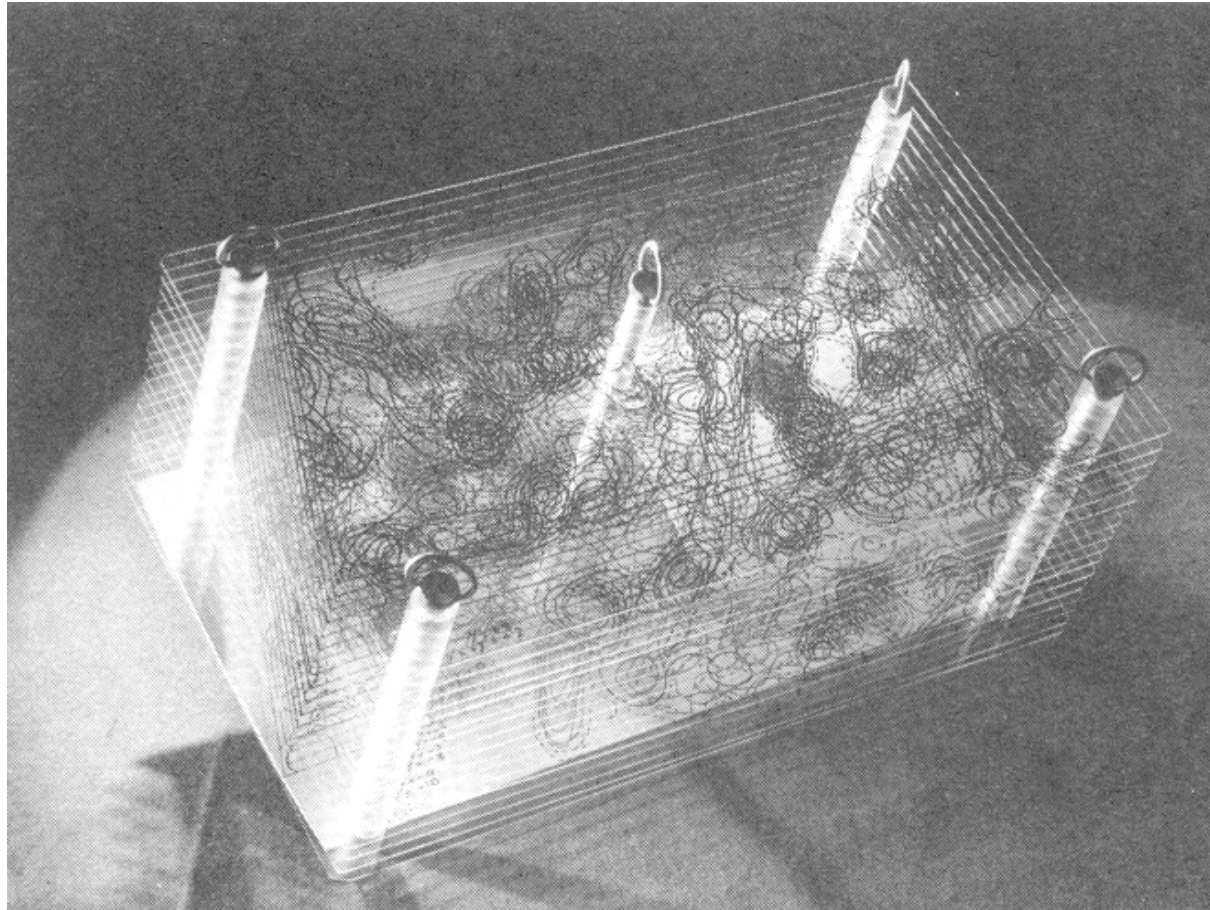
- diffraction pattern- discrete, not continuous

$$\rho(x, y, z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)}$$





Fourier Synthesis



electron density map of protein myoglobin





Electron Density Projections



- determination of relatively small molecules- 2D function $\rho(x, y)$

$$- \rho(x, y) = \int_0^c \rho(x, y, z) dZ = c \int_0^1 \rho(x, y, z) dz$$

$$\rho(x, y, z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)}$$

$$\rho(x, y) = \frac{c}{V} \int_0^1 \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)} dz$$

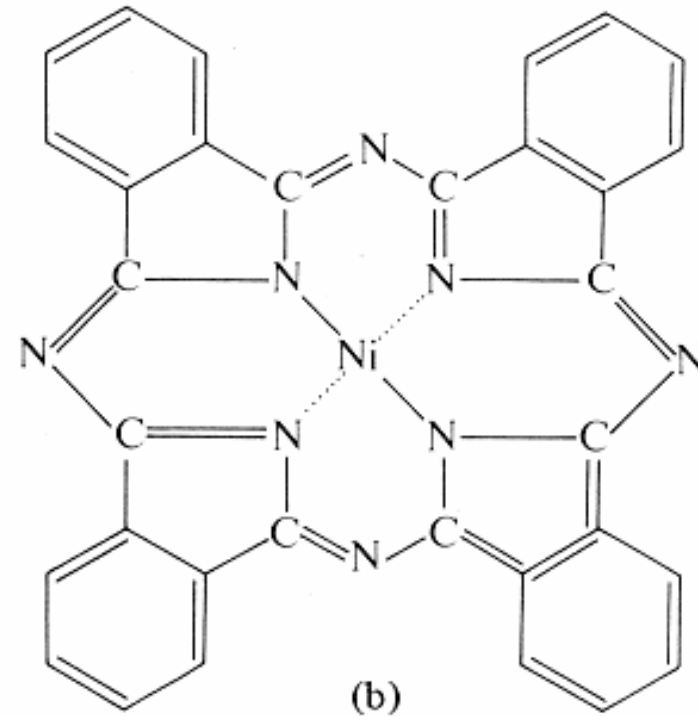
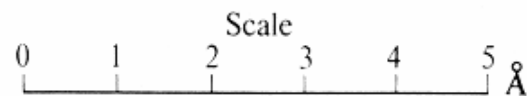
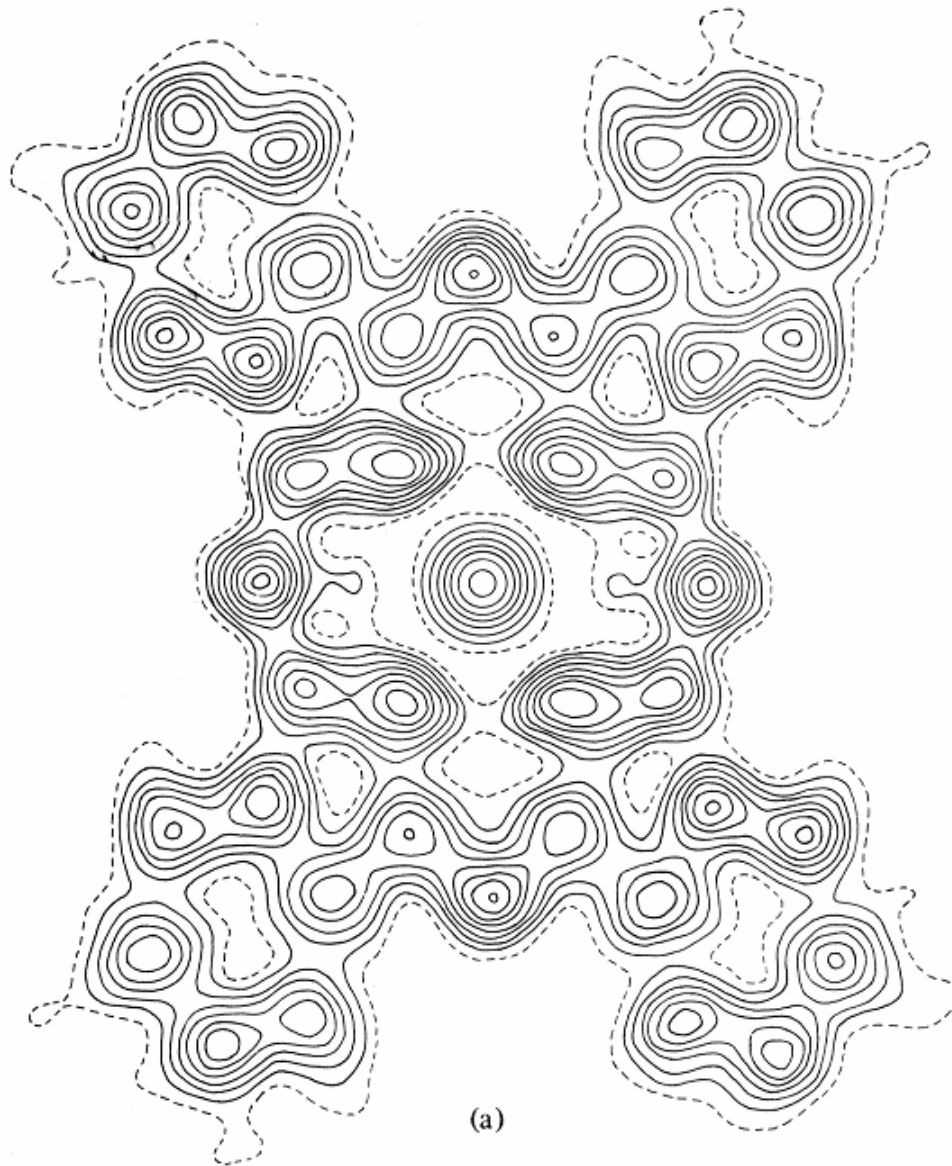
$$= \frac{1}{A} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky)} \int_0^1 e^{-2\pi ilz} dz \quad \int_0^1 e^{-2\pi ilz} dz = \delta(l)$$

$$= \frac{1}{A} \sum_h \sum_k F_{hk0} e^{-2\pi i(hx+ky)}$$





Electron Density Projections



nickel phthalocyanine



Calculation of Structure Factor

$$- F_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x, y, z) e^{2\pi i(hx+ky+lz)} dx dy dz$$

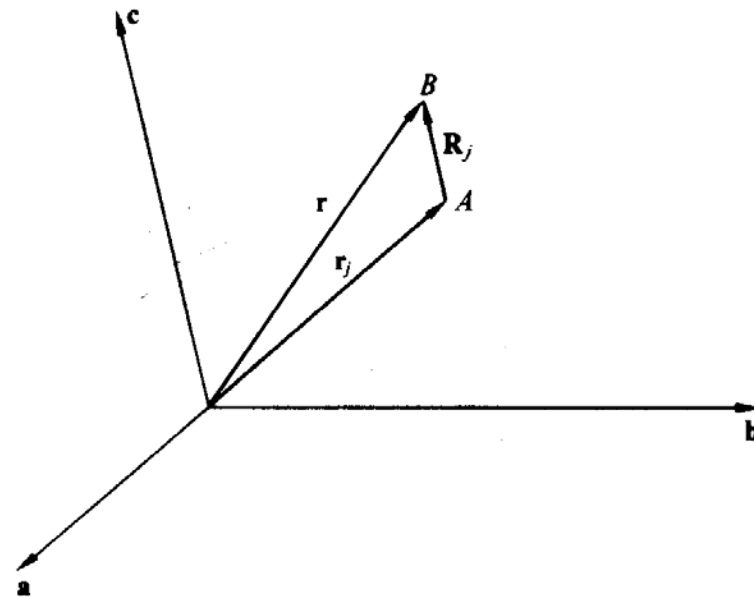
$$- \rho(x, y, z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)}$$

- only infer atomic position from the maxima in the electron density function

- alternatively, $\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$

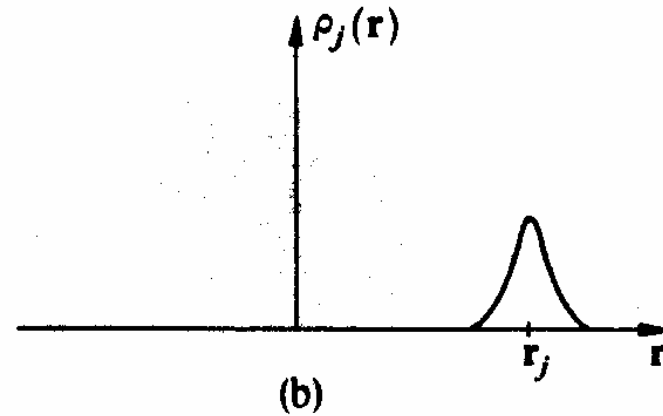
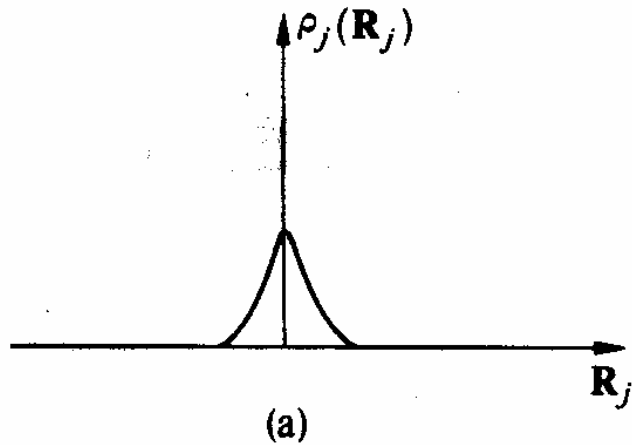
$$F_{hkl} = \int_{\text{unit cell}} \rho(\vec{r}) e^{2\pi i \vec{G}_{hkl} \cdot \vec{r}} d\vec{r}$$

- $\vec{r} = \vec{r}_j + \vec{R}_j$

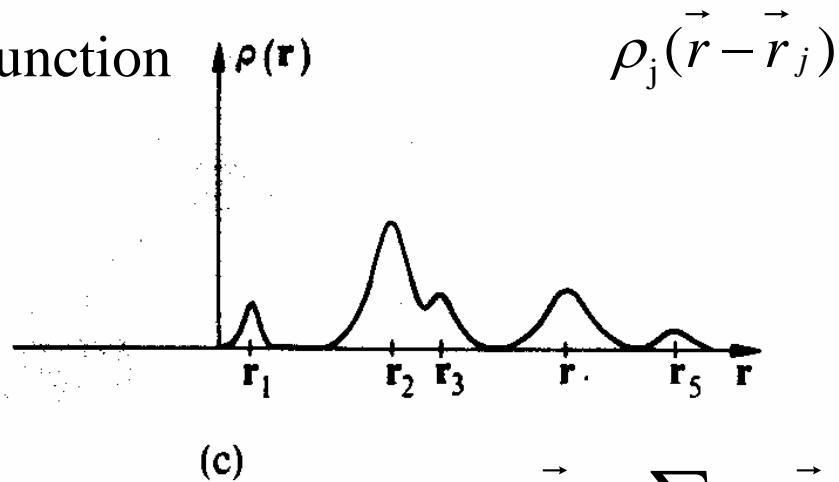




Calculation of Structure Factor



atomic electron density function



$$\rho(\vec{r}) = \sum_j \rho_j(\vec{r} - \vec{r}_j)$$





Calculation of Structure Factor

$$- F_{hkl} = \int_{\text{unit cell}} \sum_j \rho_j(\vec{r} - \vec{r}_j) e^{2\pi i \vec{G}_{hkl} \cdot \vec{r}} d\vec{r}$$

$\vec{r} = \vec{r}_j + \vec{R}_j$, positions of nuclei are constant

$$d\vec{r} = d\vec{R}_j$$

$$\begin{aligned} - F_{hkl} &= \int_{\text{unit cell}} \sum_j \rho_j(\vec{R}_j) e^{2\pi i \vec{G}_{hkl} \cdot (\vec{r}_j + \vec{R}_j)} d\vec{R}_j \\ &= \int_{\text{unit cell}} \sum_j \rho_j(\vec{R}_j) e^{2\pi i \vec{G}_{hkl} \cdot \vec{r}_j} e^{2\pi i \vec{G}_{hkl} \cdot \vec{R}_j} d\vec{R}_j \\ &= \sum_j e^{2\pi i \vec{G}_{hkl} \cdot \vec{r}_j} \int_{\text{atom}} \rho_j(\vec{R}_j) e^{2\pi i \vec{G}_{hkl} \cdot \vec{R}_j} d\vec{R}_j \end{aligned}$$





Calculation of Structure Factor



- atomic scattering factor

$$f_j = \int_{atom} \rho_j(\vec{R}_j) e^{2\pi i \vec{G}_{hkl} \cdot \vec{R}_j} d\vec{R}_j$$

- $F_{hkl} = \sum_j f_j e^{2\pi i \vec{G}_{hkl} \cdot \vec{r}_j}$

- j th atom $\vec{r}_j = x_j \vec{a} + y_j \vec{b} + z_j \vec{c}$

$$\vec{G}_{hkl} \cdot \vec{r}_j = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot (x_j \vec{a} + y_j \vec{b} + z_j \vec{c}) = (hx_j + ky_j + lz_j)$$

- $F_{hkl} = \sum_j f_j e^{2\pi i (hx_j + ky_j + lz_j)}$

- $F_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x, y, z) e^{2\pi i (hx + ky + lz)} dx dy dz$





Atomic Scattering Factor



$$-f_j = \int_{atom} \rho_j(\vec{R}_j) e^{2\pi i \vec{G}_{hkl} \cdot \vec{R}_j} d\vec{R}_j$$

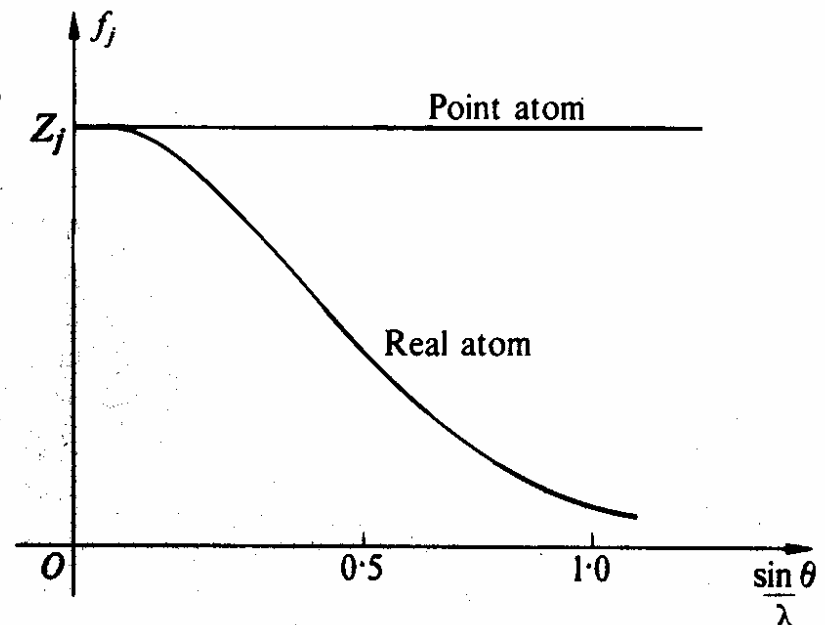
scattering ability of an atom as compared to that of a single electron (f_e)

- spherically symmetric

$$f_j = 2\pi \int_0^\infty R^2 \rho_j(R) \frac{\sin\left(\frac{4\pi}{\lambda} \sin \theta\right) R}{\left(\frac{2\pi}{\lambda} \sin \theta\right) R} dR$$

$$= 4\pi \int_0^\infty \rho_j(R) R^2 \frac{\sin sR}{sR} dR$$

$$s = \frac{4\pi \sin \theta}{\lambda}$$





Atomic Scattering Factors



$\frac{\sin \theta}{\lambda} (\text{\AA}^{-1})$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
H	1	0.81	0.48	0.25	0.13	0.07	0.04	0.03	0.02	0.01	0.00	0.00	
He	2	1.88	1.46	1.05	0.75	0.52	0.35	0.24	0.18	0.14	0.11	0.09	
Li ⁺	2	1.96	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	
Li	3	2.2	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	
Be ⁺²	2	2.0	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	
Be	4	2.9	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	
B ⁺³	2	1.99	1.9	1.8	1.7	1.6	1.4	1.3	1.2	1.0	0.9	0.7	
B	5	3.5	2.4	1.9	1.7	1.5	1.4	1.2	1.2	1.0	0.9	0.7	
C	6	4.6	3.0	2.2	1.9	1.7	1.6	1.4	1.3	1.16	1.0	0.9	
N ⁺⁵	2	2.0	2.0	1.9	1.9	1.8	1.7	1.6	1.5	1.4	1.3	1.16	
N ⁺³	4	3.7	3.0	2.4	2.0	1.8	1.66	1.56	1.49	1.39	1.28	1.17	
N	7	5.8	4.2	3.0	2.3	1.9	1.65	1.54	1.49	1.39	1.29	1.17	
O	8	7.1	5.3	3.9	2.9	2.2	1.8	1.6	1.5	1.4	1.35	1.26	
O ⁻²	10	8.0	5.5	3.8	2.7	2.1	1.8	1.5	1.5	1.4	1.35	1.26	
F	9	7.8	6.2	4.45	3.35	2.65	2.15	1.9	1.7	1.6	1.5	1.35	
F ⁻	10	8.7	6.7	4.8	3.5	2.8	2.2	1.9	1.7	1.55	1.5	1.35	
Ne	10	9.3	7.5	5.8	4.4	3.4	2.65	2.2	1.9	1.65	1.55	1.5	
Na ⁺	10	9.5	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	
Na	11	9.65	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	
Mg ⁺²	10	9.75	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	
Mg	12	10.5	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	
Al ⁺³	10	9.7	8.9	7.8	6.65	5.5	4.45	3.65	3.1	2.65	2.3	2.0	
Al	13	11.0	8.95	7.75	6.6	5.5	4.5	3.7	3.1	2.65	2.3	2.0	
Si ⁺⁴	10	9.75	9.15	8.25	7.15	6.05	5.05	4.2	3.4	2.95	2.6	2.3	
Si	14	11.35	9.4	8.2	7.15	6.1	5.1	4.2	3.4	2.95	2.6	2.3	





Crystal Symmetry and X-ray Diffraction



- symmetry of crystal \leftrightarrow symmetry of diffraction pattern

230 space group

$$- F_{hkl} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

- ex) mirror parallel to ab plane

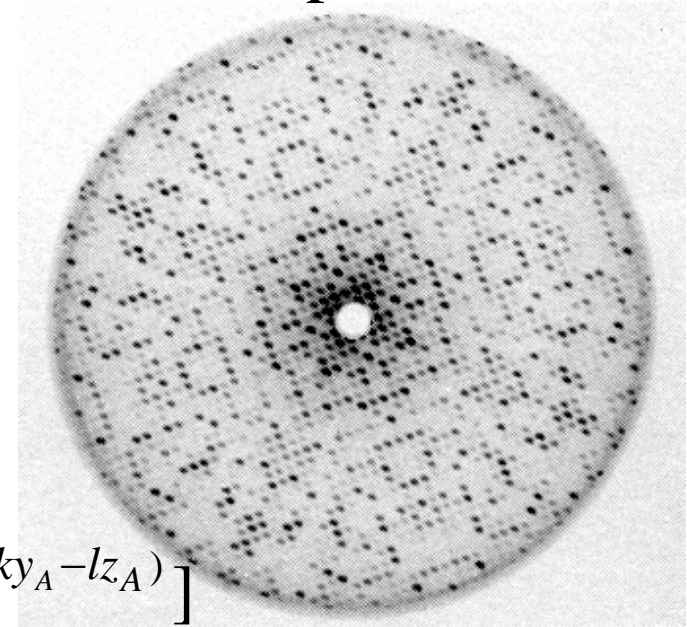
$$(x_A, y_A, z_A) \quad (x_A, y_A, -z_A)$$

$$(F_{hkl})_A = f_A [e^{2\pi i(hx_A + ky_A + lz_A)} + e^{2\pi i(hx_A + ky_A - lz_A)}]$$

$$(F_{hk\bar{l}})_A = f_A [e^{2\pi i(hx_A + ky_A - lz_A)} + e^{2\pi i(hx_A + ky_A + lz_A)}]$$

$$I_{hkl} = I_{hk\bar{l}}$$

- mirror plane, rotation axis



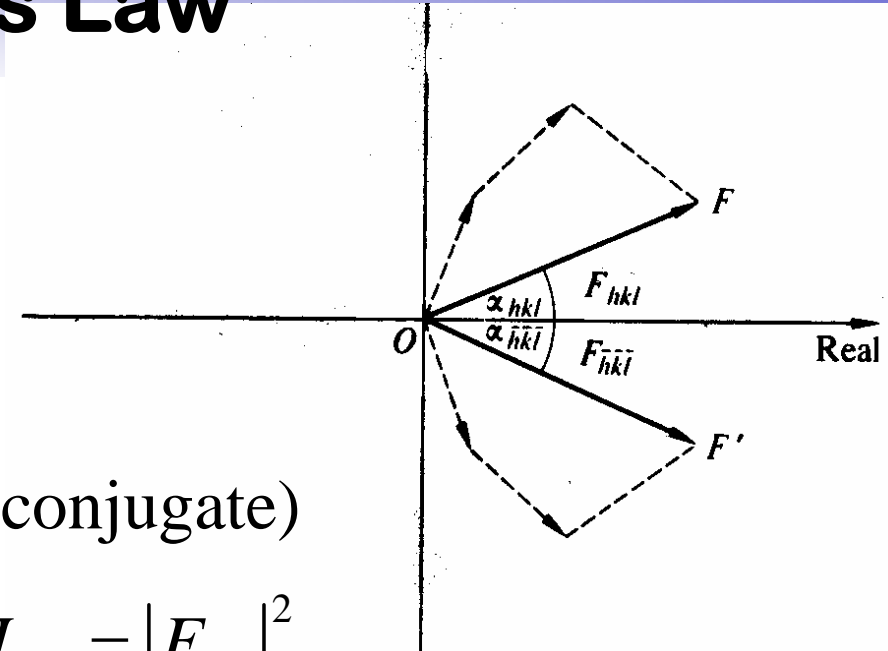


Friedel's Law



$$- F_{hkl} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

$$F_{\bar{h}\bar{k}\bar{l}} = \sum_j f_j e^{-2\pi i(hx_j + ky_j + lz_j)}$$



- f_j is real, $F_{hkl}^* = F_{\bar{h}\bar{k}\bar{l}}$ (complex conjugate)

$$|F_{hkl}| = |F_{\bar{h}\bar{k}\bar{l}}| \quad I_{hkl}^* = I_{\bar{h}\bar{k}\bar{l}} = |F_{hkl}|^2$$

- magnitude of the structure factor of centrosymmetrically related reciprocal lattice points are equal
- intensity of the diffraction maxima corresponding to centrosymmetrically related reciprocal lattice points are equal (inversion center)





- Friedel's law was proved on a perfectly general basis and its significance is that the X-ray diffraction picture in general are centrosymmetric whether or not the crystal has an inversion center
- observation of the symmetry of the diffraction pattern in general allows to identify mirror planes and proper rotation axes, but inversion centers and improper rotation axes.





Systematic Absence



- body centered cubic $(000, \frac{1}{2} \frac{1}{2} \frac{1}{2})$

$$\begin{aligned}
 F_{hkl} &= f_j e^{2\pi i(h \cdot 0 + k \cdot 0 + l \cdot 0)} + f_j e^{2\pi i(h \frac{1}{2} + k \frac{1}{2} + l \frac{1}{2})} \\
 &= f_j [1 + e^{i\pi(h+k+l)}] = 2f_j \quad \text{if } h+k+l = 2n \\
 &\quad 0 \quad \text{if } h+k+l = 2n+1
 \end{aligned}$$

- systematic absence or extinction

- a glide (\parallel (001))

$$xyz, x + \frac{1}{2} y \bar{z}$$

$$\begin{aligned}
 F_{hkl} &= f_j e^{2\pi i(hx+ky+lz)} + f_j e^{2\pi i[h(x+\frac{1}{2})+ky-lz]} \\
 &= f_j e^{2\pi i(hx+ky+lz)} [1 + e^{i\pi h} e^{-4\pi ilz}]
 \end{aligned}$$

$$l = 0 \Rightarrow hk0, \quad h = 2n + 1 \Rightarrow F_{hkl} = 0$$





Reciprocal lattice



- cubic I

$$a = b = c$$

$$\alpha = \beta = \gamma = 90^\circ$$

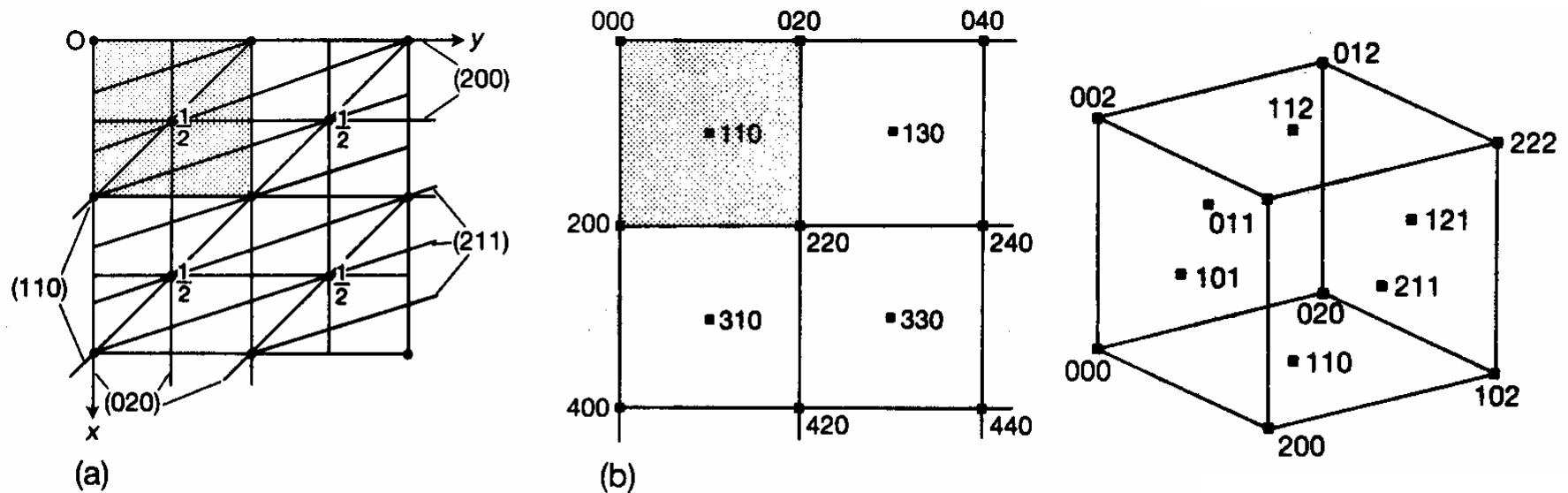


Fig. 6.4. (a) Plan of a cubic *I* crystal perpendicular to the *z*-axis and (b) pattern of reciprocal lattice points perpendicular to the *z*-axis. Note the cubic *F* arrangement of reciprocal lattice points in this plane.





Systematic Absence



- face centered cubic $(000, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0)$

$$F_{hkl} = f_j e^{2\pi i(h0+k0+l0)} + f_j e^{2\pi i(h0+k\frac{1}{2}+l\frac{1}{2})} + f_j e^{2\pi i(h\frac{1}{2}+k0+l\frac{1}{2})} \\ + f_j e^{2\pi i(h\frac{1}{2}+k\frac{1}{2}+l0)}$$

$$= f_j [1 + e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k)}]$$

$$= 4f_j \quad \text{if } h, k, l \quad \text{unmixed}$$

$$0 \quad \text{if } h, k, l \quad \text{mixed}$$

100 110 111 200 210 220 300(221) 310 311

X X O O X O X X X O





04-0836

Wavelength= 1.5405

Cu	2 θ	Int	h	k	l
Copper	43.295*	100	1	1	1
	50.431*	46	2	0	0
	74.127*	20	2	2	0
Copper, syn	89.926*	17	3	1	1
	95.135*	5	2	2	2
	116.911	3	4	0	0
	136.496	9	3	3	1
	144.700	8	4	2	0

Rad.: CuK α 1 λ : 1.5405 Filter: Ni Beta Φ d-sp:
 Cut off: Int.: Diffract. I/lor.:
 Ref: Swanson, Tatge, Natl. Bur. Stand. (U.S.), Circ. 539, I. 15 (1953)

Sys.: Cubic S.G.: Fm3m (225)
 a: 3.6150 b: c: A: C:
 α : β : γ : Z: 4 mp: 1083
 Ref: Ibid.

Dx: 8.935 Dm: 8.950 SS/FOM: F $_{\beta}$ =89(.0112, 8)

Color: Red
 Pattern taken at 26 C. Sample from metallurgical laboratory of NBS, Gaithersburg, MD, USA. CAS #: 7440-50-8. It had been heated in an H $_2$ atmosphere at 300 C. Impurities from 0.001-0.01%, Ag, Al, Bi, Fe, Si, Zn. Opaque mineral optical data on specimen from unspecified locality. R $_3$ R%=60.65. Disp.=Std., VHN100=96-104. Ref.: IMA Commission on Ore Microscopy QDF. Measured density and color from Dana's System of Mineralogy, 7th Ed., I 99. Cu type. Gold group, gold subgroup. PSC: cF4. Mwt: 63.55. Volume[CD]: 47.24.





Systematic Absence



- diamond structure $(000, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{4}\frac{1}{4}\frac{1}{4}, \frac{1}{4}\frac{3}{4}\frac{3}{4}, \frac{3}{4}\frac{1}{4}\frac{3}{4}, \frac{3}{4}\frac{3}{4}\frac{1}{4})$

$$\begin{aligned}
 F_{hkl} &= f_j e^{2\pi i(h0+k0+l0)} + f_j e^{2\pi i(h0+k\frac{1}{2}+l\frac{1}{2})} + f_j e^{2\pi i(h\frac{1}{2}+k0+l\frac{1}{2})} + f_j e^{2\pi i(h\frac{1}{2}+k\frac{1}{2}+l0)} \\
 &+ f_j e^{2\pi i(h\frac{1}{4}+k\frac{1}{4}+l\frac{1}{4})} + f_j e^{2\pi i(h\frac{1}{4}+k\frac{3}{4}+l\frac{3}{4})} + f_j e^{2\pi i(h\frac{3}{4}+k\frac{1}{4}+l\frac{3}{4})} + f_j e^{2\pi i(h\frac{3}{4}+k\frac{3}{4}+l\frac{1}{4})} \\
 &= f_j [1 + e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k)}] [1 + e^{i\pi(h+k+l)/2}]
 \end{aligned}$$

if h, k, l mixed, $F_{hkl} = 0$

if h, k, l unmixed $F_{hkl} = 4f_j (1 \pm i)$ if h, k, l are odd

$F_{hkl} = 8f_j$ if h, k, l are even multiple of 2

$F_{hkl} = 0$ if h, k, l are odd multiple of 2

100 110 111 200 210 220 300(221) 310 311 222

X X 0 X X 00 X X 0 X





06-0675

Wavelength= 1.5405

*

C	2 θ	Int	h	k	l
Carbon	43.914*	100	1	1	1
	75.298*	25	2	2	0
	91.491*	16	3	1	1
Diamond	119.514	8	4	0	0
	140.575	16	3	3	1

Rad.: CuK α 1 λ : 1.5405 Filter: Ni Beta Φ d-sp:

Cut off: Int.: Diffract. I/Icor.:

Ref: Natl. Bur. Stand. (U.S.), Circ. 539, II, 5 (1953)

Sys.: Cubic

S.G.: Fd3m (227)

a: 3.5667 b: c: A: C:

α : β : γ : Z: 8 mp:

Ref: Ibid.

Dx: 3.517 Dm: 3.511 SS/FOM: F₅=73(.0115, 6)

$\epsilon\alpha$: $\eta\omega\beta$: 2.4195 $\epsilon\gamma$: Sign: 2V:

Ref: Ibid.

Color: Colorless

Pattern taken at 26 C. Specimen was an industrial abrasive

powder. CAS #: 7782-40-3. C type. Diamond group. Also

called: bort.PSC: cF8. To replace 1-1249. Mwt: 12.01.

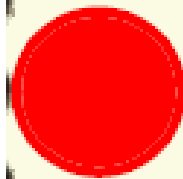
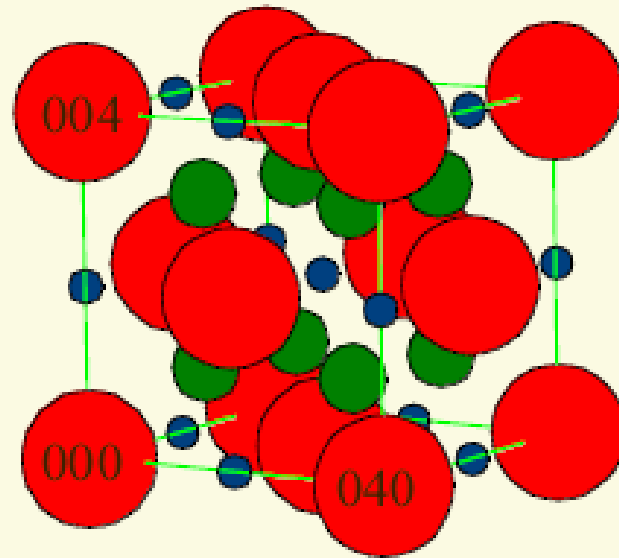
Volume[CD]: 45.37.

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Reciprocal Structure



Fundamental Diffraction Spots:
 $64f^2$



Zero intensity



Lowered intensity: $32f^2$





Table 9.1. Conditions on h , k and l for systematic absences.

Class of reflections	Condition for presence	Interpretation	Symbol	Occurrence in lattice type
		Lattice type:		
	none	primitive	P	
	$h + k + l = 2n$	body-centred	I	
	$h + k = 2n$	centred on the C face	C	
	$k + l = 2n$	centred on the A face	A	
hkl	$h + l = 2n$	centred on the B face	B	
	$h + k = 2n$	centred on all faces	F	
	$k + l = 2n$			
	$h + l = 2n$			
	$-h + k + l = 3n$	rhombohedral, obverse	R	
	$h - k + l = 3n$	rhombohedral, reverse	R	
	$h = 2n$	glide plane \parallel (001)	a	P, B, I
$hk0$	$k = 2n$		b	P, A, B
	$h + k = 2n$		n	P
	$h + k = 4n$		d	F
	$k = 2n$		b	P, B, C





$0kl$	$l = 2n$	glide plane $\parallel (100)$	c	P, C, I
	$k + l = 2n$		n	P
	$k + l = 4n$		d	F
	$h = 2n$		a	P, A, I
$h0l$	$l = 2n$	glide plane $\parallel (010)$	c	P, A, C
	$h + l = 2n$		n	P
	$h + l = 4n$		d	F, B
	$l = 2n$		e	P, C, F
hhl	$h = 2n$	glide plane $\parallel (110)$	b	C
	$h + l = 2n$		n	C
	$2h + l = 4n$		d	I
	$l = 2n$		$2_1, 4_2, 6_3$	
$00l$	$l = 3n$	screw axis $\parallel c$	$3_1, 3_2, 6_2, 6_4$	
	$l = 4n$		$4_1, 4_3$	
	$l = 6n$		$6_1, 6_5$	
	$h = 2n$		$2_1, 4_2$	
$h00$	$h = 4n$	screw axis $\parallel a$	$4_1, 4_3$	
	$k = 2n$		$2_1, 4_2$	
$0k0$	$k = 4n$	screw axis $\parallel b$	$4_1, 4_3$	
	$h = 2n$		2_1	
$hh0$		screw axis $\parallel [110]$		





Determination of Crystal Symmetry



- 230 space group
- M.J. Buerger: 122 different diffraction pattern types
- what symmetry information can be derived from the symmetry of an X-ray photograph?
 - systematic absence → lattice type
 - 11 out of 32 point group-centrosymmetric (Laue group)
 - as many as necessary for the systematic absence (glide, screw)
(diffraction symbol)
- 58 uniquely define a single space group
- 64 ambiguity as to space group





Determination of Crystal Symmetry



- of all the symmetry operations, the only one about which we can derive no information is the presence or absence of an inversion center
 - (i) breakdown of Friedel's law
 - (ii) piezoelectric effect
 - (iii) pyroelectric effect
 - (iv) optical activity

