Contents of the Unit Cell

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

$$Tf\,(crystal) = Tf\,(motif\,)\bullet[Tf\,(infinite\ lattice) * Tf\,(shape\ function)]$$

- motif (contents of the unit cell)

  envolop 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 $\vec{E}_{in}$

  $\rightarrow$ accelerate electron of charge e and mass m

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

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

$$\frac{\vec{E}_{scat}}{\vec{E}_{in}} = \frac{e^2}{4\pi\varepsilon_0 rmc^2}\frac{1+\cos^2 2\theta}{2},$$ 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

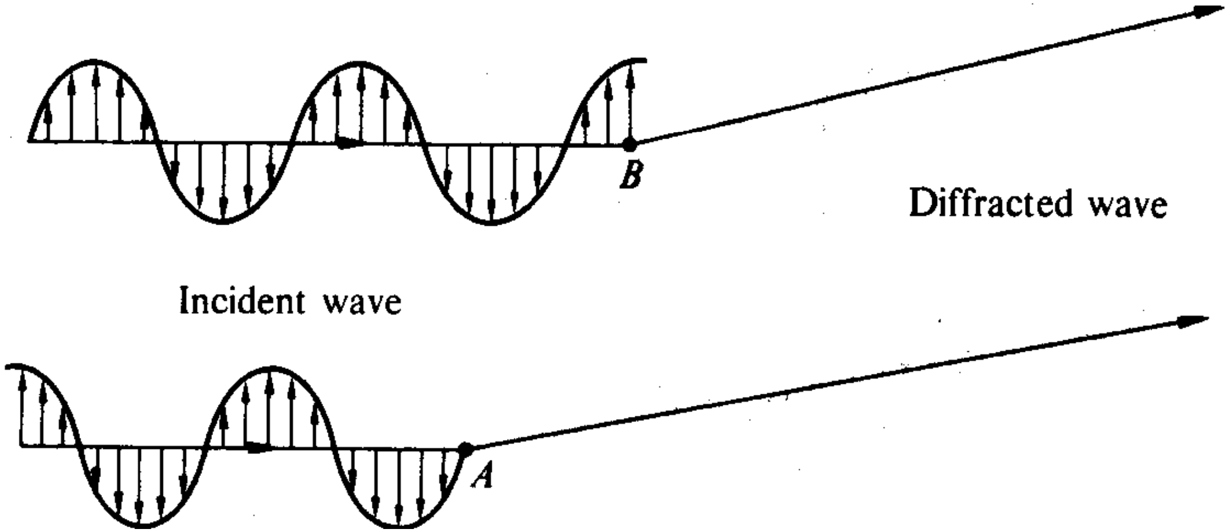
  (overall background scattering)

Scattering of X-ray by a Distribution of Electrons

- X-ray diffraction by Thomson scattering

$$\frac{\vec{E}_{scat}}{\vec{E}_{in}} = \frac{e^2}{4\pi\varepsilon_0 rmc^2}\frac{1+\cos^2 2\theta}{2} = f_e p(2\theta)$$

f_e: electronic scattring 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

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

Scattering of X-ray by a Distribution of Electrons

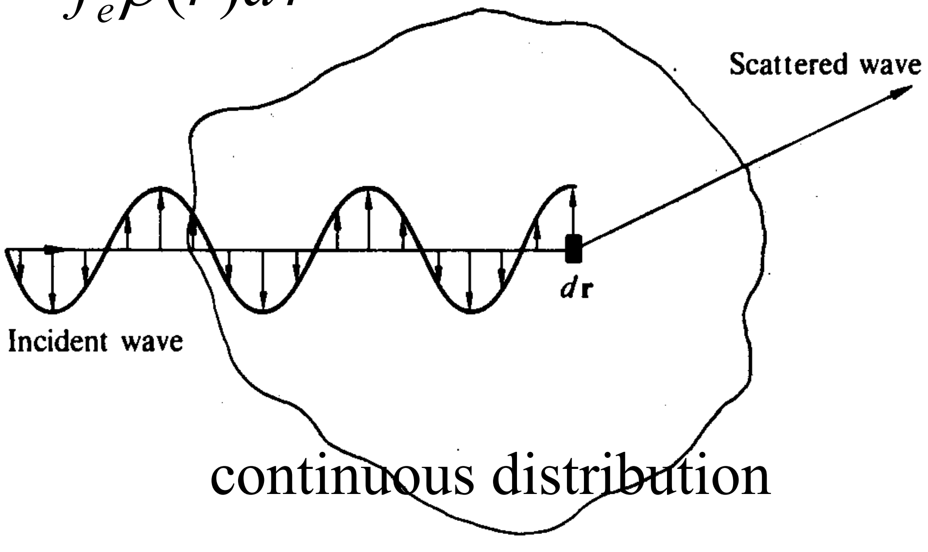
- electron density function $\rho(\vec{r})$

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

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



continuous distribution

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

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

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

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

Diffraction Pattern of the Motif

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

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

- any point within the unit cell

$$\vec{r} = X\hat{\mathrm{a}} + Y\hat{\mathrm{b}} + Z\hat{\mathrm{c}} \qquad 0 \le X \le a,\ 0 \le Y \le b,\ 0 \le Z \le c$$

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

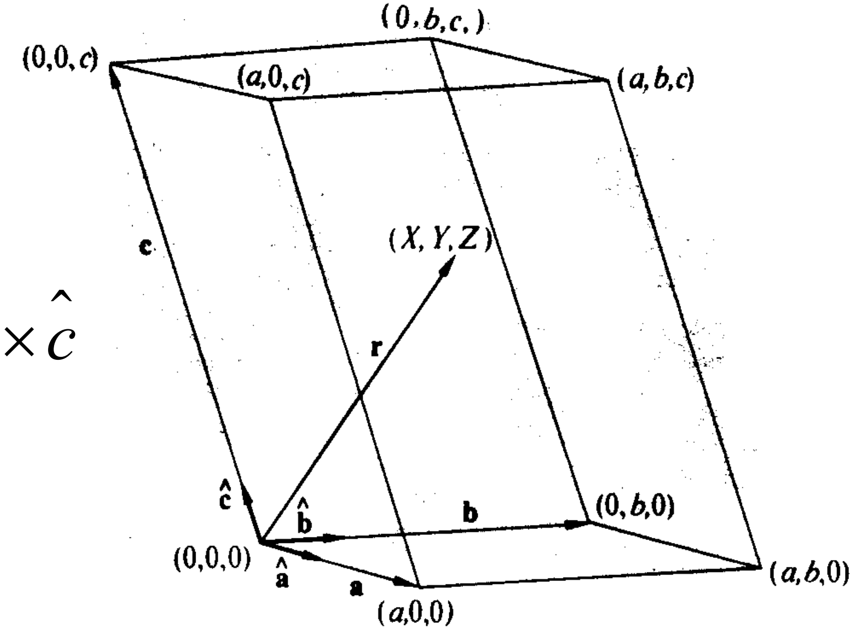
$$0 \le x \le 1,\ 0 \le y \le 1,\ 0 \le z \le 1$$

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

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

$$= dxdydz\,\vec{a}\bullet\vec{b}\times\vec{c}$$

$$= Vdxdydz$$



Diffraction Pattern of the Motif

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

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

$\Rightarrow$ envolop the diffraction pattern of the crystal lattice

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

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

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

Diffraction Pattern of the Motif

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

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

amplitude of the diffraction pattern at the point indexed as *hkl*

- structure factor

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

- in general , complex quantity

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

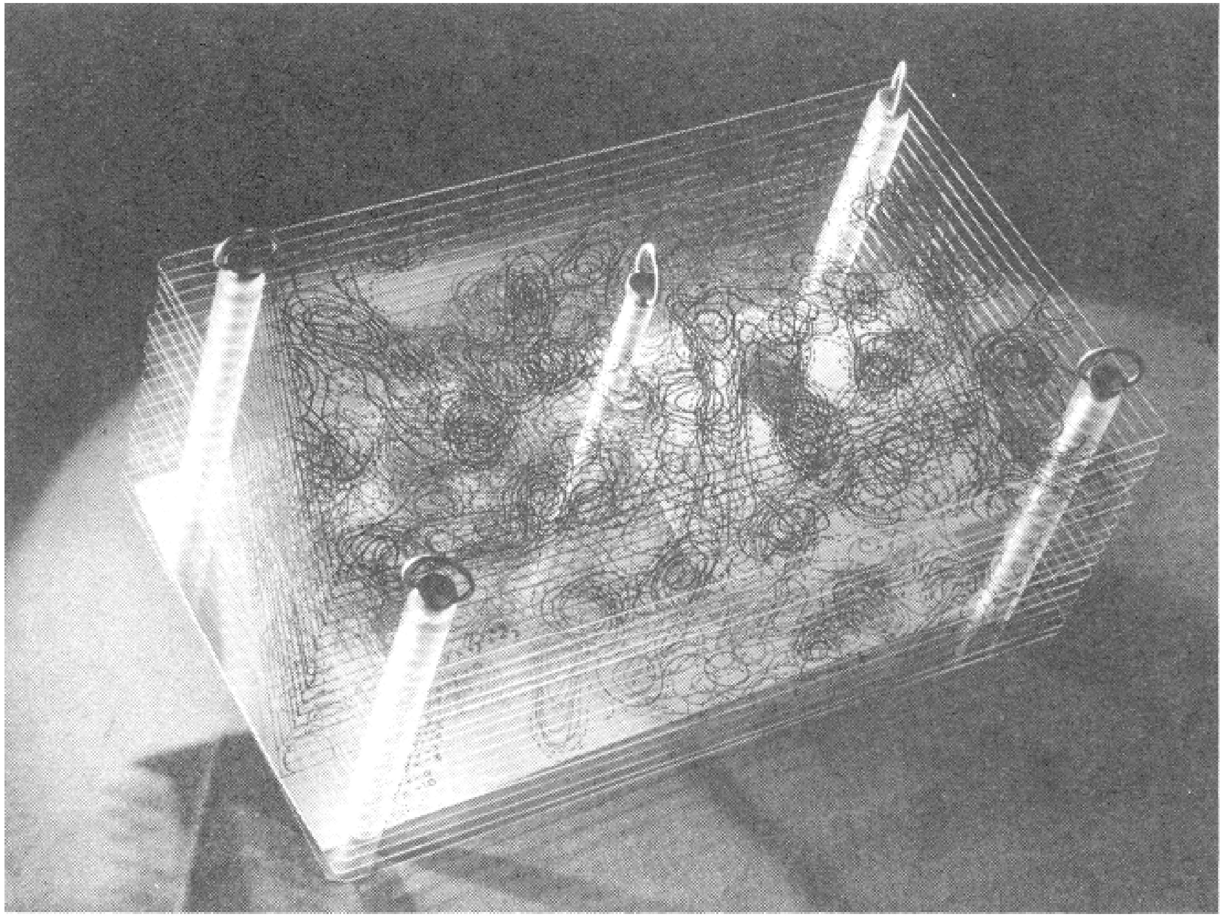
- $I_{hkl} = \left|F_{hkl}\right|^2$

Calculation of the Electron Density Function

- $F_{rel}(\Delta\vec{k}) = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x,y,z) e^{2\pi i(hx+ky+lz)} dxdydz$
- $\rho(x,y,z) = \frac{1}{V} \int_{all\ \Delta\vec{k}} F_{rel}(\Delta\vec{k}) e^{-i\Delta\vec{k}\bullet(x\vec{a}+y\vec{b}+z\vec{c})} d(\Delta\vec{k})$
- $\rho(x,y,z) = \frac{1}{V} \int_{all\ \Delta\vec{k}} F_{hkl} e^{-2\pi i(hx+ky+lz)} d(\Delta\vec{k})$
- 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 $\rho(x, y)$

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

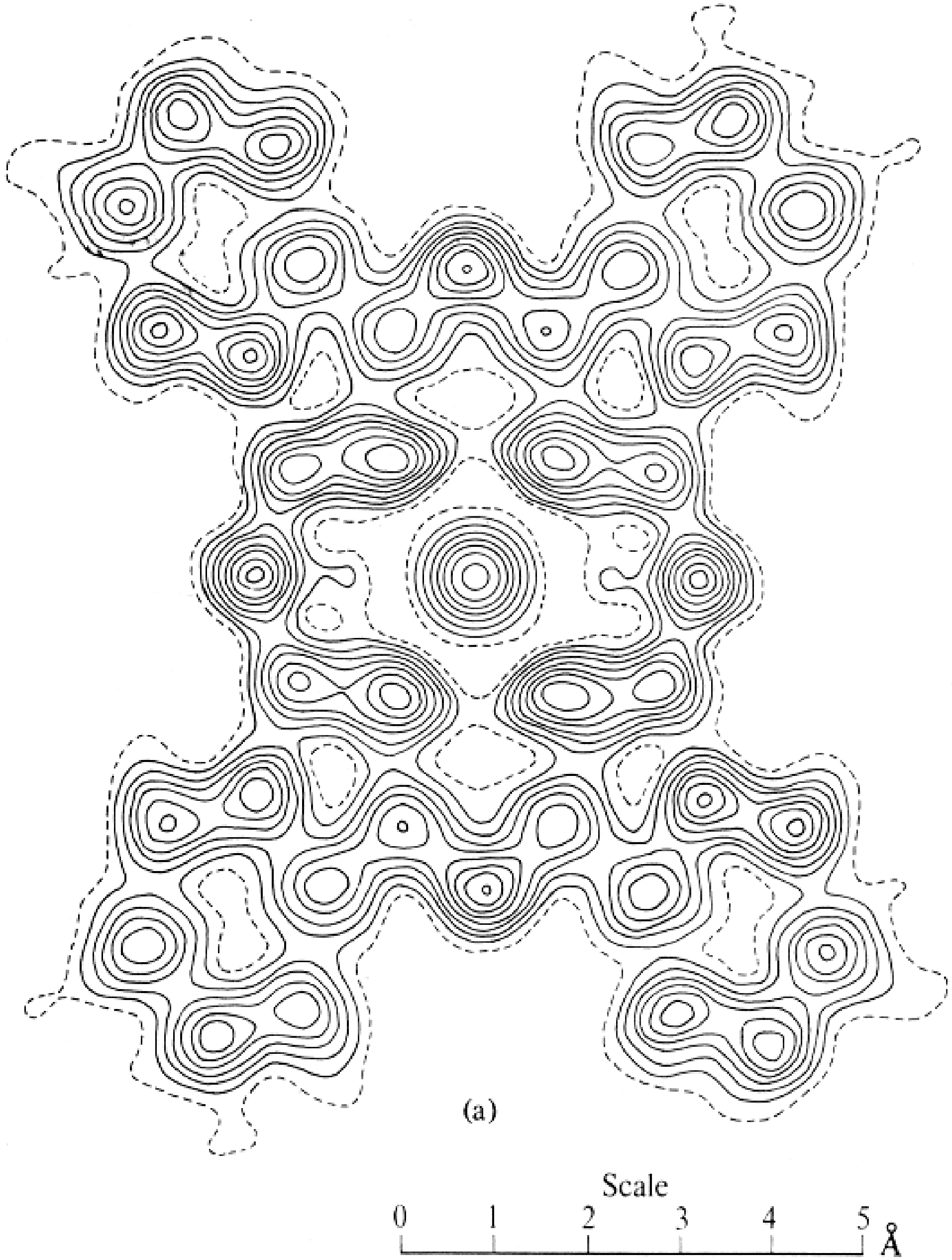
$$\rho(x, y, z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)}$$

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

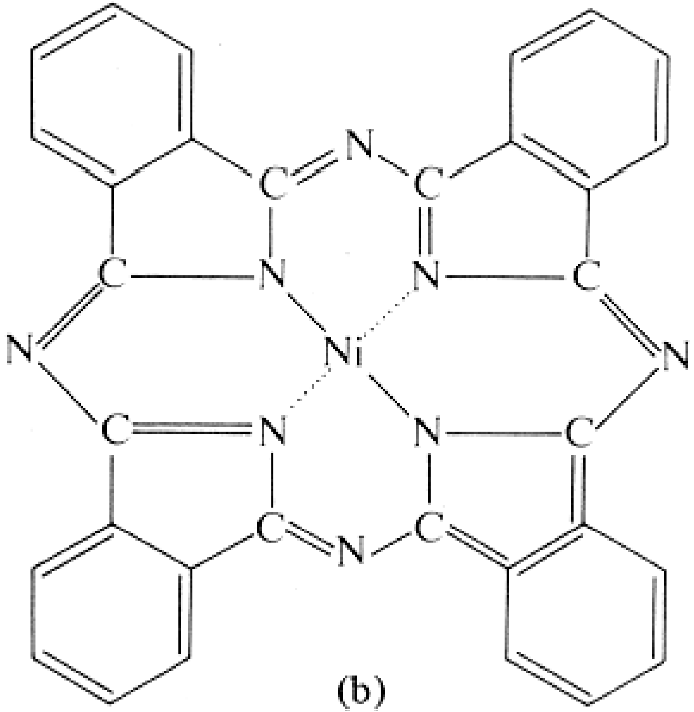
$$= \frac{1}{A} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky)} \int_0^1 e^{-2\pi ilz} dz \qquad \int_0^1 e^{-2\pi ilz} dz = \delta(l)$$

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

Electron Density Projections



(a)



(b)

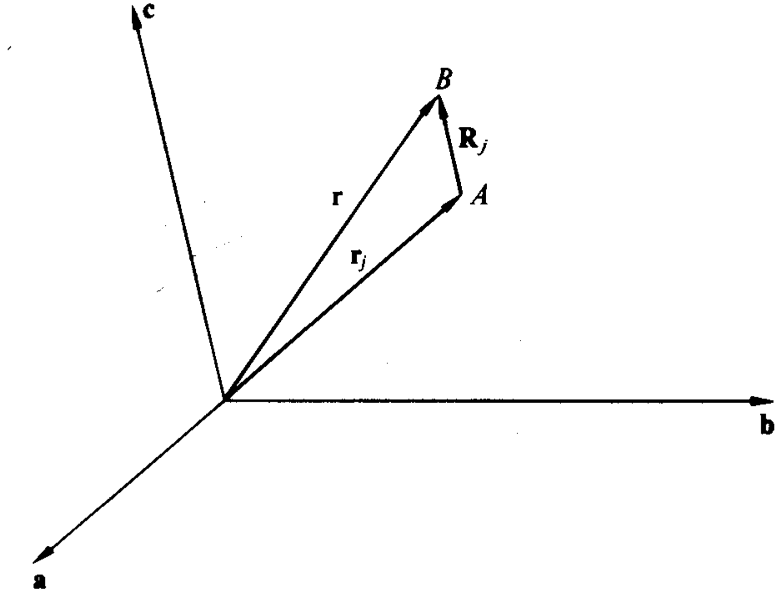
nickel phthalocyanine

Calculation of Structure Factor

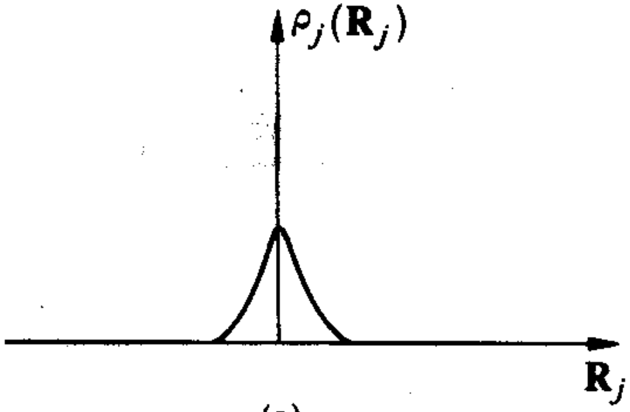
- $F_{hkl} = V \int_{x=0}^{x=1} \int_{y=0}^{y=1} \int_{z=0}^{z=1} \rho(x,y,z) e^{2\pi i(hx+ky+lz)} dxdydz$
- $\rho(x,y,z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx+ky+lz)}$
- only infer atomic position from the maxima in the electron density function
- alternatively, $\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$

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

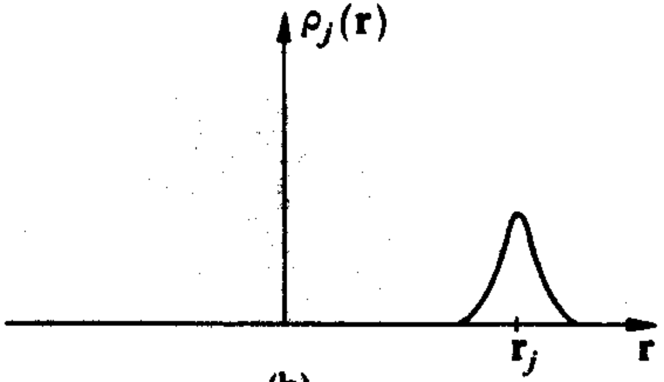
- $\vec{r} = \vec{r}_j + \vec{R}_j$



Calculation of Structure Factor



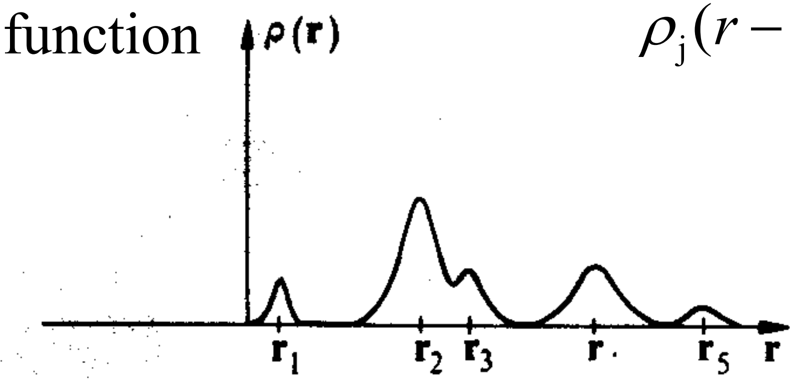
(a)



(b)

atomic electron density function

$$\rho_{\mathrm{j}}(\vec{r}-\vec{r}_j)$$



(c)

$$\rho(\vec{r}) = \sum_j \rho_{\mathrm{j}}(\vec{r}-\vec{r}_j)$$

Calculation of Structure Factor

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

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

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

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

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

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

Calculation of Structure Factor

- atomic scattering factor

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

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

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

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

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

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

Atomic Scattering Factor

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

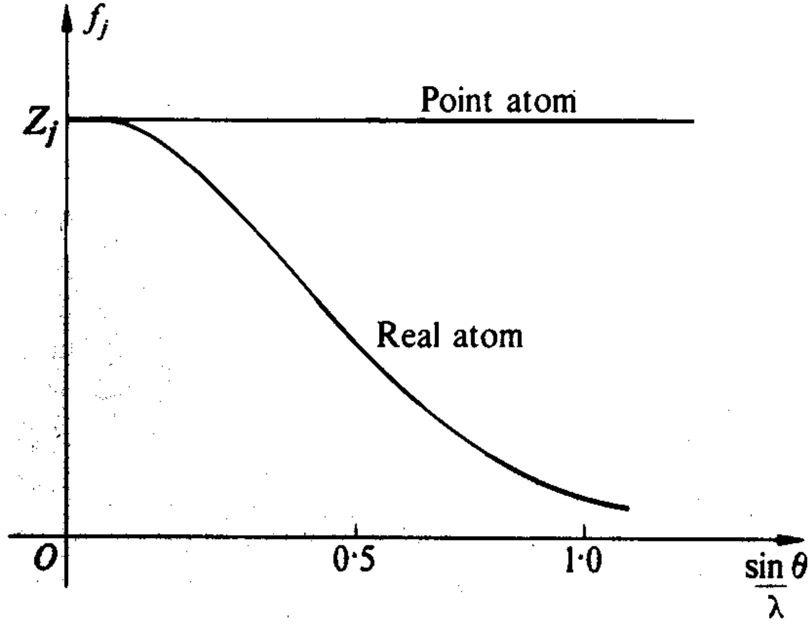
scattering ability of an atom as compared to that of a single electron (f_e)

- spherically symmetric

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

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

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



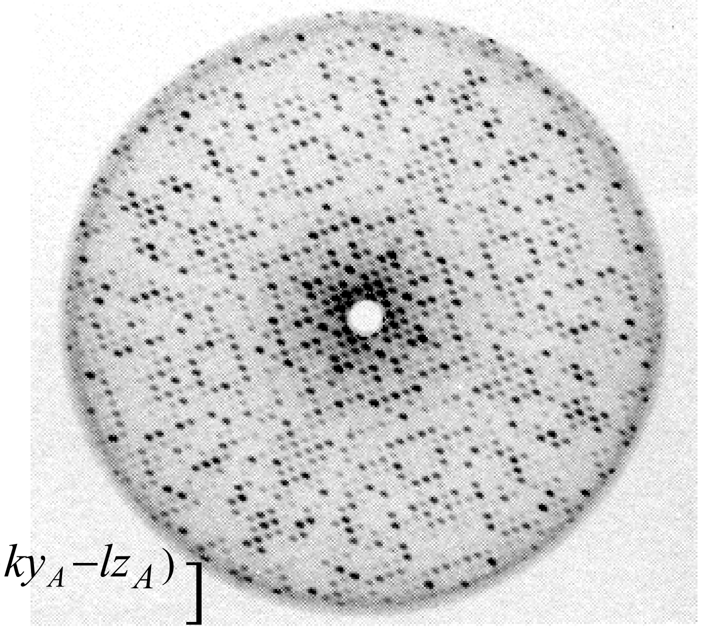
Atomic Scattering Factors

$\frac{\sin\theta}{\lambda}$ (Å^{-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 ↔ 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

$$(x_A, y_A, z_A)\ (x_A, y_A, \text{-}z_A)$$

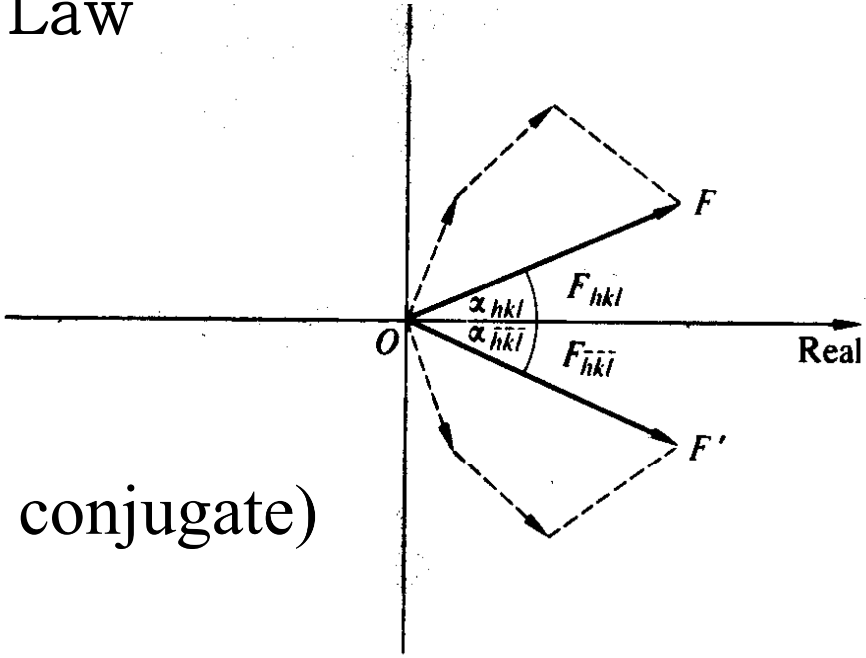
$$(F_{hkl})_A = f_A[e^{2\pi i(hx_A + ky_A + lz_A)} + e^{2\pi i(hx_A + ky_A - lz_A)}]$$

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

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

- mirror plane, rotation axis

Friedel's Law



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

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

- f_j is real, $F^*_{hkl} = F_{\overline{hkl}}$ (complex conjugate)

  $\left|F_{hkl}\right| = \left|F_{\overline{hkl}}\right|$

- 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, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$)

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

$$= f_j[1+e^{i\pi(h+k+l)}] = 2f_j \quad if\ h+k+l=2n$$

$$0 \quad if\ h+k+l=2n+1$$

- systematic absence or extinction
- a glide (|| (001))

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

$$F_{hkl} = f_j e^{2\pi i(hx+ky+lz)} + f_j e^{2\pi i[h(x+\frac{1}{2})+ky-lz)}$$

$$= f_j e^{2\pi i(hx+ky+lz)}[1+e^{i\pi h}e^{-4\pi ilz}]$$

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

Reciprocal lattice

- cubic I $a = b = c$

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

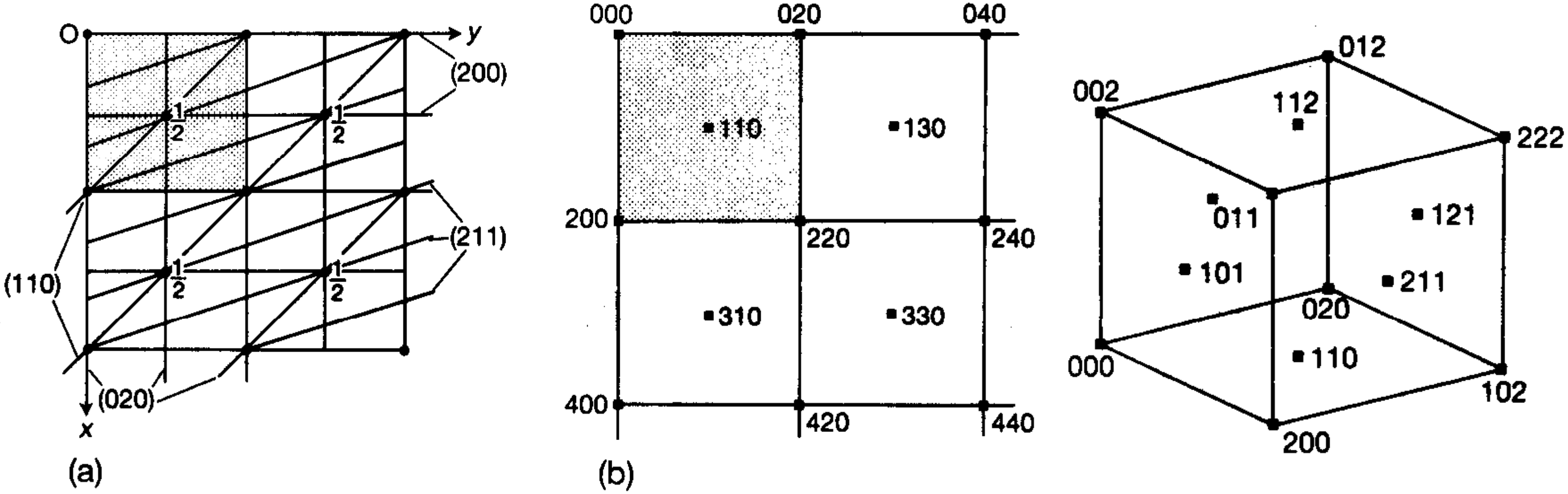


Fig. 6.4. (a) Plan of a cubic *I* crystal perpendicular to the *z*-axis and (b) pattern of reciprocal lattice points perpendicular to the *z*-axis. Note the cubic *F* arrangement of reciprocal lattice points in this plane.

Systematic Absence

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

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

$$+ f_j e^{2\pi i(h\frac{1}{2}+k\frac{1}{2}+l0)}$$

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

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

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

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

04-0836 Wavelength= 1.5405 *

Cu

Copper

Copper, syn

Rad.: CuKa1 λ: 1.5405 Filter: Ni Beta M d-sp:

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

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_8=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 H2 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, R3R%=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.

2θ	Int	h	k	l
43.295*	100	1	1	1
50.431*	46	2	0	0
74.127*	20	2	2	0
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

Systematic Absence

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

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

$$+ f_j e^{2\pi i(h\frac{1}{4}+k\frac{1}{4}+l\frac{1}{4})} + f_j e^{2\pi i(h\frac{1}{4}+k\frac{3}{4}+l\frac{3}{4})} + f_j e^{2\pi i(h\frac{3}{4}+k\frac{1}{4}+l\frac{3}{4})} + f_j e^{2\pi i(h\frac{3}{4}+k\frac{3}{4}+l\frac{1}{4})}$$

$$= f_j[1+e^{i\pi(k+l)} + e^{i\pi(h+l)} + e^{i\pi(h+k)}][1+e^{i\pi(h+k+l)/2}]$$

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

$if\ h,k,l$ unmixed $F_{hkl} = 4f_j$ (1 ± 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	o	x	x	oo	x	x	o	x

06-0675 Wavelength= 1.5405 *

C

Carbon

Diamond

Rad.: CuKa1 λ: 1.5405 Filter: Ni Beta ΦM 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.

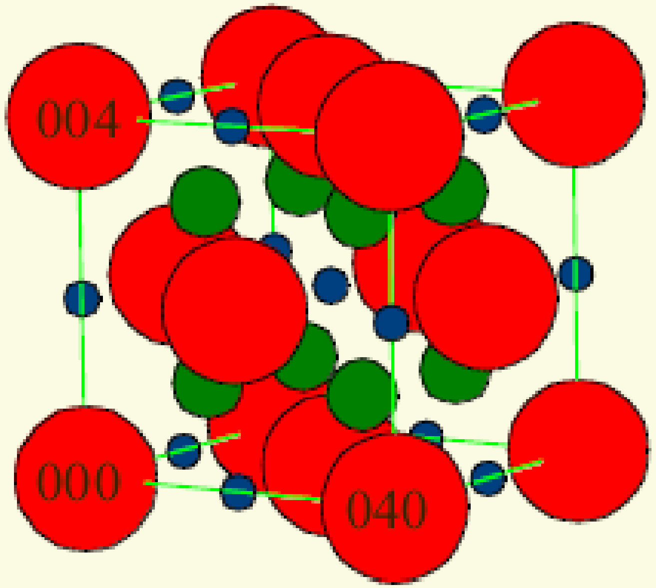
Dx: 3.517 Dm: 3.511 SS/FOM: F_5=73(.0115, 6)

εα: ηωβ: 2.4195 εγ: 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.

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

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
hkl		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	
	$h + l = 2n$	centred on the B face	B	
	$h + k = 2n$ $k + l = 2n$ $h + l = 2n$	centred on all faces	F	
	$-h + k + l = 3n$	rhombohedral, obverse	R	
	$h - k + l = 3n$	rhombohedral, reverse	R	
$hk0$	$h = 2n$	glide plane ‖ (001)	a	P, B, I
	$k = 2n$		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 ∥ (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 ∥ (010)	c	P, A, C
	$h + l = 2n$		n	P
	$h + l = 4n$		d	F, B
hhl	$l = 2n$	glide plane ∥ (110)	c	P, C, F
	$h = 2n$		b	C
	$h + l = 2n$		n	C
	$2h + l = 4n$		d	I
$00l$	$l = 2n$	screw axis ∥ c	$2_1, 4_2, 6_3$	
	$l = 3n$		$3_1, 3_2, 6_2, 6_4$	
	$l = 4n$		$4_1, 4_3$	
	$l = 6n$		$6_1, 6_5$	
$h00$	$h = 2n$	screw axis ∥ a	$2_1, 4_2$	
	$h = 4n$		$4_1, 4_3$	
$0k0$	$k = 2n$	screw axis ∥ b	$2_1, 4_2$	
	$k = 4n$		$4_1, 4_3$	
$hh0$	$h = 2n$	screw axis ∥ [110]	2_1	

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