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SPRING COLLEGE IN MATERIALS SCIENCE
ON
"CERAMICS AND COMPOSITE MATERIALS"
(17 April - 26 May 1989)

ELECTRON MICROSCOPY
(Lectures IV - VIII)

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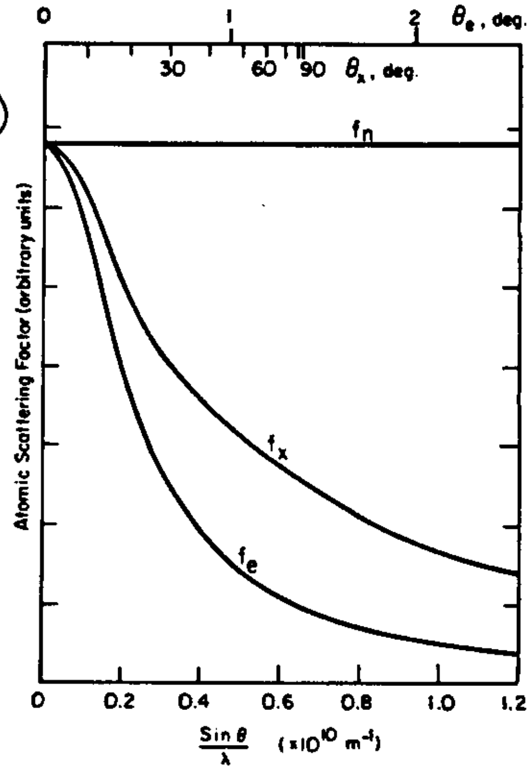
Electron Microscopy — Lecture 4 M. J. Goringe

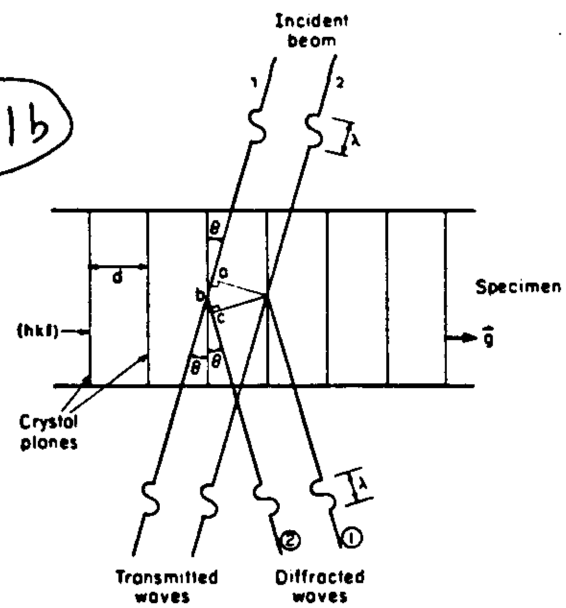
These are the diagrams used in this lecture.

4/1a



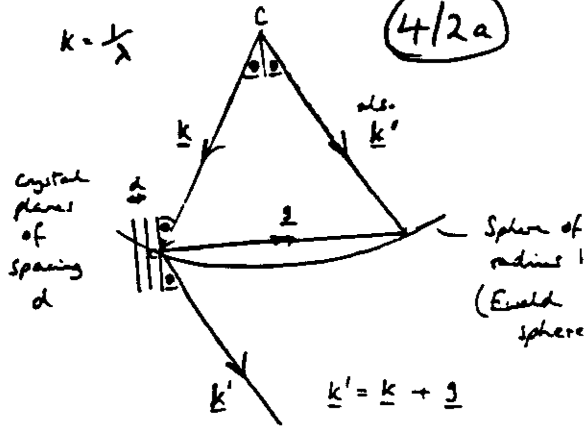
Schematic angular variation of the atomic scattering factors for electron, X-ray, and neutron diffraction. Note the differences in angular scale when plotted for typical wavelengths λ[(Cu K_α) for X-rays and neutrons, 0.037 A for electrons (100 keV)]. The three scattering factors have been arbitrarily scaled to coincide at zero scattering angle.

4/1b



Illustrating Bragg's law of scattering, for fast electrons and close-packed crystals, $\theta \simeq 1°$. The path difference between waves 1 and 2 is $abc = 2d\sin\theta$.

4/2a



$\underline{k}' = \underline{k} + \underline{g}$

If $\underline{g}$ is perpendicular to the planes

$$g = 2k\sin\theta$$

Now $k = 1/\lambda$ and if $g = 1/d$ then

$$\frac{1}{d} = 2\cdot\frac{1}{\lambda}\cdot\sin\theta$$

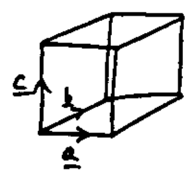
or $\lambda = 2d\sin\theta$

which is Braggs' Law again.

4/2b

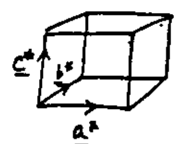
Real Lattice

cell $\underline{a}, \underline{b}, \underline{c}$



Reciprocal Lattice

$$\underline{a}^* = \frac{\underline{b} \wedge \underline{c}}{\underline{a}\cdot\underline{b}\wedge\underline{c}}$$



Properties

$$\underline{a}\cdot\underline{a}^* = \underline{b}\cdot\underline{b}^* = \underline{c}\cdot\underline{c}^* = 1$$

$$\underline{a}\cdot\underline{b}^*, \text{etc} = 0$$

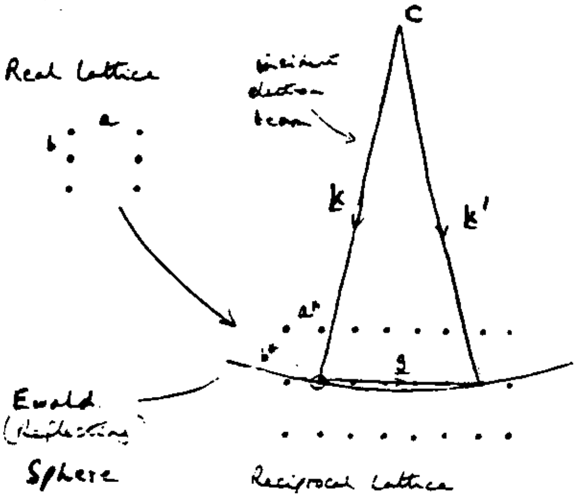
Vector $\underline{g} = h\underline{a}^* + k\underline{b}^* + l\underline{c}^*$ is perpendicular to planes (hkl) in the real crystal and is of magnitude

$$g = 1/d$$

where d is the interplanar spacing.

Reciprocal Lattice & Ewald Sphere

4/3

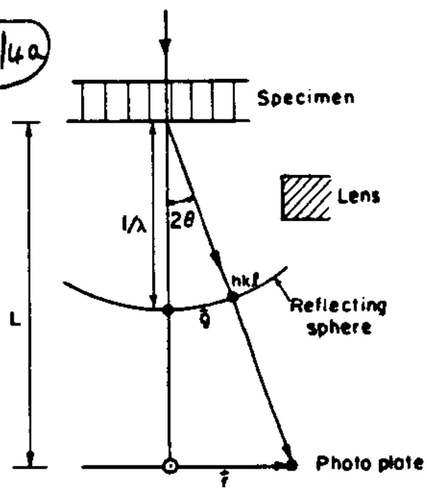


4/4b

Geometrical Structure Factor Rules for Basic Cells Containing Only One Kind of Atomic Species

Type of Crystal	Values	$F =$
Primitive	All h, k, l	f (1 atom per cell)
Body centered	$(h + k + l)$ even	$2f$ (2 atoms per cell)
Face centered	h, k, l unmixed	$4f$ (4 atoms per cell)
Base centered (e.g., ab face)	h, k, l unmixed	$2f$ (2 atoms per cell)
Hexagonal close-packed	$h + 2k = 3n$, l odd	0, e.g., 0001
	$h + 2k = 3n$, l even	$2f$, e.g., 0002
	$h + 2k = 3n \pm 1$, l odd	$\sqrt{3}\,f$, e.g., $01\bar{1}1$
	$h + 2k = 3n \pm 1$, l even	f, e.g., $01\bar{1}0$

4/4a



Schematic diagram of the formation of a diffraction pattern in the TEM, with effective camera length L.

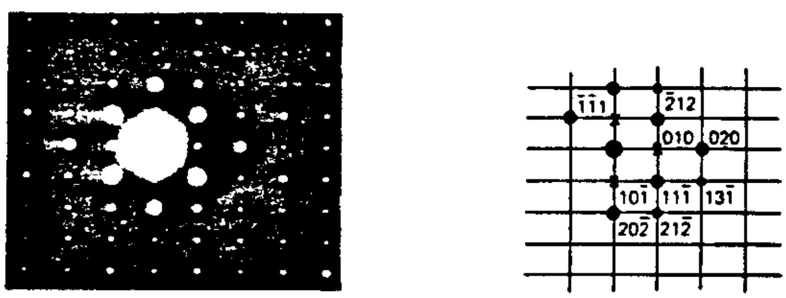
4/4c

Allowed $\{hkl\}$ Values for Cubic Crystals[a]

Bcc		Fcc		Dc		
$(h^2+k^2+l^2)$	hkl	$(h^2+k^2+l^2)$	hkl	$(h^2+k^2+l^2)$	hkl	$\sqrt{h^2+k^2+l^2}$
2	110					1.414
		3	111	3	111	1.732
4	200	4	200			2.000
6	211					2.449
8	220	8	220	8	220	2.828
10	310					3.162
		11	311	11	311	3.317
12	222	12	222			3.464
14	321					3.742
16	400	16	400	16	400	4.000
18	411					4.243
	330	19	331	19	331	4.359
20	420	20	420			4.472
22	332					4.690
24	422	24	422	24	422	4.899
26	431					5.099
	510	27	511, 333	27	511, 333	5.196
30	521					5.477
32	440	32	440	32	440	5.659

[a] All values of $(h^2+k^2+l^2)$ are possible except $4^p(8n+7)$, where p and n are integers including zero; thus, for example, 7, 15, and 23 are not possible.

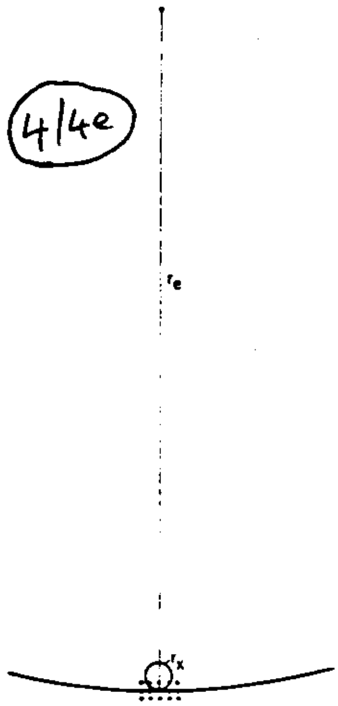
4/4d



(a) (b)

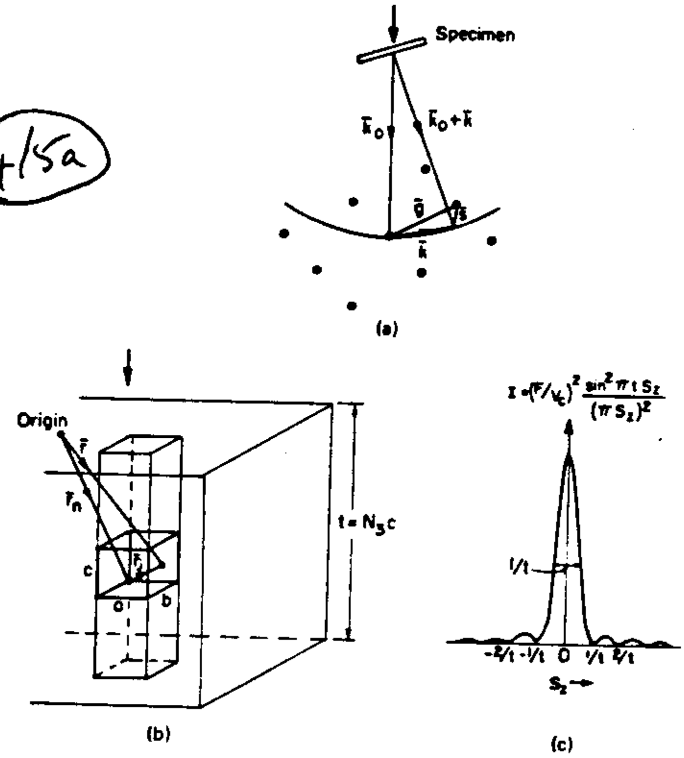
(*a*) Experimental diffraction pattern from anthracene (monoclinic $P_{21/a}$) for [101] orientation. Courtesy G. M. Parkinson. (*b*) Reciprocal lattice section relevant to (*a*) to illustrate "allowed" (·) and "forbidden" (x) diffraction spots. The size of the "allowed" spot is an indication of the strength of the reflection.

4/4e



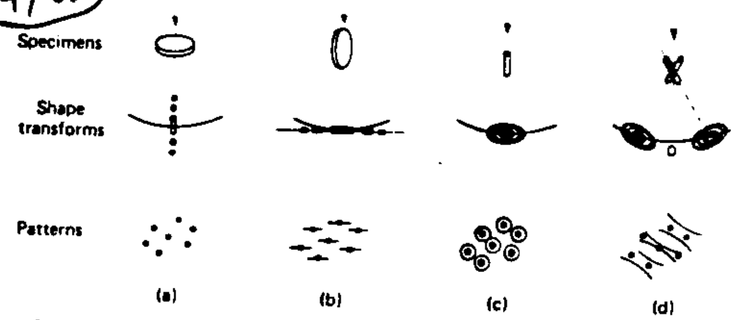
Illustrating the differences in scale of the Ewald sphere construction for conventional X-ray and electron diffraction.

4/5a



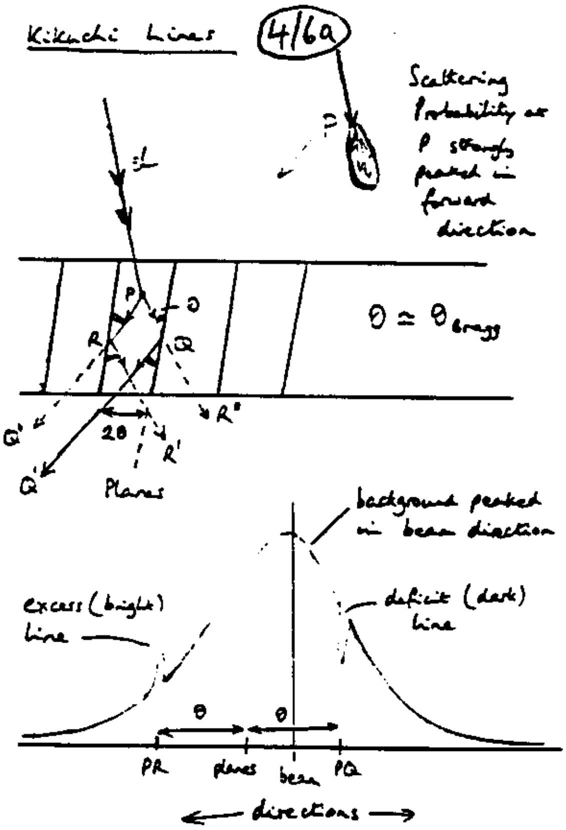
(*a*) Showing the relation between the reciprocal lattice and reflecting sphere when Bragg's law is not exactly satisfied. (*b*) Sketch of a column of unit cells in a parallelepiped crystal for calculating the interference function. (*c*) The interference function along the s_z direction, showing the kinematical intensity distribution for thin foils.

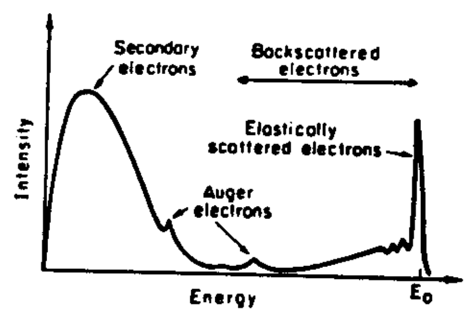
4/5b



Interference functions for crystals of small sizes, showing the effect of the shape factor on the diffraction pattern. Thin plates (*a*) normal to the beam and (*b*) parallel to the beam; needles (*c*) parallel to the beam and (*d*) inclined to the beam. Notice curved streaks in (*d*) (compare with Fig. 2.8).

Kikuchi Lines 4/6a



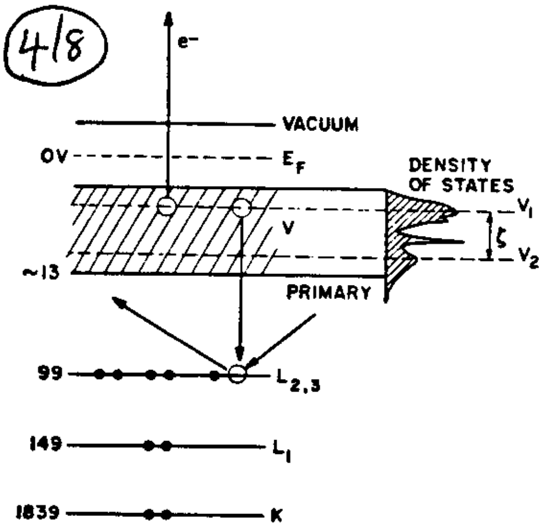


4/7b

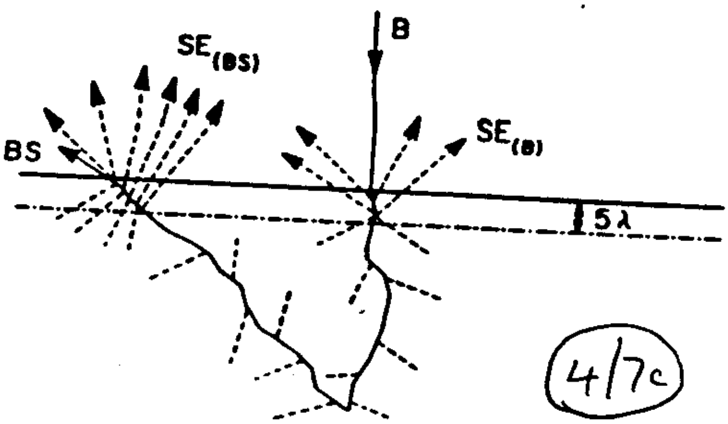
The energy spectrum of the electrons emitted from the specimen.

4/7a is fig 1.3

4/8



X-ray energy level diagram of silicon with the density of states drawn into the valence band. An $L_{2,3}VV$ Auger process is depicted.



4/7c

Secondary electron generation.

WXY notation

W – level of first ejected electron

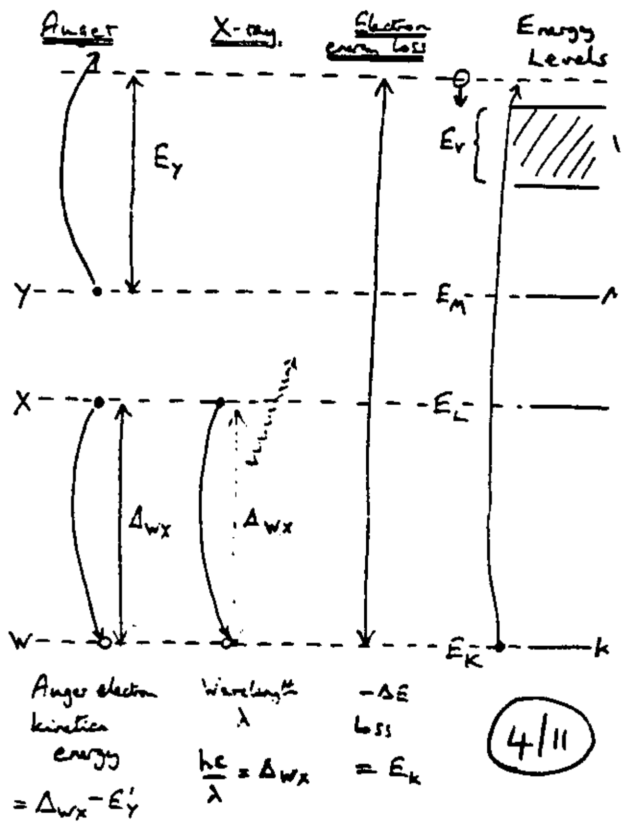
X – level from which second electron drops

Y – level from which Auger electron ejected

$$K.E.\ Auger = E_W - E_X - E_Y^{corr}$$

X-ray $\quad E = hc/\lambda = E_W - E_X$

Primary electron energy loss $\quad -\Delta E^{min} = E_W$



Electron Diffraction and Contrast Theory M.J. Goringe

The sheets of equations contain all the equations which are relevant to lectures 5–8 (but not all of them will be used!). The reference numbers are

(4·n) } as in book by Thomas & Goringe "Transmission Electron Microscopy of Materials"
(5·n) }

(6·n) are for high resolution work.

Many of the overhead projector sheets and slides will also be available later in a set of duplicated sheets.

$$\chi = \sqrt{\frac{2mE_0}{h^2}} \quad , \quad \chi_L = \sqrt{\frac{2m(E_0 + eV)}{h^2}} \qquad (4.1)$$

Reflected amplitude $A = \dfrac{\chi - \chi_L}{\chi + \chi_L} \simeq \dfrac{-eV}{4E_0}$ (4.2)

$$\chi_L \simeq \chi\left(1 + \frac{eV}{2E_0}\right) = \chi + \frac{m_0 eV}{h^2 \chi} \qquad (4.3)$$

$$\psi_i = \phi_0 \exp(2\pi i \underline{\chi} \cdot \underline{r})$$

$$\psi_e = \phi_0 \exp(2\pi i \underline{\chi} \cdot \underline{r}') \exp\left[\frac{2\pi i m_0 e V(\underline{r})\, dz}{h^2 \chi}\right] \qquad (4.4)$$

where $\underline{r}' = \underline{r} + dz$

PG integral

$$\psi_e(x,y\,t) = \phi_0 \exp(2\pi i \underline{\chi} \cdot \underline{r}') \exp\left[\frac{2\pi i m_0 e}{h^2 \chi} \int_0^t V(x,y,z)\, dz\right] \qquad (4.5)$$

valid for $t_{max} < h^2 \chi / 2\pi m_0 eV$ (4.6)

$$\psi_e(x,y,\Delta z) = \phi_0 \exp(2\pi i \underline{\chi} \cdot \underline{r}') \exp\left[\frac{2\pi i m_0 e}{h^2 \chi} \overline{V}_z(x,y)\, \Delta z\right]$$

$$= \phi_0 \exp(2\pi i \underline{\chi} \cdot \underline{r}')\left[1 + \frac{2\pi i m_0 e}{h^2 \chi} \overline{V}_z(x,y)\, \Delta z\right] \qquad (4.7)$$

Set $\overline{V}_z(x,y) = \sum_g (V_g + iV_g') \exp(2\pi i \underline{g} \cdot \underline{r})$ (4.8)

$$\psi_e(x,y,\Delta z) = \phi_0 \exp(2\pi i \underline{\chi} \cdot \underline{r}') + \phi_0 \left(\frac{2\pi i m_0 e \Delta z}{h^2 \chi}\right) \times$$

$$\times \sum_g (V_g + iV_g') \exp\left[2\pi i (\underline{\chi} + \underline{g}) \cdot \underline{r}\right] \qquad (4.9)$$

$$\Delta \phi_g \exp(2\pi i \underline{\chi}_g \cdot \underline{r}) = \phi_0 \left(\frac{2\pi i m_0 e}{h^2 \chi}\right) \Delta z (V_g + iV_g') \exp\left[2\pi i (\underline{\chi} + \underline{g}) \cdot \underline{r}\right] \qquad (4.10)$$

$$\underline{\chi}_g - \underline{\chi} = \underline{g} + \underline{s}_g \qquad (4.11)$$

$$\frac{d\phi_g}{dz} = \pi\left(\frac{i}{\xi_g} - \frac{1}{\xi_g'}\right) \phi_0 \exp(-2\pi i s_g z) \qquad (4.12)$$

where $\xi_g = \dfrac{h^2 \chi}{2m_0 eV_g}$, $\xi_g' = \dfrac{h^2 \chi}{2m_0 eV_g'}$ (4.13)

$$\frac{d\phi_0}{dz} = \pi\left(\frac{i}{\xi_0} - \frac{1}{\xi_0'}\right) \phi_0 \qquad (4.14)$$

Zero absorption ($\xi_g' \to \infty$), integration of (4.12) yields the kinematical integral for perfect crystal:

$$\phi_g = \phi_0 \left(\frac{\pi i}{\xi_g}\right) \int_0^t \exp(-2\pi i s_g z)\, dz$$

$$= \phi_0 \left(\frac{\pi i}{\xi_g}\right) \exp(-\pi i t s_g) \frac{\sin \pi s_g t}{\pi s_g}$$

Intensities $\dfrac{I_g}{I_0} = \dfrac{\pi^2 \sin^2 \pi s t}{\xi_g^2 (\pi s)^2}$ (4.15)

Comparison with X-ray scattering yields

$$\xi_g = \frac{h^2 \chi}{2m_0 eV_g} = \frac{\pi V_c}{F_g} \qquad (4.16)$$

where V_c = unit cell volume, F_g = (atomic) scattering factor

$$V(\underset{\sim}{r}) = \sum_g (V_g + iV_g') \exp\left[2\pi i \underset{\sim}{g}.(\underset{\sim}{r} - \underset{\sim}{R})\right] \qquad (4.17)$$

$$\text{Eq}(4.12) \Rightarrow \frac{d\phi_g}{dz} = \pi\left(\frac{i}{\xi_g} - \frac{1}{\xi_g'}\right)\phi_0 \exp\left[-2\pi i(s_0 z + \underset{\sim}{g}.\underset{\sim}{R})\right] \qquad (4.18)$$

Kinematical Integral for Imperfect Crystal:

$$\phi_g = \int_0^t \left(\frac{\phi_0 \pi i}{\xi_g}\right) \exp\left[-2\pi i(sz + \underset{\sim}{g}.\underset{\sim}{R})\right] dz \qquad (4.19)$$

$$\left.\begin{aligned} \frac{d\phi_0}{dz} &= \pi\left(\frac{i}{\xi_0} - \frac{1}{\xi_0'}\right)\phi_0 + \pi\phi_g\left(\frac{i}{\xi_g} - \frac{1}{\xi_g'}\right)\exp\left[2\pi i(sz + \underset{\sim}{g}.\underset{\sim}{R})\right] \\ \frac{d\phi_g}{dz} &= \pi\left(\frac{i}{\xi_g} - \frac{1}{\xi_g'}\right)\phi_0 \exp\left[-2\pi i(sz + \underset{\sim}{g}.\underset{\sim}{R})\right] + \pi\left(\frac{i}{\xi_0} - \frac{1}{\xi_0'}\right)\phi_g \end{aligned}\right\} \quad (4.20)$$

Transform $\phi_0 \rightarrow \phi_0 \exp(\pi i z/\xi_0)$

$$\phi_g \rightarrow \phi_g \exp\left(\pi i z/\xi_0 - 2\pi i s z - 2\pi i \underset{\sim}{g}.\underset{\sim}{R}\right)$$

$$\left.\begin{aligned} \frac{d\phi_0}{dz} &= -\frac{\pi}{\xi_0'}\phi_0 + \pi\left(\frac{i}{\xi_g} - \frac{1}{\xi_g'}\right)\phi_g \\ \frac{d\phi_g}{dz} &= \pi\left(\frac{i}{\xi_g} - \frac{1}{\xi_g'}\right)\phi_0 + \pi\left[2i(s + \beta_g') - \frac{1}{\xi_0'}\right]\phi_g \end{aligned}\right\} \quad (4.21)$$

where $\beta_g' = \underset{\sim}{g} \cdot \dfrac{d\underset{\sim}{R}}{dz}$ (4.22)

Try $\phi_{0,g}$ of form $\exp\left[2\pi i(\gamma_{re} + i\gamma_{im})z\right]$

$$\gamma_{re}^{(1)(2)} = \frac{w \pm \sqrt{1 + w^2}}{2\xi_g} \qquad (4.23)$$

$$\gamma_{im}^{(1)(2)} = \frac{1}{2\xi_0'} \pm \frac{1}{2\xi_g'\sqrt{1 + w^2}} \qquad (4.24)$$

where $w = s\xi_g$ (4.25)

$$\phi_0 = D_0^{(1)} \exp(2\pi i \gamma^{(1)} z) + D_0^{(2)} \exp(2\pi i \gamma^{(2)} z) \qquad (4.26)$$

$$\phi_g = D_g^{(1)} \exp(2\pi i \gamma^{(1)} z) + D_g^{(2)} \exp(2\pi i \gamma^{(2)} z) \qquad (4.27)$$

$$D_g^{(1)}/D_0^{(1)} = 2\gamma^{(1)}\xi_g = w + \sqrt{1 + w^2} \qquad (4.28)$$

$$D_g^{(2)}/D_0^{(2)} = 2\gamma^{(2)}\xi_g = w - \sqrt{1 - w^2} \qquad (4.29)$$

$$\text{At } z = 0 \quad \left.\begin{aligned} \phi_0(0) &= 1 = D_0^{(1)} + D_0^{(2)} \\ \phi_g(0) &= 0 = D_g^{(1)} + D_g^{(2)} \end{aligned}\right\} \quad (4.30)$$

Substitute $w = \cot\beta$ (4.31)

$$\left.\begin{aligned} D_0^{(1)} &= \sin^2 \beta/2, \quad D_0^{(2)} = \cos^2 \beta/2 \\ D_g^{(1)} &= \sin\tfrac{\beta}{2}\cos\tfrac{\beta}{2}, \quad D_g^{(2)} = -\sin\tfrac{\beta}{2}\cos\tfrac{\beta}{2} \end{aligned}\right\} \quad (4.32)$$

$$\phi_0(z) = \left[\sin^2\tfrac{\beta}{2}\exp(iXz) + \cos^2\tfrac{\beta}{2}\exp(-iXz)\right]\exp\left(-\frac{\pi z}{\xi_0'}\right) \qquad (4.33)$$

$$\phi_g(z) = \left[\exp(iXz) - \exp(-iXz)\right]\sin\tfrac{\beta}{2}\cos\tfrac{\beta}{2}\exp\left(-\frac{\pi z}{\xi_0'}\right) \qquad (4.34)$$

where $$X = \frac{\pi\sqrt{1 + w^2}}{\xi_g} + \frac{\pi i}{\xi_g'\sqrt{1 + w^2}} \qquad (4.35)$$

$$\Psi(\underline{r}) = \phi_o \exp(2\pi i \underline{\chi}.\underline{r}) + \phi_g \exp(2\pi i \underline{\chi}_g.\underline{r})$$

ϕ_o, ϕ_g from eqs (4.26), (4.27) ; $\underline{\chi}_g = \underline{\chi} + \underline{g}$

Set $D_o^{(j)} = \varepsilon^{(j)} C_o^{(j)}$; $D_g^{(j)} = \varepsilon^{(j)} C_g^{(j)}$, $j = 1,2$ (4.36)

$$\Psi(\underline{r}) = \varepsilon^{(1)}\left[C_o^{(1)} \exp(2\pi i \underline{k}_{xy}^{(1)}.\underline{r}_{xy}) + C_g^{(1)} \exp(2\pi i(\underline{k}_{xy}^{(1)}+\underline{g}).\underline{r}_{xy})\right]\exp(2\pi i k_z^{(1)} z)$$
$$+ \varepsilon^{(2)}\left[C_o^{(2)} \exp(2\pi i \underline{k}_{xy}^{(2)}.\underline{r}_{xy}) + C_g^{(2)} \exp(2\pi i(\underline{k}_{xy}^{(2)}+\underline{g}).\underline{r}_{xy})\right]\exp(2\pi i k_z^{(2)} z) \quad (4.37)$$

[ ] Bloch waves, normalised by $(C_o^{(j)})^2 + (C_g^{(j)})^2 = 1$ (4.38)

$$\left.\begin{aligned} \varepsilon^{(1)} = C_o^{(1)} = -C_g^{(2)} = \sin \beta/2 \\ \varepsilon^{(2)} = C_o^{(2)} = C_g^{(1)} = \cos \beta/2 \end{aligned}\right\} \quad (4.39)$$

$$\Psi(\underline{r}) = \sum_{j=1,2} b^{(j)} \varepsilon^{(j)} \exp(2\pi i \gamma^{(j)} z) \quad (4.40)$$

$$\phi_o(z) = \sum_j \varepsilon^{(j)} C_o^{(j)} \exp(2\pi i \gamma^{(j)} z) \quad (4.41)$$

$$\phi_g(z) = \sum_j \varepsilon^{(j)} C_g^{(j)} \exp(2\pi i \gamma^{(j)} z) \quad (4.42)$$

$$\Delta\gamma = \frac{\sqrt{1+w^2}}{\xi_g} = \frac{1}{\Delta z} = \frac{1}{\xi^{eff}} \quad (4.43)$$

At reflecting position : $k_{xy}^{(1)} = k_{xy}^{(2)} = -\frac{g}{2}$, $\beta = \frac{\pi}{2}$

$$b^{(1)} = \sin\frac{\beta}{2}\exp(-\pi i \underline{g}.\underline{r}) + \cos\frac{\beta}{2}\exp(\pi i \underline{g}.\underline{r})$$
$$= \sqrt{2}\cos \pi \underline{g}.\underline{r}$$
$$b^{(2)} = i\sqrt{2}\sin \pi \underline{g}.\underline{r}$$

Eq (4.20) generalises to n beams, $k = 1,2,\ldots n$

$$\frac{d\phi_k}{dz} = \sum_{j=1}^{n} \pi\left(\frac{i}{\xi_{\Delta g}} - \frac{1}{\xi'_{\Delta g}}\right)\phi_j \exp\left[-2\pi i(\Delta s_g z + \Delta \underline{g}.\underline{R})\right] \quad (4.44)$$

where $\Delta \underline{g} = \underline{g}_k - \underline{g}_j$ and $\Delta s_g = s_{gk} - s_{gj}$

$$\nabla^2\Psi(\underline{r}) + \left(\frac{8\pi^2 m}{h^2}\right)\left[E + V(\underline{r})\right]\Psi(\underline{r}) = 0 \quad (4.45)$$

$$V(\underline{r}) = \frac{h^2}{2me}\sum_g U_g \exp(2\pi i \underline{g}.\underline{r}) = \sum_g V_g \exp(2\pi i \underline{g}.\underline{r}) \quad (4.46)$$

$$\left.\begin{aligned} m &= \frac{m_o}{\sqrt{1-v^2/c^2}} = m_o\left(1 + \frac{E_o}{m_o c^2}\right) \\ E &= \frac{E_o(1 + E_o/2m_oc^2)}{1 + E_o/m_oc^2} \end{aligned}\right\} \quad (4.47)$$

$$\chi = \sqrt{2m_o E_o(1 + E_o/2m_oc^2)}/h$$

Real potential, centrosymmetric crystal

$$U_g = U_{-g} = U_g^* \quad (4.48)$$

Bloch wave solution :

$$\Psi(\underline{r}) = b(\underline{k},\underline{r}) = \sum_g C_g(\underline{k})\exp\left[2\pi i(\underline{k}+\underline{g}).\underline{r}\right] \quad (4.49)$$

$$\left[K^2 - (\underline{k}+\underline{g})^2\right]C_g(k) + \sum_{h\neq 0} U_h C_{g-h}(k) = 0 \quad (4.50)$$

$$K^2 = (2mE/h^2) + U_o \quad (4.51)$$

$$\left[\begin{aligned} (K^2 - k^2)C_o(k) + U_{-g}C_g(k) = 0 \quad (4.52) \\ U_g C_o(k) + [K^2 - (\underline{k}+\underline{g})^2]C_g(k) = 0 \quad (4.53) \end{aligned}\right.$$

$$(K^2 - k^2)[K^2 - (k+g)^2] = U_g U_{-g}$$

$$\left(K_z^2 - k_z^2\right)\left[\left(K_z^2 - k_z^2\right) - g\left(2k_{xy} + g\right)\right] = U_g U_{-g} \qquad (4.54)$$

$$\left(K_z - k_z\right)\left[K_z - k_z - \frac{g(2k_{xy}+g)}{2K_z}\right] = \frac{U_g^2}{4K_z^2} \qquad (4.55)$$

At reflecting position $k_{xy} = -g/2$, so

$$\left(K_z - k_z\right)^2 = U_g^2 / 4K_z^2$$

and, since $K_z = K\cos\theta_B$

$$k_z = K_z \pm U_g/(2K\cos\theta_B) \qquad (4.56)$$

i.e. $\Delta k_z = U_g / K\cos\theta_B = 1/\xi_g$, since

$$\xi_g = \frac{K\cos\theta_B}{U_g} \simeq \frac{K}{U_g} \qquad (4.57)$$

For general orientation $\quad s = \dfrac{-g(2k_{xy}+g)}{2K_z} \qquad (4.58)$

Thus $\quad k_z^{(1)(2)} = K_z + \dfrac{s \pm \sqrt{s^2 + U_g^2/K_z^2}}{2}$

or $\quad k_z^{(1)(2)} = K_z + \frac{1}{2}\left(s \pm \sqrt{s^2 + 1/\xi_g^2}\right) \qquad (4.59)$

$$\Delta k = k_z^{(1)} - k_z^{(2)} = \sqrt{1+w^2}/\xi_g$$

$$\frac{C_g^{(1)(2)}}{C_0^{(1)(2)}} = w \pm \sqrt{1+w^2} \qquad \text{as before}$$

$$\left[(K_z - k_z) - \frac{g(2k_{xy}+g)}{2K_z}\right]C_g + \sum_{h\neq 0}\frac{U_h C_{g-h}}{2K_z} = 0 \qquad (4.60)$$

But $K_z - k_z = -\gamma$ (say), $-g(2k_{xy}+g)/2K_z = s_g$, so

$$(s_g - \gamma)C_g + \sum_{h\neq 0}\frac{U_h C_{g-h}}{2K\cos\theta} = 0$$

$s_g = 0$ for $g = 0$

$$\underline{\underline{A}}\,\underline{C}^{(i)} = \gamma^{(i)}\underline{C}^{(i)}, \quad i = 1,2,\ldots n \qquad (4.61)$$

$$A_{00} = 0, \quad A_{gg} = s_g, \quad A_{gh} = \frac{U_{g-h}}{2K\cos\theta_{gh}} \qquad (4.62)$$

$$\text{or} \quad A_{gh} = \frac{1}{2\xi_{g-h}} \qquad (4.63)$$

For centrosymmetric crystal $\quad U_{g-h} = U_{h-g} \quad \therefore \tilde{\underline{\underline{A}}} = \underline{\underline{A}}$

U_{g-h} real $\quad \therefore \underline{\underline{A}}^* = \underline{\underline{A}}$

Thus $\underline{\underline{A}}$ is real, symmetric $\therefore$ eigenvectors $\underline{C}^{(i)}$ are real, orthogonal.

Absorption; eq (4.60) becomes

$$\left[K^2 - (\underline{k}+\underline{g})^2 + iU_0'\right]C_g(\underline{k}) + \sum_{h\neq 0}\left(U_h + iU_h'\right)C_{g-h}(\underline{k}) = 0$$

$U_h' \ll U_h \quad \therefore$ eq (4.61) stands, but with (4.62) becoming

$$A_{00} = \frac{i}{2\xi_0'}, \quad A_{gg} = s_g + \frac{i}{2\xi_0'}, \quad A_{gh} = \frac{1}{2\xi_{g-h}} + \frac{i}{2\xi_{g-h}'} \qquad (4.64)$$

Complex matrix $\underline{\underline{A}}$ can be solved, but usually perturbation instead

$$\underline{\underline{A}}_{re}\,\underline{C}^{(i)} = \gamma_{re}^{(i)}\underline{C}^{(i)}, \quad i = 1,2\ldots n \qquad (4.65)$$

$$\gamma_{im}^{(i)} = \tilde{\underline{C}}^{(i)}\underline{\underline{A}}_{im}\underline{C}^{(i)}, \quad i = 1,2\ldots n \qquad (4.66)$$

$$\underline{\phi} = \underline{\underline{C}}\,\underline{\varepsilon} \qquad (4.67)$$

i.e. $\quad \underline{\varepsilon} = \underline{\underline{C}}^{-1}\underline{\phi} = \tilde{\underline{\underline{C}}}\,\underline{\phi} \quad$ or $\quad \varepsilon^{(i)} = C_0^{(i)} \qquad (4.68)$

Bloch's theorem: $\quad \gamma^{(i)}(\underline{k}+\underline{G}) = \gamma^{(i)}(\underline{k})$

$$b'(\underline{k}+\underline{G}, \underline{r}) = b'(\underline{k}, \underline{r})$$

$$\sum C_g'(\underline{k}+\underline{G})\exp\left[2\pi i(\underline{k}+\underline{G}+\underline{g})\cdot\underline{r}\right] = \sum C_g(\underline{k})\exp\left[2\pi i(\underline{k}+\underline{g})\cdot\underline{r}\right]$$

$$C_g'(\underline{k}+\underline{G}) = C_{g+G}(\underline{k})$$

Eqs (4.41) & (4.42) rewritten

$$\begin{pmatrix} \phi_0(z) \\ \phi_g(z) \end{pmatrix} = \begin{pmatrix} C_0^{(1)} & C_0^{(2)} \\ C_g^{(1)} & C_g^{(2)} \end{pmatrix} \begin{pmatrix} \exp(2\pi i \gamma^{(1)} z) & 0 \\ 0 & \exp(2\pi i \gamma^{(2)} z) \end{pmatrix} \begin{pmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \end{pmatrix} \quad (5.1)$$

and eq (4.36) ⇒

$$\begin{pmatrix} C_0^{(1)} & C_0^{(2)} \\ C_g^{(1)} & C_g^{(2)} \end{pmatrix} \begin{pmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \end{pmatrix} = \begin{pmatrix} \phi_0(0) \\ \phi_g(0) \end{pmatrix} \quad (5.2)$$

Combining $\underline{\phi}(z) = \underline{\underline{C}} \{\exp(2\pi i \gamma z)\} \underline{\underline{C}}^{-1} \underline{\phi}(0)$ (5.3)

where $\underline{\underline{C}}$ is the matrix of $C_{0,g}^{(i)}$ and $\{\ \}$ the diagonal matrix.

Scattering matrix $\underline{\underline{P}} = \underline{\underline{C}} \{\ \} \underline{\underline{C}}^{-1}$ (5.4)

Confirm two pieces of perfect crystal t_1, t_2

$$\underline{\phi}(t) = \underline{\phi}(t_1 + t_2) = \underline{\underline{P}}(t_2)\, \underline{\underline{P}}(t_1)\, \underline{\phi}(0) \quad (5.5)$$

Faulted crystal; Bloch waves become

$$b^{(j)}(\underline{k}^{(j)} . \underline{r}) = \sum_g C_g^{(j)} \exp[2\pi i (\underline{k}^{(j)} + \underline{g}) . (\underline{r} - \underline{R})]$$

$$= \exp(-2\pi i\, \underline{k}^{(j)} . \underline{R}) \sum_g C_g^{(j)} \exp[2\pi i (\underline{k}^{(j)} + \underline{g}) . \underline{r}] . \exp(-2\pi i\, \underline{g} . \underline{R}) \quad (5.6)$$

…41), (4.42), (4.36), $C_g \rightarrow C_g{}' = C_g \exp(-i\alpha)$, $\alpha = 2\pi\, \underline{g} . \underline{R}$

Thus $\underline{\phi}(t) = \underline{\underline{P}}'(t_2)\, \underline{\underline{P}}(t_1)\, \underline{\phi}(0)$ (5.7)

Define $F^{+} = \begin{pmatrix} 1 & 0 \\ 0 & \exp(i\alpha) \end{pmatrix}$ (5.8)

$$\underline{\phi}(t) = \underline{\underline{F}}^{-} \underline{\underline{P}}(t_2) \underline{\underline{F}}^{+} \underline{\underline{P}}(t_1)\, \underline{\phi}(0) \quad (5.9)$$

Many faults $\underline{\phi}(t) = \underline{\underline{F}}_n^{-1} \underline{\underline{P}}_n \underline{\underline{F}}_n^{+} \underline{\underline{F}}_{n-1}^{-} \underline{\underline{P}}_{n-1} \underline{\underline{F}}_{n-1}^{+} \ldots\ldots \underline{\underline{F}}_2^{+} \underline{\underline{P}}_1 \underline{\phi}(0)$

Rewrite $\underline{\underline{F}}_j^{+} \underline{\underline{F}}_{j-1}^{-} = \underline{\underline{F}}_{jk}$, $j = k+1$ (5.10)

$$\underline{\phi}(t) = \underline{\underline{F}}_n^{-} \underline{\underline{P}}_n \underline{\underline{F}}_{n,n-1} \ldots \underline{\underline{F}}_{32} \underline{\underline{P}}_2 \underline{\underline{F}}_{21} \underline{\underline{P}}_1 \underline{\phi}(0) \quad (5.11)$$

$$\underline{\phi}' = \underline{\underline{A}}\, \underline{\phi} \quad (5.12)$$

$$\underline{\phi}(z + \Delta z) = \underline{\underline{P}}(s + \beta_g', \Delta z)\, \underline{\phi}(z)$$

eqs (4.37) and (5.6) ⇒ upper crystal (1) matching lower crystal (2)

$$\sum_j \varepsilon_1^{(j)} \sum_g C_g^{(j)} \exp[2\pi i (\underline{k} + \underline{g}) . \underline{r}] \exp(2\pi i \gamma^{(j)} t_1)$$

$$= \sum_j \varepsilon_2^{(j)} \sum_g C_g^{(j)} \exp(-i\alpha_{12}) \exp[2\pi i (\underline{k} + \underline{g}) . \underline{r}] \exp(2\pi i \gamma^{(j)} t_1) \quad (5.13)$$

where (4.36), corrected for refraction, is $k^{(i)} = k + \gamma^{(i)}$

Rewriting (5.13) in matrix form:

$$\underline{\underline{C}} \{\exp(2\pi i \gamma t_1)\} \underline{\varepsilon}_1 = \underline{\underline{C}}' \{\exp(2\pi i \gamma t_1)\} \underline{\varepsilon}_2$$

Thus $\underline{\varepsilon}_2 = \{\exp(-2\pi i \gamma t_1)\} \underline{\underline{C}}^{-1} \underline{\underline{F}}_{12} \underline{\underline{C}} \{\exp(2\pi i \gamma t_1)\} \underline{\varepsilon}_1$ (5.14)

$$\underline{\varepsilon} + d\underline{\varepsilon} = \{\exp(-2\pi i \gamma z)\} \underline{\underline{C}}^{-1} \underline{\underline{F}}_{slice} \underline{\underline{C}} \{\exp(2\pi i \gamma z)\} \underline{\varepsilon} \quad (5.15)$$

$$\alpha_g = 2\pi\, \underline{g} . \left(\frac{d\underline{R}}{dz} dz\right) = 2\pi \beta_g' dz$$

$$\underline{\underline{F}}_{slice} = \underline{\underline{I}} + 2\pi i \{\beta_g'\} \quad (5.16)$$

$$\frac{d\underline{\varepsilon}}{dz} = 2\pi i \{\exp(-2\pi i \gamma z)\} \underline{\underline{C}}^{-1} \{\beta_g'\} \underline{\underline{C}} \{\exp(2\pi i \gamma z)\} \underline{\varepsilon} \quad (5.17)$$

$$\underline{\phi}(z) = \{Q(z)\}^{-} \underline{\underline{C}} \{\exp(2\pi i \gamma z)\} \underline{\varepsilon}(z) \quad (5.18)$$

where $\{Q(z)\}^{-}$ is analogous to $\underline{\underline{F}}_n^{-}$ of eq (5.11)

$$2\pi \underline{R} = \underline{b}\,\Phi + \underline{b} \frac{\sin 2\Phi}{4(1-\nu)} + \underline{b}_{\wedge}\underline{u} \left[\frac{1-2\nu}{2(1-\nu)} \ln r + \frac{\cos 2\Phi}{4(1-\nu)}\right] \quad (5.19)$$

$$\phi_g(z) = \sum_i C_0^{(i)} C_g^{(i)} \exp(2\pi i \gamma^{(i)} z) \quad (5.20)$$

$$2k\Delta k = u_1 + u_3 + \left[\left(g^2 + \frac{u_1 - u_3}{2}\right)^2 + (u_1 + u_2)^2\right]^{1/2}$$

$$- \left[\left(g^2 - \frac{u_1 - u_3}{2}\right)^2 + (u_1 - u_2)^2\right]^{1/2} \quad (5.21)$$

$$M = \frac{u_1}{g^2} = \frac{K}{g^2 \xi_g} \quad (5.22)$$

$$F_{jk} = \{\exp(i\alpha_g)\}_{jk} \ , \quad \alpha_g = 2\pi\, \underline{g} . \underline{R}_{jk}$$

$$\frac{d\underline{\varepsilon}(z)}{dz} = 2\pi i \left\{\exp(2\pi i \gamma z)\right\} \underline{\underline{C}}^{-1}\left[\Delta A(z) + \beta_g'(z)\right] \underline{\underline{C}} \left\{\exp(2\pi i \gamma z)\right\} \underline{\varepsilon}(z) \quad (5.23)$$

Define $\frac{d\underline{\varepsilon}}{dz}$ or $\frac{d\underline{\phi}}{dz} = f(\underline{\varepsilon}, z)$ or $f(\underline{\phi}, z)$

$$\underline{\phi}(z+\Delta z) = \underline{\phi}(z) + \Delta\underline{\phi}(z) \simeq \underline{\phi}(z) + f(\underline{\phi}, z)\Delta z \quad (5.24)$$

(5.25) – (5.27) omitted

$$\frac{d\varepsilon^{(j)}}{dz} = 2\pi i \left[\sum_i \varepsilon^{(i)}(z) \exp\left[2\pi i(\gamma^{(i)} - \gamma^{(j)})z\right] \sum_g C_g^{(j)*} C_g^{(i)} \beta_g'\right] \quad (5.28)$$

If $\varepsilon^{(i)}(z) = \varepsilon^{(i)}(0) = C_0^{(i)} =$ const., eq (5.28) integrates

$$\Delta\varepsilon^{(j)} = \varepsilon^{(j)}(z) - \varepsilon^{(j)}(0)$$
$$= 2\pi i \sum_{i \neq g} \sum_g \varepsilon^{(i)} C_g^{(j)*} C_g^{(i)} \int_0^t \beta_g' \exp\left[2\pi i(\gamma^{(i)} - \gamma^{(j)})z\right] dz \quad (5.29)$$

$$\xi_g^{eff} = \xi_g \Big/ \sqrt{1 + s^2\xi_g^2} \quad (5.30)$$

Eq (4.19) again $\quad \phi_g = \frac{\pi i \phi_0}{\xi_g} \int_0^t \exp\left[-2\pi i(sz + \underline{g}.\underline{R})\right] dz \quad (5.31)$

phase $= -2\pi(sz + \underline{g}.\underline{R})$ (= const)

maximum when $\quad s + \frac{d}{dz}(\underline{g}.\underline{R}) = s + \beta' = 0 \quad (5.32)$

and $\quad \frac{d^2}{dz^2}(\underline{g}.\underline{R}) = \frac{d\beta'}{dz} = 0 \quad (5.33)$

$$\Delta\phi_g(t) = \sum_j \Delta\varepsilon^{(j)} C_g^{(j)} \exp(2\pi i \gamma^{(j)} t) \quad (5.34)$$

b.f. identical for: $\underline{R}_2(z) = \underline{R}_0 - \underline{R}_1(t-z) \quad (5.35)$

d.f. similar for: $\underline{R}_2(z) = \underline{R}_0 + \underline{R}_1(t-z) \quad (5.36)$

$$\phi(\underline{r}) = \sum_g \phi_g \exp\left[2\pi i\left[\theta_g(\underline{r}) + \underline{g}.\underline{r}\right]\right] \quad (5.37)$$

(5.38) – (5.41) omitted. For two beams only (5.37) becomes

$$\phi(\underline{r}) = \phi_1 \exp\left[2\pi i(\theta_1 + \underline{g}_1.\underline{r})\right] + \phi_2 \exp\left[2\pi i(\theta_2 + \underline{g}_2.\underline{r})\right]$$

Moiré: $\quad I(\underline{r}) = \phi(\underline{r})\phi^*(\underline{r}) = \phi_1^2 + \phi_2^2 + 2\phi_1\phi_2 \cos 2\pi(\Delta\theta + \Delta\underline{g}.\underline{r}) \quad$ (5.

Contrast: $\quad C = \frac{I_{max} - I_{min}}{I_{max} + I_{min}} = \frac{2\phi_1\phi_2}{\phi_1^2 + \phi_2^2} \quad (5.43)$

maximum contrast for $\phi_1 = \phi_2$

Lattice fringes: $\quad I(\underline{r}) = \phi_0^2 + \phi_g^2 + 2\phi_0\phi_g \cos 2\pi(\Delta\theta + \underline{g}.\underline{r}) \quad (5.44)$

Eq (4.7) again $\quad \Psi(x,y,\Delta z) = \phi_0 \exp(2\pi i \underline{\chi}.\underline{r}')\left[1 + i\frac{2\pi m e}{\chi}\bar{V}(x,y)\Delta z\right] \quad (6.1)$

Eq (4.10) without absorption $\quad \Delta\phi_g = i\,\phi_0 \frac{2\pi m e}{\chi} V_g \Delta z \quad (6.2)$

From (6.1) if phase change ∝ i is small term

$$I(x,y,\Delta z) = I\left(1 + \alpha\bar{V}(x,y)\right)^2 \quad (6.3)$$
$$= I\left(1 + 2\alpha\bar{V}(x,y)\right) \quad (6.4)$$

Huygens

$$\Psi'(x,y) = \iint_{-\infty}^{\infty} \frac{\Psi_e(X,Y)}{r}\, i\chi \cos(\Delta\theta).\exp(-2\pi\chi r)\, dX\,dY \quad (6.5)$$

$$r = \left[(x-X)^2 + (y-Y)^2 + (\Delta z)^2\right]^{1/2} \quad (6.6)$$

Small angles $\quad \cos\Delta\theta \simeq 1 \quad (6.7)$

$$r = \Delta z + A/2\Delta z \simeq \Delta z \quad (6.8)$$

where $\quad A = (x-X)^2 + (y-Y)^2 \quad (6.9)$

Rewrite (6.1) as $\quad \Psi_e(X,Y) = \Psi_i(X,Y).T(X,Y) \quad (6.10)$

$$(6.5) \Rightarrow \Psi'(x,y) = i\chi \iint \frac{\left[\Psi_i(X,Y).T(X,Y)\right]}{(\Delta z + A/2\Delta z)} \exp\left[-2\pi i\chi\Delta z - \frac{\pi i\chi A}{\Delta z}\right] dX\,dY \quad (6.11)$$

$$= \frac{i\chi}{\Delta z}\exp(-2\pi i\chi\Delta z)\iint\left[\Psi_e(X,Y)\right]\exp\left[-\frac{\pi i\chi}{\Delta z}\left((x-X)^2 + (y-Y)^2\right)\right] dX\,dY \quad (6.12)$$

Convolution $\quad \iint \equiv \Psi_e(X,Y) * P(x-X, y-Y) \quad (6.13)$

where Fresnel operator, $\quad P(a,b) = \exp\left[-\pi i\chi(a^2+b^2)/\Delta z\right] \quad (6.14)$

Convolution theorem: $\quad \underset{\text{convolve}}{A * B} \equiv IFT\left[FT[A].FT[B]\right] \quad (6.15)$

point multiply

(Inverse) Fourier transformation