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SECOND SCHOOL ON THE USE OF SYNCHROTRON RADIATION IN SCIENCE AND TECHNOLOGY:
"JOHN FUGGLE MEMORIAL"

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Dynamical Theory of X-Ray Diffraction by Perfect Crystals

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Dynamical Theory of X-ray Diffraction

by Perfect Crystals

deals with the propagation of waves in a periodic structure in a self-consistent way; couples the incident and diffracted waves

successive stages of accounting for the physical phenomena

geometrical theory

directions under which diffracted rays appear.

kinematical theory

combined effect of wavelets in directions other than those of maximum cooperation is taken into account; diffracted amplitudes are negligible compared to incident amplitude.

no attenuation -> energy is not conserved

good for thin crystals & imperfect crystals

dynamical theory

find conditions for a wave field exist and travel through the perfect crystal; connect fields inside the crystal to those outside.

-> solving **Maxwell equations in a Perfect Periodic** system

. . . quantum & relativistic effects . . .

historical

1912/13 Friedrich, Knipping and Laue discovered X-ray diffraction

*Annalen der Physik, **41**, 971 (1913)*

1913 Bragg relation $n\lambda = 2\,d \sin\theta$

*Proc. Camb.Phil.Soc.,**17**, 43 (1913)*

1914 Darwin : interaction of each atom in the structure with the incident wave, neglecting its interaction with the scattered waves. Good for structural crystallography; bad for diffracted intensities

*Phil.Mag., **27**, 315 (1914) (I); **27**, 675 (1914) (II)*

1916/17 Ewald : the crystal is formed by a tridimensional array of point resonators (oscilating dipoles) responsible for scattering of the electromagnetic field.

*Annalen der Physik, **49**, 1 and 117 (1916); **54**, 519 (1917)*

1931 Laue : consider a continuum electron density distribution, described by a dielectric constant - periodic and complex, similar to Bethe's devellopment for electron diffraction

*Ergeb. exakt.Naturwiss., **10**,133 (1931)*

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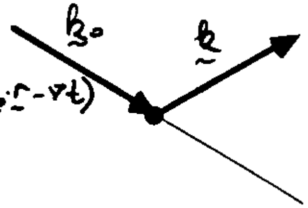
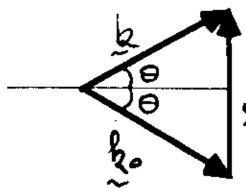
X-ray Diffraction

o scattering from electrons in an atom

λ, ν

$$E_0(\underset{\sim}{r},t) = E_0 e^{2\pi i(\underset{\sim}{k_0}\cdot\underset{\sim}{r} - \nu t)}$$





$$\underset{\sim}{S} \equiv \underset{\sim}{k} - \underset{\sim}{k_0}$$

free electron $E_e = -\frac{e^2}{mc^2}\frac{E_0(r,t)}{R}$ $\ominus$

$$|\underset{\sim}{k_0}| = \frac{1}{\lambda} = |\underset{\sim}{k}|$$

Thomson scattering

electrons in an atom (far from any resonance)

$$\frac{E_{rad}}{E_e} = f(s) = \int \rho(\underset{\sim}{r})\, e^{2\pi i\, \underset{\sim}{S}\cdot\underset{\sim}{r}}\, d^3\underset{\sim}{r}$$

$$\text{for } s=0 \quad f(0) = \int \rho(\underset{\sim}{r})\, dv = Z$$

bound electrons in an atom (resonance and absorption)

$$E_e = -\frac{e^2}{mc^2}\frac{E_0(\underset{\sim}{r},t)}{R}\cdot\frac{\omega_0^2}{\omega_0^2 - \omega^2 - i\gamma\omega_0}$$

$$\Rightarrow \quad f(s) = f_0(s) + f' + i f''$$

o periodic structure - perfect crystal (**a** , **b** , **c**)

$\rho(\mathbf{r})$: $$\rho(\underset{\sim}{r}) = \frac{1}{V} \sum_{\underset{\sim}{h}} F_h \, e^{-2\pi i \underset{\sim}{h} \cdot \underset{\sim}{r}}$$

$\underset{\sim}{\mathbf{h}}$ must be a reciprocal lattice vector : $\underset{\sim}{\mathbf{h}} = h\,\underset{\sim}{\mathbf{a}}^* + k\,\underset{\sim}{\mathbf{b}}^* + l\,\underset{\sim}{\mathbf{c}}^*$
to ensure that $\rho(\underset{\sim}{\mathbf{r}}) = \rho(\underset{\sim}{\mathbf{r}} + u\,\underset{\sim}{\mathbf{a}} + v\,\underset{\sim}{\mathbf{b}} + w\,\underset{\sim}{\mathbf{c}})$

F_h : $$F_h = \int_{\text{cell}} \rho(\underset{\sim}{r})\, e^{2\pi i \underset{\sim}{h} \cdot \underset{\sim}{r}}\, dv$$

within the assumption that the atoms behave as rigid spheres with respect to their charges densities and are not vibrating thermally

F_h : $$F_h = \sum_n f_n \, e^{2\pi i \underset{\sim}{h} \cdot \underset{\sim}{r}_n}$$

the <u>structure factor</u> is the 'sum' of the <u>scattering factor</u> of each atom in the unit cell. $\mathbf{r}_n$ is the vector fixing the center of each atom.

f_n : $\rightarrow f_n \cdot e^{-M_n}$ Debye-Waller factor

Si and Ge : $$M_n = \frac{6h^2 T}{m k_B \Theta}\left(1 + \left(\frac{\Theta}{6T}\right)^2\right)\left|\frac{1}{2}\underset{\sim}{S}\right|^2$$

Batterman and Chipman (1962)

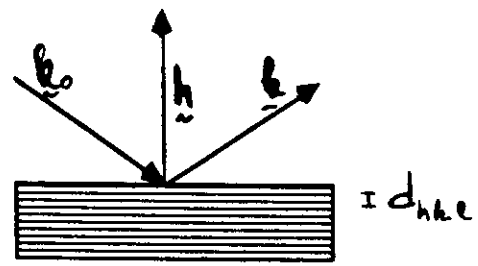
$\underset{\sim}{\mathbf{S}} = \underset{\sim}{\mathbf{k}} - \underset{\sim}{\mathbf{k}}_0 = \underset{\sim}{\mathbf{h}}$ or $\underset{\sim}{\mathbf{S}} \cdot \underset{\sim}{\mathbf{a}} = h$, etc...

Laue conditions

two useful properties of $\underset{\sim}{\mathbf{h}}$:

i) $\underset{\sim}{\mathbf{h}}$ is perpendicular to hkl plans

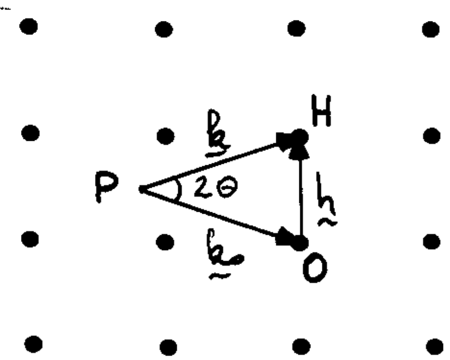
ii) $|\underset{\sim}{\mathbf{h}}| = 1/d_{hkl}$



the positions of the nodes in the reciprocal lattice give the periodicity of $\rho(r)$, hence of the crystal

Ewald's construction

reciprocal lattice



P : tie-point

$$\frac{|h|}{2} = |\underset{\sim}{k}|\sin\Theta = |\underset{\sim}{k}_0|\sin\Theta$$

$$\frac{1}{\lambda}\sin\Theta = \frac{1}{d_{hkl}}$$

Bragg's law

$$\lambda = 2 d_{hkl} \sin\Theta$$

the periodic, complex, dielectric constant :

connection to the Fourier series describing electron densities

o **E** & **H** small enough - > linear relations

$4\pi \underline{P} = \chi \underline{E}$ $\quad \underline{D} = \underline{E} + 4\pi \underline{P} = (1+\chi)\underline{E} = \epsilon \underline{E}$

$4\pi \underline{M} = \chi_m \underline{H}$ $\quad \chi_m \simeq 0$

$\chi(\underline{r})$ carries all the physical information about the crystal

$$\chi(\underline{r}) = \sum_{\underline{h}} \chi_h \exp(-2\pi i \underline{h}\cdot\underline{r})$$

$$\chi_h = \frac{1}{V}\int \chi(\underline{r}) \exp(2\pi i \underline{h}\cdot\underline{r})\, d^3\underline{r}$$

o sinusoidal field on a collection of free electrons $\quad m\ddot{\underline{x}} = e\underline{E}$

$$\to \underline{x} = -\frac{e}{m\omega_0^2}\underline{E}$$

$$\underline{P} = e\rho(\underline{r})\underline{x} = -\frac{e^2}{mc^2}\left(\frac{\lambda}{2\pi}\right)^2 \rho(\underline{r})\underline{E} \Rightarrow \chi(\underline{r}) = -\frac{e^2}{mc^2}\frac{\lambda^2}{\pi}\rho(\underline{r})$$

o bound electrons $\quad m\ddot{\underline{x}} = e\underline{E} - m\gamma\dot{\underline{x}} - m\omega_0^2 \underline{x}$

$$\chi(\underline{r}) = -\frac{e^2\lambda^2}{mc^2\pi}\rho(\underline{r})$$

$\leftarrow$ generalized density

$$\boxed{\chi_h = -\Gamma F_h} \qquad \Gamma \equiv \left(\frac{e^2}{mc^2}\right)\frac{\lambda^2}{\pi V_c}$$

which accounts for the bounded electrons and absorption

$$f \Rightarrow f + f' + i f''$$

$$F_h = \sum_n \{f_n(s) + f_n' + i f_n''\}\, e^{-M_n} e^{2\pi i \underline{h}\cdot\underline{r}_n}$$

$$F_h = F_h' + i F_h''$$

refraction index n $\quad n = \frac{c}{v} = \sqrt{\mu'\epsilon} = \sqrt{1+\chi_0}$

average of $\chi(r)$

$\chi_0 = -\Gamma F_0 \qquad hkl = 000$

$= -\Gamma F_0' - i\Gamma F_0'' \qquad |\chi_0| \approx 10^{-5} - 10^{-6}$

$n = 1 + \frac{\chi_0}{2} = 1 - \Gamma F_0' - i\Gamma F_0''$

refraction absorption

$n' = 1 \qquad \mu_0 = \left(\frac{2\pi}{\lambda}\right)\Gamma F_0''$

but $n' < 1$

CuK$_\alpha$ through Ge

$\mu_t = 350\ cm^{-1}$

$\lambda = 1.54 \times 10^{-8}$ cm

$\Rightarrow |k| < |k|_{VACUUM}$

$\Gamma F_0'' \approx 0.86 \times 10^{-6}$

total external Reflection

basic equations for possible wave-fields

Maxwell's equations

$$\nabla \times E = -\frac{1}{c}\frac{\partial H}{\partial t} \qquad \nabla \cdot H = 0$$

$$\nabla \times H = \frac{1}{c}\frac{\partial D}{\partial t} \qquad \nabla \cdot D = 0$$

$$\Rightarrow \nabla^2 D + 4\pi^2 |k|^2 D + \nabla \times (\nabla \times \chi D) = 0 \qquad |k| = \frac{1}{\lambda}$$

$|\chi|^2 \ll 1$

D sum of plane waves (Bloch's solutions)

$$D = e^{2\pi i(\nu t - k_0 \cdot r)} \sum_m D_m e^{-2\pi i h_m \cdot r}$$

or

$$D = e^{2\pi i \nu t} \sum_m D_m e^{-2\pi i k_m \cdot r}$$

with the condition $\quad k_m = k_0 + h_m \quad$ (Bragg's Law)

fundamental equation of the dynamical theory

$$\Rightarrow \frac{k_m^2 - K^2}{k_m^2} D_m = \sum_n \chi_{m-n}\, \hat{k}_m \times (\hat{k}_m \times D_n)$$

$K = \frac{1}{\lambda} = \frac{\nu}{c}$

$|\chi_{m-n}|$ very small typically $\sim 10^{-5}$

-> equation is satisfied for D_m not vanishingly small only if $k_m^2 \approx K^2$

i.e, if elastic Bragg diffraction is nearly satisfied.

one-wave case (o)

if only D_o is non-negligible, i.e. far from the Bragg condition

$$\frac{k_o^2-K^2}{k_o^2}D_o = \chi_o D_o \Rightarrow k_o^2(1-\chi_o)-K^2=0 \qquad \frac{k_o}{K}=n'$$

$$n' = \frac{1}{\sqrt{1-\chi_o}} \simeq 1+\frac{\chi_o}{2}$$

two-wave case (o,h)

Bragg condition nearly satisfied for one set of plans

$$\begin{vmatrix} \dfrac{k^2-k_o^2}{K^2} & P\chi_{\bar h} \\ P\chi_h & \dfrac{k^2-k_h^2}{K^2} \end{vmatrix} = 0$$

$$k = K\left(1+\frac{\chi_o}{2}\right)$$

$$P \equiv \frac{D_o\cdot D_h}{D_o D_h} = \begin{matrix} 1 & \sigma \\ \cos 2\theta_B & \pi \end{matrix}$$

-> spheres of radii k, centered around O and H

$$(k^2-k_o^2)(k^2-k_h^2) = P^2\chi_h\chi_{\bar h}K^2$$

$$2K\xi_o \equiv k_o^2-k^2$$

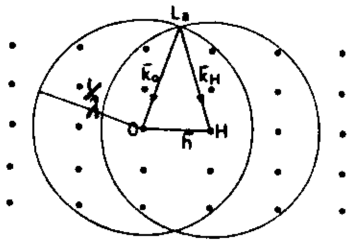
$$2K\xi_h \equiv k_h^2-k^2$$

$$\boxed{\xi_o\xi_h = \frac{P^2\chi_h\chi_{\bar h}K^2}{4} \qquad \frac{D_h}{D_o} = \frac{2\xi_o}{K\chi_{\bar h}} = \frac{K\chi_h}{2\xi_h}}$$

geometrical approach

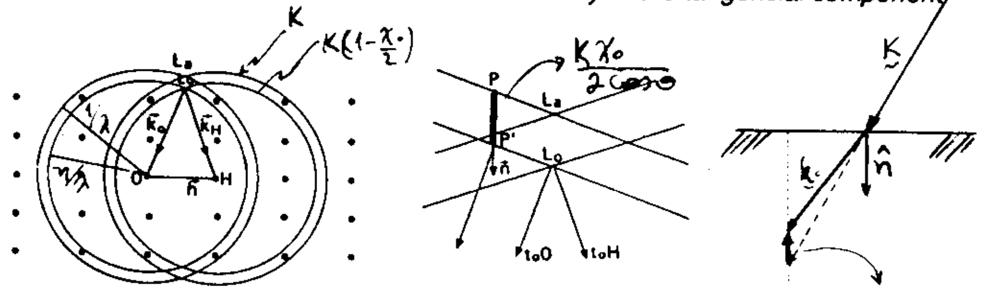
it is interesting to use Ewald's construction to better understand the dynamical parameters.

two spheres of radii k centered at O and H



refraction (n' < 1)

to match outside to inside field
continuity of the tangencial component



a) b)

$$k_o - K = -K\delta\hat{n}$$

$$|K| = \frac{1}{\lambda} \simeq |k_o|$$

what happens when we are near a Bragg condition ?

field equations near a Bragg condition (two-wave case)

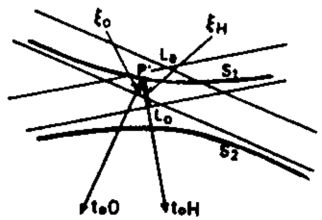
$$(k_o^2 - k^2) = \underbrace{(k_o+k)}_{\simeq 2K}\underbrace{(k_o-k)}_{\sim 10^{-5}} \simeq 2K(k_o-k)$$

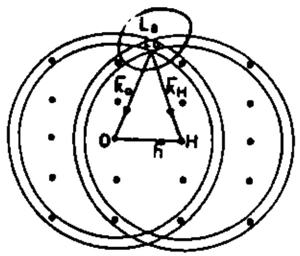
$$\xi_o \simeq k_o - k$$
$$\xi_h \simeq k_h - k$$

$$\boxed{\xi_o \xi_h = \frac{\chi_h \chi_{\bar h} K^2}{4} \qquad \frac{D_h}{D_o} = \frac{2\xi_o}{K\chi_{\bar h}} = \frac{K\chi_h}{2\xi_h}}$$

the secular equation is transformed into a hyperbola ("two branches")

"dispersion surface"





the dispersion surface contains full information about the waves which can propagate in the crystal

diameter S_1S_2 : $\frac{|\chi_h|K}{\cos\theta}$

- the amplitude ratio is proportional to the distance of the tie-points to the assymptotes.
- propagation diraction is the normal to the dispersion surface at the corresponding tie-point.
- $\xi_o' \simeq k_o' - k$

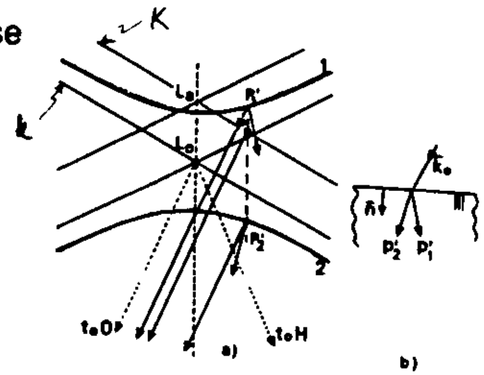
  $\xi_o'' \simeq -k_o''\cos\beta - \frac{1}{2}K\Gamma F_o''$ for $\left(\frac{k_o''}{k_o'}\right)^2 \ll 1$

boundary conditions at the crystal entrance

the tangencial component of the wave-vectors
has to be conserved

plane wave

Laue case



PO : incoming wave-vector $\mathbf{k_o}$

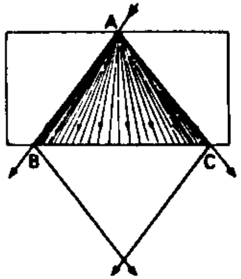
generates **two wave-fields** inside the crystal
the propagation direction is **normal** to the dispersion surface

As $\mathbf{k_o}$ changes by few seconds of arc
the wave fields change their propagation direction angle
by the very large angle 2θ

Borrmann fan

Incident wave :

sufficiently wide spatially to be considered as an almost plane wave, but sufficiently narrow to be traced as bundles of rays.



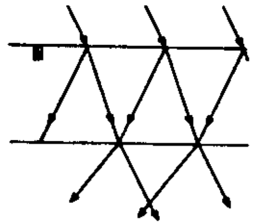
there will be wave-fields propagating in all directions between the incident and the diffracted direction

Pendellosung effects

the two-wave field excited will overlap through their propagation

O-type fields are **coherent** ; P'_1O and P'_2O differ by $P'_1P'_2$

the amplitude oscillates along the normal to the entrance surface with a period $(1/P'_1P'_2)$ as the wave-fields propagate into the crystal.



symmetrical Laue geometry and at exactly the Bragg condition we have the

Pendellosung period : $\Lambda = \frac{1}{S_1S_2} = \frac{\cos\theta}{K|\chi_h|}$ $(\Lambda \sim 10\,\mu m)$

at depth $\Lambda/2$ "O" is zero

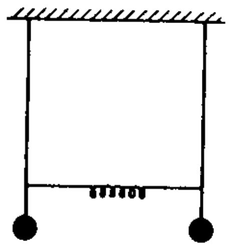
" $0, \Lambda, \ldots$ "O" is MAXIMUM

H-type fields : initial phase difference π $\therefore$ at $\Lambda/2$, MAXIMUM

at $0, \Lambda$, ZERO

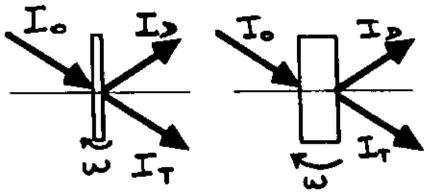
Ewald analogy

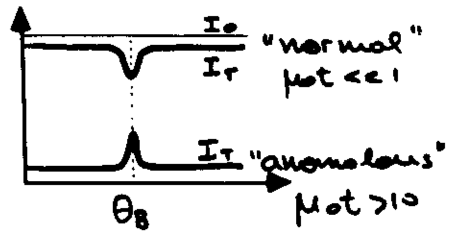
coupled pendula

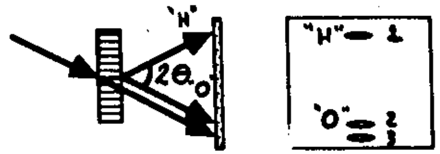


Pendellosung fringes are very sensitive to crystal distortion

Borrmann effect







some mechanism keeps the energy away from the absorbing atoms

DYNAMICAL THEORY predicts that a STANDING WAVE pattern should exist inside the crystal

tie-point on branch 1 : **nodes are on the lattice plans**

branch 1 -> branch 2 patterns are shifted by π

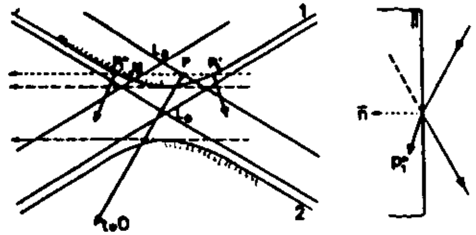
=> ***type 1 fields will be less absorbed than type 2 fields***

absorbing atoms Borrmann effect :

only branch 1 wave-fields with propagation direction along the plans survive

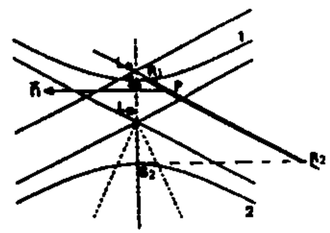
(when **nodes** becomes points of **zero intensity**)

Bragg case



P'_1 points out of the crystal and it is not a physical solution (for thick crystals)

total reflection

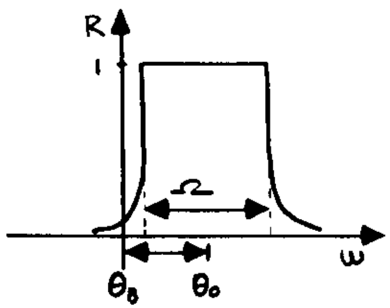


Darwin width

$$\Omega = \frac{2|\chi_h|}{\sin 2\theta}$$

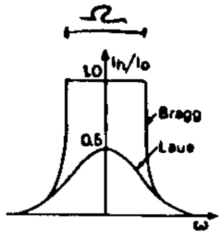
the center is not on the Laue point
the shift is just the refraction correction

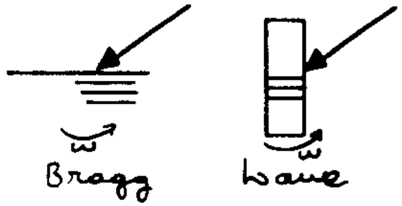
$$\frac{\chi_o}{\sin 2\theta}$$



rocking curves and integrated reflectivity

ideal case





infinitely thick; non-absorbing; symmetrical geometry

Bragg : $R'_{hkl} = \pi \frac{\Omega}{2} = \frac{\pi \chi_h}{\sin 2\theta}$

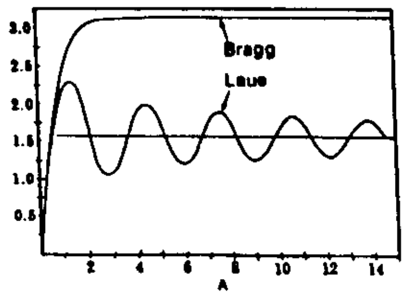
$R'_{hkl} = \frac{\pi \chi_h}{\sin 2\theta} \tanh A \qquad A = \frac{\pi t}{\Lambda}$ t: thickness; Λ: Pendellosung period

Laue : $R'_{hkl} = \{|\chi_h|/\sin 2\theta\}\, W(A) \qquad W(A) = \int_0^{2A} J_0(u)\,du$

no total reflection
MAXIMUM IS 0.5

$J_0(u)$ Bessel func.

integrated reflectivity



DYNAMICAL THEORY

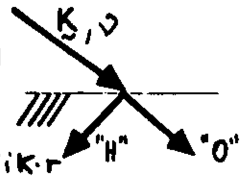
- the total wave-field inside the crystal is considered as a single entity
  energy is swapped back and forth between them
- it is necessary whenever diffraction by perfect crystals is involved
  impose corrections to the kinematical theory (extinction)
- the process is coherent

- interesting effects :
  - Bragg total reflection
  - Borrmann effect
    - anomalous transmission
    - polarization
  - Pendellosung oscilations
    - very accurate values of structure factors have been obtained
  - Standing waves

- more general presentation :
  - asymmetry
  - multiple diffraction
  - extreme situations ($\theta \approx 0$ or $\pi/2$)
    - **backdiffraction**

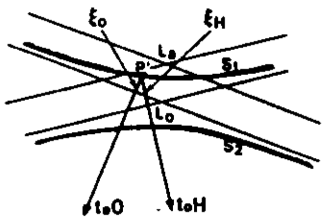
field equations in the two wave case

$$\underset{\sim}{D} = e^{2\pi i \nu t}\left[\underset{\sim}{D}_o\, e^{-2\pi i \underset{\sim}{k}_o\cdot \underset{\sim}{r}} + \underset{\sim}{D}_h\, e^{-2\pi i \underset{\sim}{k}_h\cdot\underset{\sim}{r}}\right]$$



solutions inside the crystal *when* $D_{inc} = e^{2\pi i \nu t}\, \underset{\sim}{D}_K\, e^{-2\pi i \underset{\sim}{K}\cdot \underset{\sim}{r}}$

dispersion surface



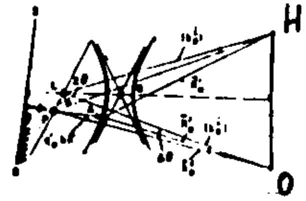
$$\xi_o \xi_h = \frac{1}{4} k^2 P^2 \chi_h \chi_{\bar h} \qquad 2k\xi_o \equiv k_o^2 - k^2$$

$$R = \frac{D_h}{D_o} = \frac{2\xi_o}{k\chi_{\bar h}} = \frac{k\chi_h}{2\xi_h} \qquad 2k\xi_h \equiv k_h^2 - k^2$$

$$\underset{\sim}{k}_o = \underset{\sim}{K} - k\delta\hat{n} \quad \to \quad \delta = -\frac{\frac{1}{2}k\chi_o + \xi_o}{\underset{\sim}{k}_o\cdot\hat{n}}$$

$$|K| = \frac{1}{\lambda} = |\underset{\sim}{k}_o| = |\underset{\sim}{k}| \qquad k = K\left(1 + \frac{\chi_o}{2}\right)$$

ξ as a function of θ



$\underset{\sim}{k}_h = \underset{\sim}{k}_o + \underset{\sim}{h}$, ξ_o, ξ_h

$a \equiv (2\underset{\sim}{k}_o\cdot b + h^2)/k^2$

$b \equiv \dfrac{\underset{\sim}{k}_o\cdot\hat{n}}{\underset{\sim}{k}_h\cdot\hat{n}} = \dfrac{\gamma_o}{\gamma_h}$

-> $\xi_h = \dfrac{k\chi_o}{2}\left(\dfrac{1-b}{b}\right) + \xi_o\dfrac{1}{b} + \dfrac{1}{2}ak$

using the dispersion relation

$$\xi_o = \frac{1}{2}k|P||b|^{1/2}\Gamma[F_hF_{\bar h}]^{1/2}\left[\eta \pm (\eta^2 + b/|b|)^{1/2}\right]$$

$$\xi_h = \frac{1}{2}k|P|(\Gamma/|b|^{1/2})[F_hF_{\bar h}]^{1/2}\Big/\left[\eta \pm (\eta^2 + b/|b|)^{1/2}\right]$$

where $\eta \equiv \dfrac{\chi_o(1-b) + a\cdot b}{2|b|^{1/2}(\chi_{\bar h}\chi_h)^{1/2}}$

- if $a \approx 2\,\Delta\theta\,\sin 2\theta_B$ -> $\eta = \dfrac{b\,\Delta\theta\,\sin 2\theta + \frac{1}{2}\Gamma F_o(1-b)}{\Gamma|P||b|^{1/2}[F_hF_{\bar h}]^{1/2}}$

- fundamentally, η is a large constant (complex) times $\Delta\theta$

$\Delta\theta$ within few seconds of arc <-> η within 0 and small integer (pos.or neg)

given $\Delta\theta$, b $\to$ $\eta \to \xi \to \xi', \xi''$ $\Rightarrow$ R, $\underset{\sim}{k}_o$ and $\underset{\sim}{k}_h$

Laue case : $b/|b| = 1$

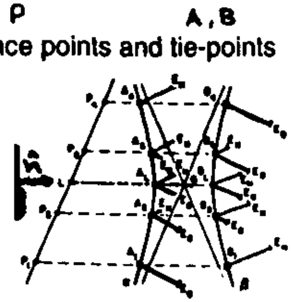
b=+1 symmetric

$$\xi_0 = \frac{1}{2}K|P||b|^{1/2}\Gamma[F_hF_{\bar h}]^{1/2}e^{\pm v}$$

$$\frac{D_h}{D_o} = \mp\left[\frac{|P||b|^{1/2}}{P}\right]\frac{[F_hF_{\bar h}]^{1/2}}{F_{\bar h}}e^{\pm v}$$

$$\eta \equiv \frac{1}{2}(e^{v}-e^{-v}) = \sinh v$$

relation between entrance points and tie-points



$$\xi_0 = \frac{1}{2}K\Delta\theta\sin 2\theta \pm \frac{1}{2}\left[K^2\Delta\theta^2\sin^2 2\theta + K^2P^2\Gamma F_hF_{\bar h}\right]^{1/2}$$

- well off Bragg angle

$$\Delta\theta^2\sin^2 2\theta \gg P^2\Gamma F_hF_{\bar h}$$

$\xi_o' \to 0$ or $\pm K|\Delta\theta|\sin 2\theta$ $\rightsquigarrow$ A, B$_4$ $\xi_o \to 0$ $\frac{D_h}{D_o} \to 0$

$\xi_o'' \to 0$ NO DIFFRACTED BEAM

and, in addition,

$$k_o' = \xi_o' + K(1-\tfrac{1}{2}\Gamma F_o') \to K(1-\tfrac{1}{2}\Gamma F_o')$$

$$k_o''\cos\beta = \tfrac{1}{2}K\Gamma F_o'' - \xi_o'' \to \tfrac{1}{2}K\Gamma F_o''$$

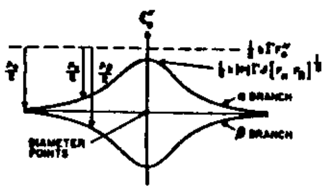
$\therefore \left(e^{-2\pi k_o\cdot r}\right)^2 \to \mu_e t = 2\pi K\Gamma F_o'' t$ $\mu_e = \mu_o = 2\pi K\Gamma F_o''$

- at Bragg angles (diameter points)

$\Delta\theta = 0$, $\eta = 0$

$$\xi_o = \xi_h = \pm\frac{1}{2}K|P|\Gamma[F_hF_{\bar h}]^{1/2} \qquad \xi_o'' = \pm\frac{1}{2}K|P|\Gamma\{Im(F_hF_{\bar h})^{1/2}\}$$

$$\frac{D_h}{D_o} = \pm\frac{|P|}{P}\frac{[F_hF_{\bar h}]^{1/2}}{F_{\bar h}}$$



effective absorption

$\left(e^{-2\pi k_o''\cdot r}\right)^2$ one of the most interesting aspect of dynamical theory

$$\mu_o(eff) = \mu_o\left[1 \pm |P|\,\epsilon\,(1-p^2)^{1/2}\right]$$

μ_o normal linear absorption coefficient

$p \equiv \frac{\tan\Delta}{\tan\theta}$ Δ the angle between the normal to the dispersion surface and lattice plans

$p \left(\begin{matrix} -1 \\ 0 \\ +1 \end{matrix} \right.$ limits of the dispersion surface

$\epsilon \approx \frac{F_h''}{F_o''}$ (exactly true for centrosymmetric crystals)

$$\mu_o(eff) = \mu_o\left\{1 \pm |P|\epsilon/[1+\eta'^2]\right\} \qquad \eta' = \frac{\Delta\theta\sin 2\theta}{\Gamma|P|F_h'}$$

o Borrmann effect

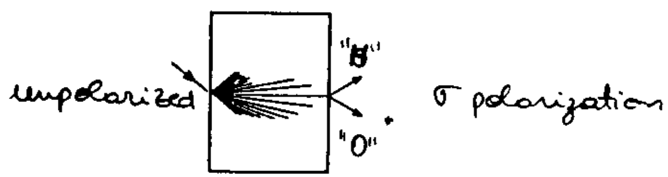
σ pol $(P=1)$; $\epsilon \approx \frac{f''(2\theta)}{f''(0)} \approx 1$

$\Delta = 0$ $(p=0,\ \Delta\theta=0)$

$\mu_o(eff) = 0$ or $2\mu_o$

branch 1   branch 2

at $\Delta\theta = 0$ $\Rightarrow$ $\mu_o(eff) = \mu_o[1 \mp |P|\epsilon]$



physical interpretation

in terms of the positional dependence of the electric field

- $\eta' = \Delta = \rho = 0$ and $F_h = F_{\bar{h}}$

$$\mathbf{D} = e^{2\pi i \nu t}\left[\mathbf{D}_0\, e^{-2\pi i \mathbf{k}_0\cdot\mathbf{r}} + \mathbf{D}_h\, e^{-2\pi i \mathbf{k}_h\cdot\mathbf{r}}\right]$$

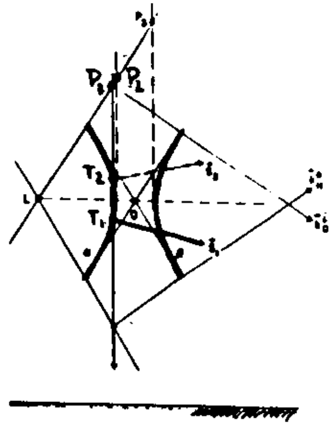
$$\xi_0 = \xi_h \Rightarrow |\mathbf{D}_0| = |\mathbf{D}_h| \qquad \frac{D_h}{D_0} = \pm 1$$

-> $$|\mathbf{D}|^2 = 2|\mathbf{D}_0|^2\left(1 \pm P\cos[2\pi\, \mathbf{h}\cdot\mathbf{r}]\right)$$

phase $2\pi\, \mathbf{h}\cdot\mathbf{r} = 2\pi \dfrac{x}{d_h}$ // *plans of equal intensity paralell to* $\mathbf{h}$

Borrmann	σ	P=1	nodes are ZERO intensity
effect	π	P=cos 2θ	nodes are NOT ZERO intensity

Bragg case



- Bragg selects two tie points on the same branch but, <u>only one is excited</u> (Kohler, Ann.Physik **18**, 265(1933))
- region which produces no intersection with the dispersion surface <u>no propagating solutions inside</u>
- $\mathbf{D}_0^i = \mathbf{D}_0$; $\mathbf{D}_H^e = \mathbf{D}_H$;
- thick crystal : internal flow is eventually attenuated $\dfrac{D_h}{D_0} \to \left|\dfrac{D_h^e}{D_0^i}\right|^2$

$$\left(\frac{D_h}{D_0}\right)^2 = \frac{\xi_0}{\xi_h}\frac{F_h}{F_{\bar h}} = |b|\left[\eta \pm (\eta^2-1)^{1/2}\right]^2 \frac{F_h}{F_{\bar h}}$$

for $F_h = F_{\bar h}$ $$\left|\frac{D_h^e}{D_0^i}\right|^2 = |b|\,|\eta \pm (\eta^2-1)^{1/2}|^2$$

→ Bragg sym (b=-1) and with no absorption

$$\eta = (-\Delta\theta \sin 2\theta + \Gamma F_0)/|P|\Gamma F_h \qquad F_0, F_h \text{ real}$$

$\eta = +1$ $\quad \Delta\theta = \dfrac{\Gamma F_0 - |P|\Gamma F_h}{\sin 2\theta}$

$\eta = -1$ $\quad \Delta\theta = \dfrac{\Gamma F_0 + |P|\Gamma F_h}{\sin 2\theta}$

$$\frac{|D_h|^2}{|D_0|^2} = 1$$

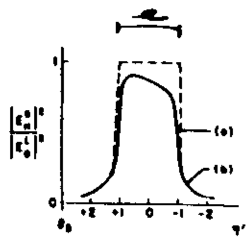
$\to \Omega = \dfrac{2|P|\Gamma|F_h|}{\sin 2\theta}$

solutions surfaces

→ with absorption

$$\eta' = (-\Delta\theta \sin 2\theta + \Gamma F_0')/|P|\Gamma F_h'$$

$$\eta'' = -(F_h''/F_h')(\eta' - 1/|P|\epsilon)$$



primary extinction

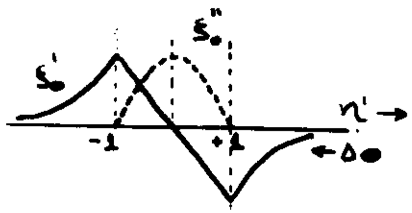
Bragg case with no absorption and $F_h = F_{\bar{h}}$

$$\xi_0 = \frac{1}{2} K |P| \Gamma F_h \left[\eta \pm (\eta^2 - 1)^{1/2} \right]$$

within the region

$$|\eta| < 1 \qquad \xi_0' = \frac{1}{2} K |P| \Gamma F_H \cdot \eta$$

$$\xi_0'' = \frac{1}{2} K |P| \Gamma F_H \, (1 - \eta^2)^{1/2}$$



with $F_0'' = 0 \quad \rightarrow \xi_0'' = -k_0'' \sin\theta$

$$\rightarrow e^{-4\pi \underset{\sim}{k_0''} \cdot \underset{\sim}{r}} = e^{[-2\pi K |P| \Gamma F_h (1-\eta^2)^{1/2} / \sin\theta] z}$$

z depth in the crystal

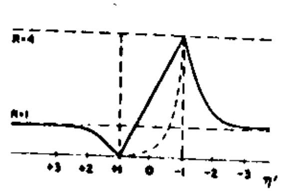
average value of the EXTINCTION FACTOR

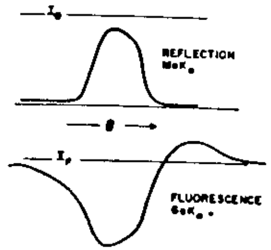
$$\exp\left[\left(-\frac{1}{2} \pi^2 K |P| \Gamma F_h / \sin\theta \right) z \right]$$

* many times greater than normal absorption

standing waves

wave fields inside the crystal





PHYSICAL REVIEW VOLUME 133, NUMBER 3A 3 FEBRUARY 1964

Effect of Dynamical Diffraction in X-Ray Fluorescence Scattering

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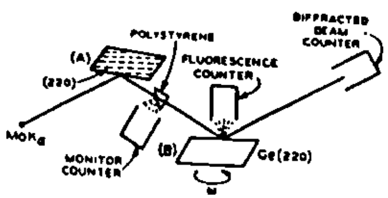
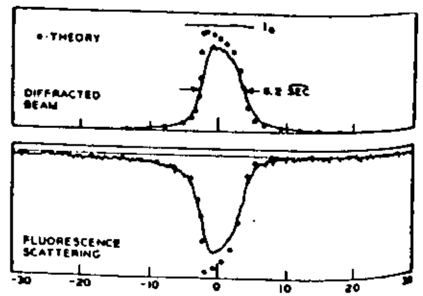
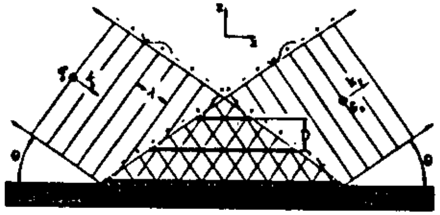
(Received 21 August 1963)



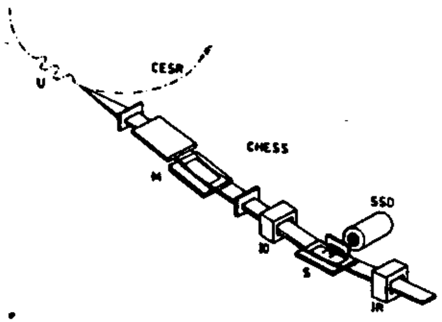


standing wave technique

- generation of a standing wave field by the interference of the incident and reflected beams.



- structutal information is obtained by measuring the fluorescence yield from foreign atoms, which depends on the position of such atoms relative to the choses diffraction planes



PHYSICAL REVIEW B VOLUME 10, NUMBER 10 15 NOVEMBER 1974

Observation of internal x-ray wave fields during Bragg diffraction with an application to impurity lattice location*

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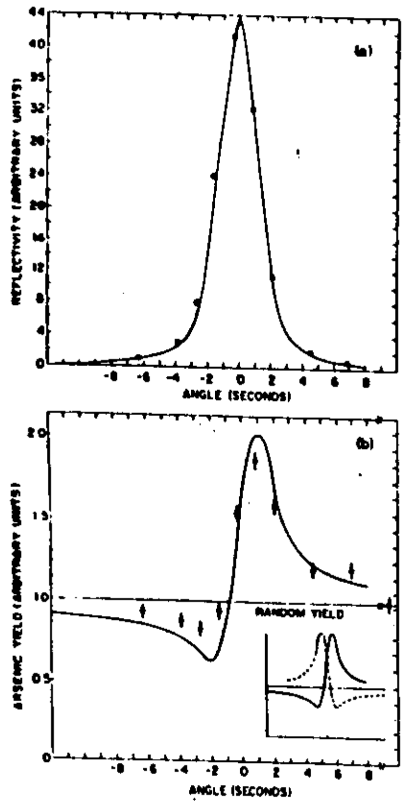
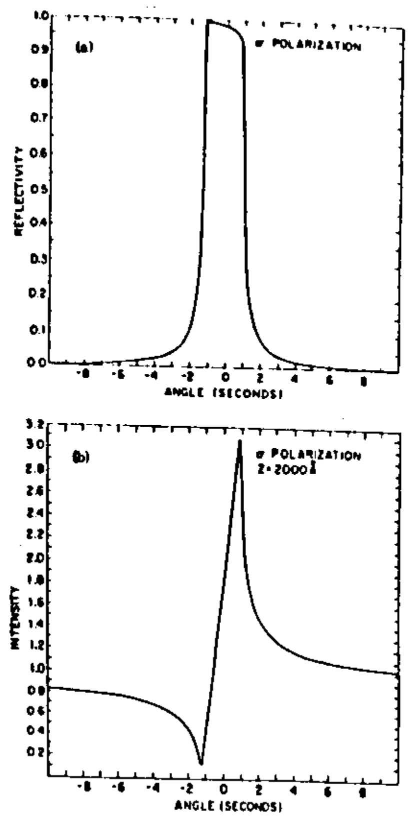
(Received 25 June 1974)





X-Ray Standing Waves at Crystal Surfaces

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(Received 17 March 1980)

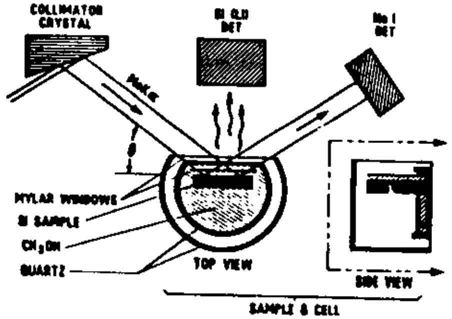
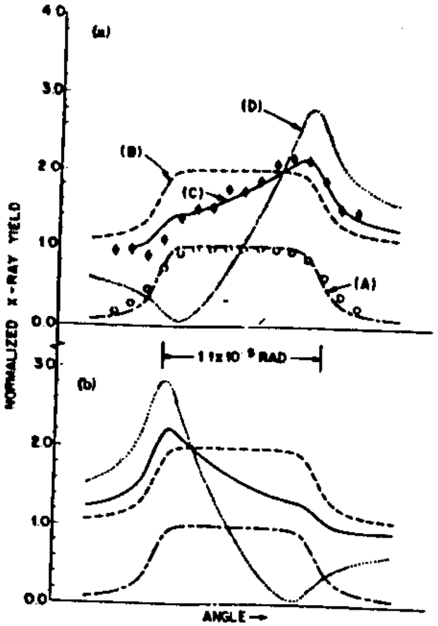


FIG. 1. Schematic layout of experimental apparatus including sample cell detail.



Simple X-Ray Standing-Wave Technique and Its Application to the Investigation of the Cu(111) $(\sqrt{3}\times\sqrt{3})R30°$-Cl Structure

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(Received 10 October 1986)

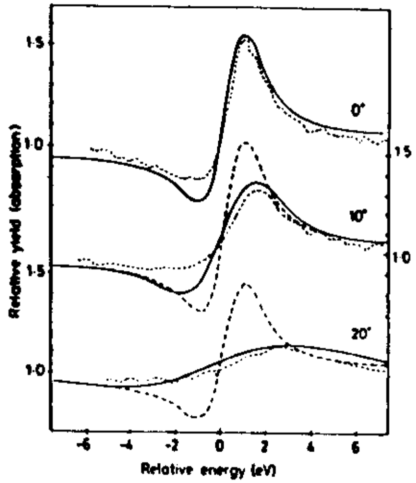

FIG. 1. Relative Cu 2p-derived Auger-electron yield (short dashed lines) from Cu(111) as the photon energy is scanned through the (111) Bragg reflection for incidence angles of 0° (normal incidence), 10°, and 20° compared with theoretical absorption profiles at the atomic planes incorporating random angular standard deviations of 0.01° (long dashed lines) and 0.1° (solid lines). For 0° incidence the two theoretical lines are indistinguishable.

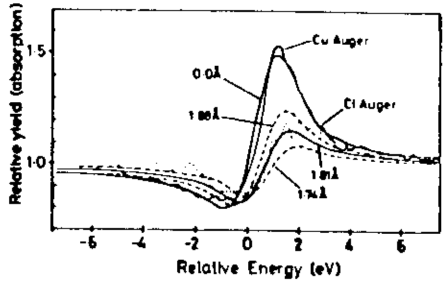

FIG 2. Relative Cu 2p-derived and Cl 1s-derived Auger-electron yields from Cu(111)$(\sqrt{3}\times\sqrt{3})R30°$-Cl as the photon energy is scanned through the (111) Bragg reflection at normal incidence. Also shown are theoretical absorption curves for absorption on the Cu atom planes and at 1.7, 1.8, and 1.88 Å above the last Cu atom plane of a perfect substrate. In these theoretical curves only 80% of the Cu or Cl absorbers are assumed to be coherently positioned relative to the substrate lattice.

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A POSSIBLE USE OF THE SOFT X-RAY STANDING WAVE METHOD FOR SURFACE AND INTERFACE STRUCTURE ANALYSIS

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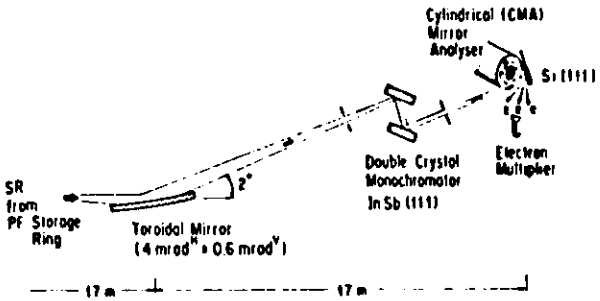

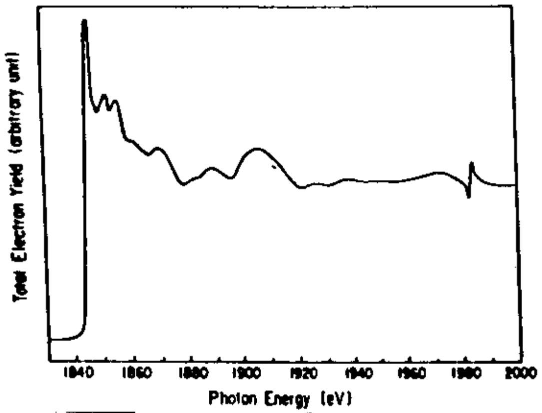

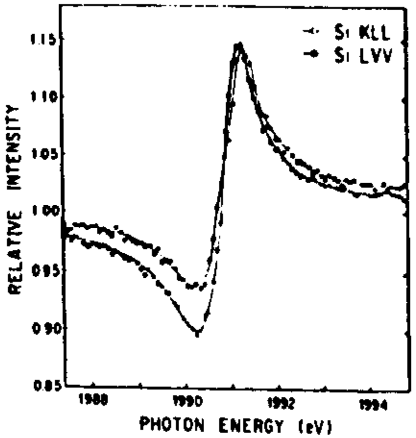

diffraction around $\pi/2$