Diffraction

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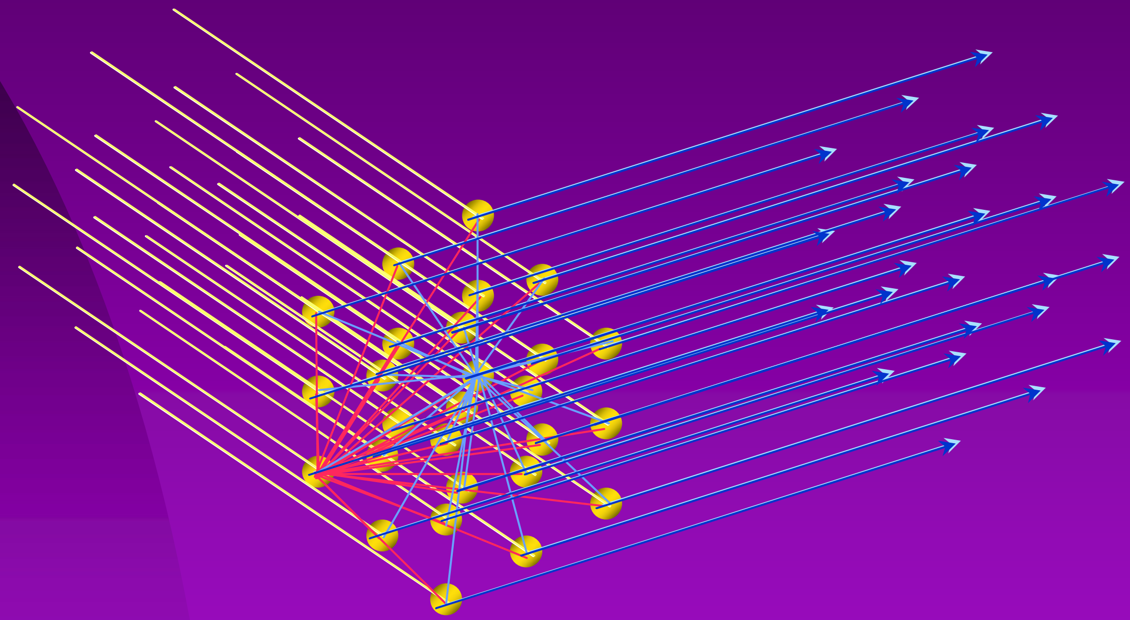
Part 2, Dynamical Diffraction

Introduction

- In the 1st part, we dealt with "Kinematical Theory" where the scattered x-rays suffer no additional scattering.
- The 2nd part is designed to give basic ideas of "Dynamical Diffraction" observed with perfect crystals as a result of multiple scattering.

Basic Idea



Kinematical Diffraction
Dynamical Diffraction

Maxwell Equation (1/2)

$$\nabla \cdot \boldsymbol{D} = \rho_{true}$$

$$\nabla \cdot \boldsymbol{B} = 0$$

$$\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \boldsymbol{j}_{true} + \frac{\partial \boldsymbol{D}}{\partial t}$$

$$\boldsymbol{D} = \varepsilon_o \boldsymbol{E} + \boldsymbol{P}$$

$$\boldsymbol{H} = \frac{\boldsymbol{B}}{\mu_o} - \boldsymbol{M}$$

$$\boldsymbol{P} = \varepsilon_o \chi \boldsymbol{E}$$

$\boldsymbol{E}$: electric field
$\boldsymbol{D}$: electric displacement
$\boldsymbol{H}$: magnetic field
$\boldsymbol{B}$: magnetic induction
ρ: charge density
$\boldsymbol{j}$: current density
$\boldsymbol{P}$: polarization
$\boldsymbol{M}$: magnetization
ε_0: permittivity of vacuum
μ_0: permeability of vacuum
χ: electric susceptibility
c: speed of light in vacuum

$$\varepsilon_o \mu_o = \frac{1}{c^2}$$

Maxwell Equation (2/2)

For periodically oscillating electromagnetic field;

$$\boldsymbol{j}_{\text{true}} = 0,\ \rho_{\text{true}} = 0.$$

For non-magnetic materials, $\boldsymbol{M}$=0 so that $\boldsymbol{B} = \mu_0 \boldsymbol{H}$.

$$\nabla \cdot \boldsymbol{D} = 0$$

$$\nabla \cdot \boldsymbol{H} = 0$$

$$\nabla \times \boldsymbol{E} = -\mu_o \frac{\partial \boldsymbol{H}}{\partial t}$$

$$\nabla \times \boldsymbol{H} = \frac{\partial \boldsymbol{D}}{\partial t}$$

Polarization

Polarization $\boldsymbol{P}$ = electric dipole moment in unit volume

$$\boldsymbol{P} = \varepsilon_o \chi \boldsymbol{E}$$

$$\boldsymbol{P} = \boldsymbol{p}\rho(r) = -e\boldsymbol{x}\rho(r) = -\frac{e^2}{m\omega^2}\rho(r)\boldsymbol{E}$$

$$\Rightarrow \chi(\boldsymbol{r}) = -\frac{e^2}{m\omega^2\varepsilon_o}\rho(\boldsymbol{r}) = -\frac{e^2\lambda^2}{4\pi^2\varepsilon_o mc^2}\rho(\boldsymbol{r}) = -r_o\frac{\lambda^2}{\pi}\rho(\boldsymbol{r})$$

$\chi(\boldsymbol{r})$ have the periodicity of crystal lattice

$$\chi(\boldsymbol{r}) = \sum_g \chi_{\boldsymbol{g}} \exp(i\boldsymbol{g}\cdot\boldsymbol{r})$$

$$\Rightarrow \rho(\boldsymbol{r}) = \frac{1}{v_c}\sum_{\boldsymbol{g}} F(\boldsymbol{g})\exp(i\boldsymbol{g}\cdot\boldsymbol{r})$$

$$\Rightarrow \chi_{\boldsymbol{g}} = -\frac{r_o\lambda^2}{\pi v_c}F(\boldsymbol{g})$$

Electromagnetic Wave in Periodic Medium

Bloch Theorem

Incident Plane Wave in Vacuum $\exp\{i(\boldsymbol{K}_o \cdot \boldsymbol{r} - \omega t)\}$

➡ Waves inside Periodic Medium $E = \exp\{i(\boldsymbol{K}_o \cdot \boldsymbol{r} - \omega t)\} u(\boldsymbol{r})$

u(***r***) has periodicity of crystal lattice

➡ u(***r***) can be expanded in a Fourier Series with reciprocal lattice vector, ***g***.

$$E = \exp\{i(\boldsymbol{K}_o \cdot \boldsymbol{r} - \omega t)\} \sum_{\boldsymbol{g}} E_{\boldsymbol{g}} \exp(i\boldsymbol{g} \cdot \boldsymbol{r})$$

Bloch Wave

$$= e^{-i\omega t} \sum_{\boldsymbol{g}} E_{\boldsymbol{g}} \exp(i\boldsymbol{K}_{\boldsymbol{g}} \cdot \boldsymbol{r})$$

$$\boldsymbol{K}_{\boldsymbol{g}} = \boldsymbol{K}_o + \boldsymbol{g}$$

Some Mathematic....

$$\frac{\partial \boldsymbol{D}}{\partial t} = -i\omega \boldsymbol{D}, \frac{\partial \boldsymbol{H}}{\partial t} = -i\omega \boldsymbol{H}$$

$$\begin{aligned} \nabla \times (\nabla \times \boldsymbol{E}) &= i\omega\mu_o \nabla \times \boldsymbol{H} \\ &= i\omega\mu_o (-i\omega) \boldsymbol{D} \\ &= \omega^2 \mu_o \varepsilon_o (1 + \chi(\boldsymbol{r})) \boldsymbol{E} \\ &= \frac{\omega^2}{c^2} (1 + \chi(\boldsymbol{r})) \boldsymbol{E} \\ &= K^2 (1 + \chi(\boldsymbol{r})) \boldsymbol{E} \end{aligned}$$

$$K = \frac{\omega}{c} = \frac{2\pi}{\lambda}; \text{X} - \text{ray wavenumber in vacuum}$$

$$\nabla \times \left\{ \boldsymbol{E}_g \exp\left(i\boldsymbol{K}_g \cdot \boldsymbol{r}\right) \right\} = i\boldsymbol{K}_g \times \boldsymbol{E}_g \exp\left(i\boldsymbol{K}_g \cdot \boldsymbol{r}\right)$$

$$\nabla \times \nabla \times \left\{ \boldsymbol{E}_g \exp\left(i\boldsymbol{K}_g \cdot \boldsymbol{r}\right) \right\} = -\boldsymbol{K}_g \times \left(\boldsymbol{K}_g \times \boldsymbol{E}_g\right) \exp\left(i\boldsymbol{K}_g \cdot \boldsymbol{r}\right)$$

Mathematics (cont'd)

$$\boldsymbol{E}_{\boldsymbol{g}[\perp \boldsymbol{K}_{\boldsymbol{g}}]} = -\frac{1}{K_g^2}\boldsymbol{K}_{\boldsymbol{g}} \times \left(\boldsymbol{K}_{\boldsymbol{g}} \times \boldsymbol{E}_{\boldsymbol{g}}\right)$$

$$\Rightarrow \nabla \times \nabla \times \left\{E_g \exp\left(ig \cdot r\right)\right\} = K_g^2 \boldsymbol{E}_{\boldsymbol{g}[\perp \boldsymbol{K}_{\boldsymbol{g}}]} \exp\left(ig \cdot r\right)$$

$$\chi\left(\boldsymbol{r}\right)E\left(\boldsymbol{r}\right) = \sum_{\boldsymbol{h}'}\sum_{\boldsymbol{h}} \chi_{\boldsymbol{h}'} \exp\left(i\boldsymbol{h}' \cdot \boldsymbol{r}\right)\boldsymbol{E}_{\boldsymbol{h}} \exp\left(i\boldsymbol{K}_{\boldsymbol{h}} \cdot \boldsymbol{r}\right)$$

$$= \sum_{\boldsymbol{g}}\sum_{\boldsymbol{h}} \chi_{\boldsymbol{g}\text{-}\boldsymbol{h}}\boldsymbol{E}_{\boldsymbol{h}} \exp\left(i\boldsymbol{K}_{\boldsymbol{g}} \cdot \boldsymbol{r}\right)$$

$$\boldsymbol{h} + \boldsymbol{h}' = \boldsymbol{g}, \boldsymbol{h}' + \boldsymbol{K}_{\boldsymbol{h}} = \boldsymbol{K}_{\boldsymbol{g}}$$

$$\sum_{g}\left\{K_g^2 \boldsymbol{E}_{\boldsymbol{g}[\perp \boldsymbol{K}_{\boldsymbol{g}}]} - K^2 \boldsymbol{E}_{\boldsymbol{g}} - K^2 \sum_{\boldsymbol{h}} \chi_{\boldsymbol{g}-\boldsymbol{h}}\boldsymbol{E}_{\boldsymbol{h}}\right\}\exp\left(i\boldsymbol{K}_{\boldsymbol{g}} \cdot \boldsymbol{r}\right) = 0 \quad (*)$$

Basic Equations for Dynamical Theory

Condition for the equation (*) should be valid for arbitrary $\boldsymbol{r}$ gives the basic equation for dynamical diffraction theory:

$$\frac{K_g^2 \boldsymbol{E}_{\boldsymbol{g}[\perp \boldsymbol{K}_g]} - K^2 \boldsymbol{E}_{\boldsymbol{g}}}{K^2} = \sum_{\boldsymbol{h}} \chi_{\boldsymbol{g}-\boldsymbol{h}} \boldsymbol{E}_{\boldsymbol{h}}$$

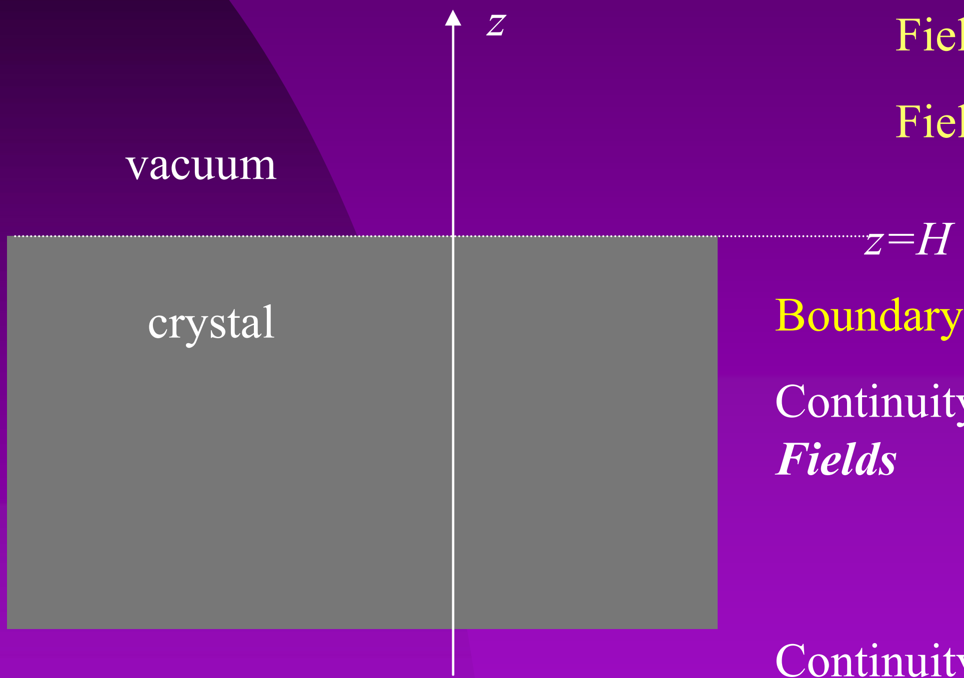
Since

$$\chi_{\boldsymbol{g}} \square 10^{-6} \Rightarrow \boldsymbol{E}_{\boldsymbol{g}[\perp \boldsymbol{k}_g]} \cong \boldsymbol{E}_{\boldsymbol{g}}$$

the basic equation is well approximated by

$$\frac{K_g^2 - K^2}{K^2} \boldsymbol{E}_{\boldsymbol{g}} = \sum_{\boldsymbol{h}} \chi_{\boldsymbol{g}-\boldsymbol{h}} \boldsymbol{E}_{\boldsymbol{h}}$$

Boundary Conditions (1/3)



Fields in vacuum: $(\boldsymbol{E}^a, \boldsymbol{D}^a)$

Fields in crystal: $(\boldsymbol{E}, \boldsymbol{D})$

Boundary conditions from Maxwell Equations:

Continuity of tangential components of ***Electric Fields***

$$E_t = E^a{}_t$$

Continuity of normal components of ***Electric Displacements***

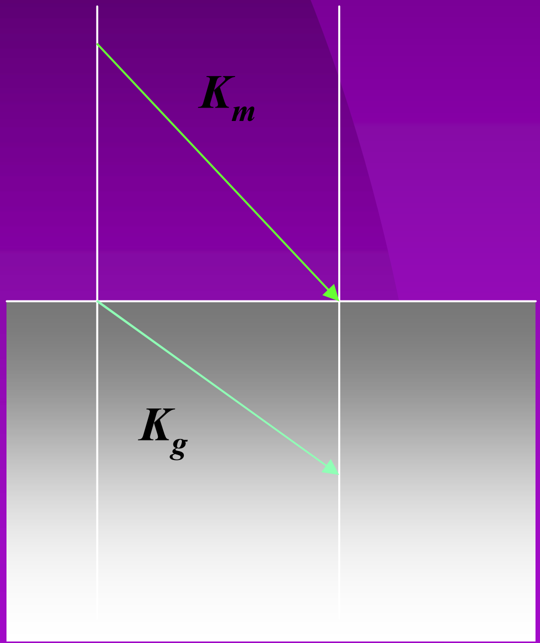
$$D_z = D^a{}_z$$

t: tangential component, z: z(=normal) component

Boundary Conditions (2/3)

Wavefield : Superposition of plane waves

$$\boldsymbol{E} = \exp(-i\omega t)\sum_{g} \boldsymbol{E}_g \exp(i\boldsymbol{K}_g \cdot \boldsymbol{r})$$



Wave Vector in Crystal: $\boldsymbol{K}_g$
Wave Vector in Vacuum: $\boldsymbol{K}_m$

$$\boldsymbol{K}_{gt} = \boldsymbol{K}_{mt}$$

crystal wave

$$\boldsymbol{E} = \sum_{g} \boldsymbol{E}_g \exp(i\boldsymbol{K}_g \cdot \boldsymbol{r}), \boldsymbol{D} = \sum_{g} \boldsymbol{D}_g \exp(i\boldsymbol{K}_g \cdot \boldsymbol{r})$$

vacuum wave

$$\boldsymbol{E}^a = \sum_{m} \boldsymbol{E}_m^a \exp(i\boldsymbol{K}_m \cdot \boldsymbol{r}), \boldsymbol{D}^a = \sum_{m} \boldsymbol{D}_m^a \exp(i\boldsymbol{K}_m \cdot \boldsymbol{r})$$

Boundary Conditions (3/3)

unit vector normal to the surface: $\hat{\boldsymbol{z}}$

unit vector tangential to the surface: $\hat{\boldsymbol{t}}$

$$\boldsymbol{K_g} = K_{gz}\hat{\boldsymbol{z}} + K_{gt}\hat{\boldsymbol{t}}$$

$$\boldsymbol{K_m} = K_{mz}\hat{\boldsymbol{z}} + K_{mt}\hat{\boldsymbol{t}}$$

Boundary Condition at $z=H$ (Crystal Surface)

$$\sum_{K_{gt}=K_{mt}} E_{gt} \exp\left(iK_{gz}H\right) = \sum_{K_{gt}=K_{mt}} E_{mt}^{a} \exp\left(iK_{mz}H\right)$$

$$\sum_{K_{gt}=K_{mt}} D_{gz} \exp\left(iK_{gz}H\right) = \sum_{K_{gt}=K_{mt}} D_{mz}^{a} \exp\left(iK_{mz}H\right)$$

$$\chi_g \ll 1 \Rightarrow \sum_{K_{gt}=K_{mt}} \boldsymbol{E_g} \exp\left(iK_{gz}H\right) = \sum_{K_{gt}=K_{mt}} \boldsymbol{E_m^a} \exp\left(iK_{mz}H\right)$$

Two-Wave Approximation (1/3)

Under usual experimental conditions, only two waves with $\boldsymbol{K_0}$ (incident direction) and $\boldsymbol{K_g}$ (diffracted direction) are strong inside the crystal.

Wavefield in crystal:

$$\boldsymbol{E} = \boldsymbol{E_0} \exp\left(i\boldsymbol{K_0} \cdot \boldsymbol{r}\right) + \boldsymbol{E_g} \exp\left(i\boldsymbol{K_g} \cdot \boldsymbol{r}\right)$$

Basic Equation:

$$\left(K_{\boldsymbol{o}}^2 - k^2\right) E_{\boldsymbol{o}} - K^2 P \chi_{\bar{\boldsymbol{g}}} E_{\boldsymbol{g}} = 0$$

$$K^2 P \chi_{\boldsymbol{g}} E_{\boldsymbol{o}} - \left(K_{\boldsymbol{g}}^2 - k^2\right) E_{\boldsymbol{g}} = 0$$

Averaged refractive index of crystal:

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

Polarization Factor

$P = 1$ for σ – polarization

$P = \cos 2\theta_{\mathrm{B}}$ for π – polarization

Two-Wave Approximation (2/3)

Condition for the basic equation,

$$\left(K_o^2 - k^2\right)E_o - K^2 P \chi_{\bar{g}} E_g = 0$$

$$K^2 P \chi_g E_o - \left(K_g^2 - k^2\right)E_g = 0$$

to have non-trivial solutions is

$$\begin{vmatrix} K_o^2 - k^2 & K^2 P \chi_{\bar{g}} \\ K^2 P \chi_g & K_g^2 - k^2 \end{vmatrix} = 0$$

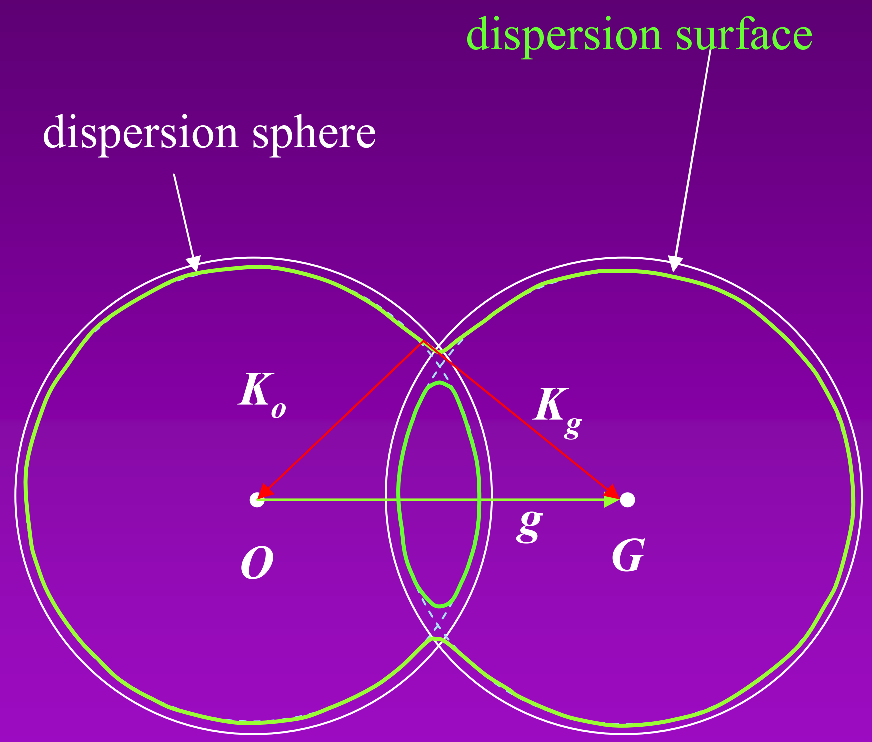
$$\boldsymbol{K}_g = \boldsymbol{K}_o + \boldsymbol{g}$$

By introducing new parameters:

$$\xi_o = K_o - k$$

$$\xi_g = K_g - k$$

$$\xi_o \xi_g = \frac{1}{4} K^2 P^2 \chi_g \chi_{\bar{g}}$$



Two Wave Approximation (3/3)

For non-absorbing crystals,

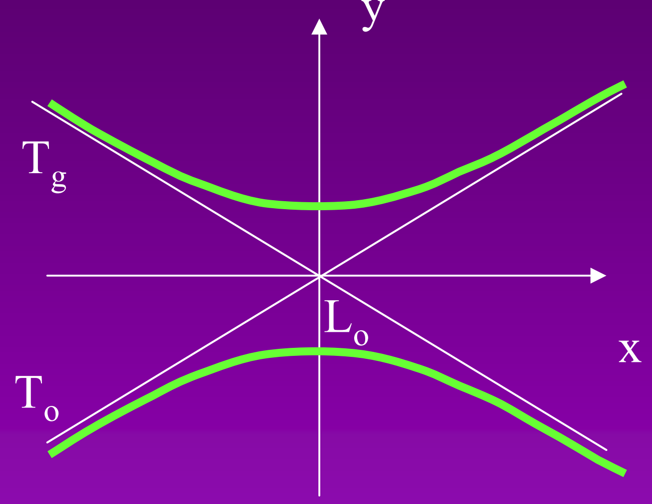
$$\chi_{\bar{g}} = \chi_g^* \text{ (complex conjugate of } \chi_g)$$

$$\chi_g \chi_{\bar{g}} = |\chi_g|^2$$

When we introduce a new parameter Λ as

$$\Lambda = \frac{2\pi \cos\theta_B}{K|P||\chi_g|} = \frac{\lambda \cos\theta_B}{|P||\chi_g|} \quad ,$$

$$\xi_o \xi_g = \frac{\pi^2 \cos^2\theta_B}{\Lambda^2}$$



Near the point L_o,

$$\xi_o = -x\sin\theta_B + y\cos\theta_B$$

$$\xi_g = x\sin\theta_B + y\cos\theta_B$$

→ **Dispersion surfaces form Hyperbolla**

$$-x^2 \sin^2\theta_B + y^2 \cos^2\theta_B = \frac{\pi^2 \cos^2\theta_B}{\Lambda^2}$$

Amplitude Ratio

$$2\xi_o E_o - KP\chi_{\bar{\mathbf{g}}} E_g = 0$$

$$KP\chi_{\mathbf{g}} E_o - 2\xi_g E_g = 0$$

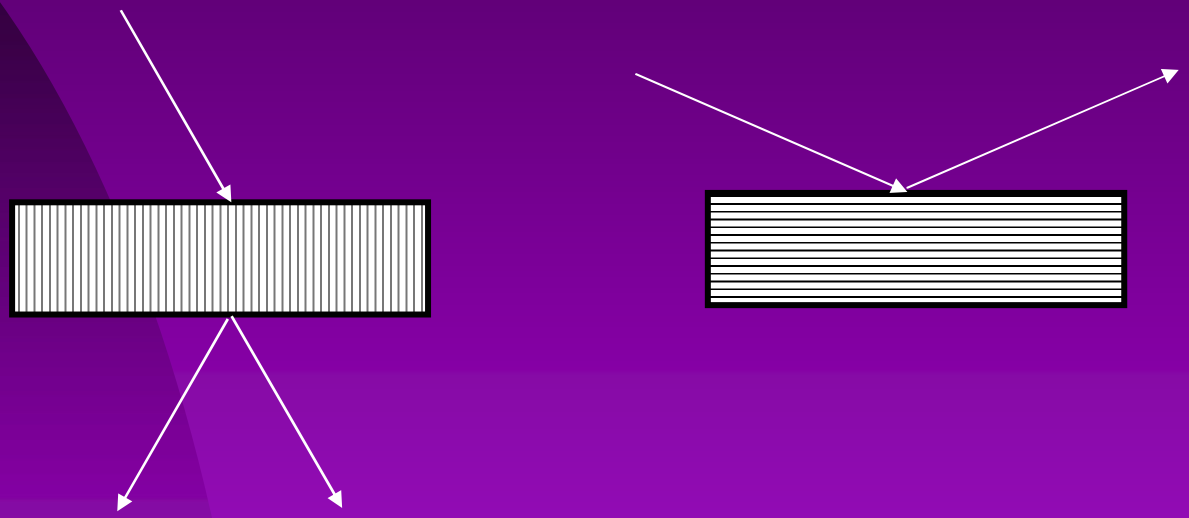
↓

Amplitude Ratio

$$r_j = \frac{E_{gj}}{E_{oj}} = \frac{2\xi_{oj}}{KP\chi_{\bar{g}}} = \frac{KP\chi_g}{2\xi_{gj}}$$

$j = 1, 2$

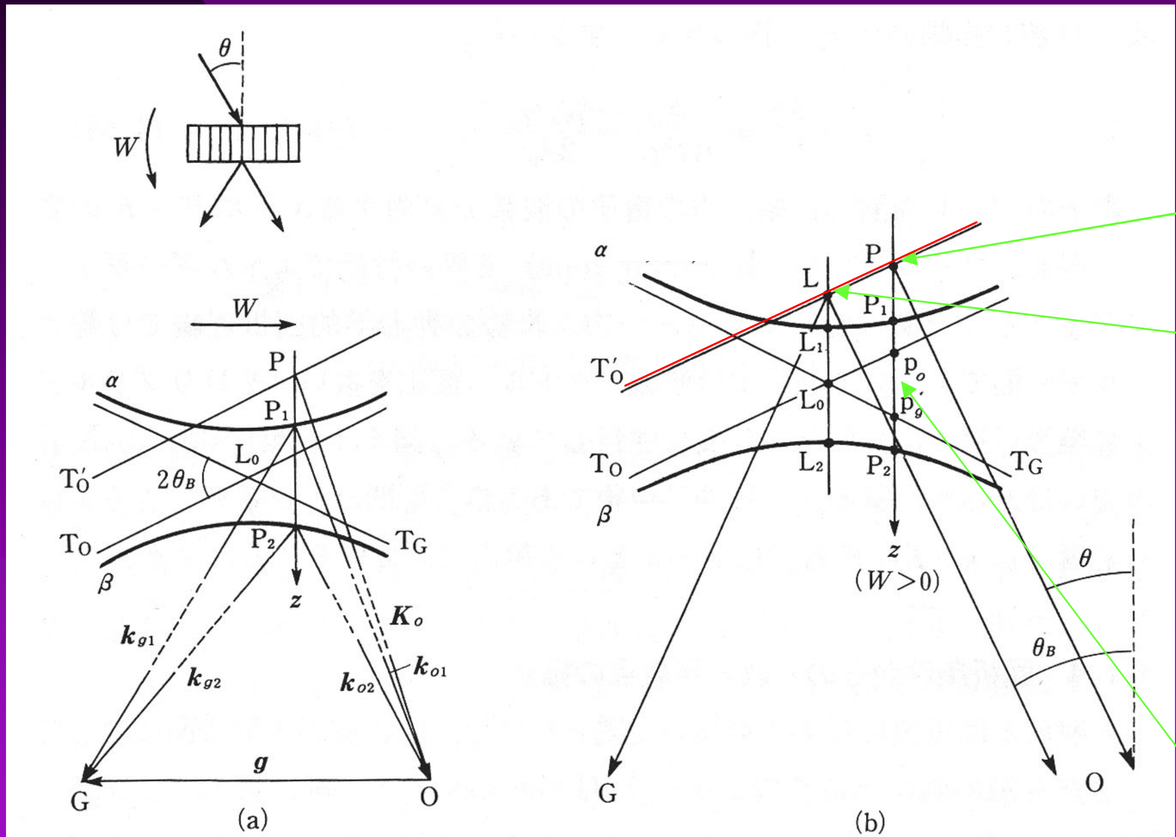
Diffraction Geometry



Symmetric Laue Case

Symmetric Bragg Case

Symmetric Laue Case



Dispersion sphere of vacuum wave (radius K)

Starting point of wave vector $\boldsymbol{K_o}$: P

Laue point: L

Deviation from Bragg Condition

$$\Delta\theta = \frac{\overline{LP}}{K}$$

$$p_o p_g = \frac{\xi_g - \xi_o}{\cos\theta_B} = 2\sin\theta_B \cdot \overline{LP}$$

$$= 2K\left(\theta_B - \theta\right)\sin\theta_B$$

Symmetric Laue Case: Deviation Parameter

Deviation Parameter *W*

$$W = \frac{p_o p_g}{L_1 L_2} = \frac{2\Lambda \sin\theta_B}{\lambda}(\theta_B - \theta)$$

$$= \frac{(\theta_B - \theta)\sin 2\theta_B}{|P||\chi_g|}$$

$\sigma - polarization$ $\quad W^{\sigma}$

$\pi - polarization$ $\quad W^{\pi}$

$$W^{\sigma} = |\cos 2\theta_B| W^{\pi}$$

Usually $W = W^{\sigma}$

$$\xi_g - \xi_o = \frac{2\pi W}{\Lambda}\cos\theta_B$$

$$\xi_g \xi_o = \frac{\pi^2 \cos^2\theta_B}{\Lambda^2}$$

Solving above equations, we can get

$$\xi_{oj} = \frac{\pi\cos\theta_B}{\Lambda}\left(-W \pm \sqrt{W^2 + 1}\right)$$

$$\xi_{gj} = \frac{\pi\cos\theta_B}{\Lambda}\left(W \pm \sqrt{W^2 + 1}\right)$$

upper sign: j=1, lower sign: j=2

Symmetric Laue Case: Amplitude Ratio

$$r_j = \frac{E_{gj}}{E_{oj}} = \frac{|P|}{P} \exp\left(i\alpha_g\right)\left(-W \pm \sqrt{W^2+1}\right)$$

$$\text{upper sign } j=1, \text{lower sign } j=2$$

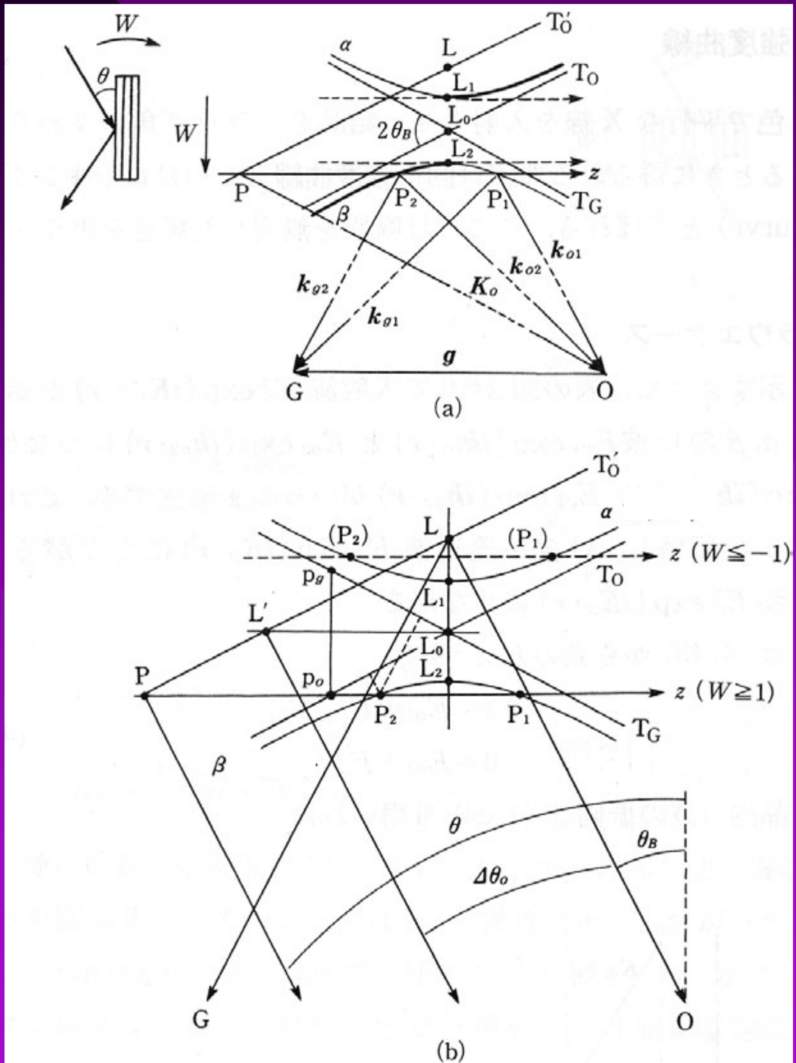
Here, $$\chi_g = \left|\chi_g\right| \exp\left(i\alpha_g\right)$$

For non-absorbing crystals,

$$\chi_{\bar{g}} = \chi_g^*, \alpha_{\bar{g}} = -\alpha_g, \left|\chi_{\bar{g}}\right| = \left|\chi_g\right|$$

$$\sqrt{\frac{\chi_g}{\chi_{\bar{g}}}} = \exp\left(i\alpha_g\right)$$

Symmetric Bragg Case (1/2)



Between L1 and L2, z has no intersections with dispersion surfaces.

Total Reflection Region

Deviation from Bragg Condition

$$\theta - \theta_B = \frac{\overline{LP}}{K}$$

$$p_o p_g = \frac{-\xi_g - \xi_o}{\cos\theta_B}$$

$$= 2\sin\theta_B \cdot \overline{L'P} = 2K\left(\theta - \theta_B - \Delta\theta_o\right)\sin\theta_B$$

Symmetric Bragg Case (2/2)

$\Delta\theta_o$: Deviation from geometrical Bragg angle by refraction

$$\Delta\theta_o = \frac{-\chi_o}{\sin 2\theta_B} = \frac{2(1-n)}{\sin 2\theta_B}$$

Deviation parameter, *W*

$$W = \frac{\overline{p_o p_g}}{\overline{L_1 L_2}} = \frac{2\Lambda \sin\theta_B}{\lambda}(\theta - \theta_B - \Delta\theta_o)$$

↓

$$\xi_g + \xi_o = -\frac{2\pi W}{\Lambda}\cos\theta_B$$

$$\xi_{oj} = \frac{\pi\cos\theta_B}{\Lambda}\left(-W \mp \sqrt{W^2 - 1}\right)$$

$$\xi_{gj} = \frac{\pi\cos\theta_B}{\Lambda}\left(W \pm \sqrt{W^2 - 1}\right)$$

upper sign: *j*=1, lower sign: *j*=2

Amplitude Ratio

$$r_j = \frac{E_{gj}}{E_{oj}} = \frac{|P|}{P}\exp(i\alpha_g)\left(-W \pm \sqrt{W^2 - 1}\right)$$

upper sign: *j*=1, lower sign: *j*=2

Rocking Curves

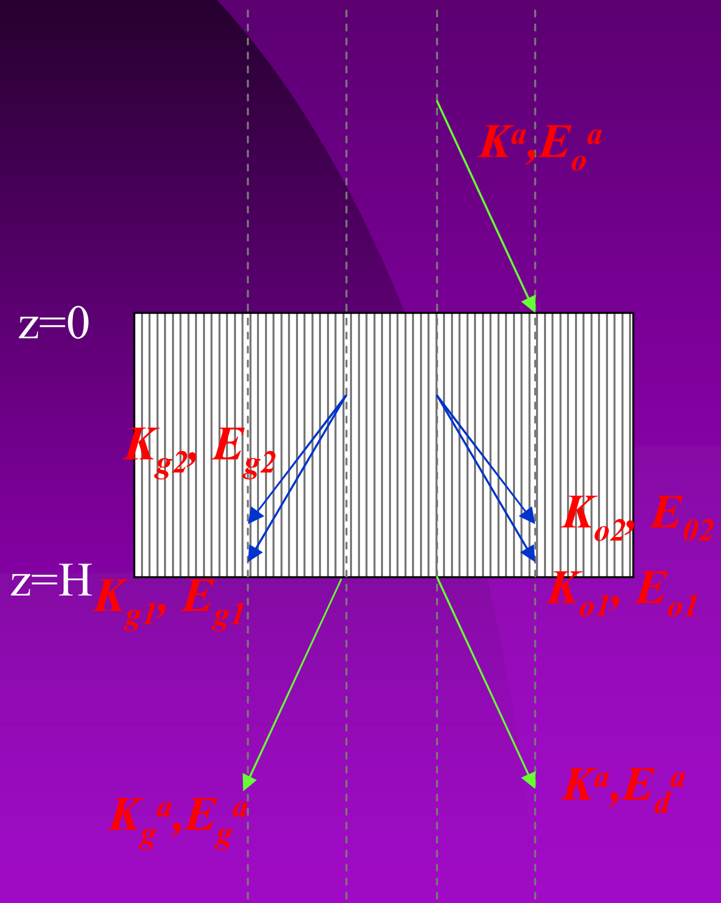
Use monochromatic plane wave as an incident beam;

Rocking the sample crystal around the Bragg angle;

↓

We can observe so-called rocking curve.

Rocking Curve: Symmetric Laue Case (1/3)



Incident Wave

$$E_o^a \exp\left(i\boldsymbol{K}^a \cdot \boldsymbol{r}\right)$$

Crystal Wave

o-wave

$$E_{o1} \exp\left(i\boldsymbol{K}_{o1} \cdot \boldsymbol{r}\right)$$

$$E_{o2} \exp\left(i\boldsymbol{K}_{o2} \cdot \boldsymbol{r}\right)$$

g-wave

$$E_{g1} \exp\left(i\boldsymbol{K}_{g1} \cdot \boldsymbol{r}\right)$$

$$E_{g2} \exp\left(i\boldsymbol{K}_{g2} \cdot \boldsymbol{r}\right)$$

Outgoing Wave

o-wave

$$E_d^a \exp\left(i\boldsymbol{K}^a \cdot \boldsymbol{r}\right)$$

g-wave

$$E_g^a \exp\left(i\boldsymbol{K}_g^a \cdot \boldsymbol{r}\right)$$

Rocking Curve: Symmetric Laue Case (2/3)

Boundary condition at z = 0
(incident surface)

$$E_o^a = E_{o1} + E_{o2}$$

$$0 = E_{g1} + E_{g2}$$

$$E_{oj} = \frac{1}{2}\left(1 \pm \frac{W}{\sqrt{1+W^2}}\right)E_o^a$$

$$E_{gj} = \frac{1}{2}\frac{P}{|P|}\exp\left(i\alpha_g\right)\frac{\pm 1}{\sqrt{1+W^2}}$$

upper sign: *j*=1, lower sign: *j*=2

At W=0 (exact Bragg condition),

$$\left|E_{oj}\right| = \left|E_{gj}\right|$$

Boundary condition at z = *H*
(exit surface)

$$E_{o1}\exp\left(iK_{o1}H\right) + E_{o2}\exp\left(iK_{o2}H\right) = E_d^a\exp\left(iK_zH\right)$$

$$E_{g1}\exp\left(iK_{g1}H\right) + E_{g2}\exp\left(iK_{g2}H\right) = E_g^a\exp\left(iK_{gz}^aH\right)$$

$$\boldsymbol{K}_{oj} = -\overline{\mathrm{PP}}_j\hat{\boldsymbol{z}} + \boldsymbol{K}^a$$

$$\boldsymbol{K}_{gj} = -\overline{\mathrm{PP}}_j\hat{\boldsymbol{z}} + \boldsymbol{K}^a + \boldsymbol{g}$$

$\hat{\boldsymbol{z}}$: inner normal vector at the incident surface

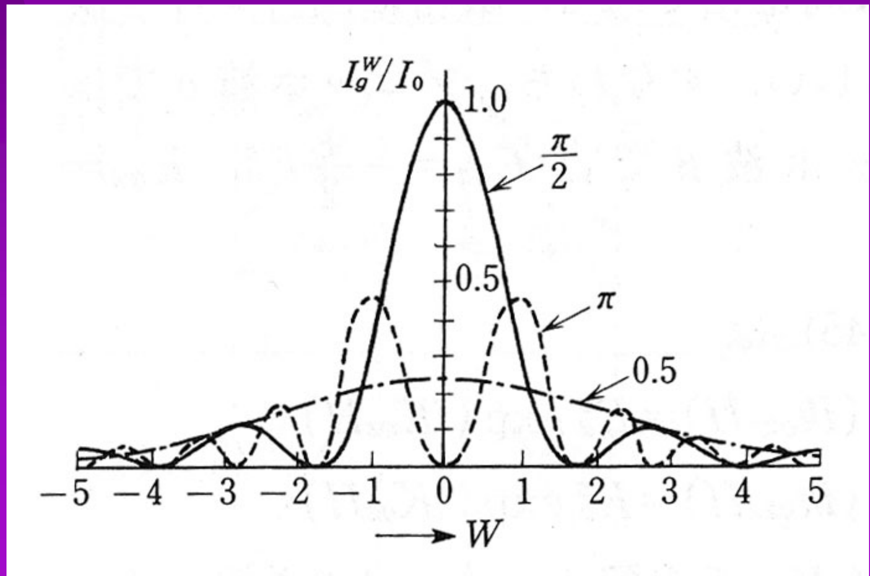
$$\overline{\mathrm{PP}}_j = \frac{-\left(\xi_{oj} + \dfrac{K\chi_o}{2}\right)}{\cos\theta_B}$$

$$\rightarrow \quad K_{ojz} = K_{gjz} = -\overline{\mathrm{PP}}_j + K_z^a$$

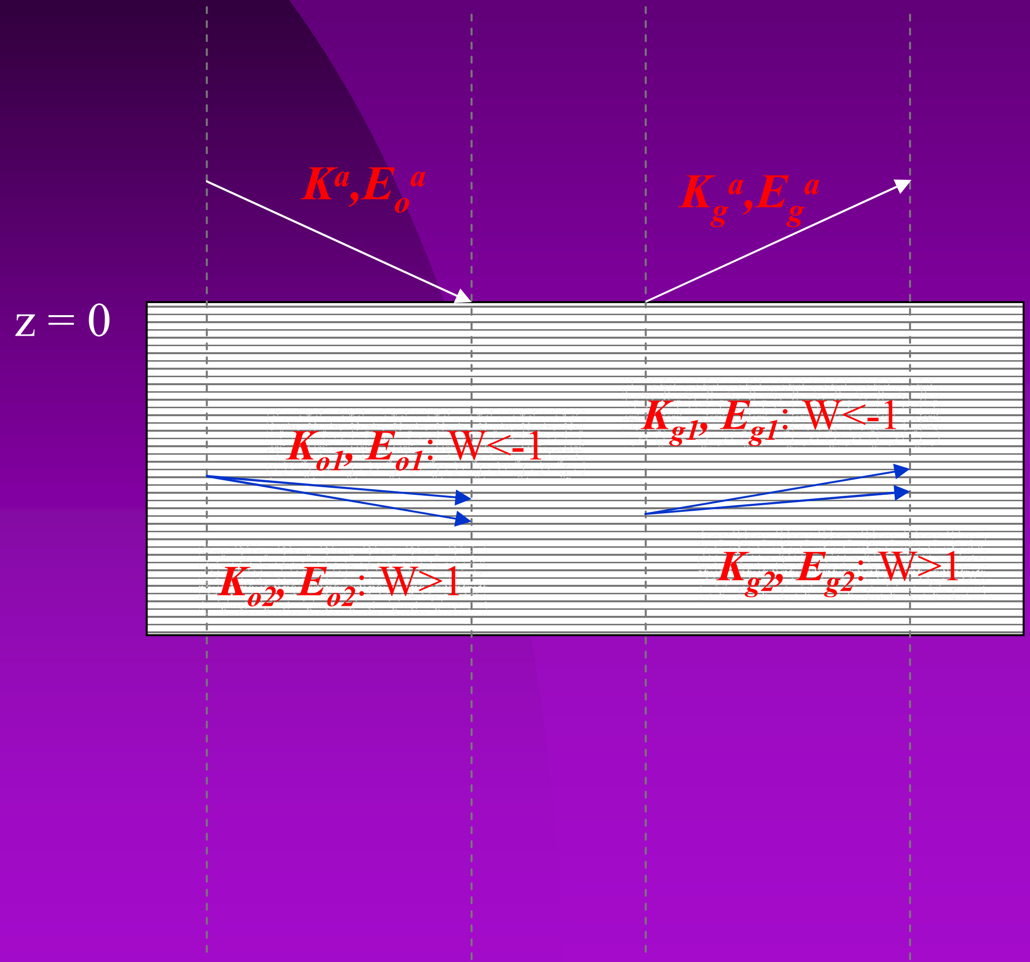
Rocking Curve: Symmetric Laue Case (3/3)

$$\frac{I_g^W}{I_o} = \left|\frac{E_g^a}{E_o^a}\right|^2 = \frac{\sin^2\left(\pi H \sqrt{W^2+1}/\Lambda\right)}{W^2+1}$$

$$\frac{I_d^W}{I_o} = \left|\frac{E_d^a}{E_o^a}\right|^2 = \frac{W^2+\cos^2\left(\pi H \sqrt{W^2+1}/\Lambda\right)}{W^2+1}$$



Rocking Curve: Symmetric Bragg Case (1/3)



Boundary condition at z = 0

$$E_o^a = E_{o1}\,(W \le -1), E_{o2}(W \ge 1)$$

$$E_g^a = E_{g1}\,(W \le -1), E_{g2}(W \ge 1)$$

$$E_g^a = \frac{|P|}{P}\exp\left(i\alpha_g\right)\left(-W \mp \sqrt{W^2-1}\right)E_o^a$$

upper sign: W<-1, lower sign: W>1

Rocking Curve: Symmetric Bragg Case (2/3)

$|W| \le 1 \Rightarrow$ z-components of $\boldsymbol{K}_o$ and $\boldsymbol{K}_g$ are complex

$$\boldsymbol{K}_{oj} = -\overline{\mathrm{PP}}_j \hat{\boldsymbol{z}} + \boldsymbol{K}$$

$$\boldsymbol{K}_{gj} = -\overline{\mathrm{PP}}_j \hat{\boldsymbol{z}} + \boldsymbol{K} + \boldsymbol{g}$$

$$\overline{\mathrm{PP}}_j = -\left(\xi_{oj} + \frac{K\chi_o}{2}\right) \Big/ \sin\theta_B$$

$$K_{oz}^i = \mathrm{Im}\left(K_{oz}\right) = K_{gz}^i = \frac{\pi\sqrt{1-W^2}}{\Lambda \tan\theta_B}$$

$$\xi_o = \frac{\pi \cos\theta_B}{\Lambda}\left(-W + i\sqrt{1-W^2}\right)$$

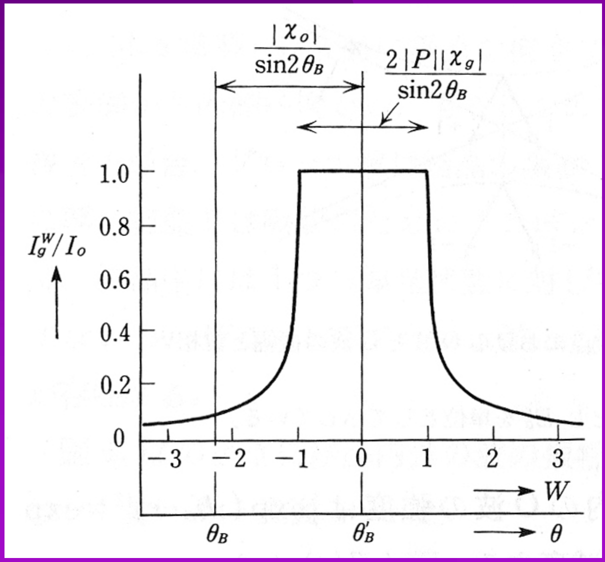
Another solution will give a divergent solution

$$E_g^a = \frac{|P|}{P} \exp\left(i\alpha_g\right)\left(-W + i\sqrt{1-W^2}\right) E_o^a$$

Rocking Curve: Symmetric Bragg Case (3/3)

Rocking curve (Darwin Curve)

$$\frac{I_g^W}{I_o} = \frac{|E_g^a|^2}{|E_o^a|^2} = \begin{cases} \left(|W| - \sqrt{W^2 - 1}\right)^2 & (|W| \geq 1) \\ 1 & (|W| \leq 1) \end{cases}$$



|W|<1: All incident energies are reflected back.

Total Reflection

$$\theta - \theta_B = \frac{|P||\chi_g|}{\sin 2\theta_B} W + \frac{|\chi_o|}{\sin 2\theta_B}$$

Center of total reflectiuon, W=0, is deviated from geometrical Bragg angle θ_B by

$$\frac{|\chi_o|}{\sin 2\theta_B}$$

Range of total reflection (-1<W<1)

$$\omega = \frac{2|P||\chi_g|}{\sin 2\theta_B} = \frac{\lambda}{\Lambda \sin \theta_B}$$

$$= \frac{2}{\pi} \frac{r_o}{v_c} |F_g| \lambda^2 \frac{|P|}{\sin 2\theta_B} \propto |\chi_g| or |F_g|$$

Darwin Width, ~microradian order

Absorbing Crystal

Absorption: Anomalous dispersion term into atomic scattering factor

$$\chi_g = \chi'_g + i\chi''_g$$

$$\chi'_g = -\frac{r_o\lambda^2}{\pi v_c}F'_g = -\frac{r_o\lambda^2}{\pi v_c}\sum_j\left(f_j^o + f'_j\right)\exp\left(-i\boldsymbol{g}\cdot\boldsymbol{r}_j\right)$$

$$\chi''_g = -\frac{r_o\lambda^2}{\pi v_c}F''_g = -\frac{r_o\lambda^2}{\pi v_c}\sum_j f''_j\exp\left(-i\boldsymbol{g}\cdot\boldsymbol{r}_j\right)$$

χ'_g, χ''_g :complex

$$\chi'_{\bar{g}} = \chi'^{*}_{g}, \chi''_{\bar{g}} = \chi'^{*}_{g}$$

Centrosymmetric Crsyatls

χ'_g, χ''_g :real

$$\chi'_{\bar{g}} = \chi'_g, \chi''_{\bar{g}} = \chi''_g$$

↓

$$\chi_g = \chi_{\bar{g}}$$

$$\chi''_g \ll \chi'_g \Rightarrow \chi_g\chi_{\bar{g}} \approx \chi'^{2}_g + 2i\chi'_g\chi''_g$$

A new parameter κ is defined as

$$\kappa = \frac{\chi''_g}{\chi'_g}$$

Symmetric Laue Case: Absorbing Crystal (1/2)

$$\frac{I_g^W}{I_o} = \frac{\exp\left(-\mu H / \cos\theta_B\right)}{W^2+1}\left\{\sin^2\left(\frac{\pi H\sqrt{W^2+1}}{\Lambda}\right) + \sinh^2\left(\frac{\kappa\pi H\sqrt{W^2+1}}{\Lambda}\right)\right\}$$

$$\Lambda = \frac{\lambda\cos\theta_B}{|P||\chi_g'|}, W = \frac{(\theta_B-\theta)\sin 2\theta_B}{|P||\chi_g'|}$$

$$\sin^2\left(\frac{\pi H\sqrt{W^2+1}}{\Lambda}\right)$$

→ Oscillating Term, Hardly to be observed experimentally without very good plane wave

averaging →

$$\frac{\overline{I_g^W}}{I_o} = \frac{1}{4(W^2+1)}\left[\exp\left\{-\frac{\mu H}{\cos\theta_B}\left(1-\frac{|P|\varepsilon}{\sqrt{1+W^2}}\right)\right\} + \exp\left\{-\frac{\mu H}{\cos\theta_B}\left(1+\frac{|P|\varepsilon}{\sqrt{1+W^2}}\right)\right\}\right]$$

$$\varepsilon = \frac{\chi_g''}{\chi_o''}$$

Bloch Wave α
small absorption

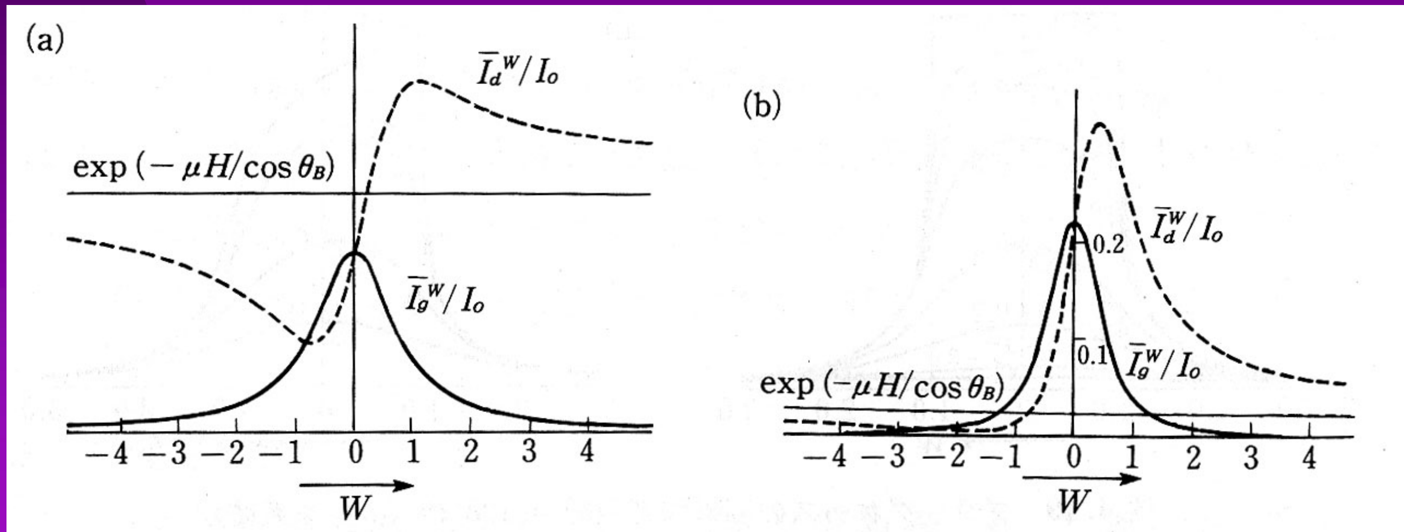
Bloch Wave β
large absorption

Anomalous Transmission (Borrman Effect)

Symmetric Laue Case: Absorbing Crystal (2/2)

Forward Diffraction

$$\frac{\overline{I_d^W}}{I_o} = \frac{1}{4}\left[\left(1+\frac{W}{\sqrt{1+W^2}}\right)^2 \exp\left\{-\frac{\mu H}{\cos\theta_B}\left(1-\frac{|P|\varepsilon}{\sqrt{1+W^2}}\right)\right\} + \left(1-\frac{W}{\sqrt{1+W^2}}\right)^2 \exp\left\{-\frac{\mu H}{\cos\theta_B}\left(1+\frac{|P|\varepsilon}{\sqrt{1+W^2}}\right)\right\}\right]$$



Thin Crystal

Thick Crystal

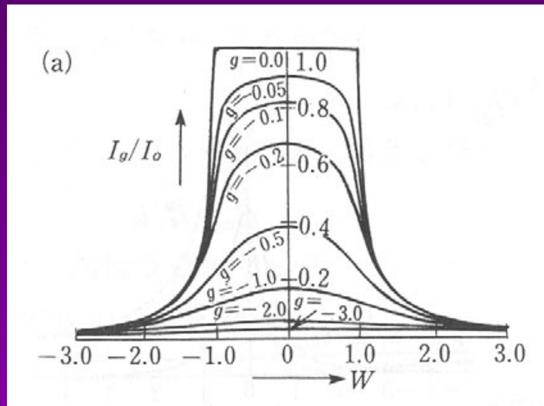
Symmetric Bragg Case: Absorbing Crystal

Rocking curve for a symmetric Bragg case diffraction from a semi-infinite absorbing crystal (with centrosymmetry)

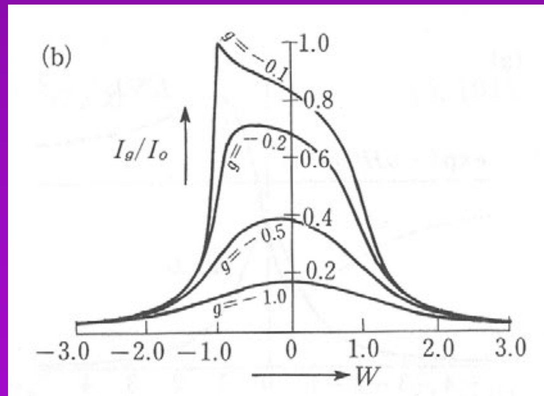
$$\frac{I_g^W}{I_o} = L - \sqrt{L^2 - 1}$$

$$L = \frac{W^2 + g^2 + \sqrt{\left(W^2 - g^2 - 1 + \kappa^2\right)^2 + 4\left(gW - \kappa\right)^2}}{1 + \kappa^2}$$

$$g = \frac{\chi_o''}{|P|\left|\chi_g'\right|}$$



κ = 0



κ = 0.1

Summary

- Very quick scan of x-ray diffraction theory was attempted.
- You may need reference text books.
- References
  - Dynamical Theory of X-Ray Diffraction, A. Authie, Oxford University Press, 2001
  - Handbook on Synchrotron Radiation Vol. 3, North-Holland, 1991.

Thank you for your attention.

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