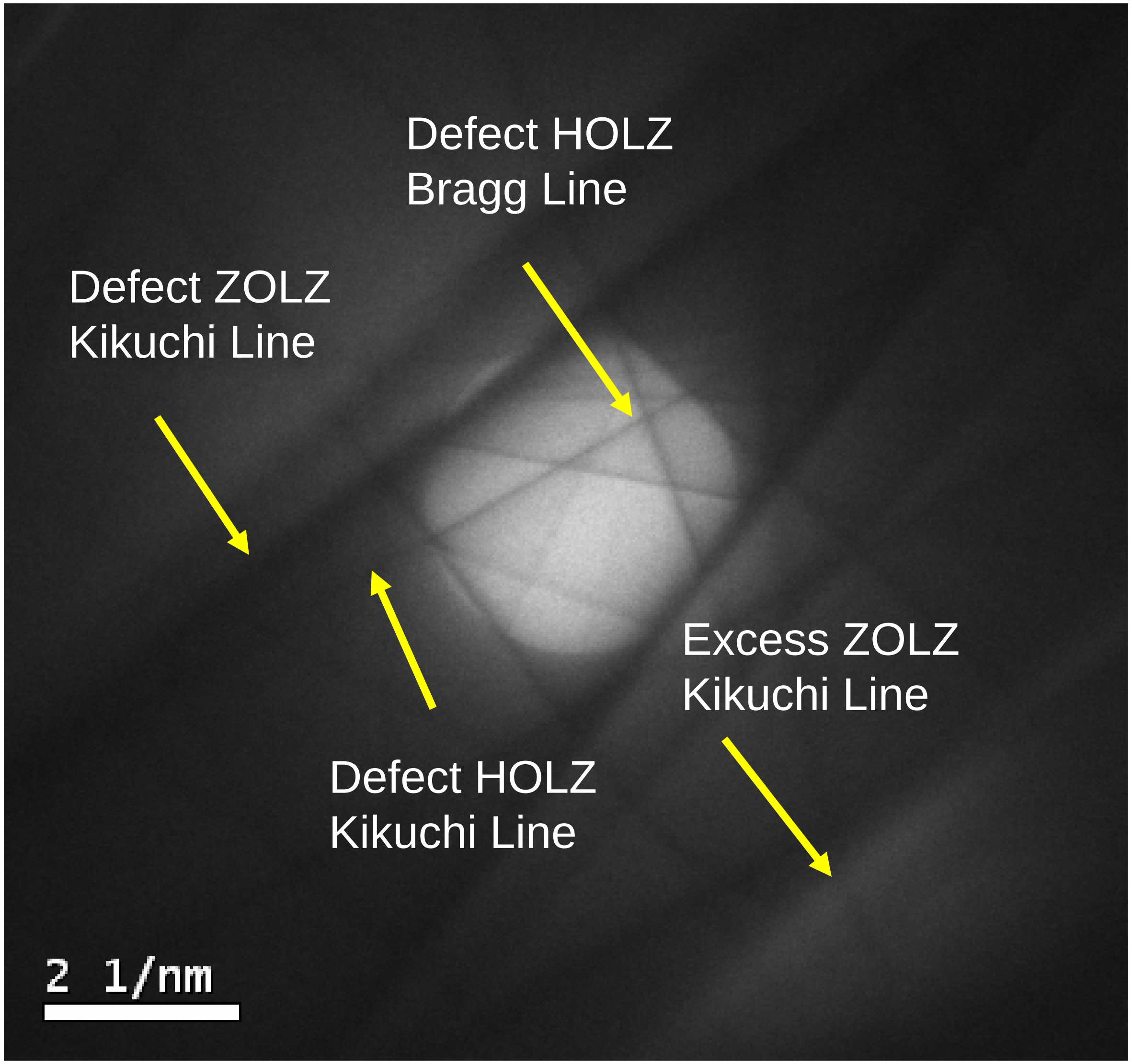
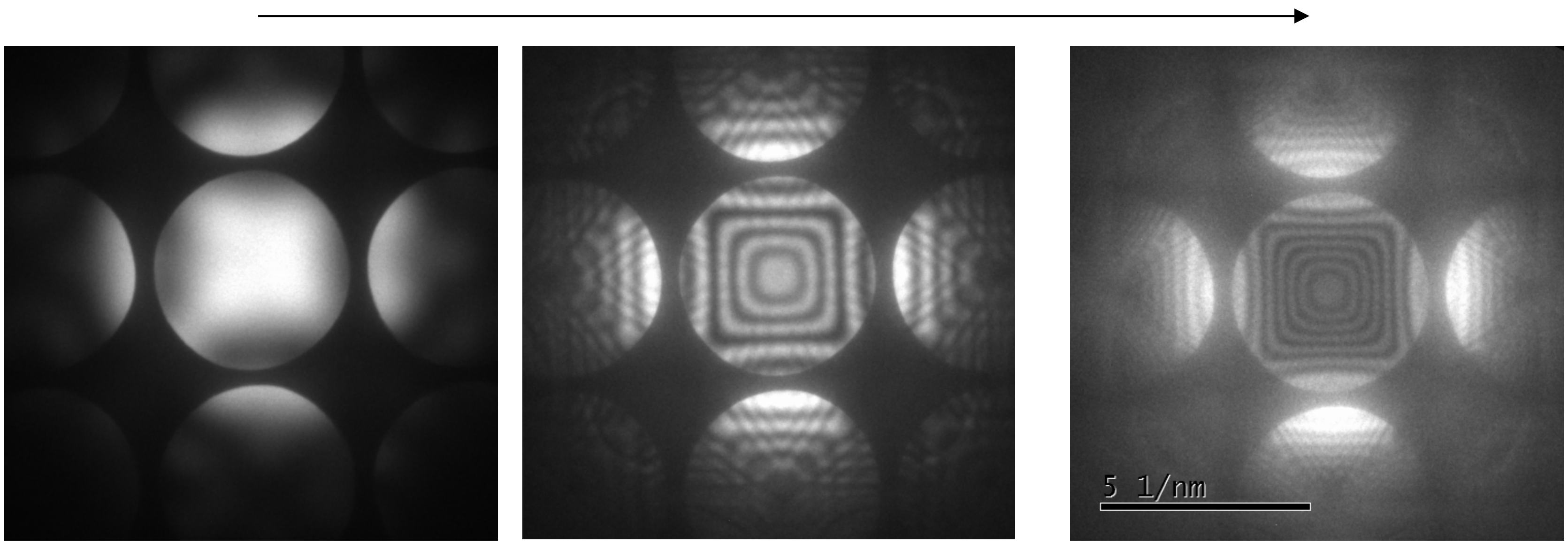
CBED Features



Influence of Thickness

thicker



K-M fringe frequency increases with thickness

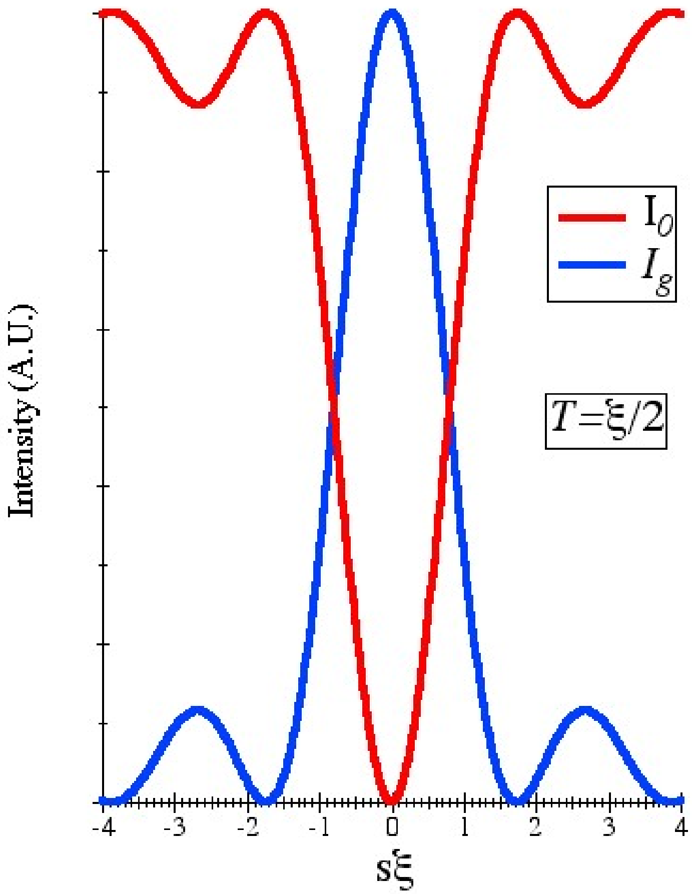
Intensity oscillation in CBED disk (I)

At a two-beam condition:

$$I_{\mathbf{g}} = \left[\frac{\sin\left(\pi s_{eff} T\right)}{s_{eff}\,\xi} \right]^2$$

$$s_{eff} \equiv \sqrt{s^2 + \left(\frac{1}{\xi^2}\right)}$$

$$I_{\mathbf{0}} = 1 - \left[\frac{\sin\left(\pi s_{eff} T\right)}{s_{eff}\,\xi} \right]^2$$



Frequency of intensity oscillation depends on T, ξ

Intensity oscillation in CBED disk (II)

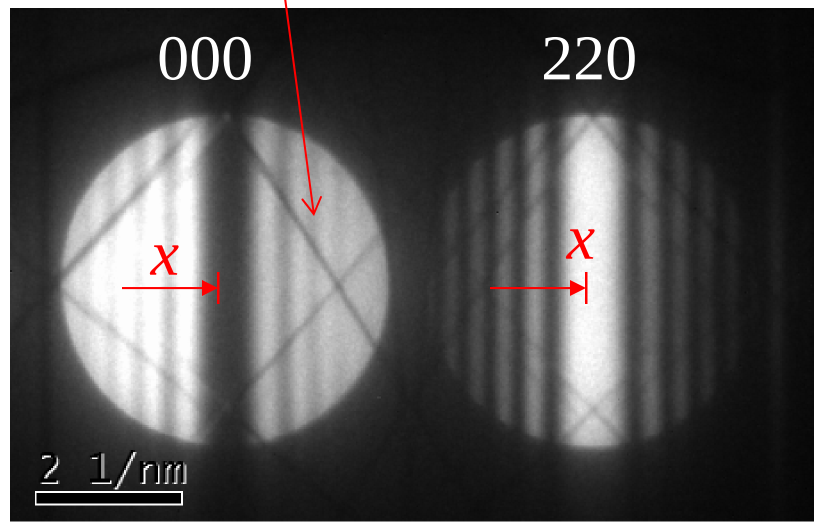
Oscillations arise from variation in s_g with beam tilt

Experiment shows absorption effects

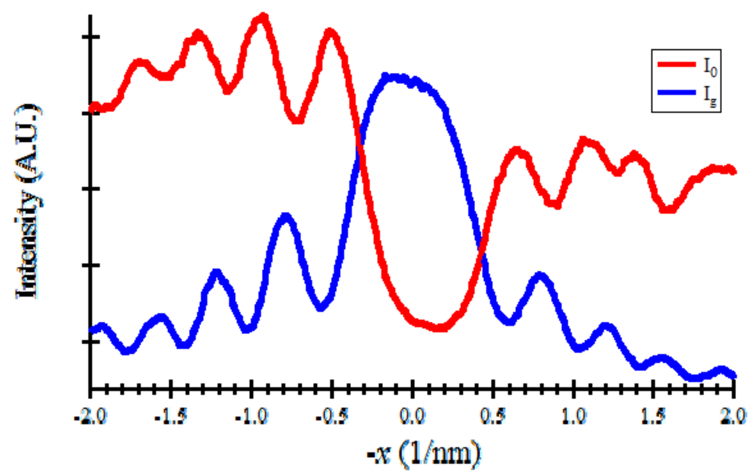
$$s = \frac{g}{k} \cdot x$$

x measures distance to Bragg condition

bright-field disk shows
"anomolous absorption"



increasing s



Absorption

Incoherent and inelastic scattering result in attenuation

What if $\Phi(\mathbf{r})$ is complex?

Simple Case: $\Phi(\mathbf{r}) = \Phi_{\mathbf{0}} + i\Phi'_{\mathbf{0}}$ $U(\mathbf{r}) = U_{\mathbf{0}} + iU'_{\mathbf{0}}$

$$\left[\nabla^2 + 4\pi^2\left(k^2 + U_{\mathbf{0}} + iU'_{\mathbf{0}}\right)\right]\psi(\mathbf{r}) = 0$$

Solution is an attenuated plane wave:

$$\psi(\mathbf{r}) = \mathrm{e}^{2\pi i(\mathbf{K}+i\mathbf{K}')\cdot\mathbf{r}} = \mathrm{e}^{2\pi i\mathbf{K}\cdot\mathbf{r}}\mathrm{e}^{-2\pi\mathbf{K}'\cdot\mathbf{r}} \qquad \nabla^2\psi(\mathbf{r}) = \left(K^2 - K'^2 + 2iKK'\right)\psi(\mathbf{r})$$

$$\left.\begin{aligned} K^2 - K'^2 &= k^2 + U_{\mathbf{0}} \\ 2KK' &= U'_{\mathbf{0}} \end{aligned}\right\}$$

Solve for K and K'

Absorption in a crystal

$$\Phi(\mathbf{r}) \to \Phi(\mathbf{r}) + i\Phi'(\mathbf{r})$$

The operator $\tilde{\mathrm{A}}$ becomes non-Hermitian:

$$\tilde{\mathrm{A}} \to \tilde{\mathrm{A}} + i\tilde{\mathrm{A}}'$$

The eigenvalues become complex:

$$\left(\tilde{\mathrm{A}} + i\tilde{\mathrm{A}}'\right)\left|\psi^{(j)}\right\rangle = \left(\gamma^{(j)} + i\gamma'^{(j)}\right)\left|\psi^{(j)}\right\rangle$$

This leads to attenuation of the Block waves:

$$\psi^{(j)}(\mathbf{r}) \to \left\{\sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} \mathrm{e}^{2\pi i \mathbf{g}\cdot\mathbf{r}}\right\} \mathrm{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}} \mathrm{e}^{2\pi i \gamma^{(j)} z} \mathrm{e}^{-2\pi\gamma'^{(j)} z}$$

$$U(\mathbf{r}) \to U(\mathbf{r}) + iU'(\mathbf{r})$$

The matrix elements are:

$$A_{g,g} = s_g$$

$$A_{\substack{g_1,g_2 \\ g_1 \neq g_2}} = \frac{1}{2\xi_{\mathbf{g}_2-\mathbf{g}_1}}$$

$$A'_{g1,g2} = \frac{1}{2\xi'_{\mathbf{g}_2-\mathbf{g}_1}}$$

Non-Hermitian: $A_{g_2,g_1} + iA'_{g_1,g_2} \neq \left(A_{g_2,g_1} + iA'_{g_2,g_1}\right)^*$

How to diagonalize a non-Hermitian matrix?

Treat Absorption as a perturbation

Typically $\Phi'_{\mathbf{g}} \approx (0.10)\Phi_{\mathbf{g}}$

$$\tilde{A}' = \begin{pmatrix} \frac{1}{2\xi'_{\mathbf{0}}} & \frac{1}{2\xi'_{\mathbf{g}_1}} & . & \frac{1}{2\xi'_{\mathbf{g}_{n-1}}} \\ \frac{1}{2\xi'^{\,*}_{\mathbf{g}_1}} & \frac{1}{2\xi'_{\mathbf{0}}} & . & \frac{1}{2\xi'_{\mathbf{g}_{n-1}-\mathbf{g}_1}} \\ . & . & . & . \\ \frac{1}{2\xi'^{\,*}_{\mathbf{g}_{n-1}}} & \frac{1}{2\xi'^{\,*}_{\mathbf{g}_1-\mathbf{g}_{n-1}}} & . & \frac{1}{2\xi'_{\mathbf{0}}} \end{pmatrix}$$

We can compute the attenuation coeffs. as a first-order perturbation:

$$\gamma'^{(j)} \approx \left\langle \psi^{(j)} \middle| \tilde{A}' \middle| \psi^{(j)} \right\rangle = \sum_{\mathbf{g},\mathbf{g}'} \left[C_{\mathbf{g}}^{(j)} \right]^* \cdot \left(\frac{1}{2\xi'_{\mathbf{g}-\mathbf{g}'}} \right) \cdot C_{\mathbf{g}'}^{(j)}$$

Two-beam simulation

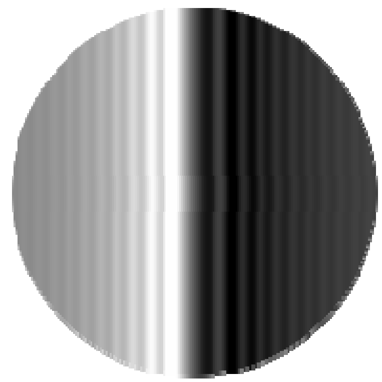
$\xi_0 = 50$ nm

$\xi_g = 100$ nm

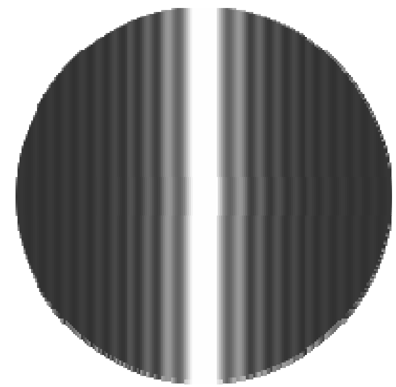
$T = 250$ nm

α=0.10

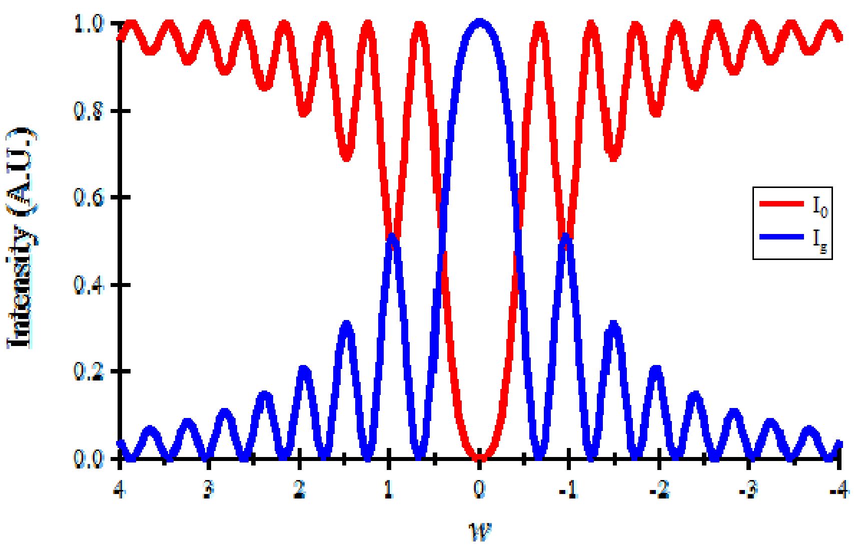
BF



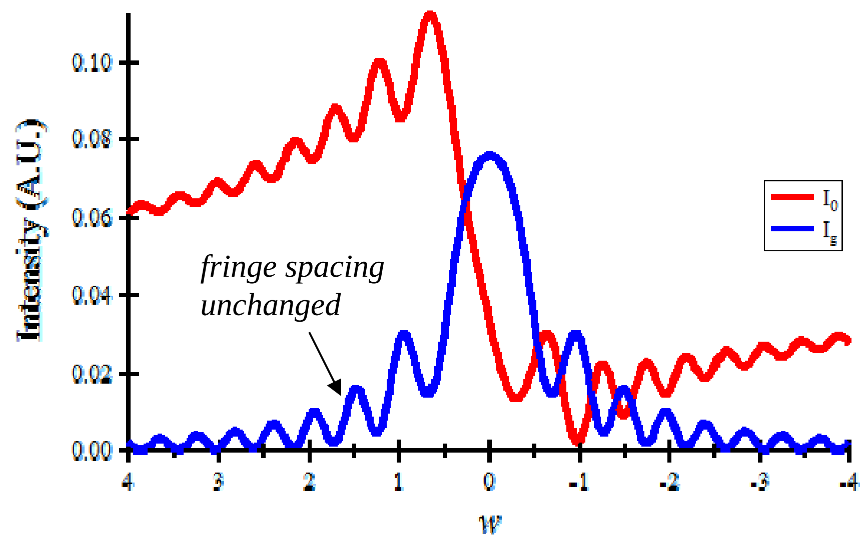
DF



No absorption



With absorption



HOLZ ring radius

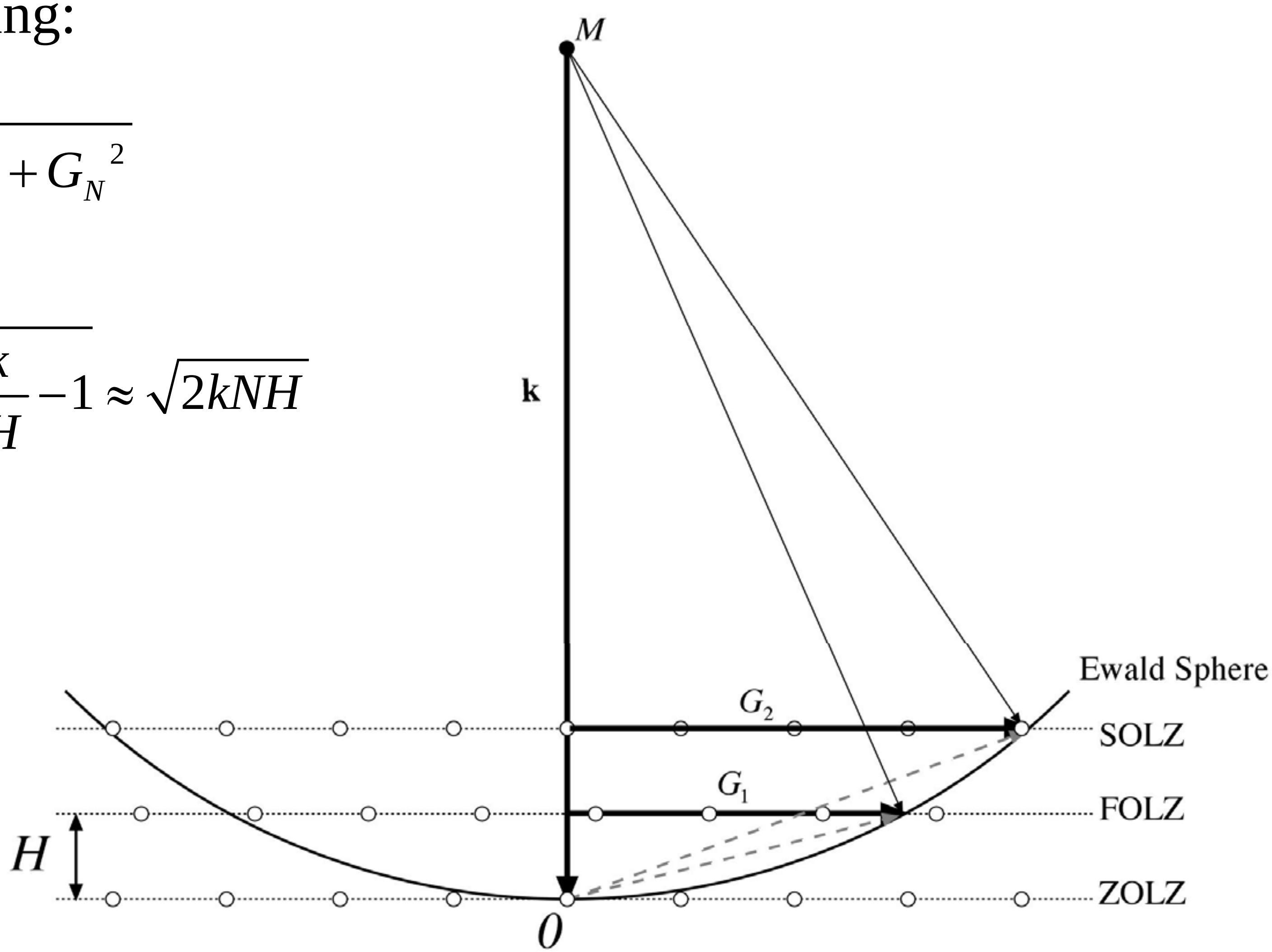
N^{th} HOLZ ring:

$$k = \sqrt{(k - NH)^2 + {G_N}^2}$$

$$G_N = NH\sqrt{\frac{2k}{NH} - 1} \approx \sqrt{2kNH}$$

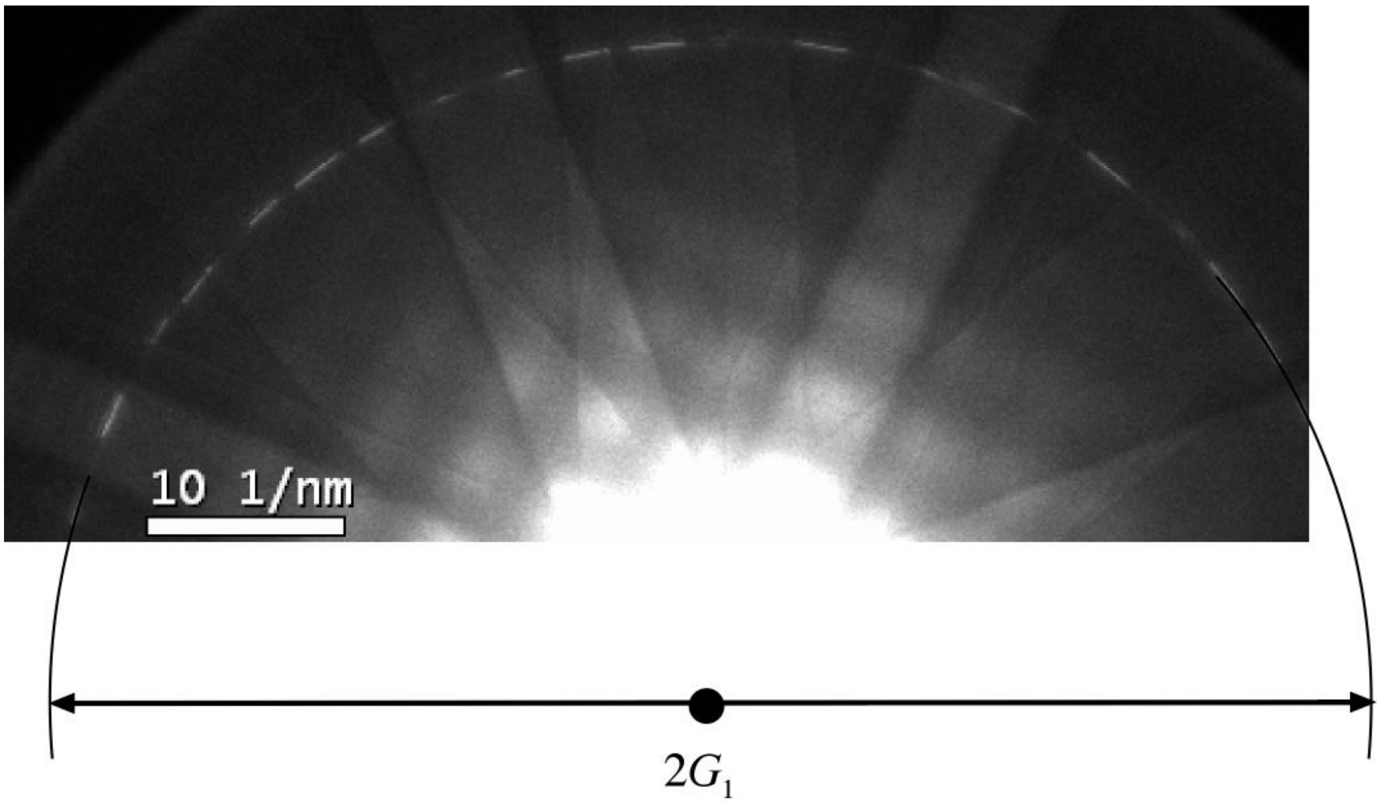
$$G_1 \approx \sqrt{\frac{2H}{\lambda}}$$

$$G_2 \approx 2\sqrt{\frac{H}{\lambda}}$$



Find H from HOLZ ring diameter

Example: Si [001] CBED pattern



$E = 125$ KeV

Find H:

$$NH = \frac{1}{\lambda} - \sqrt{\frac{1}{\lambda^2} - G_N{}^2}\left[\approx \frac{\lambda\left(G_N\right)^2}{2}\right]$$

$$2G_1 = 67.9\,\text{nm}^{-1} \rightarrow G_1 = 34.0\,\text{nm}^{-1} \rightarrow NH = 1.89\,\text{nm}^{-1}$$

We found that $H = \frac{1}{|\mathbf{r}_{uvw}|}$

fcc [001]:

FOLZ has N=1

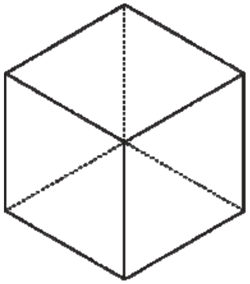
$|\mathbf{r}_{uvw}| = 1/a$

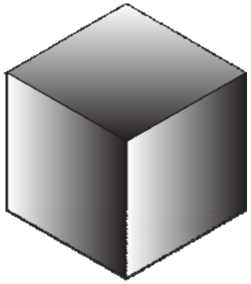
$\rightarrow H = 1/a$ $\rightarrow a = 0.53\ \text{nm}$

Actual value (Si): $a = 0.54\ \text{nm}$

Symmetry in CBED patterns

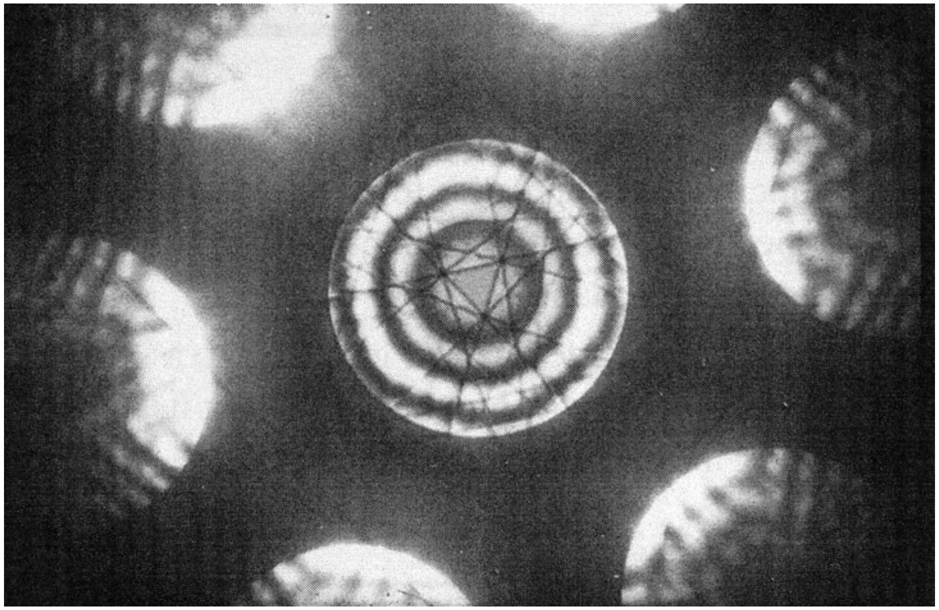
From either a K-M or K pattern:
WP: Whole-pattern symmetry



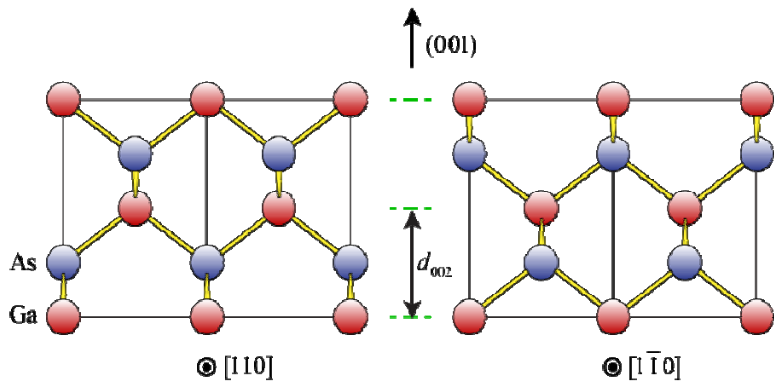


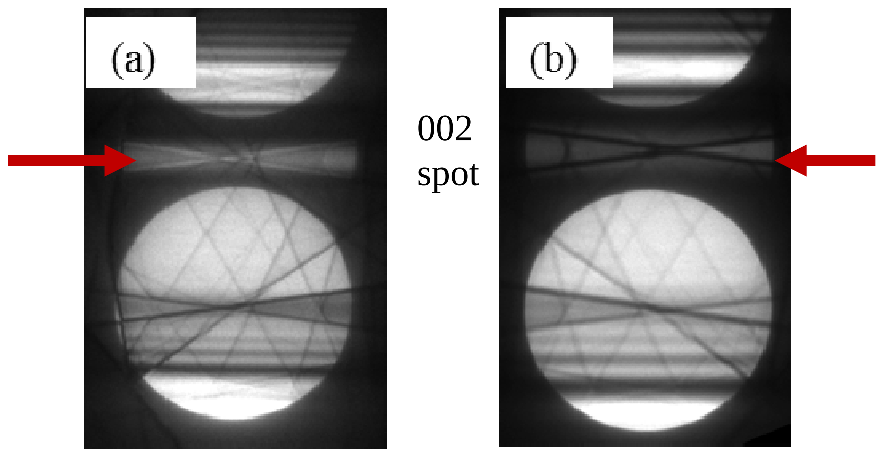
From a K-M pattern:
BF: (000) disk symmetry, including HOLZ lines
DF: (*hkl*) disk symmetry

Si [111]

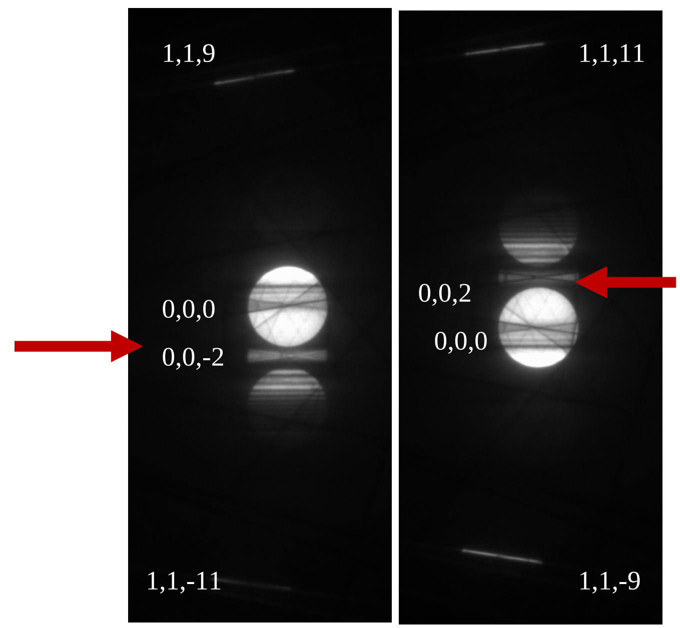


Polarity determination





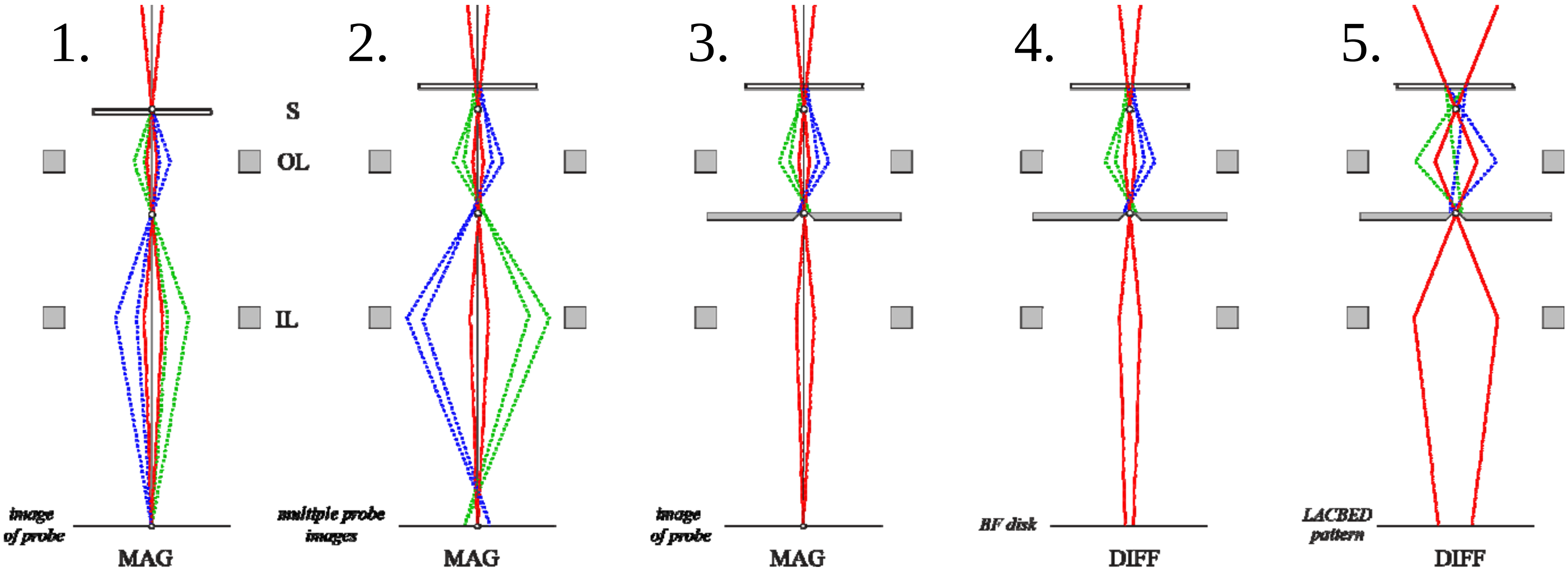
near [110]



Dynamical electron diffraction allows determination of film polarity

J. Tafto, and J.C.H. Spence, J. C. H., 1982, J. Appl. Crystallogr., 15, p. 60.

Large-angle CBED



1) focus probe on sample
2) raise sample height
3) inset diffraction aperture around *0* spot
4) switch to diffraction mode
5) increase convergence angle