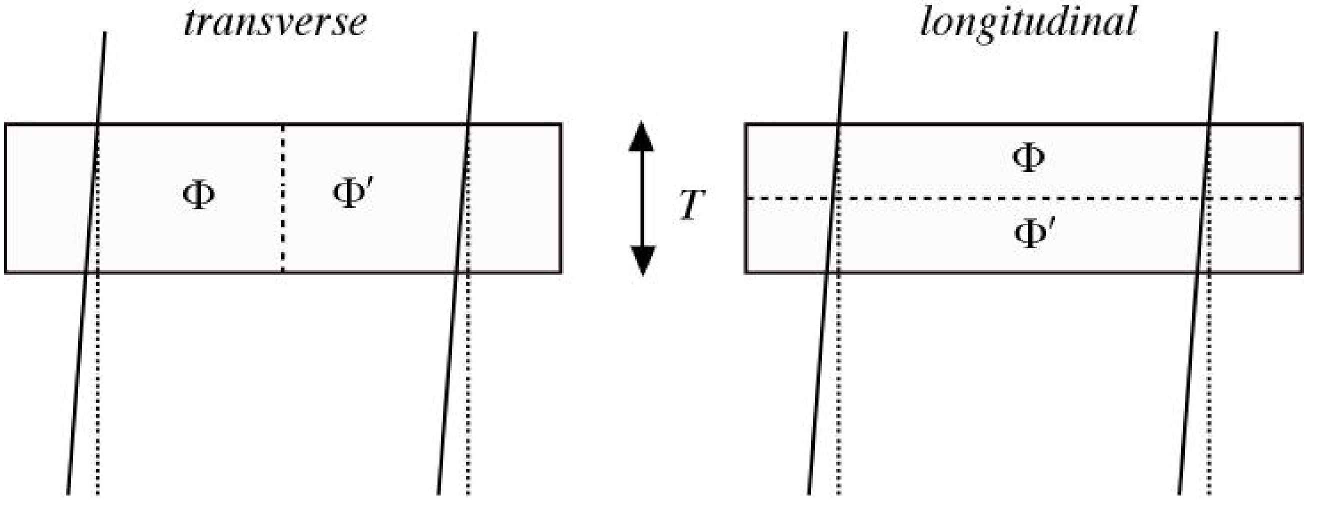
# Planar defects: orientation and types




Translation:

$$\Phi'(\mathbf{r}) = \Phi(\mathbf{r} - \mathbf{R})$$

**R**: Displacement Vector

Rotation:

$$\Phi'(\mathbf{r}) = \Phi(\tilde{M}\mathbf{r})$$

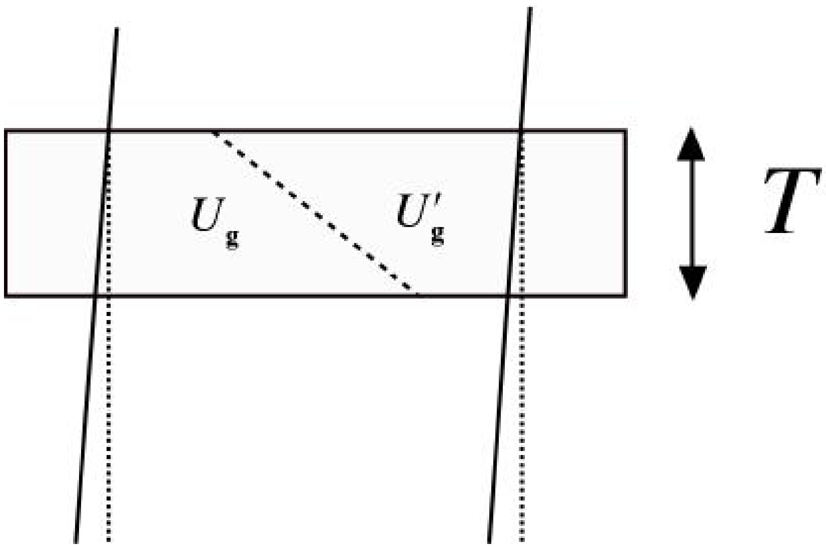
$\tilde{M}$: Rotation Matrix

# Translation: influence on Fourier coeff's

Translation:

$$U'(\mathbf{r}) = U(\mathbf{r} - \mathbf{R})$$

$$U'(\mathbf{r}) = \sum_{\mathbf{g}} U'_{\mathbf{g}} e^{2\pi i \mathbf{g}\cdot\mathbf{r}}$$




Phase factor change for each Fourier component

$$U'_{\mathbf{g}} = U_{\mathbf{g}} e^{-2\pi i \mathbf{g}\cdot\mathbf{R}} = U_{\mathbf{g}} e^{i\alpha}$$

APB: $U'_{\mathbf{g}} = -U_{\mathbf{g}}$

$$(\alpha = 180°)$$

# Translation: influence on Bloch waves

Above defect: $$\psi^{(j)}(\mathbf{r}) = \mathrm{e}^{2\pi i\mathbf{k}^{(j)}\cdot\mathbf{r}} \cdot \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} \mathrm{e}^{2\pi i\mathbf{g}\cdot\mathbf{r}}$$

Below defect:

$$\psi'^{(j)}(\mathbf{r}) = \psi^{(j)}(\mathbf{r}-\mathbf{R})$$

$$= \mathrm{e}^{2\pi i\mathbf{k}^{(j)}\cdot(\mathbf{r}-\mathbf{R})} \cdot \sum_{\mathbf{g}} C_{\mathbf{g}}^{(j)} \mathrm{e}^{2\pi i\mathbf{g}\cdot(\mathbf{r}-\mathbf{R})}$$

$$\psi'^{(j)}(\mathbf{r}) = \mathrm{e}^{2\pi i\mathbf{k}^{(j)}\cdot(\mathbf{r}-\mathbf{R})} \cdot \sum_{\mathbf{g}} C_{\mathbf{g}}'^{(j)} \mathrm{e}^{2\pi i\mathbf{g}\cdot\mathbf{r}}$$

$$C_{\mathbf{g}}'^{(j)} = C_{\mathbf{g}}^{(j)} \mathrm{e}^{-2\pi i\mathbf{g}\cdot\mathbf{R}} = C_{\mathbf{g}}^{(j)} \mathrm{e}^{i\alpha}$$

Bloch-wave coefficients are altered only if $\mathbf{g}\cdot\mathbf{R} \neq 0$

# Scattering matrix (two-beam)

The dynamical diffracted intensity can be summarized using matrices:

$$\begin{pmatrix} \Psi_{\mathbf{0}}(z) \\ \Psi_{\mathbf{g}}(z) \end{pmatrix} = \begin{pmatrix} C_{\mathbf{0}}^{(1)} & C_{\mathbf{0}}^{(2)} \\ C_{\mathbf{g}}^{(1)} & C_{\mathbf{g}}^{(2)} \end{pmatrix} \cdot \begin{pmatrix} e^{2\pi i\gamma^{(1)}z} & 0 \\ 0 & e^{2\pi i\gamma^{(2)}z} \end{pmatrix} \cdot \begin{pmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \end{pmatrix} = \tilde{C} \cdot \tilde{\Gamma}(z) \cdot \begin{pmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \end{pmatrix}$$

$$\begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix} = \tilde{C} \cdot \begin{pmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \end{pmatrix} = \left(\tilde{C}\right)^{-1} \cdot \begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix}$$

$$\begin{pmatrix} \Psi_{\mathbf{0}}(z) \\ \Psi_{\mathbf{g}}(z) \end{pmatrix} = \tilde{C} \cdot \tilde{\Gamma}(z) \cdot \left(\tilde{C}\right)^{-1} \cdot \begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix}$$

Scattering Matrix: $\tilde{P}(z) = \tilde{C} \cdot \tilde{\Gamma}(z) \cdot \tilde{C}^{-1}$

$$\begin{pmatrix} \Psi_{\mathbf{0}}(z) \\ \Psi_{\mathbf{g}}(z) \end{pmatrix} = \tilde{P}(z) \cdot \begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix}$$

# Propagation across a planar defect (I)

Below the fault: $$\begin{pmatrix} \Psi'_{\mathbf{0}}(z) \\ \Psi'_{\mathbf{g}}(z) \end{pmatrix} = \tilde{C}' \cdot \tilde{\Gamma}'(z-t) \cdot \begin{pmatrix} \varepsilon'^{(1)} \\ \varepsilon'^{(2)} \end{pmatrix}$$

Same eigenvalues:

Different Bloch wave coefficients:

$$\Gamma'(z-t) = \Gamma(z-t) = \begin{pmatrix} e^{2\pi i \gamma^{(1)}(z-t)} & 0 \\ 0 & e^{2\pi i \gamma^{(2)}(z-t)} \end{pmatrix}$$

$$\tilde{C}' = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \cdot \tilde{C}$$

$$\begin{pmatrix} \Psi'_{\mathbf{0}}(t) \\ \Psi'_{\mathbf{g}}(t) \end{pmatrix} = \tilde{C}' \cdot \begin{pmatrix} \varepsilon'^{(1)} \\ \varepsilon'^{(2)} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon'^{(1)} \\ \varepsilon'^{(2)} \end{pmatrix} = \left(\tilde{C}'\right)^{-1} \cdot \begin{pmatrix} \Psi'_{\mathbf{0}}(t) \\ \Psi'_{\mathbf{g}}(t) \end{pmatrix}$$

Scattering Matrix: $\tilde{P}'(z-t) = \tilde{C}' \cdot \tilde{\Gamma}'(z-t) \cdot \left(\tilde{C}'\right)^{-1}$

$$\begin{pmatrix} \Psi'_{\mathbf{0}}(z) \\ \Psi'_{\mathbf{g}}(z) \end{pmatrix} = \tilde{P}'(z-t) \cdot \begin{pmatrix} \Psi'_{\mathbf{0}}(t) \\ \Psi'_{\mathbf{g}}(t) \end{pmatrix}$$

# Propagation across a planar defect (II)

Boundary condition at the buried phase boundary interface ($z = t$):

$$\begin{pmatrix} \Psi'_{\mathbf{0}}(t) \\ \Psi'_{\mathbf{g}}(t) \end{pmatrix} = \begin{pmatrix} \Psi_{\mathbf{0}}(t) \\ \Psi_{\mathbf{g}}(t) \end{pmatrix} = \tilde{P}(t) \cdot \begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix}$$

$$\begin{pmatrix} \Psi'_{\mathbf{0}}(z) \\ \Psi'_{\mathbf{g}}(z) \end{pmatrix} = \tilde{P}'(z-t) \cdot \begin{pmatrix} \Psi'_{\mathbf{0}}(t) \\ \Psi'_{\mathbf{g}}(t) \end{pmatrix} = \tilde{P}'(z-t) \cdot \tilde{P}(t) \cdot \begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix}$$

$$\begin{pmatrix} \Psi_{\mathbf{0}}(0) \\ \Psi_{\mathbf{g}}(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

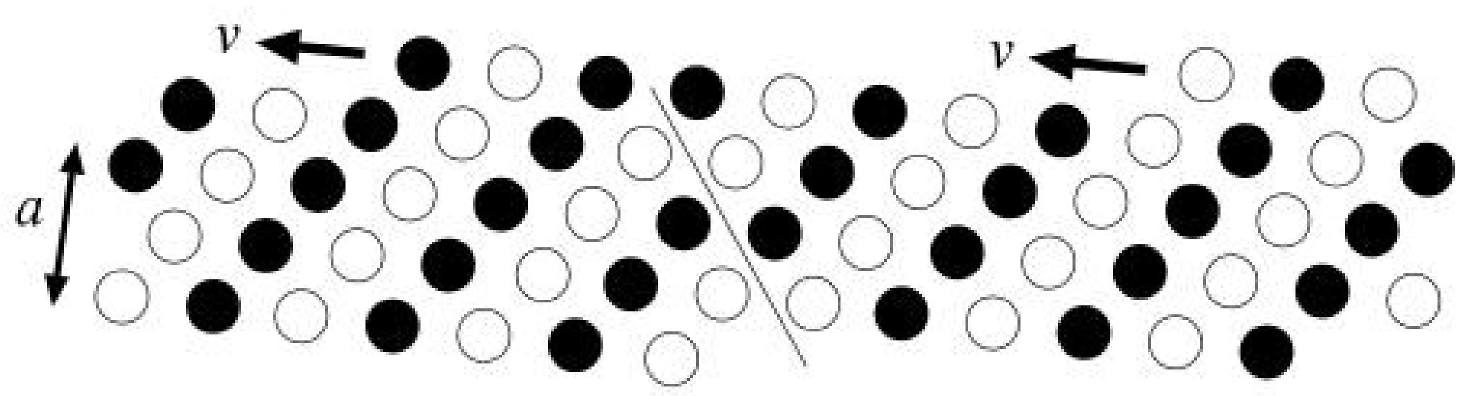
$$\begin{pmatrix} \Psi'_{\mathbf{0}}(T) \\ \Psi'_{\mathbf{g}}(T) \end{pmatrix} = \tilde{P}'(T-t) \cdot \tilde{P}(t) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

# Antiphase boundary

180° phase shift in ordering sequence

$$\alpha = 180°$$

$$F_{\mathbf{g}} = f_A - f_B \qquad F'_{\mathbf{g}} = f_B - f_A = -F_{\mathbf{g}}$$




*Depiction of APB propagation via step-flow-driven crystal growth*

# Propagation across an APB (I)

General two-beam result:

$$\Gamma(z) = e^{\pi i w z/\xi} \cdot \begin{pmatrix} e^{\pi i \sqrt{1+w^2}\, z/\xi} & 0 \\ 0 & e^{-\pi i \sqrt{1+w^2}\, z/\xi} \end{pmatrix}$$

$$w = 1/s\xi$$

$$\sin(\beta) = 1/\sqrt{1+w^2}$$

$$\cos(\beta) = w/\sqrt{1+w^2}$$

$$\tilde{C} = \begin{pmatrix} \sin(\beta/2) & -\cos(\beta/2) \\ \cos(\beta/2) & \sin(\beta/2) \end{pmatrix}$$

$$\tilde{C}' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdot \tilde{C} = \begin{pmatrix} \sin(\beta/2) & -\cos(\beta/2) \\ -\cos(\beta/2) & -\sin(\beta/2) \end{pmatrix}$$

Scattering matrices:

$$\tilde{P}(z) = \tilde{C} \cdot \tilde{\Gamma}(z) \cdot \tilde{C}^{-1}$$

$$\tilde{P}'(z-t) = \tilde{C}' \cdot \tilde{\Gamma}'(z-t) \cdot (\tilde{C}')^{-1}$$

# Propagation across an APB (II)

Strong-beam result: $\gamma^{(1,2)} = \pm 1/2\xi$

$$\Gamma(z) = \begin{pmatrix} e^{\pi i z/\xi} & 0 \\ 0 & e^{-\pi i z/\xi} \end{pmatrix} \qquad \tilde{C} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \qquad \tilde{C}' = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}$$

Define: $a = \pi t/\xi$ $\quad b = \pi T/\xi$

Above the APB: $\tilde{\Gamma}(t) = \begin{pmatrix} e^{ia} & 0 \\ 0 & e^{-ia} \end{pmatrix}$

$$\tilde{P}(t) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} e^{ia} & 0 \\ 0 & e^{-ia} \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} \cos(a) & i\sin(a) \\ i\sin(a) & \cos(a) \end{pmatrix}$$

Below the APB: $\tilde{\Gamma}(T-t) = \begin{pmatrix} e^{i(b-a)} & 0 \\ 0 & e^{-i(b-a)} \end{pmatrix}$

$$\tilde{P}'(T-t) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix} \cdot \begin{pmatrix} e^{i(b-a)} & 0 \\ 0 & e^{-i(b-a)} \end{pmatrix} \cdot \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix} = \begin{pmatrix} \cos(b-a) & -i\sin(b-a) \\ -i\sin(b-a) & \cos(b-a) \end{pmatrix}$$

# Propagation across an APB (III)

Apply boundary condition at entrance surface:

$$\tilde{\mathrm{P}}(t)\cdot\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}\cos(a)\\ i\sin(a)\end{pmatrix}$$

$$\tilde{\mathrm{P}}(T-t)\cdot\tilde{\mathrm{P}}(t)\cdot\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}\cos(b-a) & -i\sin(b-a)\\ -i\sin(b-a) & \cos(b-a)\end{pmatrix}\cdot\begin{pmatrix}\cos(a)\\ i\sin(a)\end{pmatrix}=\begin{pmatrix}\cos(2a-b)\\ i\sin(2a-b)\end{pmatrix}$$

Diffracted-beam amplitudes:

$$\begin{pmatrix}\Psi'_{\mathbf{0}}(T)\\ \Psi'_{\mathbf{g}}(T)\end{pmatrix}=\begin{pmatrix}\cos[\pi(2t-T)/\xi]\\ i\sin[\pi(2t-T)/\xi]\end{pmatrix}$$

# Diffracted Intensity Across an APB

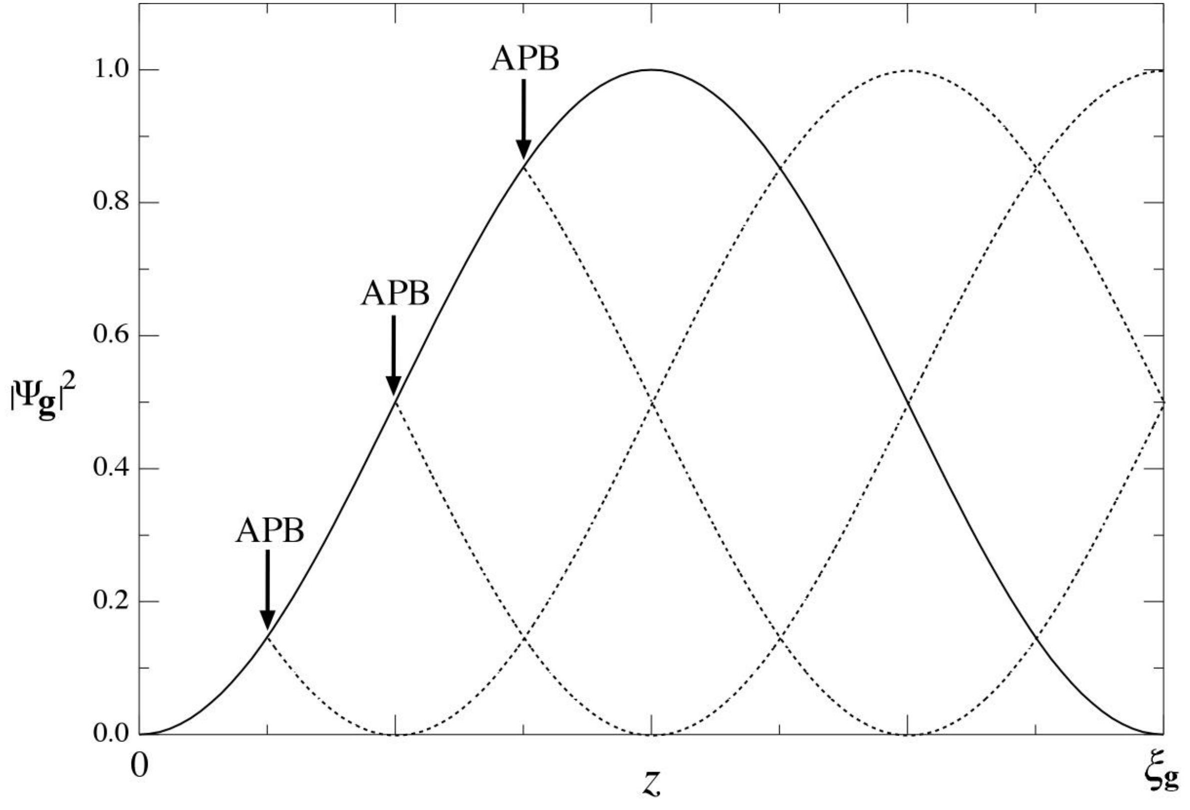
Strong-Beam Case:

Above:

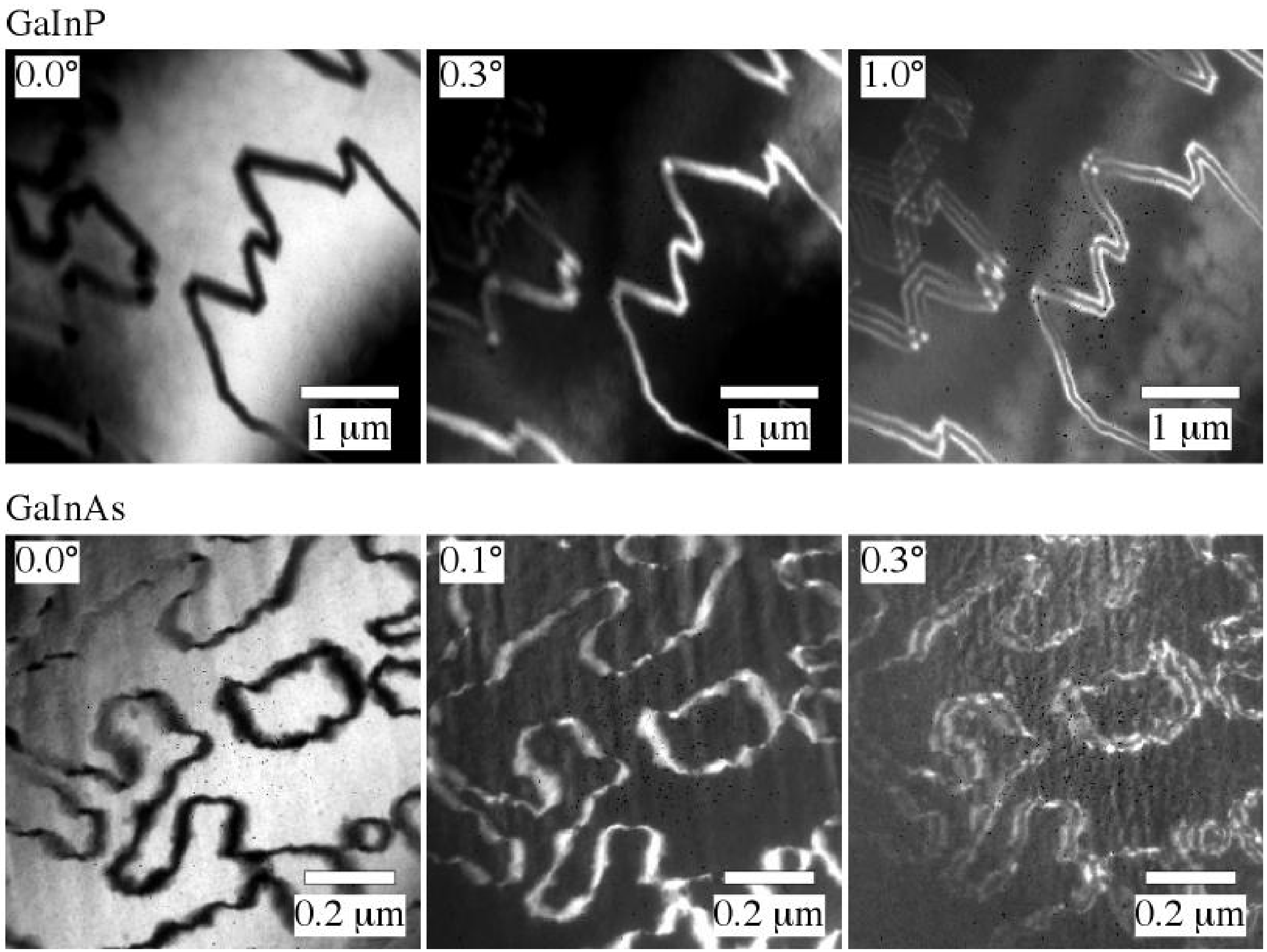
$$\left|\Psi_{\mathbf{g}}(z)\right|^2 = \sin^2(\pi z/\xi)$$

Below:

$$\left|\Psi'_{\mathbf{g}}(z)\right|^2 = \sin^2\left[\pi(2t - z)/\xi\right]$$



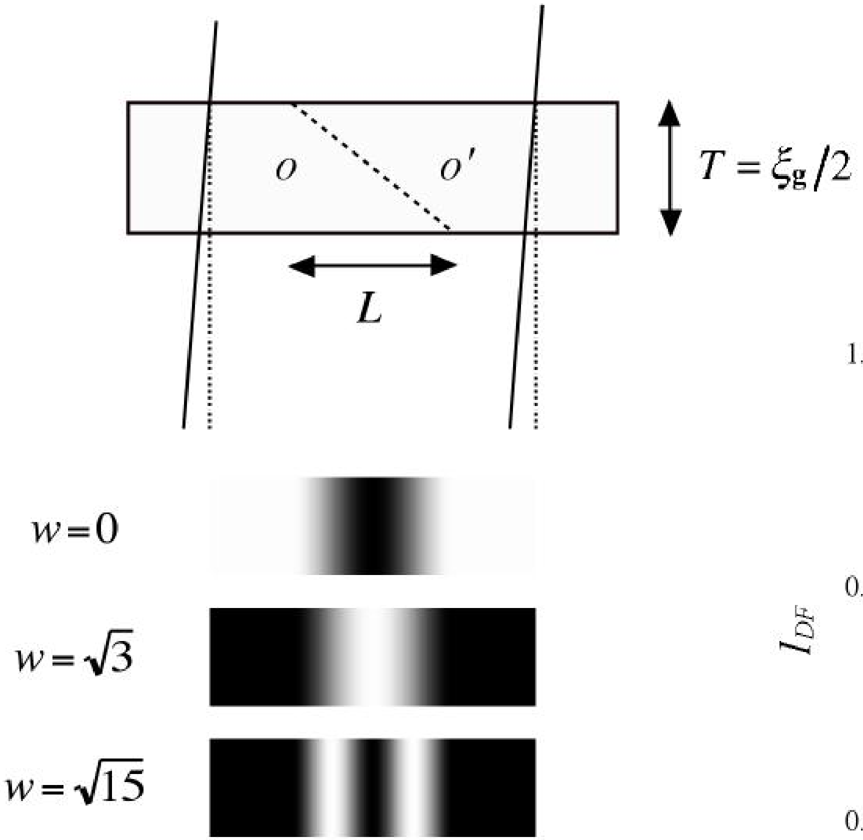
# DF images of inclined APBs: influence of tilt

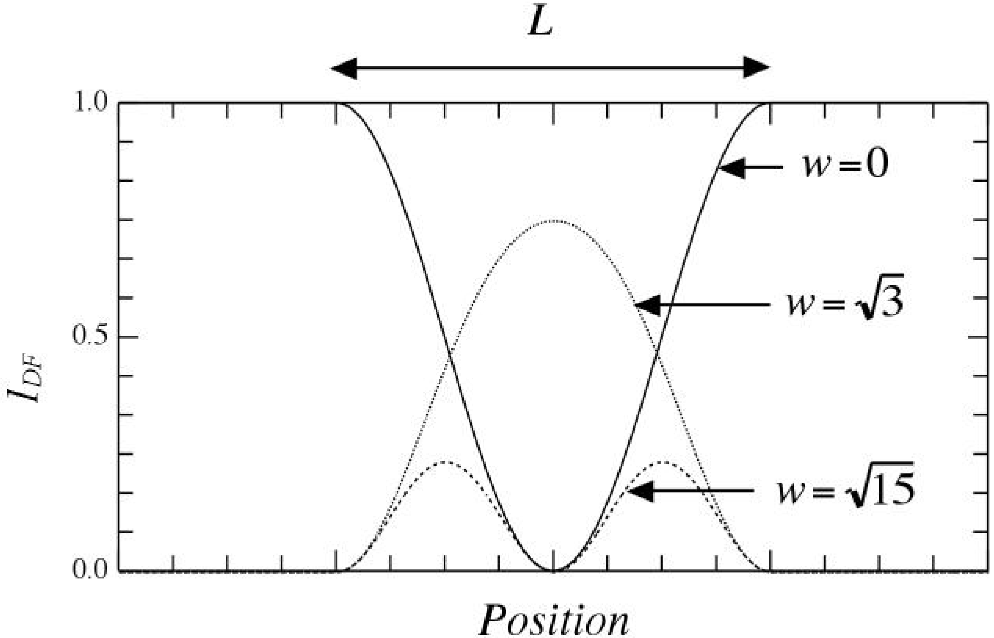


# Inclined APBs: two-beam analysis

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

$$\omega^2 + 1 = N^2$$

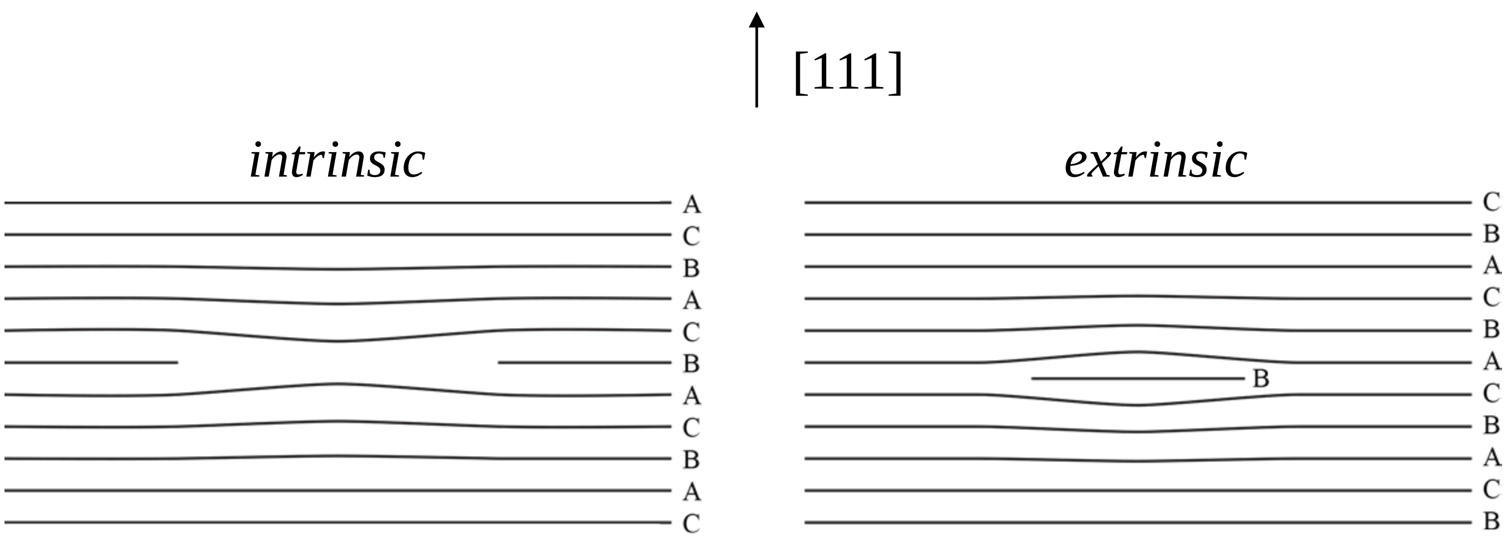


# Stacking faults in fcc crystals

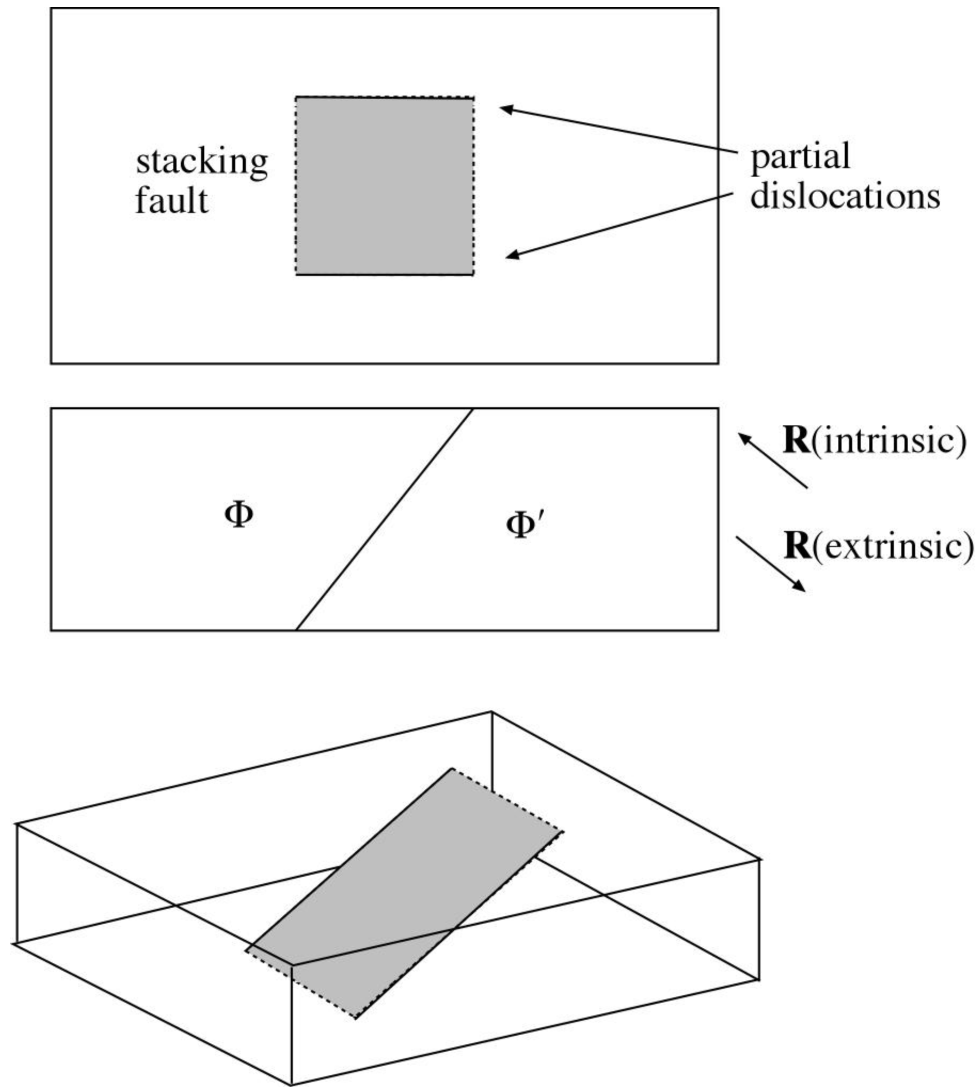
Two types:

Intrinsic and Extrinsic



# Stacking fault geometry

Partial dislocations border fault

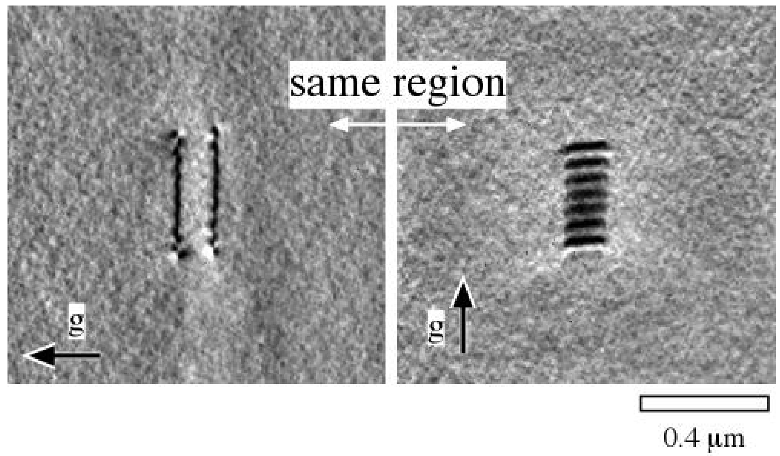



Fault is observed with $\mathbf{g} \cdot \mathbf{R} \neq 0$

# Stacking fault images

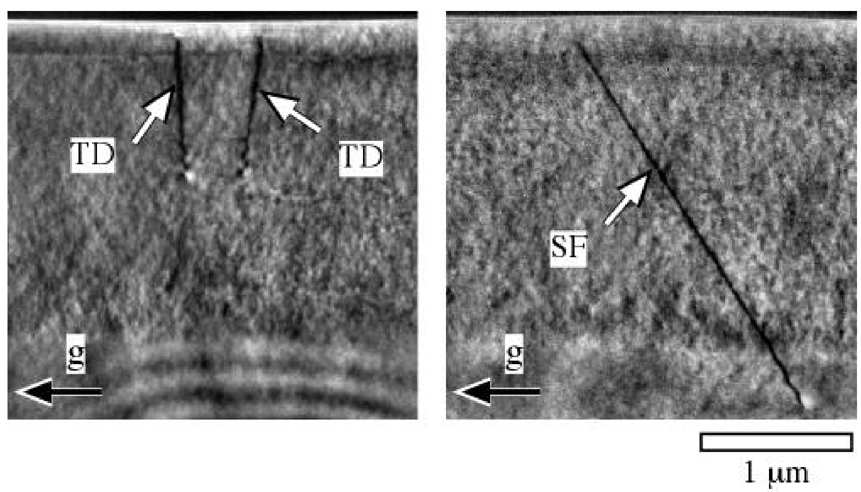
[001]
Plan view

{220} DF




[110]
Cross section

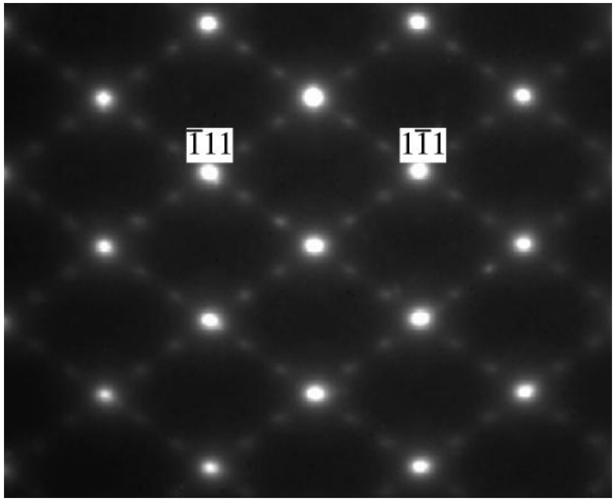
{220} DF



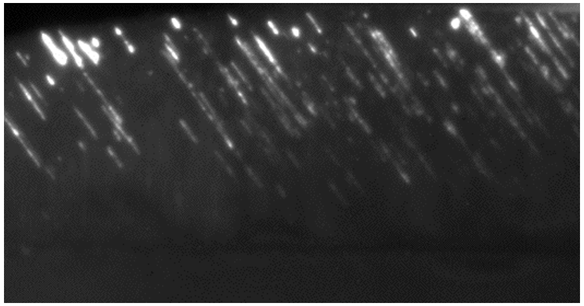

*Sometimes hard to distinguish threading dislocations from partial dislocations*

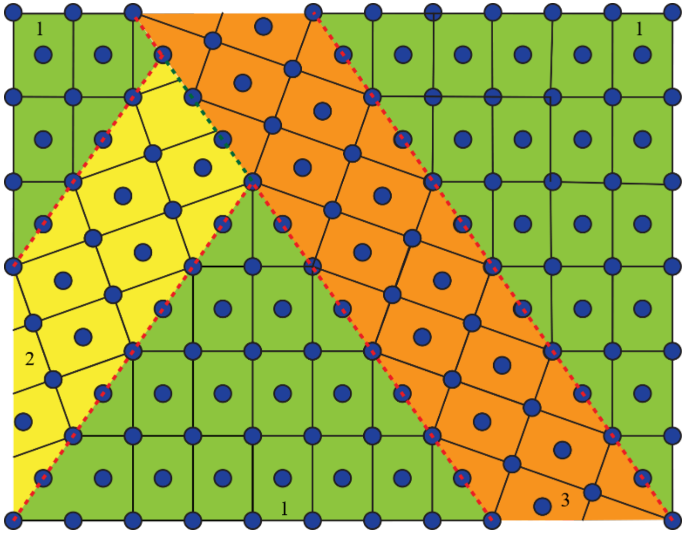
# Twin boundaries in fcc crystals

[110]




1/3(111) dark-field image

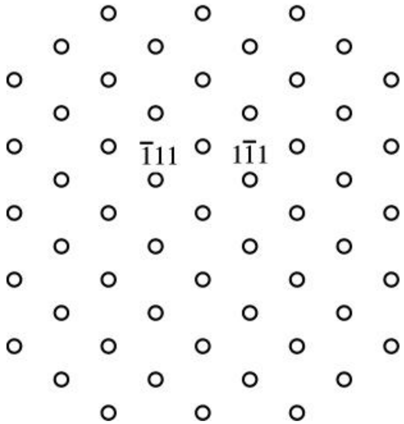





Give rise to extra spots at 1/3(111) positions

# Origin of 1/3 position spots

Matrix

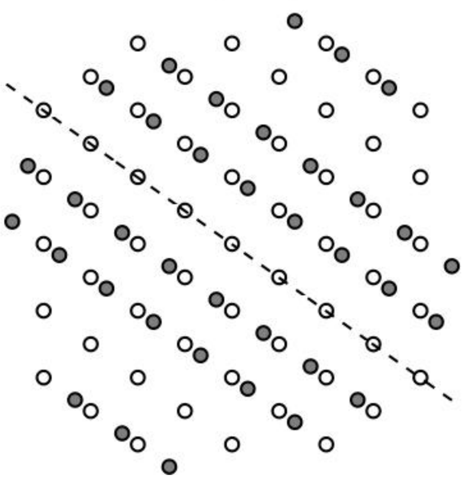



[110] fcc

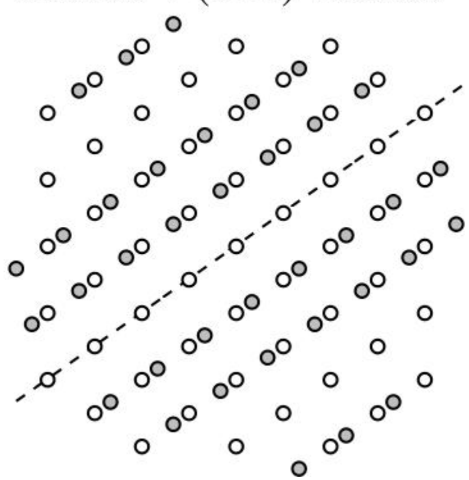
180° Rotation about (111) directions

Dynamical diffraction gives complete pattern

Matrix + ($\bar{1}11$) variant



Matrix + ($1\bar{1}1$) variant



Matrix + Both Variants