



## POWDER DIFFRACTION

### Principles

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### BRAGG'S LAW

The diagram shows two waves, wave 1 (green) and wave 2 (red), hitting a series of parallel horizontal lines representing atomic planes. The distance between these planes is labeled  $d$ . The incident angle of wave 1 is  $\theta$ , and its reflected angle is  $\theta'$ . The path difference between the reflections from two adjacent planes is labeled  $d \sin \theta$ . The diagram illustrates how the waves interfere constructively at a specific angle, leading to a reflection. A label  $n=2$  indicates the order of the reflection.

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$$2 d_{hkl} \sin \theta_{hkl} = n \lambda$$

(Geometric interpretation of diffraction)

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### SINGLE- VS. MULTI-CRYSTAL DIFFRACTION

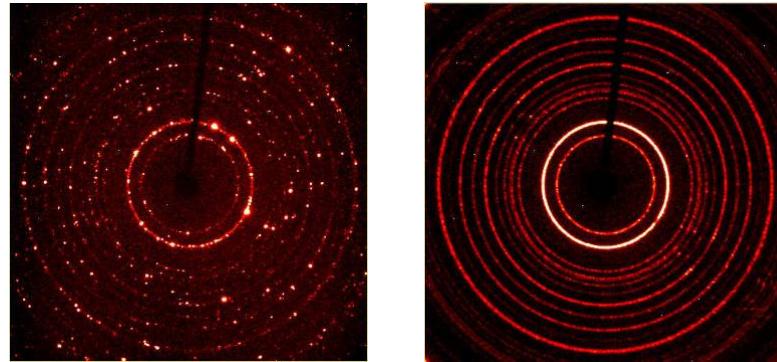
The diagram shows three types of diffraction patterns:

- One crystal:** Shows a few sharp spots on a 2D grid.
- Four crystals:** Shows more spots than the single crystal case.
- Powder:** Shows a continuous halo or a series of concentric rings.

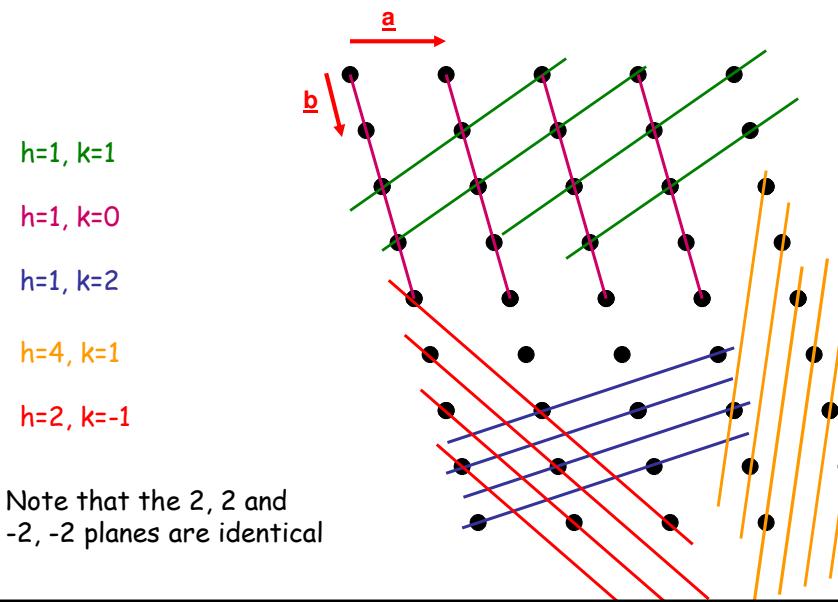
Below the patterns, a schematic shows a sample source emitting X-rays, which converge into a cone labeled "Debye-Scherrer cones". An "image plate detector" is positioned to record the diffraction pattern.



## POWDER DIFFRACTION



## CRYSTAL PLANES – MILLER INDICES



**CRYSTAL PLANES – d-VALUES**

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Isometric      Hexagonal      Tetragonal      Trigonal      Orthorhombic      Monoclinic      Triclinic

a    b    c (Å)    α    β    γ (°)

$$\frac{1}{d_{hkl}^2} = [h^2 \sin^2\alpha/a^2 + k^2 \sin^2\beta/b^2 + l^2 \sin^2\gamma/c^2 + 2kl(\cos\beta \cos\gamma - \cos\alpha)/(bc) + 2hl(\cos\alpha \cos\gamma - \cos\beta)/(ac) + 2hk(\cos\alpha \cos\beta - \cos\gamma)/(ab)] / [1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha \cos\beta \cos\gamma]$$

$$\frac{1}{d_{hkl}^2} = (h^2 + k^2 + l^2) / a^2$$

The diagram shows a 3D coordinate system representing Real space with vectors  $\mathbf{a}$  and  $\mathbf{b}$ . The angle between  $\mathbf{a}$  and  $\mathbf{b}$  is  $\gamma$ . A plane perpendicular to  $\mathbf{c}$  defines the boundary between Real space (shaded grey) and Reciprocal space (dark grey). The origin of Reciprocal space is marked. Several reciprocal lattice points are plotted, labeled 01, 02, 10, 11, 12, 20, 21, and 22. The distance from the origin to point 10 is labeled  $d_{10}$ , and the distance to point 01 is labeled  $d_{01}$ .

**RECIPROCAL SPACE**

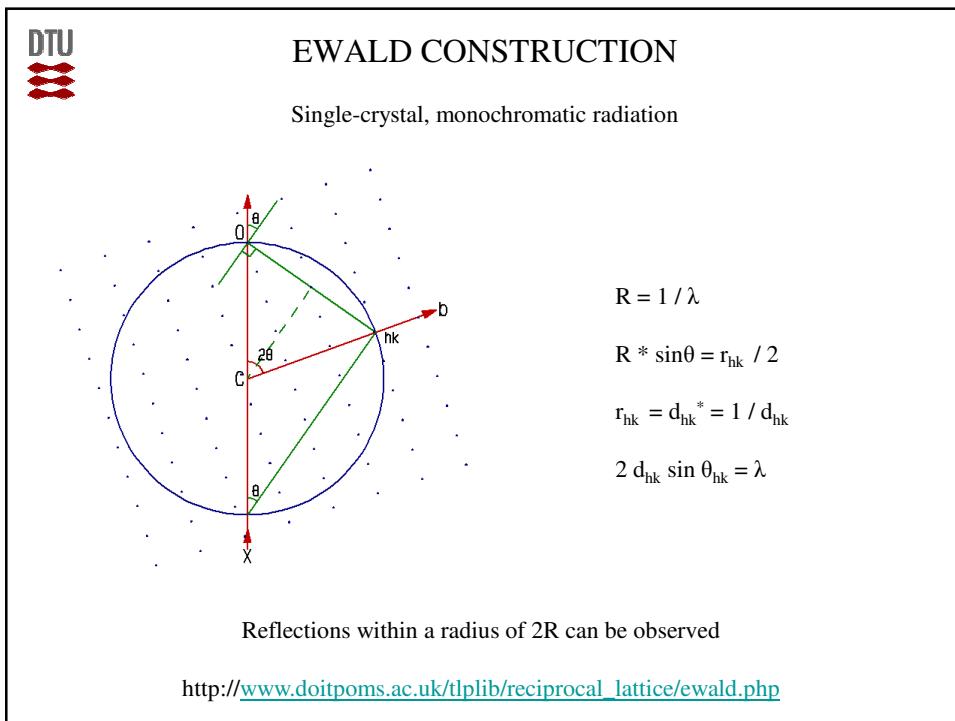
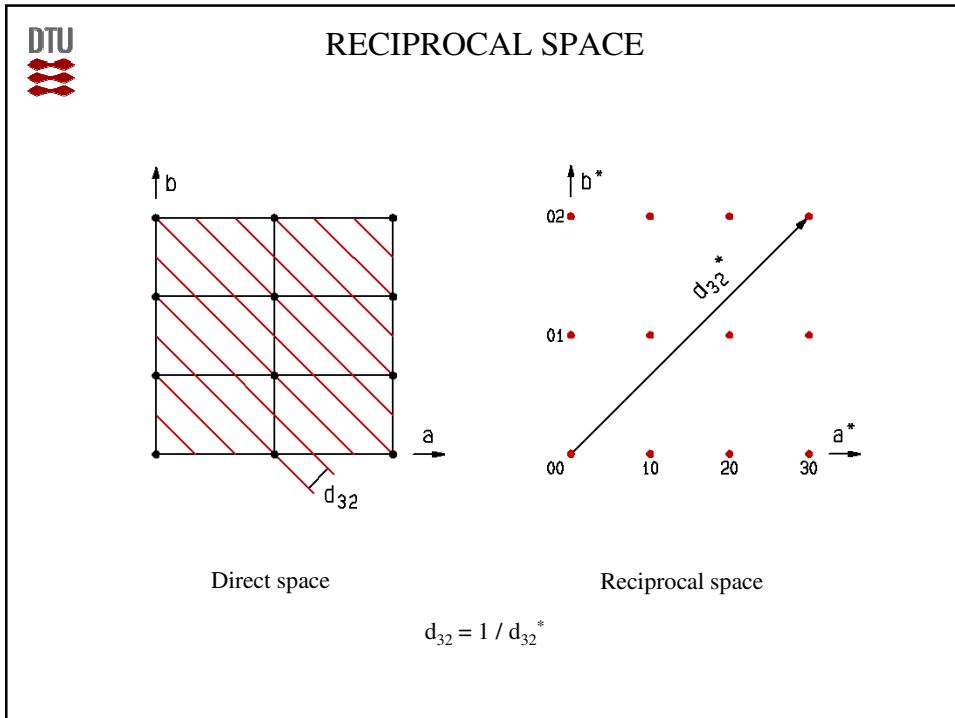
$a^* = b \otimes c / V_{\text{cell}}$  ( $= b c \sin\alpha / V_{\text{cell}}$ )

$b^* = a \otimes c / V_{\text{cell}}$  ( $= a c \sin\beta / V_{\text{cell}}$ )

$c^* = a \otimes b / V_{\text{cell}}$  ( $= a b \sin\gamma / V_{\text{cell}}$ )

$a \cdot a^* = 1 \quad a \cdot b^* = 0$

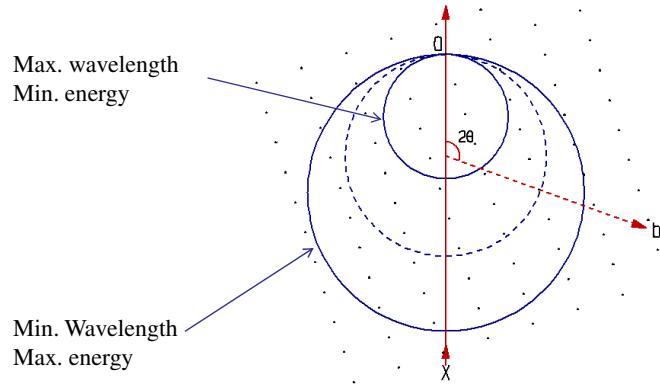
$d_{\text{hkl}} = 1 / d_{\text{hkl}}^*$





## SINGLE-CRYSTAL LAUE DIFFRACTION

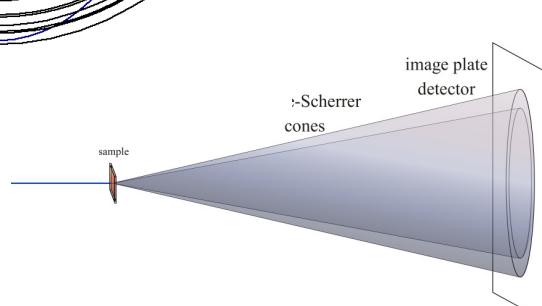
Single-crystal, white or "pink" radiation

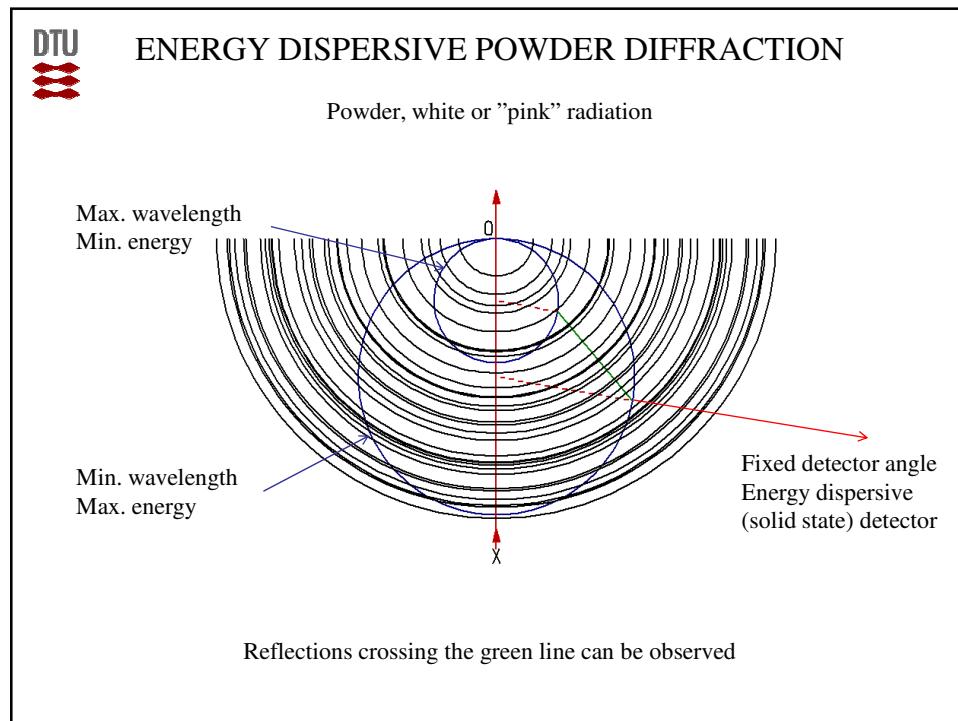
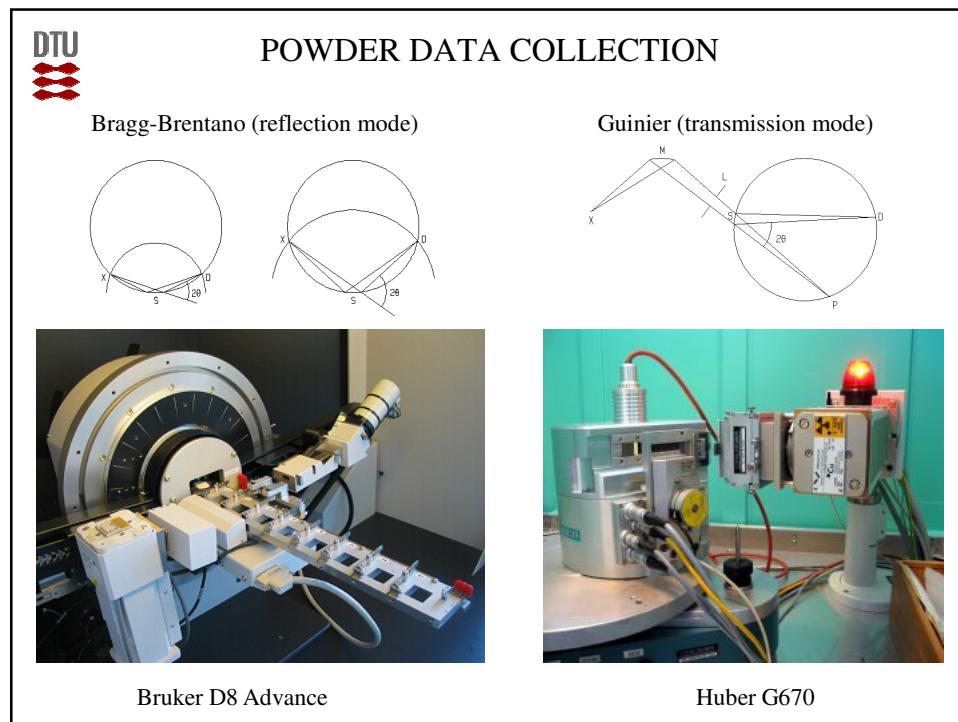


All reflections between the two Ewald spheres can be observed.



## POWDER DIFFRACTION







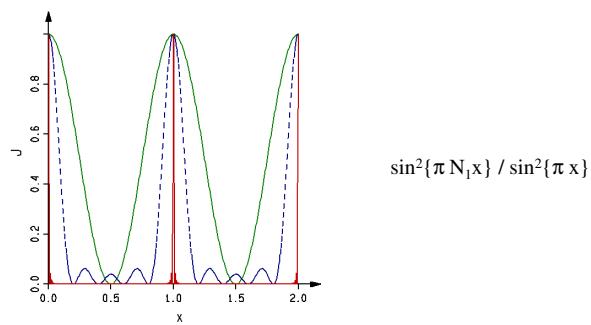
## INTERFERNCE FUNCTION

$$f_j = f_j \exp\{2\pi i(\mathbf{r} + \mathbf{v}) \cdot \mathbf{r}^*\}$$

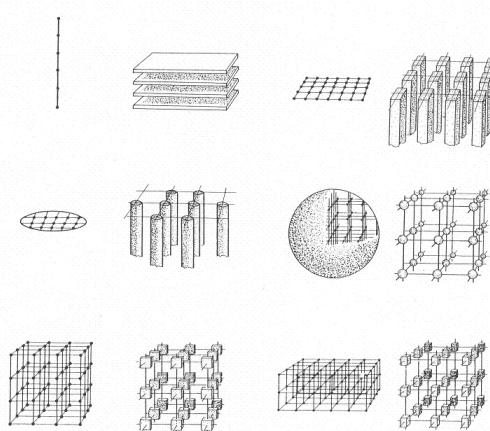
$$\mathbf{v} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$$

$$\mathbf{F}_{\text{cryst}} = \sum_{\text{cryst}} \exp\{2\pi i \mathbf{v} \cdot \mathbf{r}^*\} \cdot \mathbf{F}_{\text{hkl}} = J(\mathbf{r}^*) \cdot \mathbf{F}_{\text{hkl}}$$

$$\sum_{N_1} \exp\{2\pi i N_1 \mathbf{a} \cdot \mathbf{r}^*\} = (1 - \exp\{2\pi i N_1 \mathbf{a} \cdot \mathbf{r}^*\}) / (1 - \exp\{2\pi i \mathbf{a} \cdot \mathbf{r}^*\}) = \sin\{\pi N_1 \mathbf{a} \cdot \mathbf{r}^*\} / \sin\{\pi \mathbf{a} \cdot \mathbf{r}^*\}$$

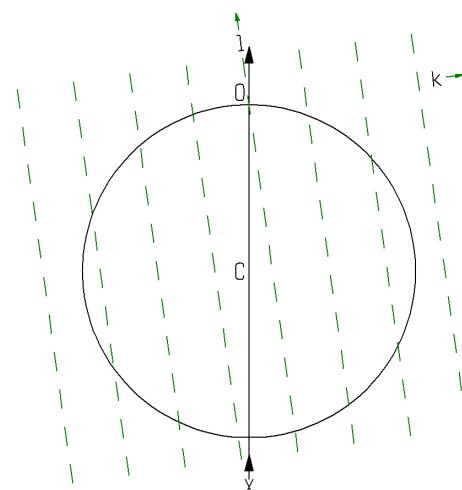


## INTERFERENCE FUNCTION





## ANISOTROPIC SIZE EFFECTS



## ANISOTROPIC SIZE EFFECTS

