Zone Axis

Lattice planes \((hkl)\) of the zone \([mnp]\)

Use plane normals...

\[
\begin{vmatrix}
  i & j & k \\
  h_1 & k_1 & l_1 \\
  h_2 & k_2 & l_2 \\
\end{vmatrix} = (h_1k_2l_3 - h_1k_3l_2)
\]

\[
\begin{vmatrix}
  h_1 & k_1 & l_1 \\
  h_2 & k_2 & l_2 \\
  h_3 & k_3 & l_3 \\
\end{vmatrix} = (h_1k_2l_3 - h_1k_3l_2 - h_2k_1l_3 + h_2k_3l_1 - h_3k_1l_2 + h_3k_2l_1)
\]

...to find perpendicular vector.

Crystal Shape Factor

Real space

Reciprocal space

rel rod

Primärstrahl

Probe

Rods vertical to plane

Rods parallel to plane

R. Ubic
Structure Factor

\[ d_{000} = d = a/h \]

for constructive interference:
\[ \delta_{11} = 2 \sin \theta = \lambda \]
\[ \delta_{21} = 2 \sin \theta = (x/d) \lambda = (xh/a) \lambda. \]

Now remove \( \lambda \) by switching from path difference to phase difference:
\[ \phi = (\delta/\lambda) 2\pi \quad \text{[radians]} \ldots \] \[ \therefore \theta_{21} = (2 \pi x h / a) \]

Express \( x \) as fractional coordinate \( u = x/a \), then:
\[ \theta_{21} = 2 \pi hu \]

In 3D this expression expands to:
\[ \phi = 2 \pi (hu + kv + lw) \]

EM wave: \[ E = E_0 e^{i \phi} \]
\[ \therefore E = E_0 \exp[2 \pi i ((hu + kv + lw)] \]

\( E_0 \) = amplitude
- atomic scattering factor
- scattering due to one atom
\[ \therefore \]

Now add up all such waves for all atoms in a unit cell:
\[ F_{hkl} = \sum f_i e^{2 \pi i (hu + kv + lw)} \]

Complex – amplitude & phase

Intensity of diffracted beam is proportional to \( |F|^2 \), so imaginary part always vanishes.