X-Ray generation and measurement set up

\[ E = h\nu = \frac{hc}{\lambda} \]

- a copper target X-ray tube produces an X-ray beam with the principle wavelengths:
- Cu K-alpha₁: 1.5405 Å (transition from 2s to 1s, used for HRXRD)
- Cu K-alpha₂: 1.5443 Å (transition from 2p to 1s)
The Diffraction condition

- Bragg’s law gives the correlation between the minimum distance between parallel planes \( d \) and the angular position of the X-Ray peak in the two theta-omega scan.

Points to note:

The minimum distance between planes \((k_1, k_2, k_3)\) in a cubic lattice is given by

\[
d = \frac{a}{\sqrt{k_1^2 + k_2^2 + k_3^2}}
\]

Distance between planes \((k_1, k_2, k_3)\) in hexagonal lattice is given by

\[
\frac{1}{d_{k_1,k_2,k_3}^2} = \frac{4}{3} \left( \frac{k_1^2 + k_1 k_2 + k_2^2}{a^2} \right) + \frac{k_3^2}{c^2}
\]
Symmetric and asymmetric scan types

- Symmetric scans can give us information regarding \textit{c lattice constant} (assuming \(\Delta a/a = 0\) for accuracy), and the length of a period and total length of superlattice layers.
- It can also give us information about the quality of the material.
- Two basic types of symmetric scans:
  - Omega-two theta scan
  - Omega scan or rocking curve
- Asymmetric scans are useful for measuring \textit{a lattice constant} and reciprocal space maps used to determine crystalline quality.

Symmetric scan: (002) (004) diffraction

Asymmetric scan: (102), (104), (114) etc.
The omega - two theta scan

- Source fixed, but if sample rotates $\theta$, then detector rotates $2\theta$ (note here $\omega = \theta$, and hence this is also called $\theta$ - $2\theta$ scan)
- The intensity of peaks usually proportional to the thickness of the layers
- The $\omega$-$2\theta$ scans give the composition of the respective layers in the entire structure
The omega scan or rocking curve

- The source is fixed, the detector is fixed but the sample is rocked around the Bragg peak slightly.
- The FWHM of the rocking curve is an important indicator of the material crystalline quality.

\[ \Delta k \]

\[ k_i \rightarrow k_f \]

\[ \Delta k \]

Normal

\[ k_i \rightarrow k_f \]

GaN Thin Film (002) Reflection

Intensity (Counts/s)

0 8000 16000

16.995 17.195 17.395 17.595 17.795

Omega (deg)
GaN/InGaN multi quantum well XRD

- The distances between the major satellite peaks (marked by numbers) are proportional to the width of one repeat, while the distances between the smaller peaks are related to the total thickness of the superlattice.
- The major satellite peaks become sharper for larger quantum well due to stricter conditions for interference.

**X-ray spectra of InGaN/GaN MQW**

**FIG. 1.** Experimental (002) data on QW structures, 1 repeat (bottom), 5 (middle), and 10 (top) all grown at 750 °C (with the analyzer crystal). (Other data for this 10QW sample are shown in Figs. 12 and 13).
Reciprocal space maps for crystalline quality

- For symmetric scans q is always perpendicular to the sample surface. $q_\perp$ is varied to measure c lattice constant.
- For obtaining reciprocal space maps both the $q_\perp$ and $q_\parallel$ are varied.
- AlGaN in (a) and (b) are both pseudomorphic, but (b) has much worse quality. AlGaN in (c) is not pseudomorphic as it does not have the same $q_\parallel$. 

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Reflection high energy electron diffraction (RHEED)

- At a grazing incidence the incident wave vector cannot penetrate deep into the crystal, so the crystal seems to have a 2D lattice.
- The reciprocal space of a 2D lattice consists of rods separated by the reciprocal lattice spacing.
- Usual electron energy of ~100 keV used can give the radius of the Ewald sphere of 1000 Å⁻¹ which is much larger than the reciprocal lattice spacing of ~1 Å⁻¹.
- Due to thermal vibration and lattice imperfections, the rods have finite thickness.
- Due to divergence and dispersion of the electron beam, the Ewald sphere has finite thickness.

Real RHEED patterns are elongated

Ideal RHEED pattern

Real RHEED pattern
Growth process monitoring

From the period of the growth oscillations the growth rate can be calculated.

The oscillation reduce in magnitude as layer grows thicker due to initiation of many growth fronts (growth proceeding in different layers, a monolayer growth starting before one is complete).

Only good for MBE due to requirement of high vacuum.

Layer by layer growth