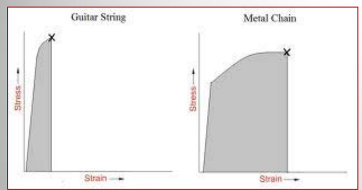
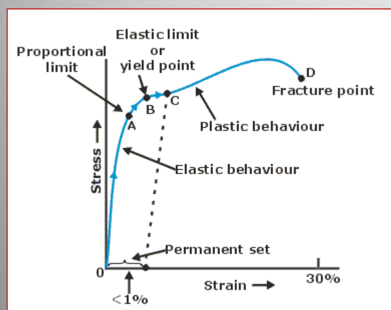




A typical stress-strain curve for a ductile metal

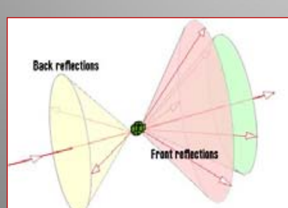
PHYS485

Materials Physics

Dr. Gregory W. Clark
Manchester University

X-ray Methods

- The Laue Method: scatter from single Xtal using range of wavelengths from λ_1 to λ_o
- The Rotating Crystal Method: monochromatic X-rays with rotating sample
- The Powder (Debye-Sherrer) Method: equivalent to rot. Xtal method but with rot. axis varied over all possible orientations

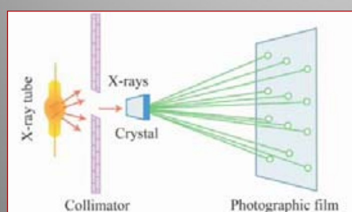


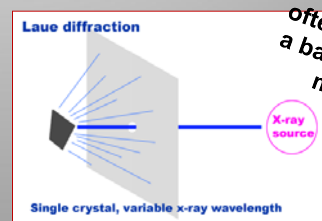
$$G = 2k\sin(\phi/2) = 2k\sin(\theta)$$

Note: scattering angle $\phi \equiv 2\theta$

where θ is the Bragg angle

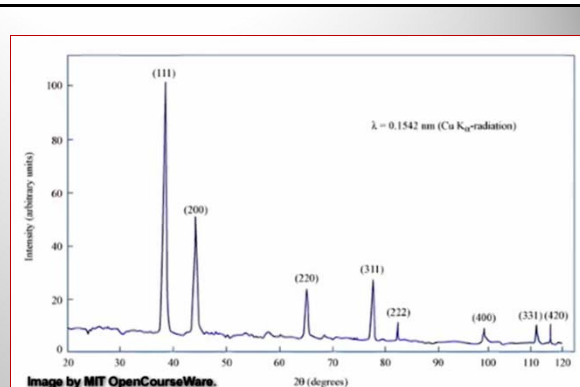
- XRD: Laue pattern:
  - white X-rays; do not know λ
  - useful for orienting Xtals

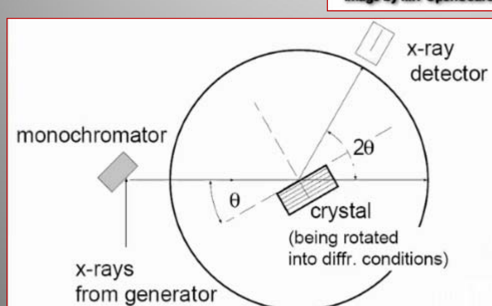




often used in a backscatter mode

XRD: Rotating Xtal



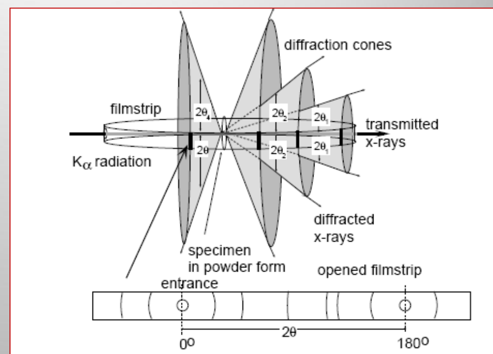


Note:

$\phi \equiv 2\theta$

XRD: Powder Method

- Debye-Scherrer method



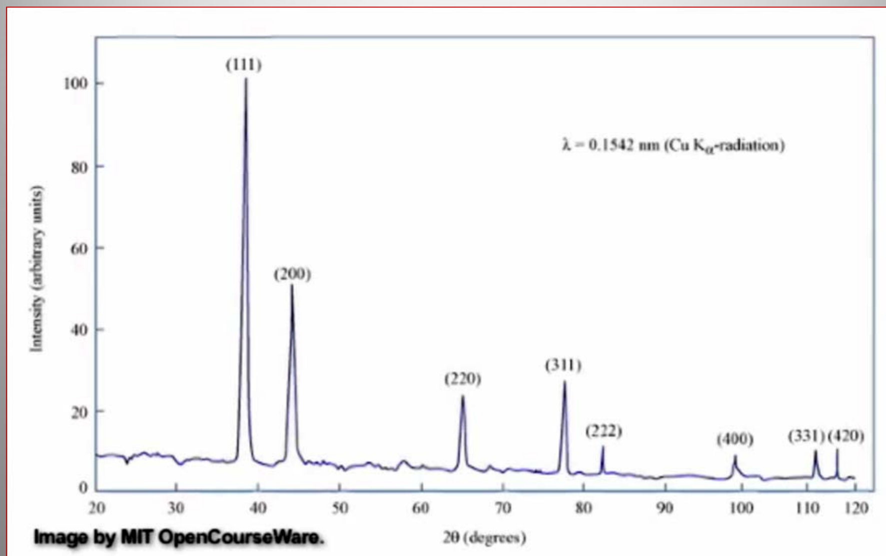
XRD Selection Rule Chart for reflection in cubic systems

- SC: all allowed
- BCC: h + k + l = even
- FCC: h, k, l all even or all odd ("unmixed")
- Diamond? FCC + basis

(hkl)	$h^2+k^2+l^2$	SC	BCC	FCC
100	1	Y	N	N
110	2	Y	Y	N
111	3	Y	N	Y
200	4	Y	Y	Y
210	5	Y	N	N
211	6	Y	Y	N
220	8	Y	Y	Y
300	9	Y	N	N
310	10	Y	Y	N
311	11	Y	N	Y
222	12	Y	Y	Y
320	13	Y	N	N
321	14	Y	Y	N
400	16	Y	Y	Y

Diamond: the red circled FCC bits + (331)

Rotating Xtal data:



One method of attack:

(1) Start with 2θ values and generate a set of $\sin^2\theta$ values.

(2) Normalize the $\sin^2\theta$ values by generating $\sin^2\theta_n/\sin^2\theta_1$

(3) Clear fractions from the "normalized" column.

(4) Speculate on the hkl values that would seem as $h^2+k^2+l^2$ to generate the sequence of the "clear fractions" column.

(5) Compute for each θ the value of $\sin^2\theta/(h^2+k^2+l^2)$ on the basis of the assumed hkl values. If each entry in this column is identical, then the entire process is validated.

Diffraction with Real Atoms

- The amplitude of a scattered wave is given by

$$\mathrm{A} \propto \left[\sum_R \exp(i\vec{R}\cdot\Delta\vec{k})\right]\left[\sum_p f_{ap}(\theta)\exp(i\vec{r}_p\cdot\Delta\vec{k})\right]$$

or $$A \propto \sum_R e^{i\vec{R}\cdot\vec{G}} S_k$$ for constructive interference

[We'll show this shortly!]

[$\vec{R}$ points to unit cells, $\vec{r}_p$ to atoms in unit cell; $\vec{r}'$ is the integration variable for e- density]

where $$S_{\vec{G}} = \sum_p f_{ap}(\theta) e^{i\vec{G}\cdot\vec{r}_p} = \text{geometric structure factor}$$

$$f_{ap}(\theta) = f_e(\theta)\int_p \rho(\vec{r}')\exp(i\vec{r}'\cdot\Delta\vec{k})d^3\vec{r}'$$

$f_{ap}(\theta)$ is the atomic form factor (atomic scattering function)

$f_e(\theta)$ is the electron form factor (electron scattering function)

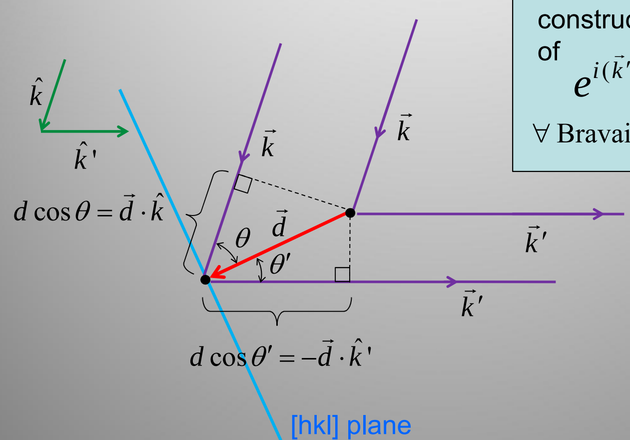
Back to X-rays! Laue formulation:

Path difference: $d\cos\theta + d\cos\theta' = \vec{d}\cdot(\hat{k}-\hat{k}') = m\lambda$

Leads to Laue condition for constructive interference of

$$e^{i(\vec{k}'-\vec{k})\cdot\vec{R}} = e^{i\vec{G}\cdot\vec{R}} = 1$$

$\forall$ Bravais lattice vectors $\vec{R}$



for $\vec{G} = \vec{k}' - \vec{k} = \Delta\vec{k}$

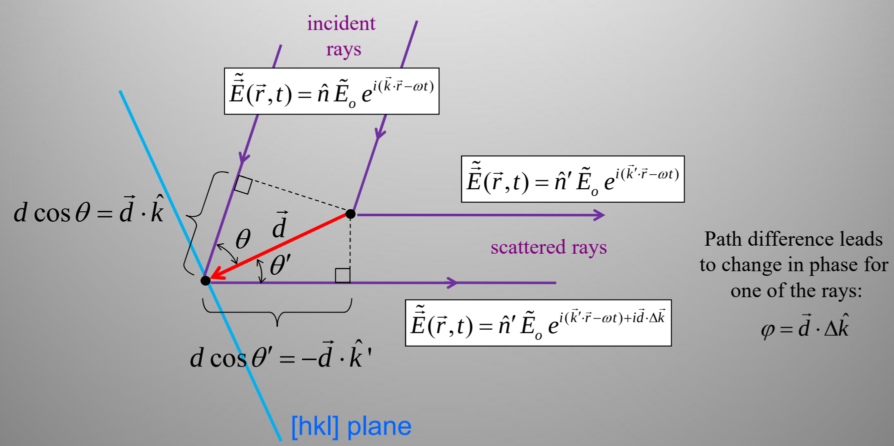
Note: scattering is elastic, so $|\vec{k}'| = |\vec{k}|$

Laue formulation:

The intensity of an electromagnetic wave is proportional to the amplitude of the electric field; for the incident rays

$$I \propto \left| \tilde{E}_o\, e^{i(\vec{k}\cdot\vec{r}-\omega t)} \right|^2$$

$$= \left| \tilde{E}_o e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t} \right|^2 = \left| \tilde{E}_o e^{i\vec{k}\cdot\vec{r}} \right|^2$$



Laue formulation:

The intensity of the scattered electromagnetic wave is superposition of x-rays scattered by the two atoms:

$$\tilde{\vec{E}}(\vec{r},t) = \hat{n}'\,\tilde{E}_o\, e^{i(\vec{k}'\cdot\vec{r}-\omega t)} + \hat{n}'\,\tilde{E}_o\, e^{i(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}\cdot\Delta\vec{k}}$$

So we have $I_{scatt} \propto \left| e^{i(\vec{k}'\cdot\vec{r}-\omega t)} + e^{i(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}\cdot\Delta\vec{k}} \right|^2 = \left| e^{i\vec{k}'\cdot\vec{r}} + e^{i\vec{k}'\cdot\vec{r}} e^{i\vec{d}\cdot\Delta\vec{k}} \right|^2$

$$= \left| e^{i\vec{k}'\cdot\vec{r}} (1 + e^{i\vec{d}\cdot\Delta\vec{k}}) \right|^2 = \left| 1 + e^{i\vec{d}\cdot\Delta\vec{k}} \right|^2$$

If the second term is -1, then we have completely destructive interference;

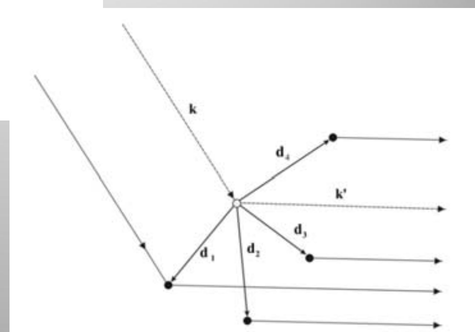
if the second term is +1, then we have completely constructive interference

Laue formulation:

For multiple scattering – from more than two atoms:

$$\left|\tilde{\vec{E}}'(\vec{r},t)\right| \sim e^{-(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}_0\cdot\vec{K}} + e^{-(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}_1\cdot\vec{K}} + e^{-(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}_2\cdot\vec{K}} + e^{-(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}_3\cdot\vec{K}} + e^{-(\vec{k}'\cdot\vec{r}-\omega t)+i\vec{d}_4\cdot\vec{K}}$$

$$= e^{-(\vec{k}'\cdot\vec{r}-\omega t)}\left(\sum_{j=0}^{4} e^{i\vec{d}_j\cdot\vec{K}}\right)$$



If all the scattering centers are identical, we define the *Structure Factor*:

$$S(\vec{d}_j,\Delta\vec{k}) = \sum_{j=0}^{4} e^{i\vec{d}_j\cdot\Delta\vec{k}}$$

So, we have $I_{scatt} \propto \left|\tilde{\vec{E}}'(\vec{r},t)\right|^2 \propto \left|S(\vec{d}_j,\Delta\vec{k})\right|^2$

Laue formulation:

In general, if all the scattering are not the same, we write the *Structure Factor* as:

$$S(\vec{d}_j,\Delta\vec{k}) = \sum_{j=0}^{4} f_{aj}(\Delta\vec{k})e^{i\vec{d}_j\cdot\Delta\vec{k}}$$

where $f_{aj}(\Delta k)$ is the atomic form factor (atomic scattering function) and the sum is over the atoms in the unit cell. Thus, we have

$$I_{scatt} \propto \left|\tilde{\vec{E}}'(\vec{r},t)\right|^2 \propto \left|S(\vec{d}_j,\Delta\vec{k})\right|^2$$

If $\Delta\vec{k} = \vec{k}' - \vec{k} = \vec{G}$ then we have constructive interference!

For cubic structures, the $\vec{d}_j = \vec{a}_j$, our lattice vectors, with

$$\vec{G} = m_1\frac{2\pi}{a}\hat{i} + m_2\frac{2\pi}{a}\hat{j} + m_3\frac{2\pi}{a}\hat{k} \qquad \vec{a}_i\cdot\vec{G} = 2\pi\, m_i$$

Laue Formulation

Note that $\vec{a}_i \cdot \vec{G} = 2\pi m_i$ for integer m_i

So $\vec{R} \cdot \vec{G} = 2\pi n$ for integer n

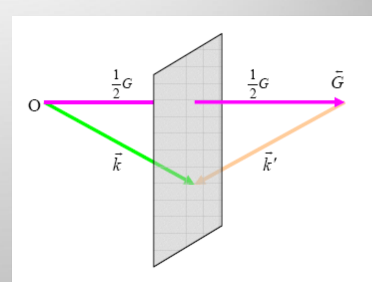
or $$\boxed{e^{i\vec{G}\cdot\vec{R}} = 1}$$

Laue condition for constructive interference

The reciprocal lattice is the set of all vectors $\vec{G}$ satisfying this relation for all $\vec{R}$ in the Bravais lattice.

Laue formulation – alternate form

$$\boxed{\vec{k} \cdot \hat{G} = \frac{1}{2} G}$$



The component of the incident wavevector along G is equal to hale the "length" of G

Laue condition satisfied **iff** the tip of the incident wavevector lies in a plane that is the perp. bisector of a line joining the origin of k-space to a reciprocal lattice point.

These planes are referred to as BRAGG PLANES

Diffraction: constructive interference

- Laue Formulation vs. Bragg Condition: One can show that they are equivalent!
- Combining these tools with an understanding of the reciprocal lattice, one can interpret XRD data

$$\left|\vec{G}\right| = \frac{2\pi}{d} = \sqrt{h^2 + k^2 + l^2} \qquad 2d\sin\theta = n\lambda$$

Mechanical Properties

- <u>Tension/Compression</u>
  - Stress $\sigma = \dfrac{F}{A}$
  - Strain $\varepsilon = \dfrac{\Delta l}{l}$
  - Related by $\boxed{\sigma = Y\varepsilon}$

where Y is Young's modulus (the gradient of a σ vs. ε plot)

A property of the <u>material</u>; independent of size/shape!