PHYS485

Materials Physics

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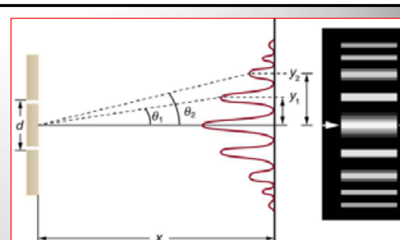
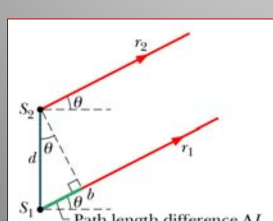
Scattering

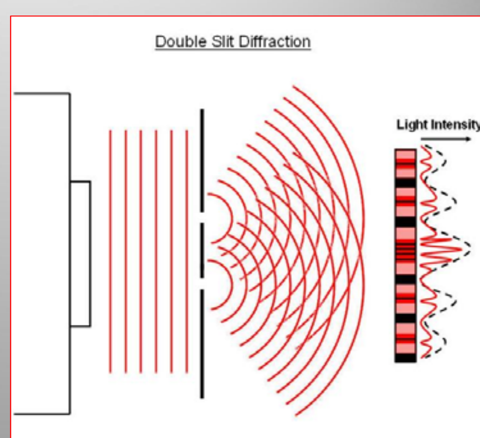
- Double slit diffraction:



  - Constructive interference

$$d \sin\theta = n\lambda$$



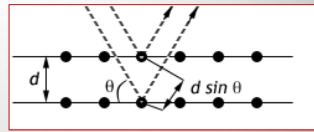


Bragg Scattering

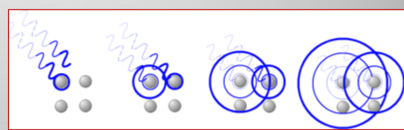
- X-ray diffraction:
  - Bragg's Law: constructive interference

$$2d\sin\theta = n\lambda$$

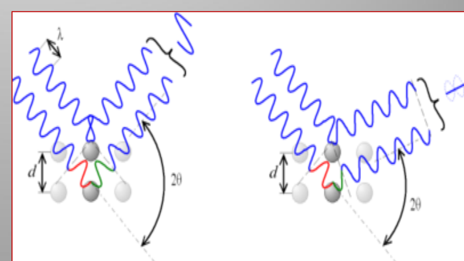
  - Actually, quite general!



Bragg formulation

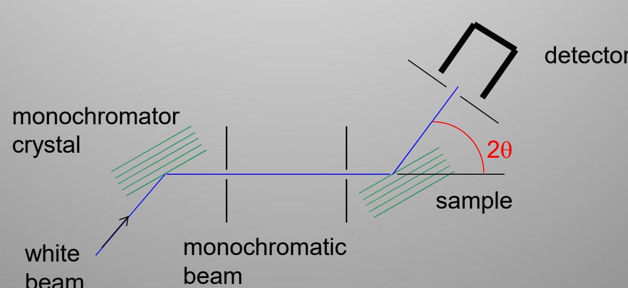


Laue formulation



Diffraction experiments

- **Requirements:**
  - a monochromatic beam (well-collimated) of X-rays, neutrons, electrons, *etc.*
  - a detector that can scan
  - a way of aligning the crystal so that the selected Miller planes are oriented with respect to the incident and diffracted beams



X-ray Methods

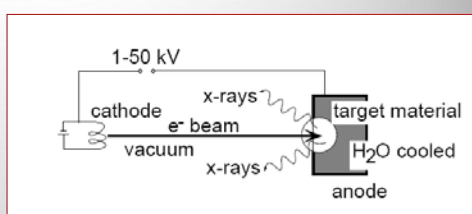
- The Laue Method: scatter from single Xtal using range of wavelengths from λ_1 to λ_o
- The Rotating Crystal Method: monochromatic X-rays with rotating sample
- The Powder (Debye-Sherrer) Method: equivalent to rot. Xtal method but with rot. axis varied over all possible orientations

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

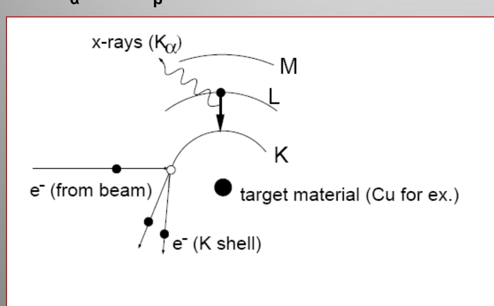
Note: scattering angle $\phi \equiv 2\theta$

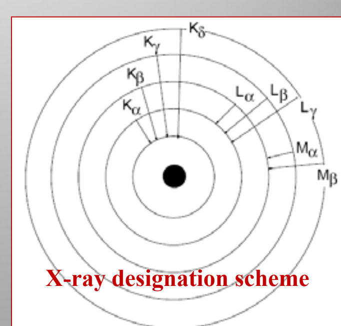
where θ is the Bragg angle

Generating X-rays



- e^- beam incident on metal target (e.g., Cu, Mo) liberates core e^-
- “characteristic” X-rays from core transitions
- Generally, two sharp peaks: K_α and K_β



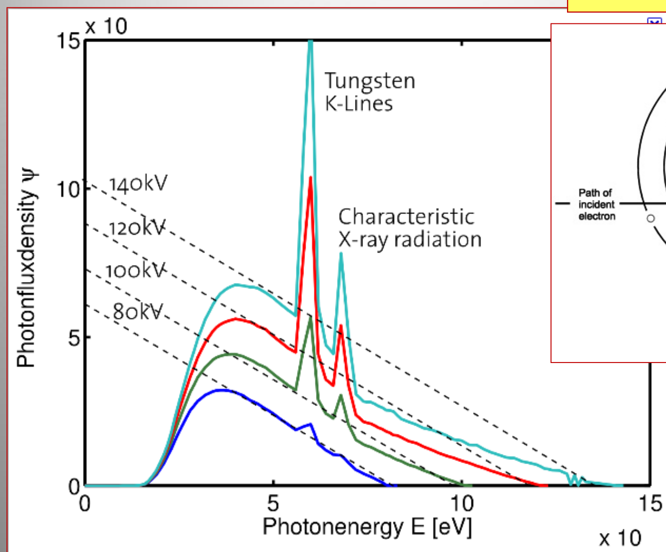


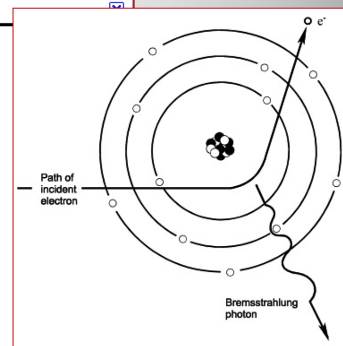
X-ray designation scheme

http://ocw.mit.edu/courses/materials-science-and-engineering/3-091sc-introduction-to-solid-state-chemistry-fall-2010/syllabus/MIT3_091SCF09_aln05.pdf

Generating X-rays

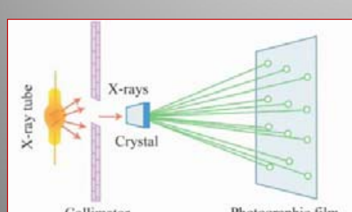
Bremsstrahlung
=braking radiation

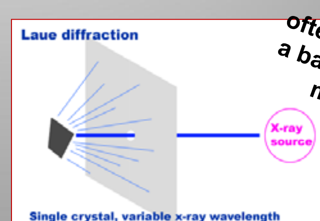




http://people.ee.ethz.ch/~pcattin/2008-BIA-UniBas/03-Modalities-I.html#%2816%29

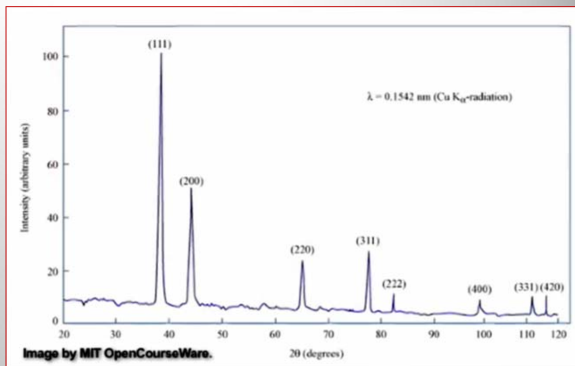
- XRD: Laue pattern:
  - white X-rays; do not know λ
  - useful for orienting Xtals

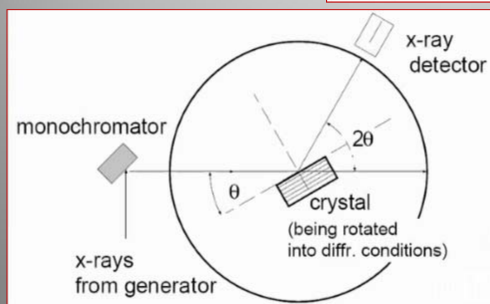




often used in
a backscatter
mode

XRD: Rotating Xtal



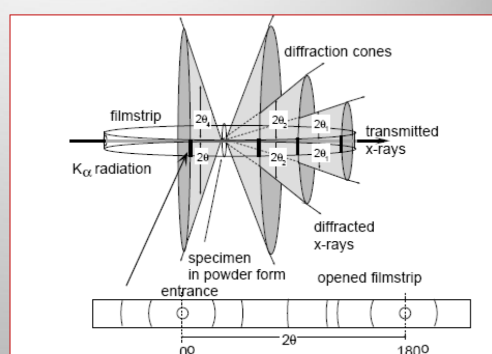


Note:

$\phi \equiv 2\theta$

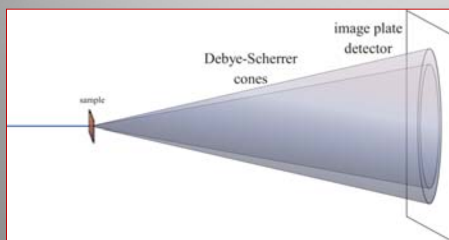
XRD: Powder Method

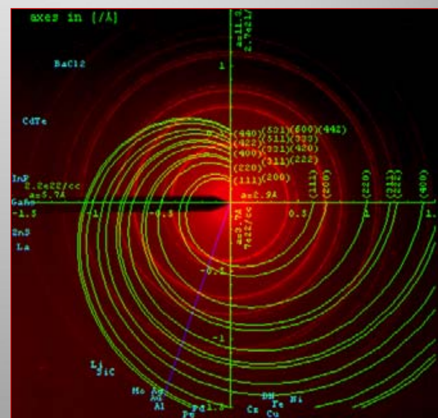
- Debye-Scherrer method



XRD: Powder Method

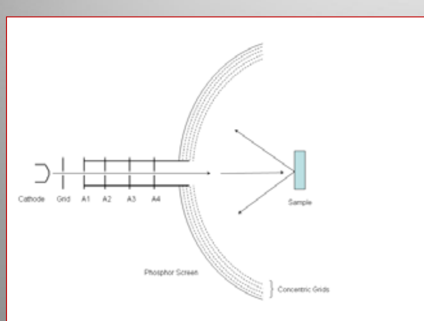
- Al film with FCC overlay



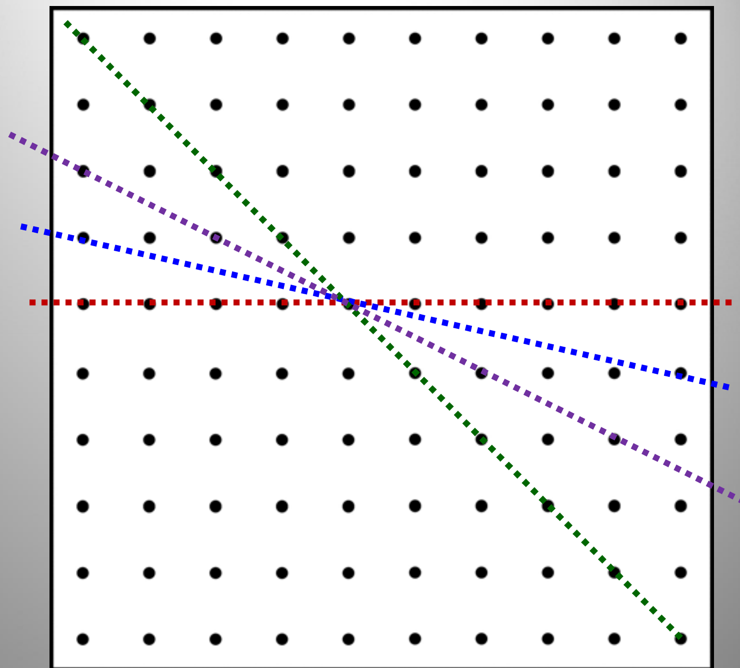


Low Energy Electron Diffraction

- LEED – surface technique
- Similar physics



Some planes of atoms will produce stronger reflections than others
(we will parameterize with "structure factors")



- **Example:**
- The (4,4,0) diffraction peak of silicon is measured experimentally to occur at a diffraction angle 2θ of 43.2° when using x-rays of wavelength 0.707 Å. Calculate the cubic unit cell parameter a for silicon.
- If this unit cell has 8 atoms per unit cell, determine the density of silicon.

Electromagnetic Waves

- Recall that monochromatic plane E&M waves can be written

$$\tilde{\vec{E}}(\vec{r},t) = \hat{n}\,\tilde{E}_o\,e^{i(\vec{k}\cdot\vec{r}-\omega t)} \qquad \tilde{\vec{B}}(\vec{r},t) = \frac{1}{c}\hat{k}\times\tilde{\vec{E}}$$

- or

$$\vec{E}(\vec{r},t) = \hat{n}\,E_o\cos(\vec{k}\cdot\vec{r}-\omega t+\delta)$$

$$\vec{B}(\vec{r},t) = \frac{1}{c}(\hat{k}\times\hat{n})\,E_o\cos(\vec{k}\cdot\vec{r}-\omega t+\delta)$$

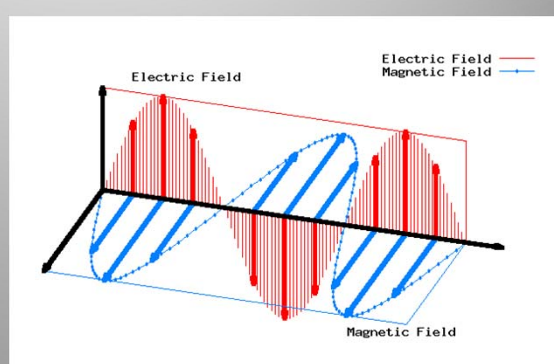
Note that if we know the electric field, we know the magnetic field!

Electromagnetic Waves

- Wavevector, $\vec{k}$, points in the direction of propagation
- Polarization given by direction of $\hat{n}$

$$\tilde{\vec{E}}(\vec{r},t) = \hat{n}\,\tilde{E}_o\,e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

$$\tilde{\vec{B}}(\vec{r},t) = \frac{1}{c}\hat{k}\times\tilde{\vec{E}}$$



EM Waves and the Lattice

- A plane wave $\tilde{\vec{E}}(\vec{r},t) = \hat{n}\,\tilde{E}_o\, e^{i(\vec{k}\cdot\vec{r}-\omega t)}$ travels through a Bravais lattice (set of points $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$)
- For certain choices of wavevector the wave will have the same periodicity as the lattice.
- The set of all wavevectors $\vec{G} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$ that yield plane waves with the periodicity of the Bravais lattice is known as the **reciprocal lattice**

The Reciprocal Lattice

- Motivation …
- Recall the Fourier Series: any periodic function, f(t), can be expanded in

$$f(t) = \frac{a_o}{2} + \sum_{n=1}^{\infty}[a_n\cos(n\omega t) + b_n\sin(n\omega t)]$$

where

$$a_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\cos(n\omega t)\,dt, \quad n = 0, 1, 2, \ldots$$

$$b_n = \frac{2}{T}\int_{-T/2}^{T/2} f(t)\sin(n\omega t)\,dt, \quad n = 1, 2, 3, \ldots$$

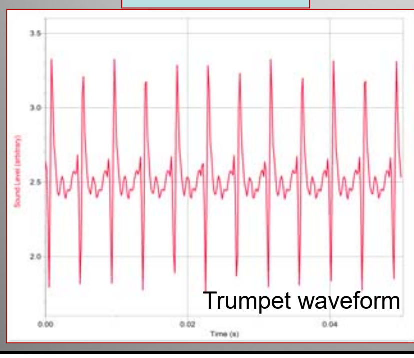
- The Fourier Series can also be written as

$$f(t) = \sum_{n=-\infty}^{\infty} c_n\, e^{in\omega t} = \sum_{n=-\infty}^{\infty} c_n\, e^{i2\pi n t/T}, \quad n = 0, \pm 1, \pm 2, \ldots$$

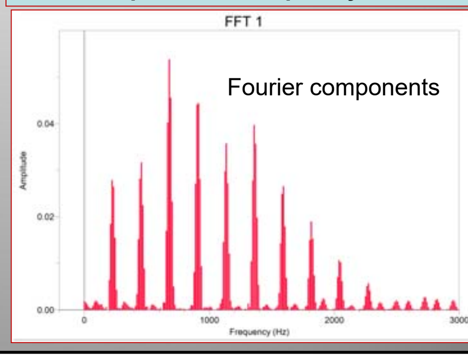
where $$c_n = \frac{1}{T}\int_{-T/2}^{T/2} f(t)\, e^{-in\omega t}\, dt$$

- One context: **sound**

"time domain"

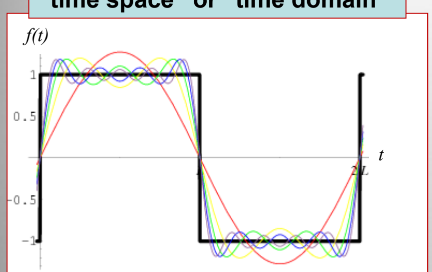


"Fourier space" or "frequency domain"

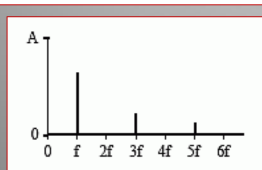


- Other examples:

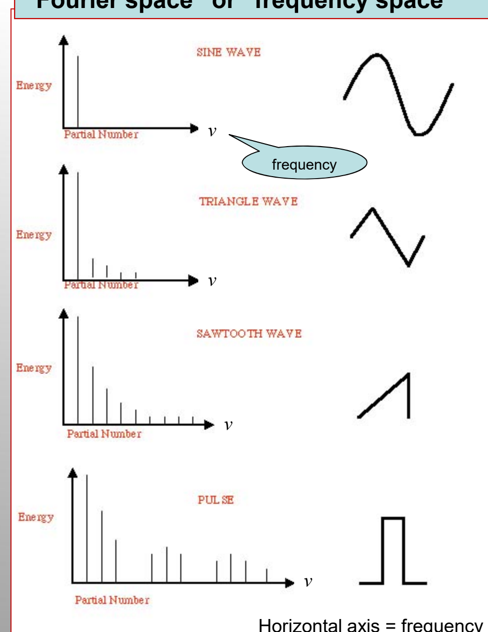
"time space" or "time domain"



$$f(t) = \frac{4}{\pi}\sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n}\sin\left(\frac{n\pi t}{T}\right)$$



"Fourier space" or "frequency space"



Reciprocal Lattice Vectors

- Look at the vectors, $\vec{G}$

- Construct axis vectors of the reciprocal lattice:

$$\vec{b}_1 = \frac{2\pi\, \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \qquad \vec{b}_2 = \frac{2\pi\, \vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)} \qquad \vec{b}_3 = \frac{2\pi\, \vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

Note that $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$

For cubic lattice
$$\begin{cases} \vec{a}_i = a\,\hat{e}_i \\ \vec{b}_i = \dfrac{2\pi}{a}\hat{e}_i \end{cases}$$