Phys 446:
Solid State Physics / Optical Properties

Fall 2007

Solid State Physics

Lecture 2

(Ch. 2.1-2.3, 2.6-2.7)
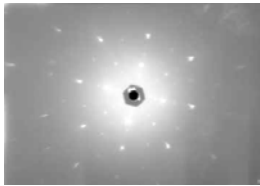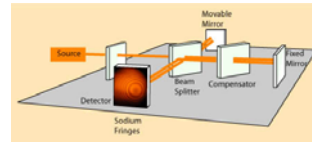
Last week:

• Crystals,

• Crystal Lattice,

• Reciprocal Lattice, and

• Types of bonds in crystals

Today:

• Diffraction from crystals
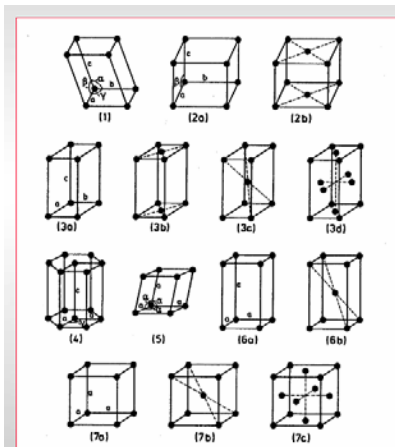
• Importance of the *reciprocal lattice* concept

Crystal Lattice

14 Bravais Lattices which can be assigned to **7 different Crystal Systems**

(1) triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
(2) monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$
a) primitive	
b) base centered	
(3) orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$
a) primitive	
b) base centered	
c) space centered	
d) face centered	
(4) hexagonal	$a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$
(5) trigonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$
(6) tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$
a) primitive	
b) space centered	
(7) cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$
a) primitive	
b) space centered	
c) face centered	

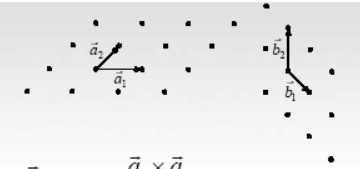### *Reciprocal Lattice*

crystal lattice point: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

reciprocal lattice point: $\vec{G} = h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3$

primitive translations of the reciprocal lattice:

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

properties: $\vec{a}_i \cdot \vec{b}_k = 2\pi\delta_{ik}$ **or** $\vec{R} \cdot \vec{G} = m2\pi$

fundamental property of a crystal lattice:
translation invariance of electron- / scattering-density: $\boxed{\rho(\vec{r}) = \rho(\vec{r} + \vec{R})}$

$$\rho(\vec{r}) = \sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \quad \textbf{with} \quad \rho(\vec{r} + \vec{R}) = \sum_{\vec{G}} \rho_{\vec{G}} e^{i(\vec{G}\cdot\vec{r} + \vec{G}\cdot\vec{R})} = \sum_{\vec{G}} \rho_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = \rho(\vec{r})$$

Diffraction of waves by crystal lattice

- Most methods for determining the atomic structure of crystals are based on scattering of particles/radiation.
- X-rays is one of the types of the radiation which can be used
- Other types include electrons and neutrons
- The wavelength of the radiation should be comparable to a typical interatomic distance of a few Å   (1 Å = 10^{-10} m)

$$E = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E}$$

$\lambda(\text{Å}) = 12398/E(\text{eV}) \Rightarrow$

few keV is suitable energy for λ = 1 Å

- X-rays are scattered mostly by electronic shells of atoms in a solid. Nuclei are too heavy to respond.
- Reflectivity of x-rays $\sim10^{-3}$-10^{-5} $\Rightarrow$ deep penetration into the solid $\Rightarrow$ x-rays serve as a bulk probe

The Bragg Law

Conditions for a sharp peak in the intensity of the scattered radiation:

1) the x-rays should be specularly reflected by the atoms in one plane

2) the reflected rays from the successive planes interfere constructively
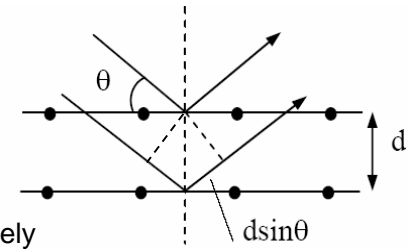
The path difference between the two x-rays: $2d\cdot\sin\theta \Rightarrow$

the Bragg formula: $2d\cdot\sin\theta = m\lambda$

The model used to get the Bragg law are greatly oversimplified (but it works!).

- It says nothing about intensity and width of x-ray diffraction peaks
- neglects differences in scattering from different atoms
- assumes single atom in every lattice point
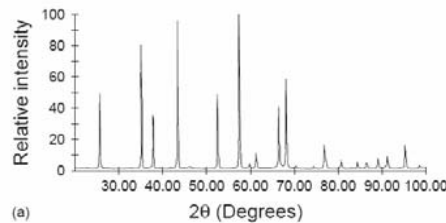- neglects distribution of charge around atoms

The Bragg Law and Diffraction grating

Compare Bragg Law

$$2d\cdot\sin\theta = m\lambda$$
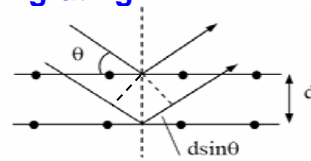
X-ray Diffraction

Diffraction Grating

A diffraction grating is the tool of choice for separating the colors in incident light.
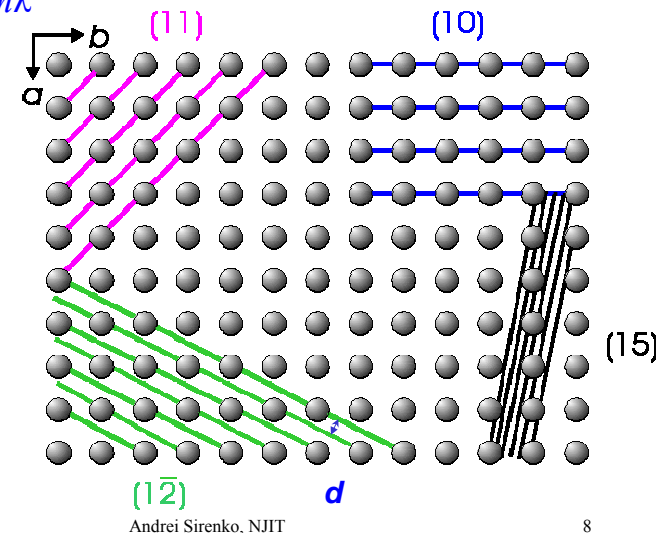
The condition for maximum intensity is the same as that for a double slit. However, angular separation of the maxima is generally much greater because the slit spacing is so small for a diffraction grating.
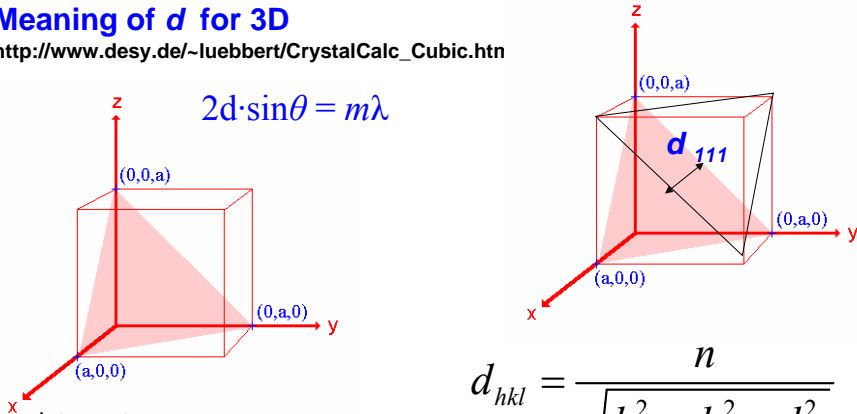
$d \sin\theta = m\lambda$

Meaning of *d* for 2D

$$2d\cdot\sin\theta = m\lambda$$

(11)   (10)   (15)   (1$\bar{2}$)   *d*

Meaning of *d* for 3D

$$2d \cdot \sin\theta = m\lambda$$

(0,0,a)

z
x
y
(a,0,0)
(0,a,0)

d_{111}

z
(0,0,a)
(a,0,0)
(0,a,0)
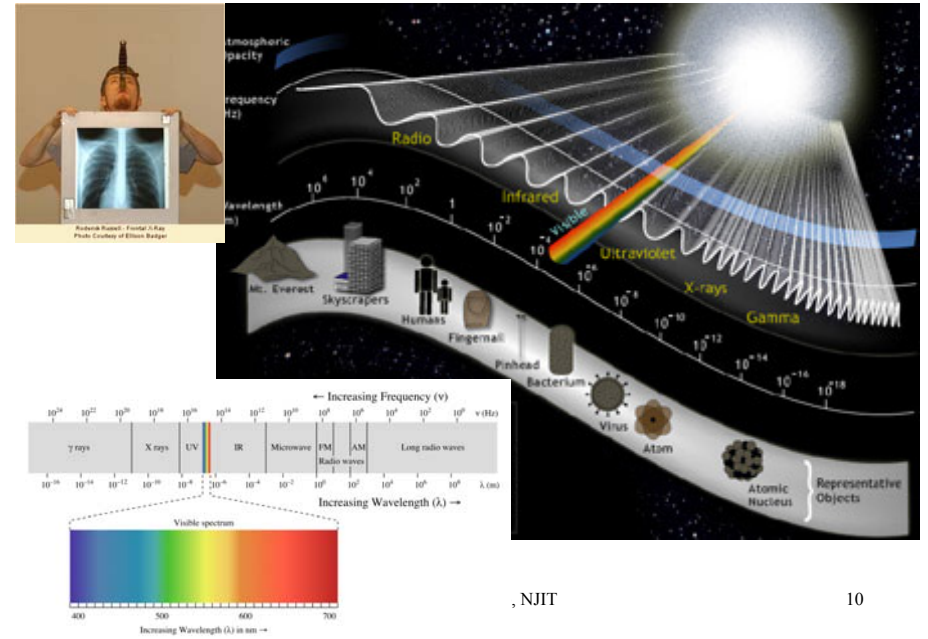x
y

Intercepts: a,a,a
Reciprocals: a/a, a/a, a/a
= 1, 1, 1
Miller index for this plane : (1 1 1)

$$d_{hkl} = \frac{n}{\sqrt{\dfrac{h^2}{a^2} + \dfrac{k^2}{b^2} + \dfrac{l^2}{c^2}}}$$

$$d_{111} = \frac{n \cdot a}{\sqrt{3}} \approx 3.13 \text{ A for Si with } a = 5.431 \text{ A}$$
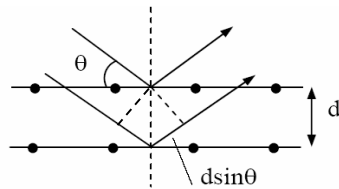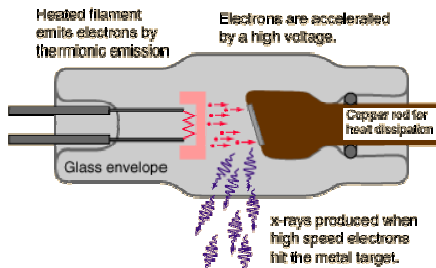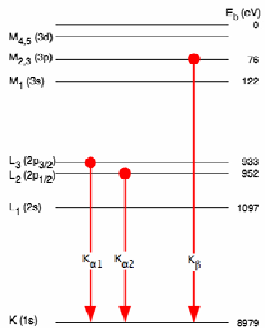

X-rays are EM waves

X-rays and X-ray tube

Bragg Law

$$2d \cdot \sin\theta = m\lambda$$

for $m=1$ $2d > \lambda$

θ
d
dsinθ

X-ray tube

Electronic
transitions

Heated filament emit electrons by thermionic emission

Electrons are accelerated by a high voltage.

Copper rod for heat dissipation

Glass envelope

x-rays produced when high speed electrons hit the metal target.

X-ray K-series spectral line wavelengths (nm)
for some common target materials.[5]

Target	Kβ₁	Kβ₂	Kα₁	Kα₂
Fe	0.17566	0.17442	0.193604	0.193998
Ni	0.15001	0.14886	0.165791	0.166175
Cu	0.139222	0.138109	0.154056	0.154439
Zr	0.070173	0.068993	0.078593	0.079015
Me	0.063229	0.062099	0.070930	0.071359

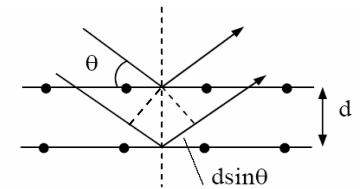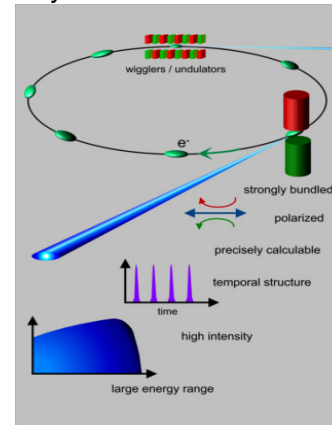## X-rays and Synchrotrons

Bragg Law

$$2d \cdot \sin\theta = m\lambda$$

θ
d
dsinθ

Synchrotron radiation

wigglers / undulators
e⁻
strongly bundled
polarized
precisely calculable
temporal structure
time
high intensity
large energy range

Natural Synchrotron Radiation
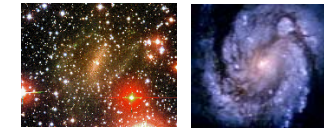
Stars and Galaxies

Synchrotron Radiation
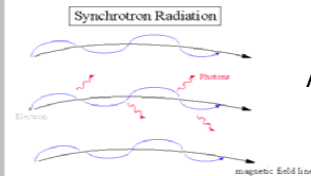
Accelerating electron emits light

magnetic field lines

SYNCHROTRON RADIATION

$v \ll c$ $\qquad$ $v \approx 0.99999999\ c$

$\theta = 4\pi\ srad$ $\qquad$ $\theta \approx \sqrt{1-\dfrac{v^2}{c^2}} \approx 0.001\ srad$
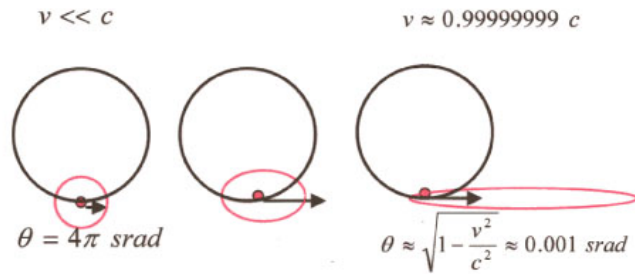
Synchrotron Radiation produced by relativistic electrons in accelerators (since 1947)

<u>NSLS:</u>
- 50 m circumference,
- Current = 1 A,
- f=6 MHz,
- E=800MeV (restmass energy $E_0 \approx 0.5$MeV)
- $I \propto \lambda^{-7/3}$

•**Synchrotron Radiation from a storage ring is the most bright manmade source of white light**
•**Useful for materials studies from Far Infrared and UV to X-ray**

Diffraction condition and reciprocal lattice

Von Laue approach:
– crystal is composed of identical atoms placed at the lattice sites T
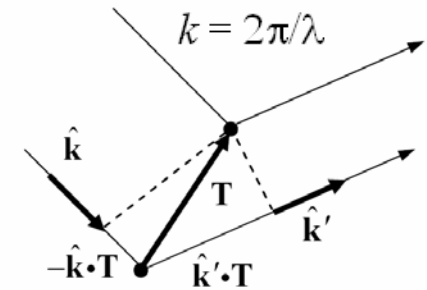– each atom can reradiate the incident radiation in all directions.
– Sharp peaks are observed only in the directions for which the x-rays scattered from all lattice points interfere constructively.

$k = 2\pi/\lambda$

Consider two scatterers separated by a lattice vector **T**.
Incident x-rays: wavelength λ, wavevector **k**; $|\mathbf{k}| = k = 2\pi/\lambda$;
Assume *elastic* scattering: scattered x-rays have same energy (same λ) $\Rightarrow$ wavevector **k'** has the same magnitude $|\mathbf{k'}| = k = 2\pi/\lambda$

$$\hat{\mathbf{k}} = \frac{\mathbf{k}}{|\mathbf{k}|} \qquad \hat{\mathbf{k}}' = \frac{\mathbf{k}'}{|\mathbf{k}'|}$$

Condition of constructive interference: $(\hat{\mathbf{k}}'-\hat{\mathbf{k}})\cdot\mathbf{T} = m\lambda$ or $(\mathbf{k}'-\mathbf{k})\cdot\mathbf{T} = 2\pi n$

Define $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$ - *scattering wave vector*

Then $\Delta\mathbf{k} = \mathbf{G}$, where **G** is defined as such a vector for which $\mathbf{G}\cdot\mathbf{T} = 2\pi m$

We obtained the *diffraction (Laue) condition*: $\Delta\mathbf{k} = \mathbf{G}$ where $\mathbf{G}\cdot\mathbf{T} = 2\pi m$

Vectors **G** which satisfy this relation form a ***reciprocal lattice***

A reciprocal lattice is defined with reference to a particular Bravais lattice, which is determined by a set of lattice vectors **T**.

Constricting the reciprocal lattice from the direct lattice:

Let $\mathbf{a_1},\ \mathbf{a_2},\ \mathbf{a_3}$ - primitive vectors of the direct lattice; $\mathbf{T} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$

Then reciprocal lattice can be generated using the primitive vectors

$$\mathbf{b}_1 = \frac{2\pi}{V}\mathbf{a}_2\times\mathbf{a}_3,\quad \mathbf{b}_2 = \frac{2\pi}{V}\mathbf{a}_3\times\mathbf{a}_1,\quad \mathbf{b}_3 = \frac{2\pi}{V}\mathbf{a}_1\times\mathbf{a}_2$$

where $V = \mathbf{a_1}\cdot(\mathbf{a_2}\times\mathbf{a_3})$ is the *volume of the unit cell*

Then vector $\mathbf{G} = m_1\mathbf{b_1} + m_2\mathbf{b_2} + m_3\mathbf{b_3}$ $\qquad$ We have $\mathbf{b}_i\cdot\mathbf{a}_j = \delta_{ij}$

Therefore, $\mathbf{G}\cdot\mathbf{T} = (m_1\mathbf{b_1} + m_2\mathbf{b_2} + m_3\mathbf{b_3})\cdot(n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}) =$
$\qquad\qquad 2\pi(m_1 n_1 + m_2 n_2 + m_3 n_3) = 2\pi m$

The set of reciprocal lattice vectors determines the possible scattering wave vectors for diffraction

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We got $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k} = \mathbf{G}$ $\Rightarrow$ $|\mathbf{k}'|^2 = |\mathbf{k}|^2 + |\mathbf{G}|^2 + 2\mathbf{k}\cdot\mathbf{G}$ $\Rightarrow$ $G^2 + 2\mathbf{k}\cdot\mathbf{G} = 0$
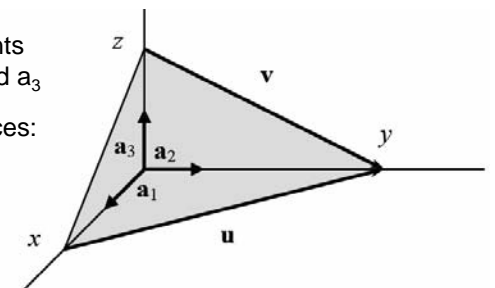
$\quad 2\mathbf{k}\cdot\mathbf{G} = G^2$ – another expression for diffraction condition

Now, show that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ is orthogonal to the plane represented by Miller indices (hkl)

plane (hkl) intercepts axes at points $x, y,$ and z given in units a_1, a_2 and a_3

By the definition of the Miller indices:

$$(h,k,l) = \left(\frac{1}{x},\frac{1}{y},\frac{1}{z}\right)$$

define plane by two non-collinear vectors **u** and **v** lying within this plane:

$$\mathbf{u} = y\mathbf{a}_2 - x\mathbf{a}_1 \ \text{ and }\ \mathbf{v} = y\mathbf{a}_2 - z\mathbf{a}_3$$

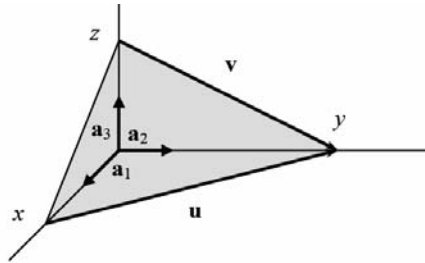prove that **G** is orthogonal to **u** and **v**:

$\mathbf{u}\cdot\mathbf{G} = (y\mathbf{a}_2 - x\mathbf{a}_1)\cdot(h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}) = 2\pi(yk - xh) = 0$

analogously show
$\mathbf{v}\cdot\mathbf{G} = 0$ 16

Now, prove that the distance between two adjacent parallel planes of the direct lattice is $d = 2\pi/G$.

The interplanar distance is given by the projection of the one of the vectors $x\mathbf{a}_1, y\mathbf{a}_2, z\mathbf{a}_3$, to the direction normal to the (hkl) plane, which is the direction of the unit vector $\mathbf{G}/G$
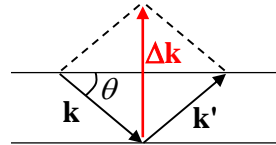
$$\Rightarrow \quad d = x\mathbf{a}_1 \cdot \mathbf{G}/G = 2\pi x h/G = 2\pi/G$$

The reciprocal vector $G(hkl)$ is associated with the crystal planes (hkl) and is normal to these planes. The separation between these planes is $2\pi/G$
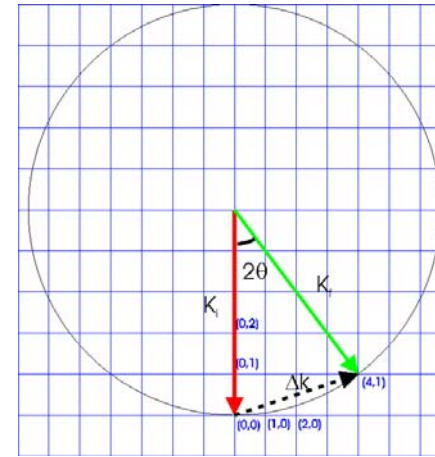
$$2\mathbf{k}\cdot\mathbf{G} = G^2 \Rightarrow 2|\mathbf{k}|G\sin\theta = G^2$$
$$\Rightarrow 2\cdot 2\pi\sin\theta/\lambda = 2\pi/d \Rightarrow 2d\sin\theta = \lambda$$

$2d\sin\theta = m\lambda$ - get Bragg law

Ewald Construction for Diffraction Condition and reciprocal space
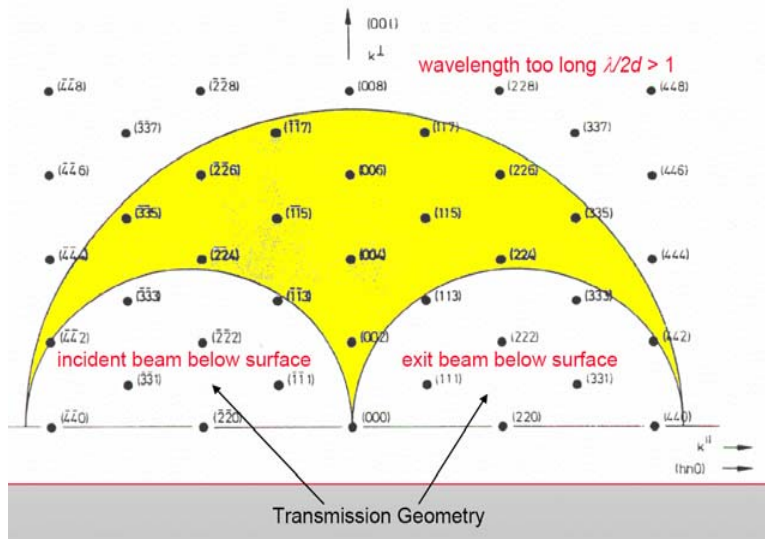

Diffraction occurs for:

$$\vec{k} + \vec{G} = \vec{k'}$$
Or
$$\vec{k'} - \vec{k} = \vec{G}$$

$$k = 2\pi/\lambda$$


Reciprocal Space: Accessible Area for Diffraction

Summary $\qquad k = 2\pi/\lambda$

❖ Various statements of the Bragg condition:

$$2d\cdot\sin\theta = m\lambda \;; \qquad \Delta\mathbf{k} = \mathbf{G} \;; \qquad 2\mathbf{k}\cdot\mathbf{G} = G^2$$

❖ Reciprocal lattice is defined by primitive vectors:

$$\mathbf{b}_1 = \frac{2\pi}{V}\mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V}\mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V}\mathbf{a}_1 \times \mathbf{a}_2$$

❖ A reciprocal lattice vector has the form $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$
It is normal to (hkl) planes of direct lattice

❖ Only waves whose wave vector drawn from the origin terminates on a surface of the Brillouin zone can be diffracted by the crystal

First BZ of bcc lattice   First BZ of fcc lattice
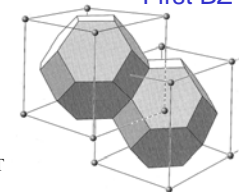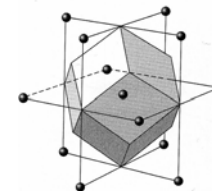
Atomic and structure factors

Experimental techniques

Neutron and electron diffraction

Diffraction process:
1) Scattering by individual atoms
2) Mutual interference between scattered rays

Scattering from atom

Consider single electron. Plane wave $\quad u = Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \quad k = |\mathbf{k}| = \dfrac{2\pi}{\lambda}$

Scattered field: $\quad u' = f_e \dfrac{A}{R} e^{i(kR-\omega t)} \quad f_e$ – *scattering length of electron*
$\qquad\qquad\qquad\qquad\qquad\qquad\qquad R$ – radial distance

Two electrons: $\quad u' = f_e \dfrac{A}{R} e^{ikR}\left[1 + e^{i\Delta\mathbf{k}\cdot\mathbf{r}}\right]$

or, more generally $\quad u' = f_e \dfrac{A}{R} e^{ikR}\left[e^{i\Delta\mathbf{k}\cdot\mathbf{r}_1} + e^{i\Delta\mathbf{k}\cdot\mathbf{r}_2}\right]$

many electrons: $\quad u' = f_e \dfrac{A}{R} e^{ikR}\sum_l e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l}$ $\qquad$ similar to single electron with

$$f = f_e \sum_l e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l}$$

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intensity: $\quad I \sim |f| = f_e^{2}\left|\sum_l e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l}\right|^{2}$

this is for coherent scatterers. If random then $\quad I \sim N f_e^{2}$

Scattering length of electron: $\quad f_e = \left[(1+\cos^2 2\theta)/2\right]^{1/2} r_e$

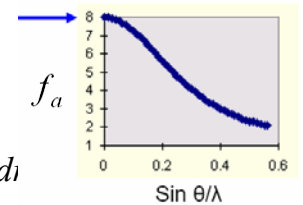classical electron radius $\quad r_e = \dfrac{1}{4\pi\varepsilon_0}\dfrac{e^2}{mc^2} \approx 2.8\times10^{-15}$ m

In atom, $\quad f_e \sum_l e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l} \rightarrow f_e \int n(\mathbf{r})e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l} d^3r$
$\qquad\qquad\qquad\qquad\qquad\qquad n(\mathbf{r})$ – electron density

$f_a = \int n(\mathbf{r})e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l} d^3r$ **- atomic scattering factor (form factor)**

Atomic scattering factor (dimensionless) is determined by electronic distribution.

If $n(\mathbf{r})$ is spherically symmetric, then

$$f_a = \int_0^{r_0} 4\pi r^2 n(r)\frac{\sin(\Delta k \cdot r)}{\Delta k \cdot r}dr$$

in forward scattering $\Delta k = 0$ so $\qquad f_a = 4\pi\int r^2 n(r)dr = Z$

Z - total number of electrons

Atomic factor for forward scattering is equal to the atomic number

(all rays are in phase, hence interfere constructively)

Scattering from crystal

crystal scattering factor:
$$f_{cr} = \sum_l e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l} = \sum_l f_{al} e^{i\Delta\mathbf{k}\cdot\mathbf{R}_l}$$

$\mathbf{R}_l$ - position of lth atom, f_{al} - corresponding atomic factor

rewrite $f_{cr} = F \cdot S$

where $F = \sum_j f_{aj} e^{i\Delta\mathbf{k}\cdot\mathbf{s}_j}$ - *structure factor* of the basis, summation over the atoms in unit cell

and $S = \sum_l e^{i\Delta\mathbf{k}\cdot\mathbf{R}_l^c}$ - lattice factor, summation over all unit cells in the crystal

Where $\mathbf{R}_l = \mathbf{R}_l^c + \mathbf{s}_j$

Since $\Delta\mathbf{k} = \mathbf{G}$, the lattice factor becomes
$$S = \sum_l e^{i\mathbf{G}\cdot\mathbf{R}_l^c} = \sum_l e^{i2\pi m} = N$$

Then scattering intensity $I \sim |f_{cr}|^2$ where $f_{cr} = F \cdot N = N\sum_j f_{aj} e^{i\mathbf{G}\cdot\mathbf{s}_j}$

$\mathbf{G} = \mathbf{G}_{hkl} = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ if $\mathbf{s}_j = u_j\mathbf{a_1} + v_j\mathbf{a_2} + w_j\mathbf{a_3}$

Then $F = \sum_j f_{aj} e^{i(u_j\mathbf{a_1}+v_j\mathbf{a_2}+w_j\mathbf{a_3})(h\mathbf{b_1}+k\mathbf{b_2}+l\mathbf{b_3})} = \sum_j f_{aj} e^{2\pi i(hu_j+kv_j+lw_j)}$

structure factor

Example: structure factor of bcc lattice (identical atoms)

structure factor $F = \sum_j f_{aj} e^{2\pi i(hu_j+kv_j+lw_j)}$

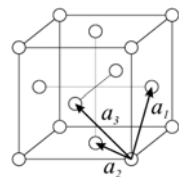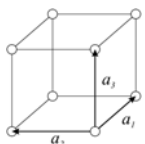Two atoms per unit cell: $\mathbf{s}_1 = (0,0,0)$; $\mathbf{s}_2 = a(1/2,1/2,1/2)$

$$F = f_a\left[1 + e^{\pi i(h+k+l)}\right]$$

$\Rightarrow F=2f_a$ if $h+k+l$ is even, and $F=0$ if $h+k+l$ is odd

Diffraction is absent for planes with odd sum of Miller indices

For allowed reflections in fcc lattice *h,k,and l* are all even or all odd

4 atoms in the basis.

What about simple cubic lattice ?

## Structure factor of the BCC lattice

- What does this mean? Metallic sodium, for example, is BCC. The diffraction pattern does not contain lines such as (100), (300), (111), etc. – whenever the sum of integers hkl is odd. However, there are lines such as (200), (110), (222), etc.

- The physical reason is that reflections with $v_1 + v_2 + v_3$ = odd refer to planes of atoms where the rays are out of phase by π, so that each ray, from plane to plane, cancels out the next ray, and the net intensity is zero.

- An example: (100) reflection in the BCC cell:

0 phase
π phase
2π phase

d_{100}

1st plane
2nd plane
3rd plane
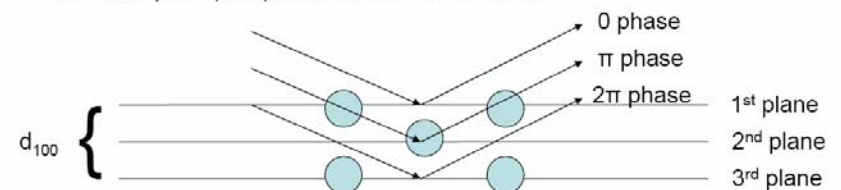
Structure factor of the FCC lattice

- For the FCC lattice, we have the basis (identical atoms at both positions):

$$x_1 = 0 \; y_1 = 0 \; z_1 = 0$$
$$x_2 = 0 \; y_2 = \tfrac{1}{2} \; z_2 = \tfrac{1}{2}$$
$$x_3 = \tfrac{1}{2} \; y_3 = 0 \; z_3 = \tfrac{1}{2}$$
$$x_4 = \tfrac{1}{2} \; y_4 = \tfrac{1}{2} \; z_4 = 0$$
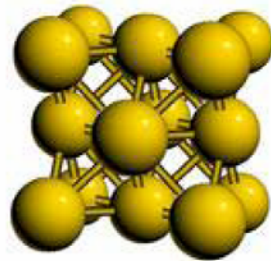
- So, this means that $S(v_1, v_2, v_3)$ is:

$$S(v_1, v_2, v_3) = f\,[1 + \exp[-i\pi(v_2 + v_3)] + \exp[-i\pi(v_1 + v_3)] + \exp[-i\pi(v_1 + v_2)]]$$

- Therefore, if all the indices are even integers, or all are odd S = 4f. If 1 is even, and 2 are odd, then S = 0. If 1 is odd, and 2 are even, then S is zero. This means that no reflections can occur for which the indices are partly even and partly odd.

Structure factor of the FCC lattice

- Nickel has an FCC structure:
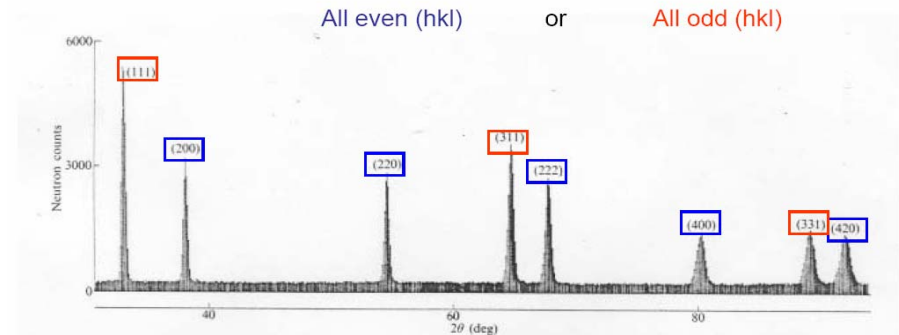
All even (hkl)   or   All odd (hkl)

FIG. 58. A section of a powder diffraction pattern for nickel at a wavelength of 1·14 Å recorded on the PANDA diffractometer at A.E.R.E.-Harwell using a germanium monochromator. Counts are made at intervals of 0·1° of 2θ. (Courtesy of R. F. Dyer.)

Note: There are no reflections with mixtures of odd and even indices (eg. (110))

Structure factor of the SC lattice

- The structure factor S does not have to be real, because the intensity of the x-ray goes like S*S. However, S*S must be real.
- For a simple cubic lattice, the structure factor is easy to calculate:
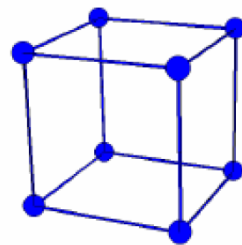
The basis is one atom, at (0, 0, 0).
(This will produce all the atoms in the unit cell by translation)

So: $S(v_1, v_2, v_3) = f\,[\exp 0] = f$

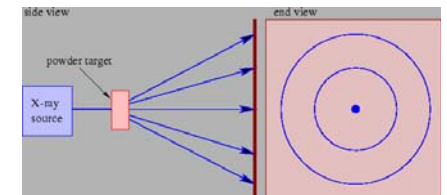This means all of the reflections where $\overrightarrow{\Delta k} = \overrightarrow{G}$ are allowed (so we see all reflections of the form (hkl), eg. (100), (110), any combination of integers). We will see that this is not true for the BCC and FCC lattice
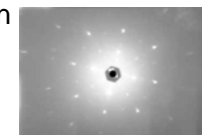

Experimental XRD techniques

Rotating crystal method –
for single crystals, epitaxial films
θ-2θ, rocking curve, φ - scan
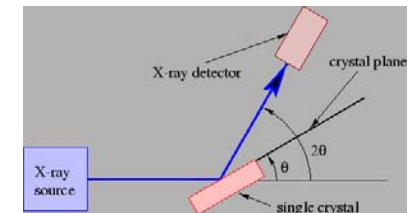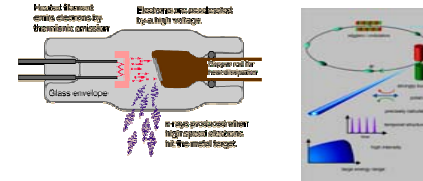
Powder diffraction

Laue method – *white* x-ray beam used most often used for mounting single crystals in a precisely known orientation

Laue Equations

- Another way of expression the diffraction condition $\Delta\vec{k} = \vec{G}$ is by the Laue equations, which can be derived by taking the scalar product of $\Delta\vec{k}$ and $\vec{G}$ with $\vec{a_1}$, $\vec{a_2}$, and $\vec{a_3}$

$$\vec{a_1} \cdot \Delta\vec{k} = 2\pi v_1 \qquad \vec{a_2} \cdot \Delta\vec{k} = 2\pi v_2 \qquad \vec{a_3} \cdot \Delta\vec{k} = 2\pi v_3$$

(Laue Equations)

- These equations have a simple interpretation: for a Bragg reflection, $\Delta\vec{k}$ must lie on a certain cone about the direction of $\vec{a_1}$ (for example). Likewise, it must be on a cone for $\vec{a_2}$ and $\vec{a_3}$. Thus, a Bragg reflection which satisfies all three conditions must lie at the intersection of these three cones, which is at a <u>point</u> in reciprocal space.

Geometric interpretation of Laue condition:

$$2\mathbf{k} \cdot \mathbf{G} = G^2 \Rightarrow \mathbf{k} \cdot \left(\frac{1}{2}\mathbf{G}\right) = \left(\frac{1}{2}\mathbf{G}\right)^2$$
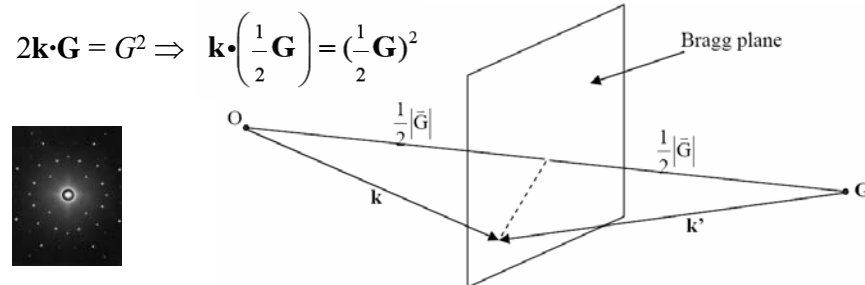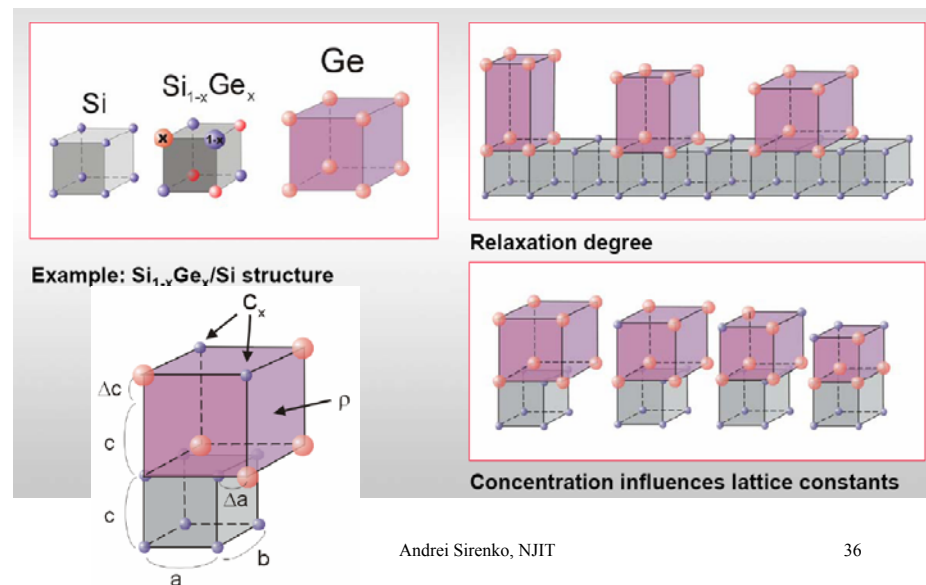

- Diffraction is the strongest (constructive interference) at the perpendicular bisecting plane (Bragg plane) between two reciprocal lattice points.
- true for any type of waves inside a crystal, including electrons.
- Note that in the original real lattice, these perpendicular bisecting planes are the planes we use to construct Wigner-Seitz cell

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Applications of X-ray Diffraction for crystal and thin-film analysis
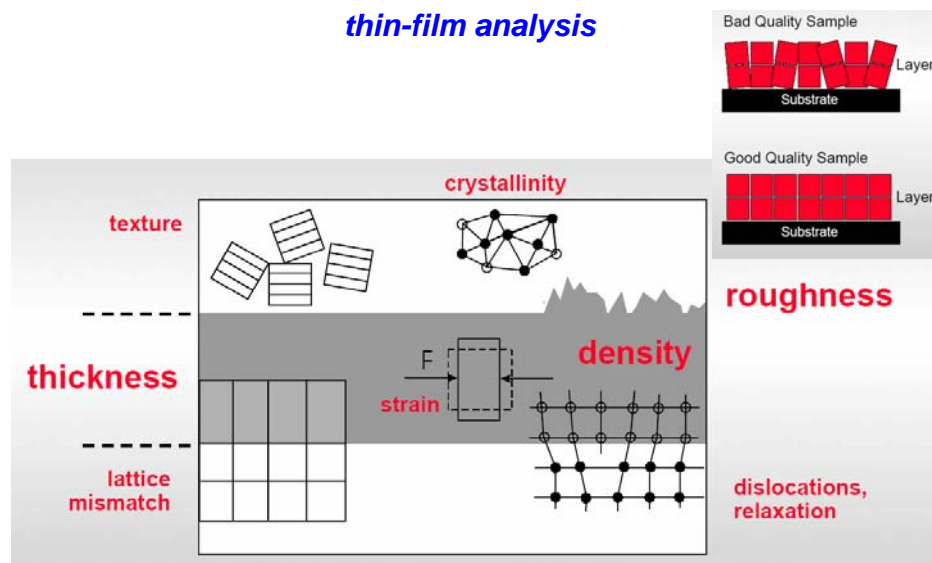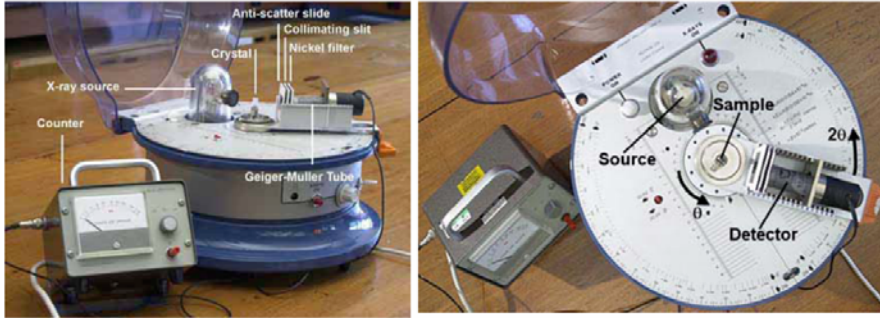

Applications of X-ray Diffraction for hetero-structures (one or more crystalline films grown on a substrate)
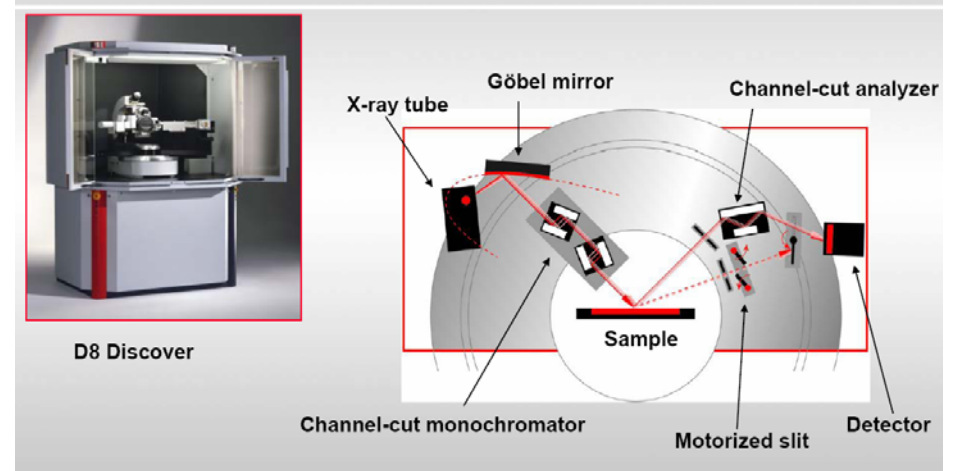
Example: $Si_{1-x}Ge_x/Si$ structure

Relaxation degree

Concentration influences lattice constants

How are diffraction experiments done?

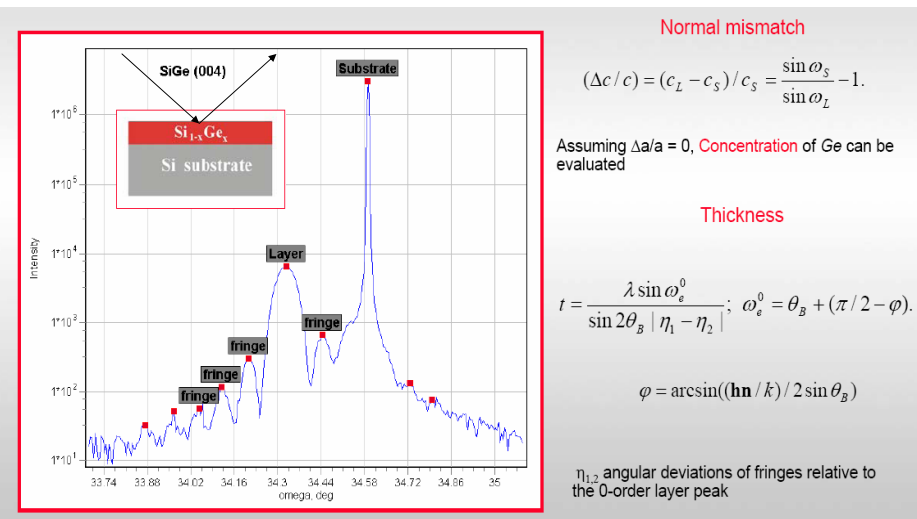### *X-ray Diffraction Setup*

High Angular Resolution X-ray Diffraction Setup

B11 Tiernan

### *Example of High Angular Resolution X-ray Diffraction analysis of a SiGe film on Si substrate*

Normal mismatch

$$(\Delta c / c) = (c_L - c_S)/c_S = \frac{\sin \omega_S}{\sin \omega_L} - 1.$$

Assuming $\Delta a/a = 0$, Concentration of Ge can be evaluated

Thickness

$$t = \frac{\lambda \sin \omega_e^0}{\sin 2\theta_B \mid \eta_1 - \eta_2 \mid}; \quad \omega_e^0 = \theta_B + (\pi / 2 - \varphi).$$

$$\varphi = \arcsin((\mathbf{hn} / k) / 2 \sin \theta_B)$$

$\eta_{1,2}$ angular deviations of fringes relative to the 0-order layer peak

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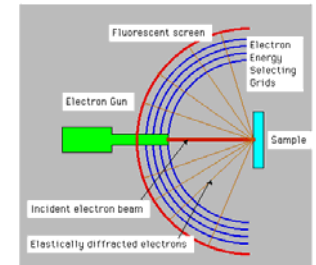### Low Energy Electron Diffraction (LEED)

$\lambda = h/p = h/(2mE)^{1/2}$

$E = 20$ eV $\rightarrow \lambda \approx 2.7$Å;
200 eV $\rightarrow 0.87$ Å

Small penetration depth (few tens of Å) – surface analysis
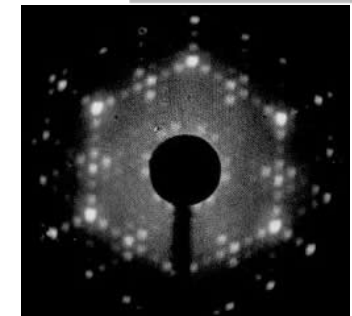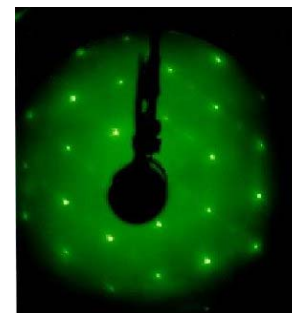
Reflection high Energy Electron Diffraction (RHEED)

- Glancing incidence: despite the high energy of the electrons (5 – 100 keV), the component of the electron momentum perpendicular to the surface is small

- Also small penetration into the sample – surface sensitive technique

- No advantages over LEED in terms of the quality of the diffraction pattern

- However, the geometry of the experiment allows much better access to the sample during observation of the diffraction pattern. (important if want to make observations of the surface structure during growth or simultaneously with other measurements

- Possible to monitor the atomic layer-by-atomic layer growth of epitaxial films by monitoring oscillations in the intensity of the diffracted beams in the RHEED pattern.

MBE and Reflection high Energy Electron Diffraction (RHEED)
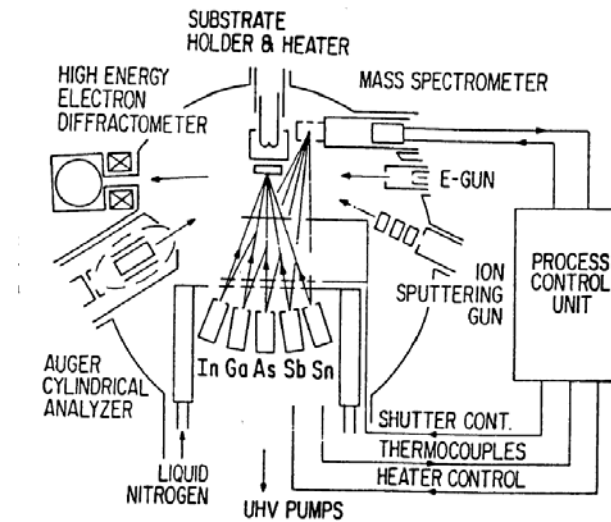
Real time growth control by
Reflection High Energy Electron Diffraction (RHEED)

Growth start

Growth end

110 azimuth
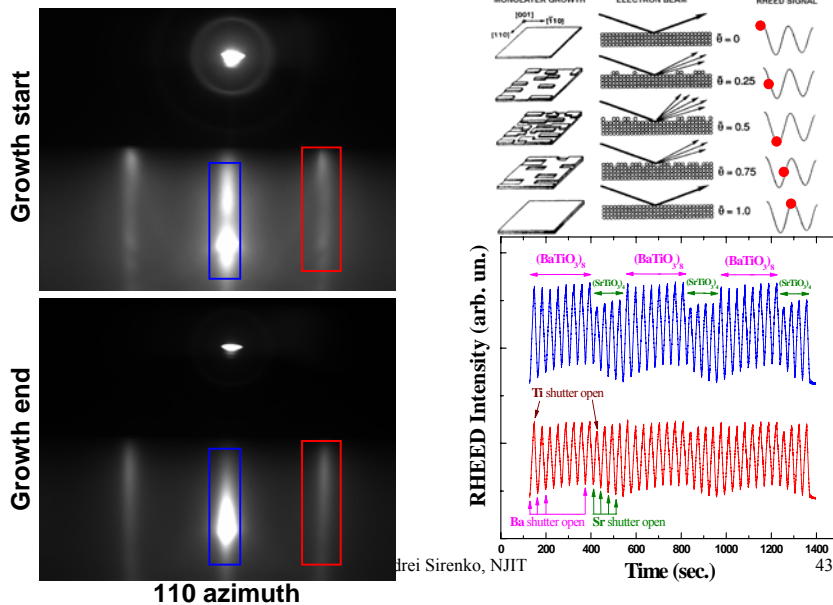
Neutron Diffraction

- $\lambda = h/p = h/(2mE)^{1/2}$ mass much larger than electron $\Rightarrow$

  $\lambda \approx 1\text{Å} \rightarrow 80$ meV   Thermal energy kT at room T: 25 meV

  called "cold" or "thermal' neutrons

- Don't interact with electrons. Scattered by nuclei

- Better to resolve light atoms with small number of electrons, e.g. Hydrogen

- Distinguish between isotopes (x-rays don't)

- Good to study lattice vibrations

  Disadvantages:

- Need to use nuclear reactors as sources; much weaker intensity compared to x-rays – need to use large crystals

- Harder to detect

Summary

❖ Diffraction amplitude is determined by a product of several factors: atomic form factor, structural factor

❖ Atomic scattering factor (form factor): reflects distribution of electronic cloud.

$$f_a = \int n(\mathbf{r}) e^{i\Delta\mathbf{k}\cdot\mathbf{r}_l} d^3 r$$

In case of spherical distribution

$$f_a = \int_0^{r_0} 4\pi r^2 n(r) \frac{\sin(\Delta k \cdot r)}{\Delta k \cdot r} dr$$

Atomic factor decreases with increasing scattering angle

❖ Structure factor

$$F = \sum_j f_{aj} e^{2\pi i (hu_j + kv_j + lw_j)}$$

where the summation is over all atoms in unit cell

❖ Neutron diffraction – "cold neutrons" - interaction with atomic nuclei, not electrons

❖ Electron diffraction – surface characterization technique