Intro. to Electro-physics The basics of crystalline structure

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Basics of crystals (1/2)

- Crystal
 - 3D periodic array of identical building blocks (e.g. atoms, groups of atoms, or even molecules)

 - Why X-ray?

 - X-ray can interact with (or be diffracted by) an array of atoms (Neutron and electron diffractions work in a similar manner)





The periodicity of a crystal experimentally observed by X-Ray Diffraction by the crystal (Laue in 1912)

- X-ray : an electromagnetic wave with a wavelength comparable to the interatomic spacing ($\sim 1.5 {
m A}$)

X-ray diffractometer (wikipedia)

Interactions of X-ray with atoms



Basics of crystals (2/2)

- Importance of crystals
 - **Periodic atomic model** + quantum theory = the birth of solid state physics -
 - de Broglie wavelength for electrons, $\lambda = h/mv \sim 1 \text{\AA}$ (interatomic distance!)
 - "Electronic waves" respond dramatically to the periodic array of atoms of the crystal
 - Electronic properties (thermal, electrical, ...) determined by the crystal structure!
- Crystal structure \bullet
 - A crystal is constructed by the infinite repetition of identical groups -
 - A group = **basis**
 - The set of points where the basis is attached = lattice







Lattice

Mathematical representation of lattice

r' = r + T, where $T = (u_1a_1 + u_2a_2 + u_3a_3) \cdots (1)$

- The arrangement of atoms looks the same when viewed from *r* as when viewed from $m{r}'$ translated by $m{T}$ (an **integral multiple** of the $m{a}_i$'s) from $m{r}$
- Lattice is said **primitive** if (1) satisfies with any choice of **integers** (u_1, u_2, u_3) —
 - Primitive translation vectors : (a_1, a_2, a_3)
 - Primitive cell : the unit cell defined by (a_1, a_2, a_3)

Important characteristics of <u>primitive cell</u>

- The primitive cell is a **minimum-volume cell** (with a volume of $a_1 \cdot a_2 \times a_3$)
- The definition of the primitive cell is **not unique!** • Q) What are not primitive cells?
- There is only "one" lattice point per primitive cell.









Bravias lattice

System	Simple	Base-centered	Body-centered	Fa
Triclinic $a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$	α β			
Monoclinic $a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^\circ \neq \beta$				
Orthorhombic $a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$				
Tetragonal $a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$				
Rhombohedral $a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ$	$ \begin{array}{c} \alpha \\ \alpha \\ \alpha \\ \alpha \\ a \end{array}^{\alpha} a \end{array}^{a} $			
Hexagonal $a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	$\gamma = 120^{\circ}$			
Cubic $a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$				

Bravais lattice

- Distinct lattice type in 3D (there are total 14 types) \bullet
- **Simple** : lattice points on the <u>cell corners only</u>
- **Base-centered** : Lattice points on the cell corners ulletwith an additional pair in the parallel faces of the cell
- **Body-centered** : Lattice points on the cell corners, \bullet with one additional point at the center of the cell
- **Face-centered** : Lattice points on the cell corners, \bullet with one additional point at the center of each of the faces of the cell













The characteristics of cubic lattices



a١ a





Simple cubic (SC)	Body-centered cubic (BCC)	Face-centered cubic (FCC)
$\begin{cases} \boldsymbol{a}_1 = a\hat{\boldsymbol{x}} \\ \boldsymbol{a}_2 = a\hat{\boldsymbol{y}} \\ \boldsymbol{a}_3 = a\hat{\boldsymbol{z}} \end{cases}$	$\begin{cases} \boldsymbol{a}_1 = \frac{1}{2}a\left(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}}\right) \\ \boldsymbol{a}_2 = \frac{1}{2}a\left(-\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}\right) \\ \boldsymbol{a}_3 = \frac{1}{2}a\left(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}\right) \end{cases}$	$\begin{cases} \boldsymbol{a}_1 = \frac{1}{2}a\left(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}\right) \\ \boldsymbol{a}_2 = \frac{1}{2}a\left(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}\right) \\ \boldsymbol{a}_3 = \frac{1}{2}a\left(\hat{\boldsymbol{z}} + \hat{\boldsymbol{x}}\right) \end{cases}$
a ³	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
6	8	12
a	$\frac{\sqrt{3}}{2}a$	$\frac{a}{\sqrt{2}}$
$\frac{\pi}{6} \sim 0.524$	$\frac{\sqrt{3}\pi}{8} \sim 0.680$	$\frac{\sqrt{2}\pi}{6} \sim 0.740$

* The maximum proportion of the available volume that can be filled with hard spheres



Index system for crystal planes

- The rules finding the orientation of a plane
 - Find the intercepts on the axes in terms of the primitive lattice vectors (a_1, a_2, a_3) . (The axes may be those of a primitive or non primitive cell)
 - Taking the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest three integers. The result, enclosed in parentheses (hkl), is called the Miller index of the plane







X-ray diffraction by crystals (1/2)

- Crystal structure identified by diffraction of X-ray, electron and neutron • (X-ray is most common!)
 - _ All can have λ comparable to interatomic distance ($d \sim$
 - $\lambda \gg d$: Incident radiation undergoes the ordinary optical refraction
 - $\lambda \sim d$: Diffraction occurs in directions quite different from the incident beam
- The X-ray beams with $\lambda \sim d$ obliquely incident on a crystal •
 - The crystal = a set of discrete, parallel planes separated by d
 - The X-ray can undergo specular (mirror-like) reflection by an array of atoms
 - Reflection \approx Elastic scattering where the energy of X-ray is not changed
 - Each plane reflects only a small fraction of the radiation (e.g. $10^{-5} \sim 10^{-3}$ absorbed $\rightarrow 10^{3} \sim 10^{5}$ planes undergo reflection)
 - Multiple reflected beams are resulted

10 10 electromagnetic X-ray 10³ wave 10 10 electron E/eV10⁰ - 1 eV $E = h^2/2m_e\lambda^2$ 10 light energy 10-2 $E = hc/\lambda$ 10⁻³ −1 meV neutron 10 $E = h^2/2m_n\lambda^2$ 10 10 1 µe\ deBrogue 10 wave 10 1 Å 1 nm lμm 1 mm 10⁻¹⁰ 10-12 10-8 10-6 10-4

wavelength, λ / m

Energy dispersion of X-ray, neutron, electron





X-ray diffraction by crystals (2/2)

Bragg's law ullet

- The diffraction occurs when the reflected beams "interfere constructively" (intensified due to reflection by successive planes)
- Such constructive interference occurs only if the path difference

between the reflected beams = an integral multiple of wavelength as

$$2d\sin\theta = n\lambda, \ (n = 1, 2, \cdots)$$

- θ : glancing angle, λ : X-ray wavelength, n : the diffraction order
- The Bragg's law satisfies only when $\lambda \leq 2d$
- Intense peaks of reflected radiation occur at only certain values of θ

The Bragg's law = a consequence of the periodicity of the lattice



XRD of Silicon powder

 $dsin\theta$



XRD principle

