# Intro. to Electro-physics <br> The basics of crystalline structure 

Jaesang Lee<br>Dept. of Electrical and Computer Engineering<br>Seoul National University<br>(email: jsanglee@snu.ac.kr)

## Basics of crystals $(1 / 2)$

- Crystal
- 3D periodic array of identical building blocks (e.g. atoms, groups of atoms, or even molecules)
- The periodicity of a crystal experimentally observed by X-Ray Diffraction by the crystal (Laue in 1912)
- Why X-ray?
- X-ray : an electromagnetic wave with a wavelength comparable to the interatomic spacing ( $\sim 1.5 \AA$ )
- X-ray can interact with (or be diffracted by) an array of atoms
(Neutron and electron diffractions work in a similar manner)



X-ray diffractometer (wikipedia)


## Basics of crystals (2/2)

- Importance of crystals
- Periodic atomic model + quantum theory = the birth of solid state physics
- de Broglie wavelength for electrons, $\lambda=h / m v \sim 1 \AA$ (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
- 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

$$
\boldsymbol{r}^{\prime}=\boldsymbol{r}+\boldsymbol{T}, \text { where } \boldsymbol{T}=\left(u_{1} \boldsymbol{a}_{1}+u_{2} \boldsymbol{a}_{2}+u_{3} \boldsymbol{a}_{3}\right) \quad \cdots \quad \text { (1) }
$$

- The arrangement of atoms looks the same when viewed from $r$ as when viewed from $\boldsymbol{r}^{\prime}$ translated by $\boldsymbol{T}$ (an integral multiple of the $\boldsymbol{a}_{i}$ 's) from $\boldsymbol{r}$
- Lattice is said primitive if $(1)$ satisfies with any choice of integers $\left(u_{1}, u_{2}, u_{3}\right)$
- Primitive translation vectors : $\left(a_{1}, a_{2}, a_{3}\right)$

- Primitive cell : the unit cell defined by $\left(\boldsymbol{a}_{1}, \boldsymbol{a}_{2}, \boldsymbol{a}_{3}\right)$


## Important characteristics of primitive cell

- The primitive cell is a minimum-volume cell (with a volume of $\boldsymbol{a}_{1} \cdot \boldsymbol{a}_{2} \times \boldsymbol{a}_{3}$ )
- 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
Triclinic
$a_{1} \neq a_{2} \neq a_{3}$
$\alpha \neq \beta \neq \gamma$

## Bravais lattice

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


## The characteristics of cubic lattices



| Type | Simple cubic (SC) | Body-centered cubic (BCC) | Face-centered cubic (FCC) |
| :---: | :---: | :---: | :---: |
| Primitive Translation Vector | $\left\{\begin{array}{l}\boldsymbol{a}_{1}=a \hat{\boldsymbol{x}} \\ \boldsymbol{a}_{2}=a \hat{\boldsymbol{y}} \\ \boldsymbol{a}_{3}=a \hat{\boldsymbol{z}}\end{array}\right.$ | $\left\{\begin{array}{l}a_{1}=\frac{1}{2} a(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}-\hat{\boldsymbol{z}}) \\ a_{2}=\frac{1}{2} a(-\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}}) \\ a_{3}=\frac{1}{2} a(\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}})\end{array}\right.$ | $\left\{\begin{array}{l} \boldsymbol{a}_{1}=\frac{1}{2} a(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}) \\ \boldsymbol{a}_{2}=\frac{1}{2} a(\hat{\boldsymbol{y}}+\hat{\boldsymbol{z}}) \\ \boldsymbol{a}_{3}=\frac{1}{2} a(\hat{z}+\hat{\boldsymbol{x}}) \end{array}\right.$ |
| Volume | $a^{3}$ | $\frac{1}{2} a^{3}$ | $\frac{1}{4} a^{3}$ |
| Number of nearest neighbors | 6 | 8 | 12 |
| nearest neighbor distance | $a$ | $\frac{\sqrt{3}}{2} a$ | $\frac{a}{\sqrt{2}}$ |
| Packing fraction* | $\frac{\pi}{6} \sim 0.524$ | $\frac{\sqrt{3} \pi}{8} \sim 0.680$ | $\frac{\sqrt{2} \pi}{6} \sim 0.740$ |

* 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 $\left(\boldsymbol{a}_{1}, \boldsymbol{a}_{2}, \boldsymbol{a}_{3}\right)$.
(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 $(h k l)$, is called the Miller index of the plane

(1) Intercepts are at $\left(1 a_{1}, 2 a_{2}, 3 a_{3}\right)$
(2) Reciprocals are $\left(\frac{1}{1}, \frac{1}{2}, \frac{1}{3}\right)$
(3) The index of the plane is (632)



## 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 $\lambda$ comparable to interatomic distance $(d \sim 1.5 \AA)$
- $\lambda \gg d$ : 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)


## Energy dispersion of X-ray, neutron, electron



## X-ray diffraction by crystals (2/2)

## - Bragg's law

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

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

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


XRD of Silicon powder


XRD principle

