EE20011 2025 Fall

Homework - Problem Set #1

Due: September 22nd, 11:59 pm

Please scan your homework and upload it on the KLMS website.

Problem 1 Terminologies (12 points)

Answer the following questions as concisely as possible.

(a) Give definitions of unit cell, primitive cell, Wigner Seitz cell. (3 points)

- A unit cell is the smallest repeating unit of a crystal lattice that, when translated in three dimensions, can generate the entire crystal.
- A primitive cell is a special type of unit cell that contains exactly one lattice point.
- A Wigner-Seitz cell is a specific type of primitive cell constructed by bisecting the lines connecting a central lattice point to all its nearest neighbors with perpendicular planes.

(b) How many lattice points are there in a simple cubic unit cell? in a bcc unit cell? in a fcc unit cell? How many Si atoms in a fcc unit cell? (3 points)

- Simple cubic (SC): 1 lattice point per unit cell. The eight corners each contribute 1/8 of a lattice point ($8 \times 1/8=1$).
- Body-centered cubic (BCC): 2 lattice points per unit cell. The eight corners contribute 1, and the center contributes 1 ($8 \times 1/8+1=2$).
- Face-centered cubic (FCC): 4 lattice points per unit cell. The eight corners contribute 1, and the six faces each contribute 1/2 ($8 \times 1/8+6 \times 1/2=4$).
- Si atoms in an FCC unit cell: 8 Si atoms per unit cell.

(c) How many nearest-neighbor atoms are there in silicon? (3 points)

- Silicon has a diamond cubic structure. Each atom in this structure is tetrahedrally bonded to four nearest neighbors.

(d) Which plane has the highest surface density in silicon? (3 points)

- (110) has the highest surface density.

Problem 2 Atomic distance and lattice constant (10 points)

In terms of the lattice constant *a*, what is the distance between nearest-neighbor atoms in:

(a) a bcc lattice? (5 points)

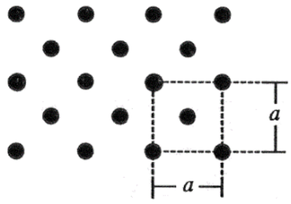
$$\frac{a\sqrt{3}}{2}$$

(b) a fcc lattice? (5 points)

$$\frac{a}{\sqrt{2}}$$

Problem 3 Surface density (15 points)

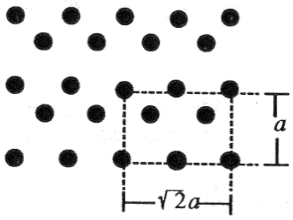
The figure shown below is the placement of Si atoms on the surface of the (100) Si wafer.



(a) Determine the number of atoms per cm^2 at the surface of the (100) wafer. (a = 5.43 x 10^{-8} cm) (5 points)

- area size : a^2
- atoms in area : 2
- the number of atoms per cm2 : 6.78 x 10^{14}(atoms/cm2)

The figure shown below is the placement of Si atoms on the surface of the (110) Si wafer.



(b) Determine the number of atoms per cm^2 at the surface of the (110) wafer. (5 points)

- area size : $\sqrt{2}a^2$
- atoms in area : 4
- the number of atoms per cm2 : 9.59x10^{14}(atoms/cm2)

(c) Determine the number of atoms per cm^2 at the surface of the (111) wafer. (5 points)

- area size : $\frac{\sqrt{3}}{2}a^2$
- atoms in area : 2
- the number of atoms per cm2 : 7.83x10^{14}(atoms/cm2)

Problem 4 Miller index (5 points)

When the fundamental translational vectors in a cubic crystal are **a**, **b**, and **c**, show the spacing between two adjacent (h,k,l) planes is d.

$$d = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}}$$

Plane equation : $\frac{x}{a/h} + \frac{y}{b/k} + \frac{z}{c/l} = 1$

Distance between two adjacent : $d = \frac{\left|\frac{h}{a}\times 0+\frac{k}{b}\times 0+\frac{l}{c}\times 0-1\right|}{\sqrt{(\frac{h}{a})^2+(\frac{k}{b})^2+(\frac{l}{c})^2}} = \frac{1}{\sqrt{(\frac{h}{a})^2+(\frac{k}{b})^2+(\frac{l}{c})^2}}$

Problem 5 Silicon structure (20 points)

Silicon has the diamond structure which you learn in chapter 1. The lattice constant of Si is 5.43Å and the atomic weight is 28.09. Calculate **(a)** distance of Si atoms, **(b)** density (g/cm^3) and **(c)** number density ($1/cm^3$) of Si. **(d)** the density of valance electrons in silicon.

(a) Nearest-neighbor distance for Si atoms

- Distance = $a\sqrt{3}/4 \approx 2.35$ Å

(b) Density

- $\rho = \frac{n \times M/N_A}{a^3} \approx 2.33\ g/cm^3$

(c) Number Density

- Number Density = $\frac{n}{a^3} = 8/(5.43\times10^{-8})^3 \approx 5.00\times10^{22}$ atoms/cm³

(d) Valence electron density

- Valence electron density = (Number Density) × (4 valence electrons per atom)
- 2.00×10^{23} atoms/cm³

Problem 6. Diamond structure (10 points)

The lattice constant of GaAs is a= 5.65Å. Calculate **(a)** the distance between the centers of the nearest Ga and As atoms, and **(b)** the distance between the centers of the nearest As atoms.

(a) Distance between the centers of the nearest Ga and As atoms

Distance = $a\sqrt{3}/4 \approx 2.45$ Å

(b) **Distance between the centers of the nearest As atoms.**

$a\sqrt{2}/2 \approx 3.99$ Å

Problem 7. Atomic packing factor (10 points)

(a) Find the atomic packing factor of a fcc lattice.

(b) Find the atomic packing factor of a bcc lattice.

(a) FCC lattice

- APF=$\frac{\frac{16\pi}{3}R^3}{a^3}=\frac{\pi}{3\sqrt{2}}\approx 0.74$

(b) BCC lattice

- APF=$\frac{\frac{8\pi}{3}R^3}{a^3}=\frac{\pi\sqrt{3}}{8}\approx 0.68$