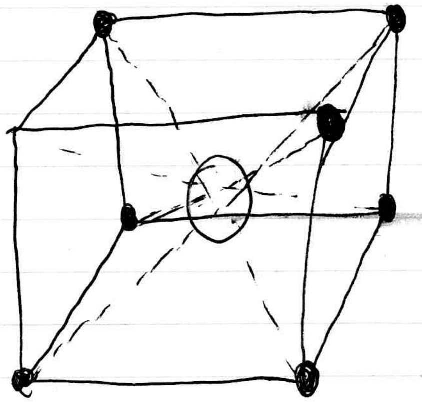
Example: Cesium Chloride crystal structure

(Q): The crystal structure of CsCl is shown below. The dark spheres represent atoms of Cl.



Identify the crystal system:

(A): Cubic

(Q): Identify the Bravais Lattice:

(A): Simple cubic

(Q): Identify the basis of the crystal structure:

(A): $Cs^+ Cl^-$ pair

Example: Palladium Structure

(Q): • Calculate the lattice constant a in Pd. Use only the information available in the class periodic table, and express your answer in angstroms.

• Calculate the distance between adjacent (110) planes in palladium (Pd). Hint: Use your work from the first part.

(A): • We see of the formula

$$a = \left(\frac{4 \cdot V_{molar}}{N_{Av}}\right)^{1/3} = \left(\frac{(4\,\text{atoms} \cdot (8.85\ cm^3/mol))}{6.022 \cdot 10^{23}\ \text{atoms}/mol}\right)^{1/3} \simeq 3.89 \cdot 10^{-8}\ cm \simeq 3.89\ \mathring{A}$$

• We found that $a = 3.89\ \mathring{A}$, then since

$$d = \frac{a}{\sqrt{h^2+k^2+L^2}}$$

$$d_{(110)} = \frac{3.89\ \mathring{A}}{\sqrt{2}} = 2.79\ \mathring{A}$$

Example: N-type ~~silicon~~ Silicon

(Q): • You wish to make n-type silicon. Select all suitable dopant atoms from the following list:

- X | P
- | B
- | Mg
- | Ga
- X | As
- | In
- X | Sb
- | Al
- | Tl
- | H

• Name the majority charge carrier in the doped material.

- | Holes
- X | Electrons
- | Electron-hole pairs
- | The dopant ion

• The conduction band is at a higher energy than the valence band.

- X | True
- | False

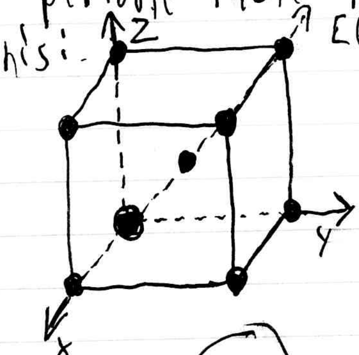
• No electronic states lie between the conduction and valence bands in n-type silicon.

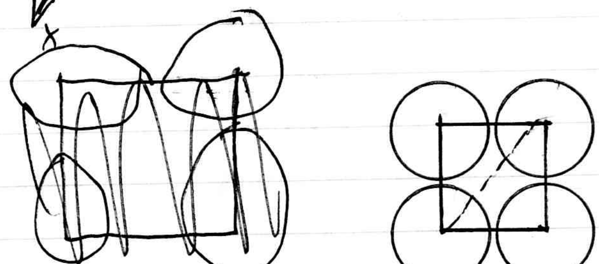
- | True
- X | False

Example: Molybdenum Density

(Q): Calculate the density of atoms along [011] in Mo. Use only the information provided in your class periodic table and express your answer in units of atoms/cm.

(A): We see by the periodic table that Palladium has a BCC structure; lets draw this:





We see by the figures that along the [011] vector, there ~~are~~ is 1 atom every $\sqrt{2}\,a$, thus

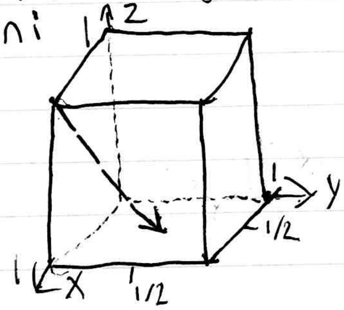
$$\frac{1\text{ atom}}{\sqrt{2}\,a} = \cancel{\frac{1}{\sqrt{2}}\left(\frac{2\cdot \text{molar volume}}{\text{avogadros number}}\right)^{1/3}}$$

$$= \cancel{\frac{1}{\sqrt{2}}\left(\frac{2\cdot 6.022\cdot 10^{23}}{\quad}\right)^{1/3}}$$

$$= \frac{1}{\sqrt{2}}\left(\frac{2\cdot \text{molar volume}}{\text{avogadros number}}\right)^{1/3} \approx 2.24\cdot 10^{7}$$

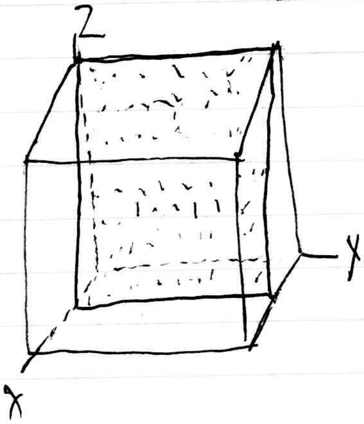
Example: Directions and planes

(Q): • Name the following ~~features~~ crystallographic features below using proper crystallographic notation:



(A): $[\bar{1}\,1\,\bar{2}]$

(Q):



(A): (2 0 1)

Example: Structure of CdO

(Q): CdO is cubic with a lattice constant $a = 4.695 \text{ Å}$ and a density $\rho = 8.15\ g/cm^3$. Determine the crystal structure of CdO.

(A): Recall the formula

$$\frac{x \text{ bases}}{a^3} = \frac{N_{Av}}{V_{molar}}$$

and

$$V_{molar} = \frac{m_a}{\rho}$$

Then,

$$x \text{ bases} = \frac{(4.695 \text{ Å})^3 \cdot (6.022 \cdot 10^{23}) \cdot (8.15\ g/cm^3)}{128.4\ g} = 3.96 \text{ bases}$$

Note that the Face Centered Cubic shape has 4 bases;

$$3.96 \approx 4,$$

thus the CdO has FCC structure

Example: Free carrier density in Ge

(Q): Chemical analysis of a germanium crystal reveals indium at a level of 0.000 3091 %. Assuming that the concentration of thermally excited charge carriers from the Ge matrix is negligible, what is the density of free charge carriers (carriers/cm³) in this Ge crystal?

(A): ~~Let the volume be $1\,cm^3$;~~ let $\phi = 0.000003091$; then ~~the mass of this crystal is~~

$$\phi \cdot 7.31\ g/cm^3 \cdot 1\ cm^3 = 2.26 \cdot 10^{-5}\ g \text{ indium}$$

$$2.26 \cdot 10^{-5}\ g \cdot \frac{1\ mole}{114.818\ g} = 1.968 \cdot 10^{-7}\ mole \cdot \frac{6.022 \cdot 10^{23}\ carriers}{mole}$$

$$= 1.185 \cdot 10^{17}\ carriers.$$

Since we assume a volume of $1\,cm^3$, then the carrier density is

$(1.185 \cdot 10^{17}\ carriers/cm^3)$

Example: Boron doping

(Q): Determine the amount (in grams) of boron that when substantially incorporated into 1 kg of silicon will establish a charge carrier density of $3.091 \cdot 10^{17}$ carriers/cm³.

(A): We see that 1 kg of silicon has volume 394.85 cm^3;
Then we want x grams B such that

$394.85 \text{ cm}^3 \cdot$

$$x \text{ grams } B \cdot \frac{1 \text{ mole}}{10.811 \text{ g}} \cdot \frac{6.022 \cdot 10^{23} \text{ atoms}}{1 \text{ mole}} \doteq 3.091 \cdot 10^{17} \text{ carriers/cm}^3$$

$$X = 0.00219 \text{ g}$$