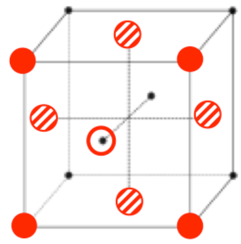
Question 1 Basic crystal properties

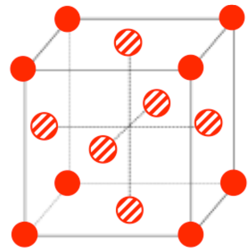
Face-centred cubic (fcc)

Nearest neighbour atoms:



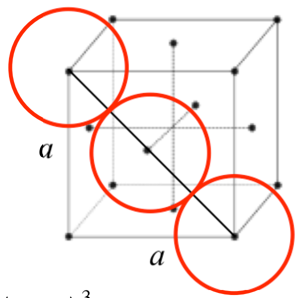
If you look at the circled atom, the nearest neigbours are on the same plane (filled circles, 4 atoms) as well as on the neighbouring planes (circles with oblique lines, 4 atoms on the plane behind and another 4 atoms on that behind (not shown), 8 atoms in total). As a result, the nearest neighbours are 12 atoms.

Atoms in a unit cell:



In a unit cell, filled atoms are shared with 8 neighbouring unit cells (1/8 × 8 = 1), and circles with oblique lines are shared with 2 neighbouring unit cells (1/2 × 6 = 3). As a sum, a unit cell contains 4 atoms.

Filling rate:

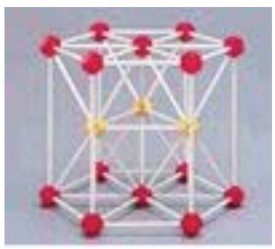


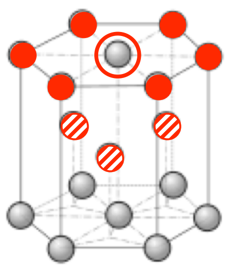
As shown in the right figure, 3 atoms are connected with each other along the diagonal axis in a unit cell plane, indicating that the radius of the atoms is $\sqrt{2}a/4$. Therefore, the filling rate is calculated to be

$$\frac{(\text{atoms in unit cell})\times(\text{atom sphere volume})}{(\text{unit cell volume})}=\frac{4\times\frac{4}{3}\pi r^3}{a^3}=\frac{4\times\frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3}=\frac{2\sqrt{2}}{12}\pi=74\%.$$

Hexagonal close-packed (hcp)

Nearest neighbour atoms:

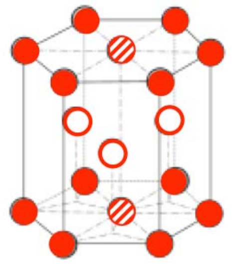




If you look at the circled atom, the nearest neigbours are on the same plane (filled circles, 6 atoms) as well as on the neighbouring planes (circles with oblique lines, 3 atoms on the plane below and another 3 atoms on that above (not shown), 6 atoms in total). As a result, the nearest neighbours are 12 atoms.

Atoms in a unit cell:

In a unit cell, filled atoms are shared with 6 neighbouring unit cells (1/6 × 12 = 2), circles with oblique lines are shared with 2 neighbouring unit cells (1/2 × 2 = 1), and open circles are not shared with the other unit cells (3 atoms). As a sum, a unit cell contains 6 atoms.



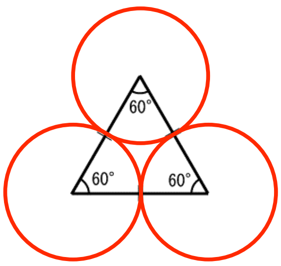
Filling rate:

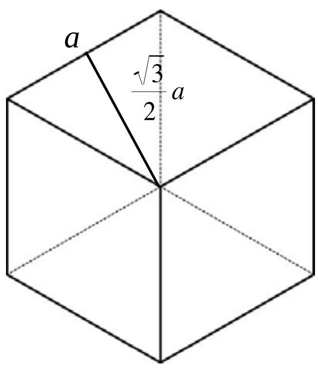
As shown in the bottom figure, 3 atoms are connected with each other in an equilateral triangle plane in the bottom unit cell plane, indicating that the radius of the atoms is *a*/2.

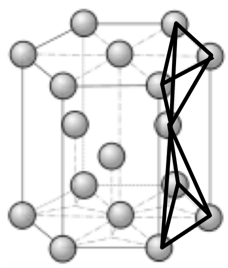
Here, the area of this equilateral triangle is $(1/2)\times\left(\sqrt{3}a/2\right)\times a$, resulting the surface area of the bottom unit cell plane to be $(1/2)\times\left(\sqrt{3}a/2\right)\times a\times 6$. Since the hcp unit cell contains a pair of regular tetrahedrons in the vertical direction, the unit cell height is calculated to be $\sqrt{a^2-(2/3)\times\left(\sqrt{3}a/2\right)}\times 2$ Therefore, the filling rate is calculated to be as follows:

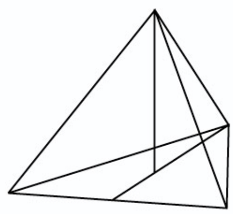
$$\frac{(\text{atoms in unit cell})\times(\text{atom sphere volume})}{(\text{unit cell volume})}=\frac{6\times\frac{4}{3}\pi r^3}{\left(\frac{1}{2}\times\frac{\sqrt{3}a}{2}\times a\right)\times 6\times\sqrt{a^2-\left(\frac{2}{3}\frac{\sqrt{3}a}{2}\right)^2}\times 2}$$

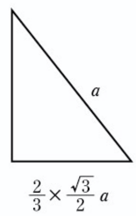
$$=\frac{\pi a^3}{3\sqrt{2}a^3}=\frac{1}{3\sqrt{2}}\pi=74\%.$$



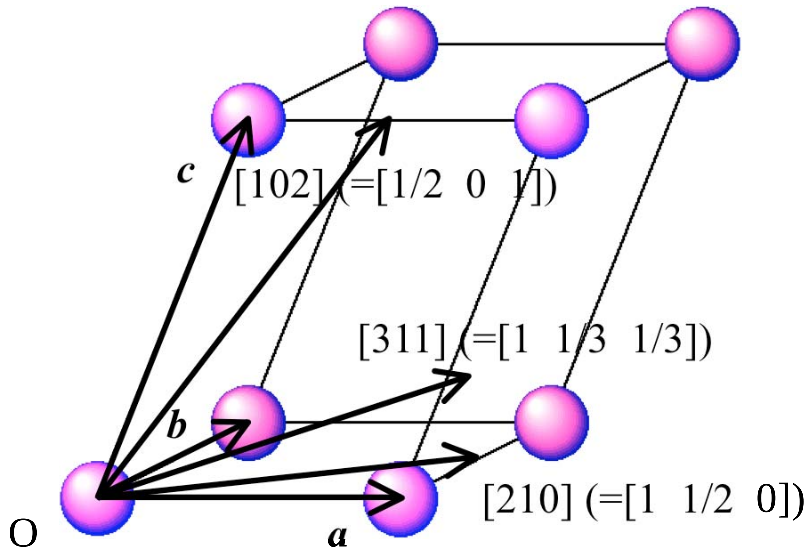


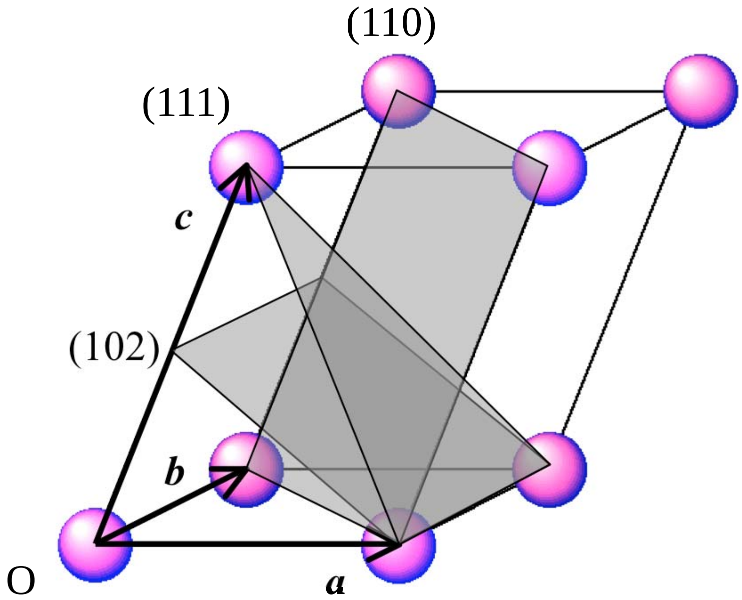






Question 2 Miller indices

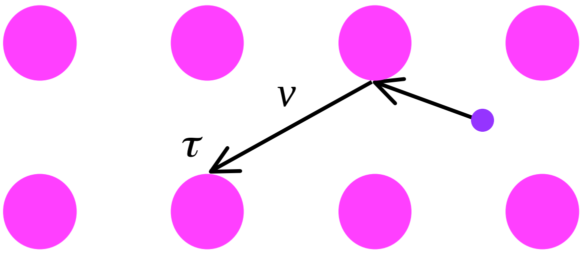




Question 3 Relaxation time

Equation of motion of an electron with resistive force mv/τ is

$$m\frac{dv}{dt} = -qE - \frac{m}{\tau}v$$



$$\frac{dv}{dt} + \frac{1}{\tau}v = -\frac{qE}{m}$$

Multiplying $e^{t/\tau}$ for both sides,

$$e^{t/\tau}\frac{dv}{dt} + \frac{1}{\tau}e^{t/\tau}v = -\frac{qE}{m}e^{t/\tau}$$

$$e^{t/\tau}\frac{dv}{dt} + \left(\frac{d}{dt}e^{t/\tau}\right)v = -\frac{qE}{m}e^{t/\tau}$$

By using integration by parts: $\frac{d}{dx}f(x)g(x) = \frac{df(x)}{dx}g(x) + f(x)\frac{dg(x)}{dx}$,

$$\frac{d}{dt}\left(e^{t/\tau}v\right) = -\frac{qE}{m}e^{t/\tau}$$

$$\therefore e^{t/\tau}v = -\int\frac{qE}{m}e^{t/\tau}dt + C$$

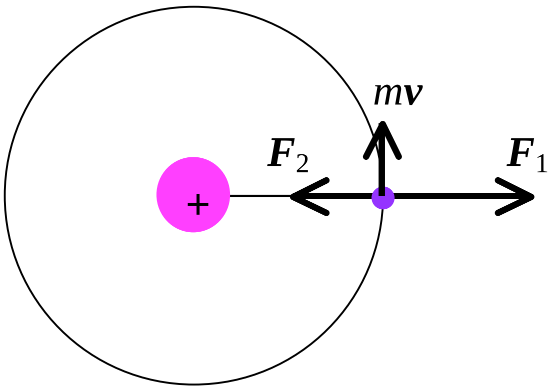
Therefore,

$$\begin{aligned} v &= -\frac{qE}{m}e^{-t/\tau}\left\{\int e^{t/\tau}dt + C'\right\} \\ &= -\frac{qE}{m}e^{-t/\tau}\left(\tau e^{t/\tau} + C'\right) \\ &= -\frac{q\tau E}{m}\left(1 - C''e^{-t/\tau}\right) \end{aligned}$$

For v=0 at t=0,

$$v = -\frac{q\tau E}{m}\left(1 - e^{-t/\tau}\right)$$

Question 4 Electron potential energy



Centrifugal force $\boldsymbol{F}_1$ is

$$\boldsymbol{F}_1 = \frac{mv^2}{r}$$

Coulomb force $\boldsymbol{F}_2$ is

$$\boldsymbol{F}_2 = -\frac{Zq^2}{4\pi\varepsilon_0 r^2}$$

For a stable electron rotation, $|\boldsymbol{F}_1|=|\boldsymbol{F}_2|$ and hence,

$$\frac{mv^2}{r} = \frac{Zq^2}{4\pi\varepsilon_0 r^2}$$

Accordingly, electron kinetic energy is obtained as

$$\frac{1}{2}mv^2 = \frac{1}{2}\frac{Zq^2}{4\pi\varepsilon_0 r}$$

Here, potential energy V is defined as $-\frac{dV}{dr} = F_2$, and therefore,

$$\begin{aligned} V &= \int_r^\infty \left(-\frac{dV}{dr}\right)dr = \int_r^\infty F_2 dr \\ &= \int_r^\infty \left(-\frac{Zq^2}{4\pi\varepsilon_0 r^2}\right)dr \\ &= \left[-\frac{Zq^2}{4\pi\varepsilon_0}\left(-\frac{1}{r}\right)\right]_r^\infty \\ &= 0 - \frac{Zq^2}{4\pi\varepsilon_0 r} \\ &= -\frac{Zq^2}{4\pi\varepsilon_0 r} \\ &\propto -\frac{A}{r} \end{aligned}$$

(A: constant)