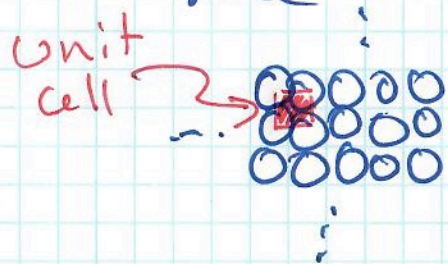


Solids (crystals)

We recognize that compounds such as LiF , NaCl , or Al_2O_3 (sapphire) exist only in the solid state. It makes no sense to speak of a "NaCl molecule".

Amorphous or glassy solids do not possess long-range order. However most solids are crystalline & have a unit cell



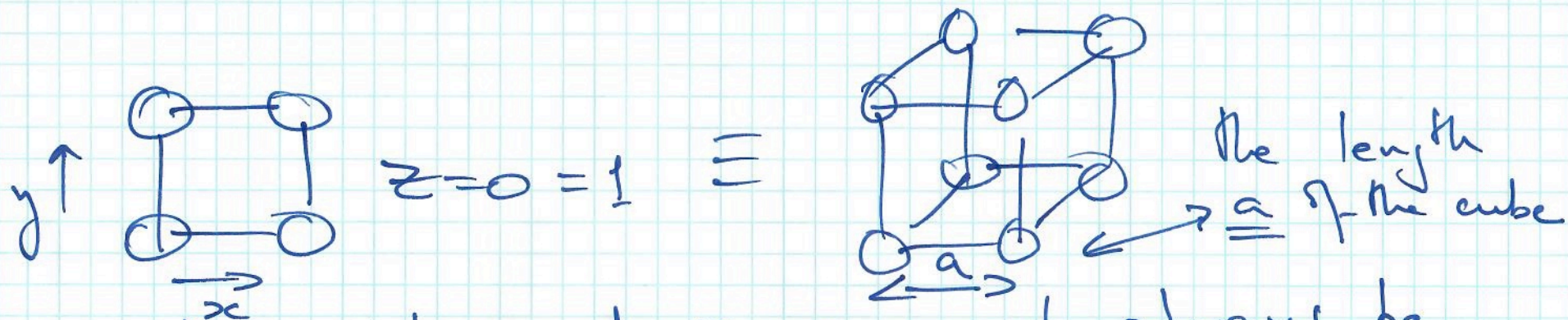
crystal

The whole crystal is created by stacking the unit cell in 3D

Some simple structures

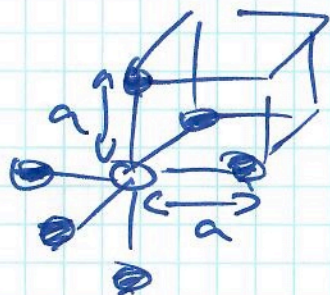
②

1. α -Po (polonium): The simple cubic (SC) crystal structure (we only consider cubes)



The section at $z=0$ must always be equal to the section at $z=1$

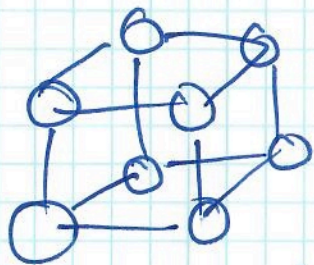
Questions: How many near neighbors



$\equiv 6$ at the distance a

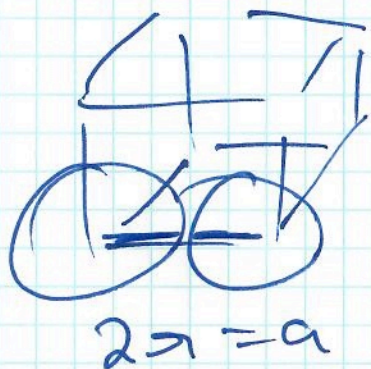
How many atoms in the cell?

Only 1



each shared between eight unit cells, so each corner atom is $\frac{1}{8} \Rightarrow 8 \times \frac{1}{8} = 1$ atom per cell

How is the radius r of the atom related to the length of the cell, a ?



The atoms touch along the length of the cell.

▣ Packing Efficiency :

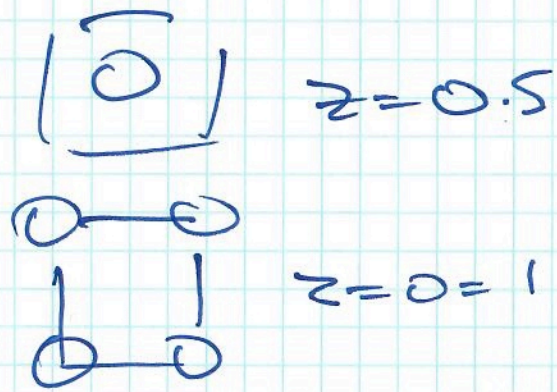
$$\frac{\text{Volume of atoms}}{\text{Volume of cell}}$$

(4)

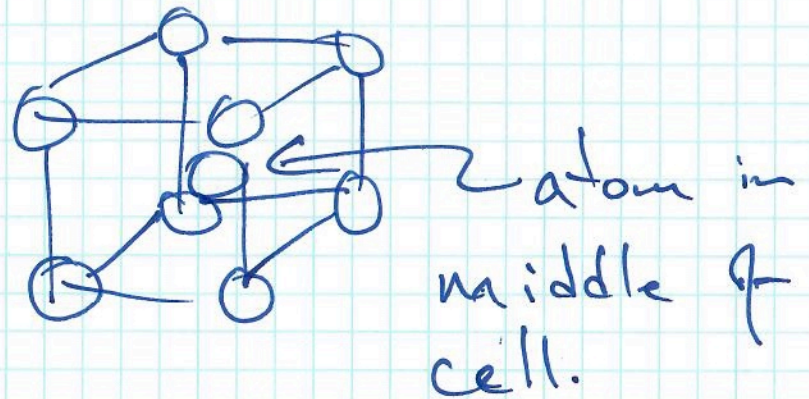
$$\begin{aligned} & \xrightarrow{1 \text{ atom per cell}} \frac{1 * \frac{4}{3} \pi r^3}{a^3} = \frac{\frac{4}{3} \pi r^3}{(2r)^3} = \frac{4 \pi r^3}{3 * 8 r^3} \\ & = \frac{\pi}{6} = 0.524 = 52.4\% \end{aligned}$$

2. α -Fe (Body-Centered Cubic)

(5)



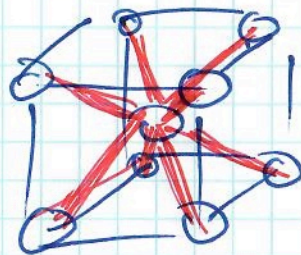
\equiv



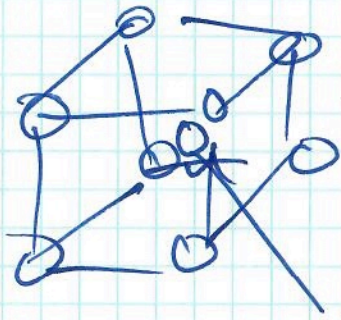
All atoms are identical. The one in the middle just has its origin shifted by $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

How many near neighbors?

8



How many atoms in the cell?

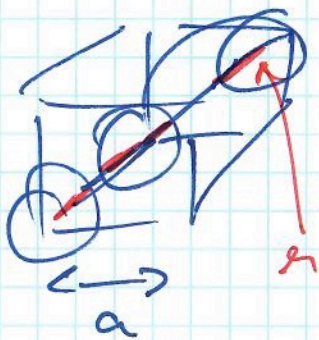


← corners $8 * \frac{1}{8} = 1$

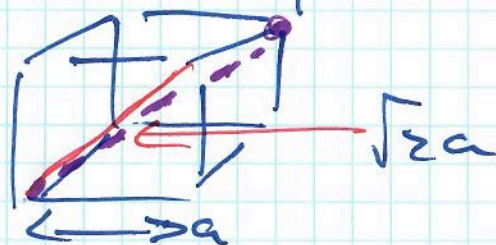
atom in center = $1 * 1 = 1$

total 2

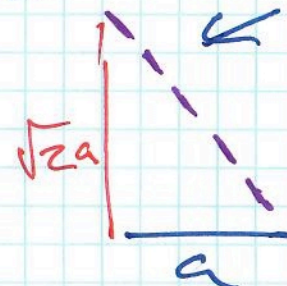
How is r related to a ?



The atoms touch along the body-diagonal that connect opposite corners of the cube



=

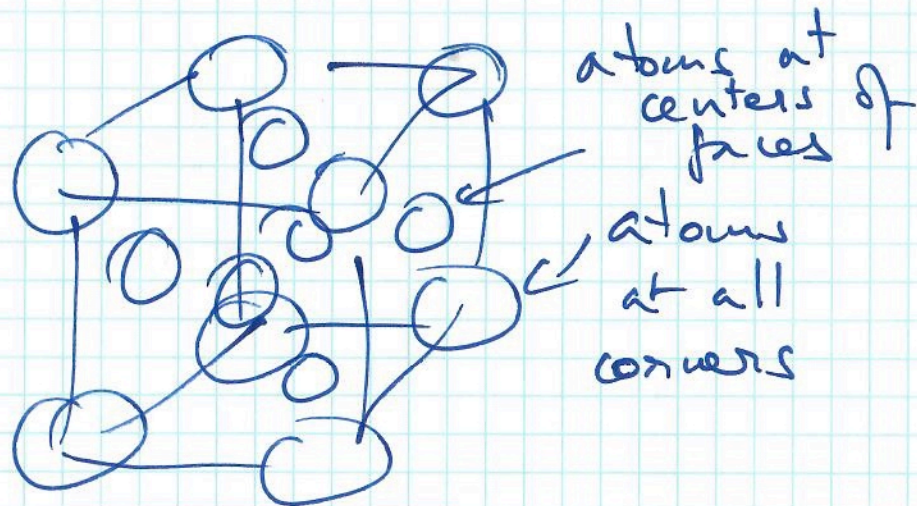
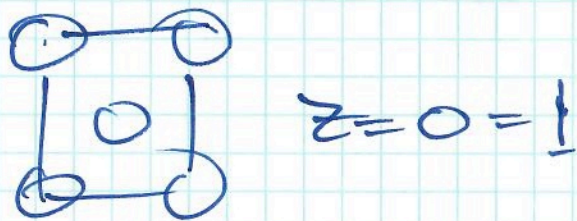


← body diagonal = $\sqrt{3} a$

$4r = \sqrt{3} a$

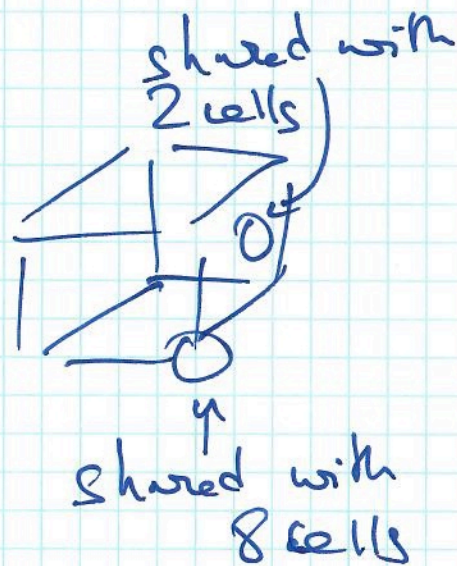
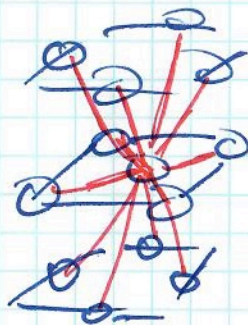
3. Au (Gold) Face-centered Cube

⑧



All atoms are actually the same!

⇒ Near-neighbors: 12

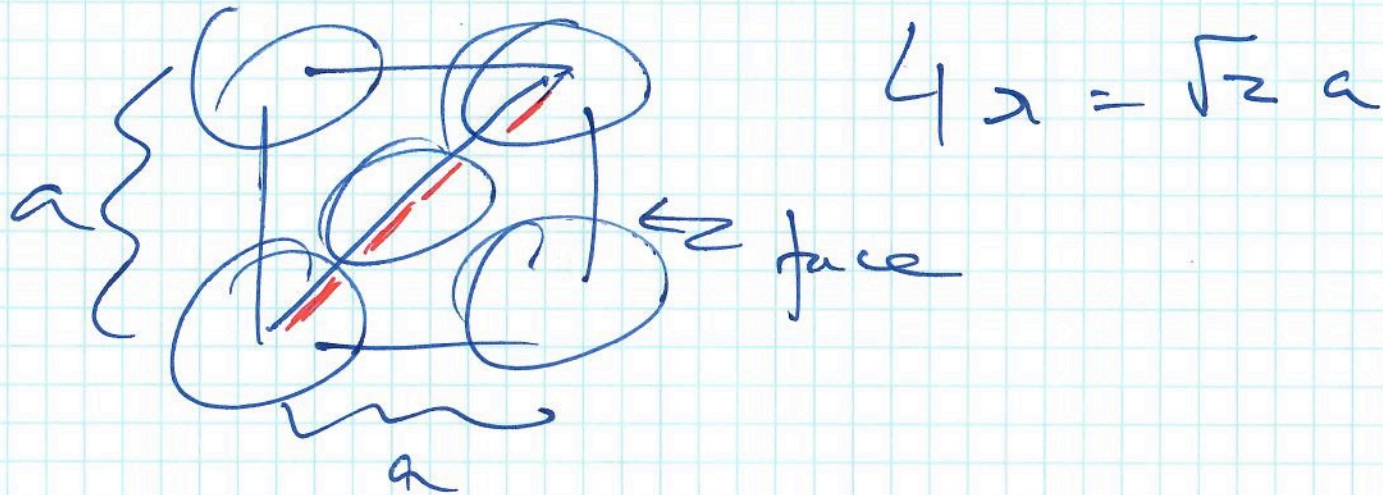


⇒ How many atoms?

$$8 * \frac{1}{8} (\text{corner}) + 6 * \frac{1}{2} (\text{face}) = \underline{\underline{4}}$$

⇒ How are r & a related?

9



⇒ Packing Efficiency

$$= \frac{4 * \frac{4}{3} \pi r^3}{\left(\frac{4}{\sqrt{2}}\right)^3 \frac{1}{3}} = \frac{\left(\frac{16}{3}\right) \pi}{\left(\frac{64}{2\sqrt{2}}\right) \pi} = 0.740 = 74\%$$

Density of Au

$$= \frac{\text{contents of unit cell}}{\text{Volume of unit cell}}$$

$$a = 4.067 \text{ \AA for Au}$$

$$= 4.067 \times 10^{-10} \text{ m} = 4.067 \times 10^{-8} \text{ cm}$$

$$\rho = \frac{4 \times 196.97}{6.0221 \times 10^{23}} \text{ g} / \underbrace{(4.067 \times 10^{-8})^3}_{a^3 = \text{volume}} \text{ cm}^3$$

mass of 4 atoms of gold

$$\rho = 19.45 \text{ g cm}^{-3}$$