Workshop Tutorials for Physics

Solutions to PR7: **Solids II – Crystals and Bonding**

A. Qualitative Questions:

1. The three types of strong bonds that form between atoms are ionic, covalent and metallic bonds.

a. Elements that form ionic bonds are those which will easily lose or gain an electron. These are those to the far left and right of the periodic table (but not the last column). Those to the left have only one or two electrons in their outer shells, which can easily be removed, and those to the far right have an almost full outer shell and will easily accept an extra electron. (The last column has a full outer shell and will not readily form bonds at all.)

b. In an ionic solid some atoms are negatively charged from gaining electrons while others are positively charged from donating electrons. Charges interact via an electric field, and the strength of interaction decreases with the square of the distance between them, hence all the atoms in an ionic solid interact with all the others (within a reasonable distance), giving long range Coulomb interactions. In a covalent solid the atoms share the electrons, so they are not charged, and there is no long range interaction.

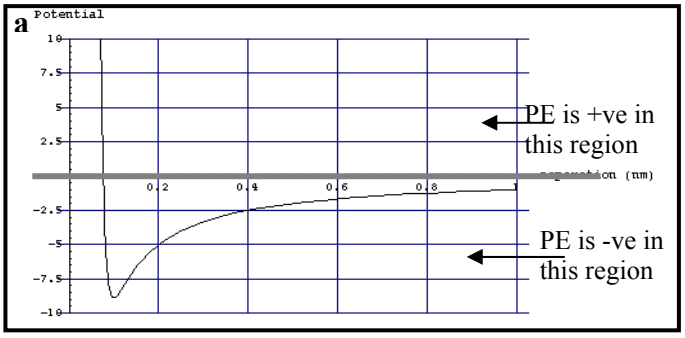
c. Metals from bonds by sharing many electrons with many atoms, hence the electrons are approximately free. The metallic bonds have neither charge nor direction restrictions, so the atoms can move relatively easily relative to each other, making metals very malleable. Ionic solids, such are salt, have charge restrictions on their bonds, so small movements tend to bring positive ions nearer to other positive ions, while moving them further away from negative ions, which can break down many bonds, making these solids brittle.

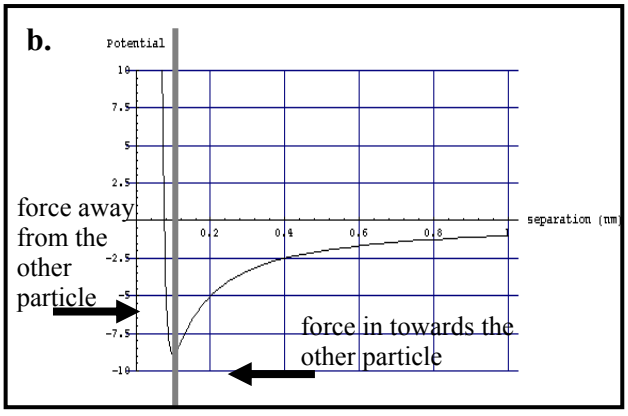
d. Metals like copper have free electrons, which can move in response to an electric field, making them good conductors. Ionic and covalent solids have electrons localized, and bound so that they are not free to move about, hence they are poor conductors.

2. In ionic solids there are charge and directional restrictions because the atoms are charged, like charges repel, so nearest neighbours have to be oppositely charged. In covalent solids there are directional restrictions because the electron clouds which form the bonds between atoms are charged and repel, so that the angle between bonds is maximized. These restrictions limit how the atoms can be arranged, and prevent the atoms from being packed very closely together. In metals there are no direction or charge restrictions on the bonds, so that the atoms can be packed very closely together, making metals very dense compared to ionic and covalent solids.

B. Activity Questions:

1. Lenard - Jones potential

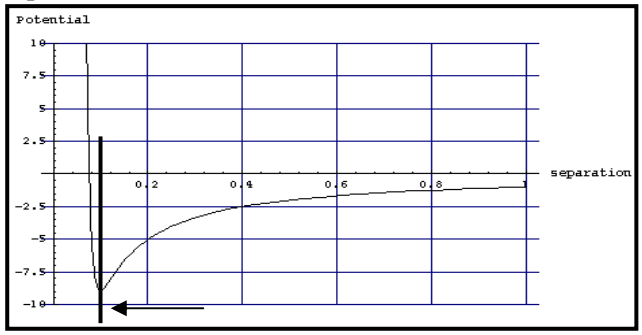




b. See diagram above right. The force is the negative of the gradient of the potential, $F = -dP/dr$, so where the slope is positive the force is negative, ie towards $r = 0$. If you look at the graph it's easy to tell which way the force is because the particle will move down hill on the potential plot, in the direction of the force.

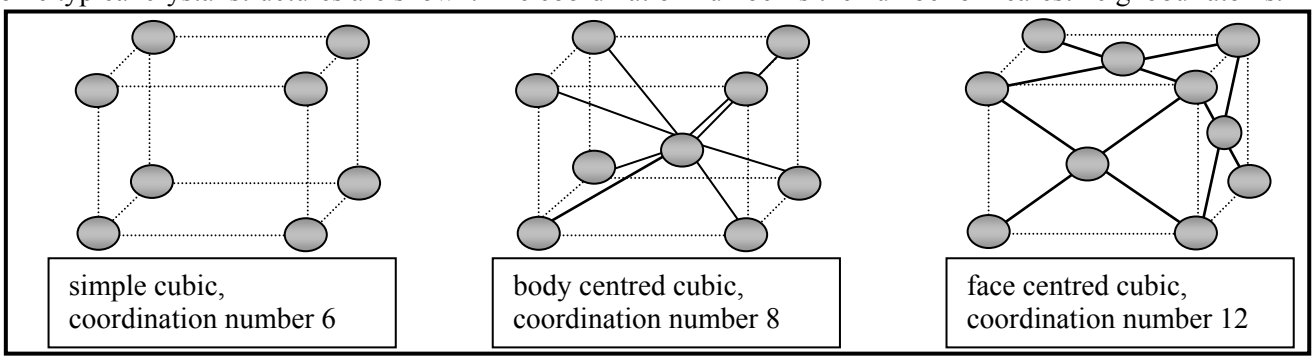
c. The equilibrium distance for this pair of atoms is where the potential energy is a minimum, ~0.1 nm. See diagram.

d. Binding energy is the difference in energy between being bound together and completely separated (infinitely far apart). It is the amount of energy you have to put into a system to unbind it. The maximum binding energy is at the point of minimum potential energy, where the equilibrium position is.



2. Crystal structures

Some typical crystal structures are shown. The coordination number is the number of nearest neighbour atoms.



3. Bend and Stretch

Chalk is held together by covalent bonds, so it is brittle. Chalk is strong to compression, but breaks easily when stretched, bent or twisted because the atoms cannot move easily relative to each other. Stretching, bending and twisting the chalk also opens up micro-cracks in the material, which compression tends to close.

The bonds in ionic solids have charge requirements, and those in covalent solids have directional requirements, making them both generally brittle.

The metal is much more plastic, it can be bent without breaking. This is because the metallic bonds have fewer restrictions than ionic or covalent bonds, they have neither charge nor direction requirements.

C. Quantitative Questions:

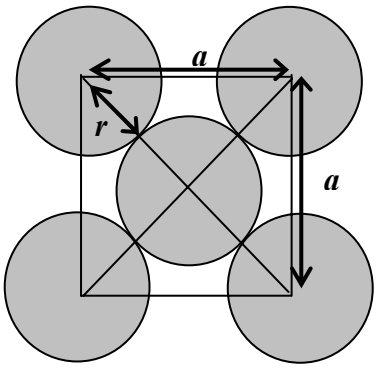
1. The potential energy function for two ions, one with a charge of $+e$ and the other with a charge of $-e$ is given by

$$V(r) = -\frac{Ae^2}{r} + \frac{B}{r^9} .$$

The equilibrium separation distance, r_o, is at the equilibrium position, ie where the force is zero on the ions. This happens when the potential energy is a minimum, as the force is the gradient of the potential energy. To find this point we take the derivative of the potential energy with respect to distance: $dV(r)/dr = \frac{d}{dr}\left(-\frac{Ae^2}{r} + \frac{B}{r^9}\right) = \frac{Ae^2}{r^2} - \frac{9B}{r^{10}}$. The minimum value of the potential energy, where the force is equal to zero, occurs when $dV/dr = 0$, ie when:

$\frac{Ae^2}{r^2} - \frac{9B}{r^{10}} = 0$ or $\frac{Ae^2}{r^2} = \frac{9B}{r^{10}}$ rearranging for r gives $r = r_o = \left(\frac{9B}{Ae^2}\right)^{\frac{1}{8}}$.

2. A single side of a face centred cubic crystal has atoms arranged as shown if we model the atoms as rigid spheres sitting up against their nearest neighbours. The diagonal distance across the square is 4 atomic radii, r, and the length of the unit cell is a.



The volume of the unit cell is $V_{cell} = a^3$.

Each unit cell encloses 4 complete atoms, hence the volume taken up by the spherical atoms is $V_{atoms} = 4 \times \frac{4}{3}\pi r^3$.

By trigonometry we can say that $a^2 + a^2 = r^2$. We can rearrange this for $r = a/2\sqrt{2}$ and write the volume taken up by the atoms as

$V_{atoms} = 4\times\frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3 = \frac{16}{3}\pi\frac{1}{16\sqrt{2}}a^3 = \frac{\pi}{3\sqrt{2}}a^3 = \frac{\pi}{3\sqrt{2}}V_{cell} = 0.74\ V_{cell}$.

Hence the packing fraction is 74%.