Workshop Tutorials for Introductory Physics

Solutions to PI5: **Solids II – Bonding and Crystals**

A. Review of Basic Ideas:

Bonding in solids

Bonds can be divided into two main types, primary or **strong** bonds and secondary or weak bonds. The strong bonds are what holds **solids** together, these are ionic bonds, covalent bonds and metallic bonds. The two types of weak bonds are **hydrogen** bonds and van der Waals bonds.

The three types of primary bonding reflect the ways in which atoms can group together by gaining or losing or sharing electrons.

Atoms near the left or right sides of the periodic table can lose or gain 1 (or 2) electrons to form charged ions. For example, a sodium atom can **lose** one electron and become a positively charged cation. A chlorine atom can **gain** one electron to become a negatively charged anion. These two ions then will be attracted to each other by non-directional **electrostatic** force and form an ionic bond. When large numbers of such ion pairs come together an ionic solid is formed, such as table **salt**, NaCl. In ionic solids there is a charge requirement for stacking atoms. Each ion must have nearest neighbours of **opposite** charge. There are no directional requirements, so stacking depends on meeting charge and size requirements and the bonding can be at any angle. However there are long range requirements because they attract or repel other ions beyond the nearest and next-nearest neighbours.

Atoms at the centre of the periodic table find it difficult to lose or gain electrons and end up sharing. These atoms form **covalent** bonds. When large numbers of such atom pairs come together, all sharing some of their electrons, a covalent solid is formed, for example **diamond**. In covalent bonding there are no charge requirements - each atom does not have to have nearest neighbours of opposite charge, and there are no long range requirements. The bonds act only between those nearest-neighbour atoms sharing electrons. However there are strong directional requirements which determine structural geometries.

Metals have atoms that release some electrons to be shared by all the atoms of the solid, often referred to as a bed of atoms with a "**sea** of electrons". Metallic bonding occurs between the positive atom cores and the "free" electrons. In metallic bonding there are no charge requirements, or directional requirements, but there are long range effects. This means that the atoms pack together as closely as possible.

B. 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.

2. The properties of a solid depend on the bonding between the atoms that make up the solid.

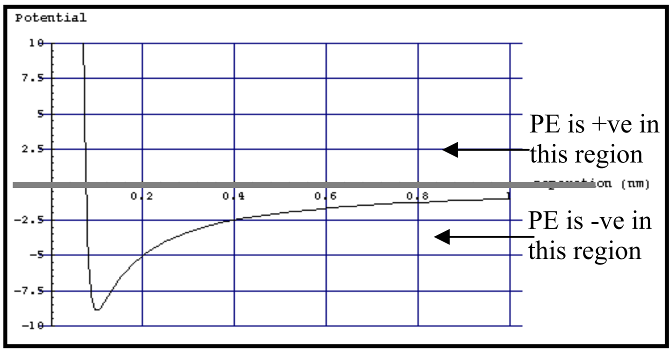
a. Metals form bonds by sharing many electrons with many atoms, hence the electrons are approximately free. The metallic bonds have neither charge nor direction restrictions, so the atoms can move easily relative to each other, making metals very malleable. Ionic solids, such as salt, have nearest neighbour and charge restrictions on their bonds, so small movements tend to break down many bonds, making these solids brittle.

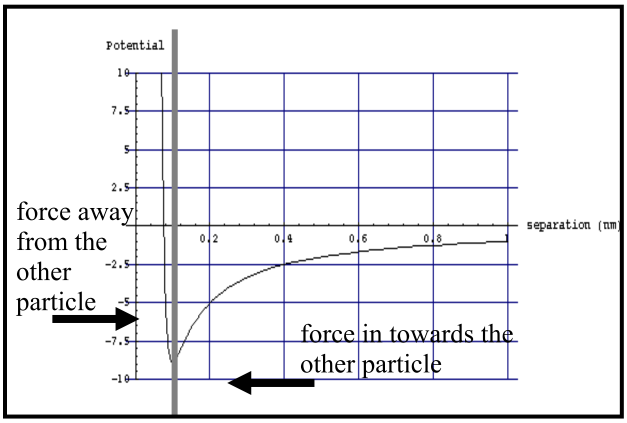
b. Metals like copper have free electrons, which can move in response to an electric field, making them good conductors. Ionic and covalent solids have electrons localised and bound so that they are not free to move about, hence they are poor conductors.

C. Activity Questions:

1. Lenard - Jones potential

a.

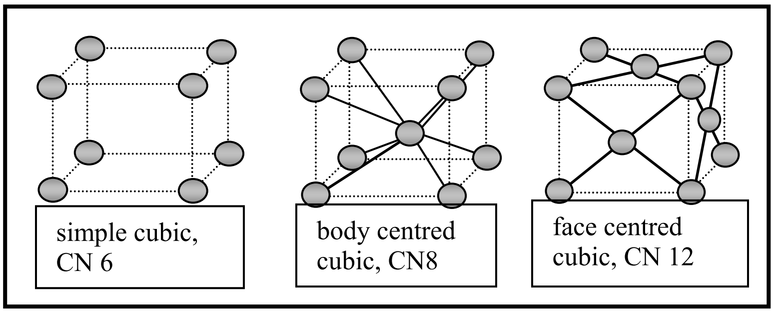




b. See diagram above right. The force is the negative of the gradient of the potential, $F = -dP/dr$, so where the slope is positive the force is negative, ie towards $r = 0$. If you look at the graph it's easy to tell which way the force is because the particle will move down hill on the potential plot,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

2. Crystal structures

Some typical cubic crystal structures are shown. The coordination number, CN, is the number of nearest neighbour atoms for each atom.



simple cubic, CN 6

body centred cubic, CN8

face centred cubic, CN 12

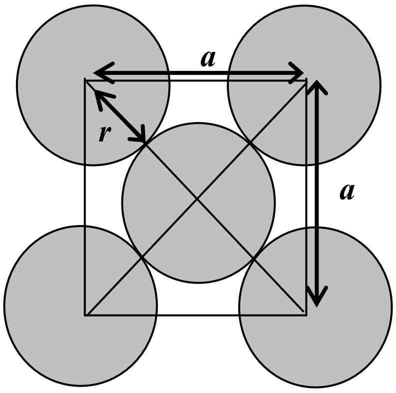
3. Bend and Stretch

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.

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.

D. Quantitative Question:



a. Write an expression for the atomic radius, r = ¼ the diagonal across the square. By trigonometry we can say that $a^2 + a^2 = r^2$. We can rearrange this for $r = a/2\sqrt{2}$.

b. Each unit cell encloses 4 complete atoms, ½ an atom from each face plus $\frac{1}{8}$ from each corner.

c. The volume of atoms contained in each unit cell is

$V_{\text{atoms}} = 4\times\frac{4}{3}\pi r^3$.

d. The volume of the unit cell is a^3.

e. To find the packing fraction we can write the atom volume using $r = a/2\sqrt{2}$ as

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

Hence the packing fraction is 74%.