Atomic Structure of Solids

2.1 Atomic Bonding

The structural elements of matter are the atoms, which consist of a nucleus and the atomic shell. The properties of solids are essentially determined by the electron shell structure. According to the Bohr model of an atom, the electrons occupy specific orbitals (Fig. 2.1) the configuration of which, i.e. number of electrons and their spatial arrangement, follows the laws of quantum mechanics. The most important electrons for the properties of a solid are the electrons in the outermost orbital, because they determine the interaction with other atoms. The dominant principle of atomic interaction is the tendency of an atom to have its outermost shell filled with eight electrons, i.e. the noble gas configuration. This simple principle is the foundation of chemical bonding. If an atom has already a complete outer shell with eight electrons, like the noble gases, then its tendency to interact with other atoms, i.e. for chemical bonding or even for solidification is very small. Helium has to be cooled to 0.1 K to make the interaction forces between the atoms sufficiently large compared to thermal vibrations to generate a solid. All elements which do not have a noble gas configuration have the tendency (since associated with an energy gain) to accept, to donate, or to share the outermost electrons, also referred to as valence electrons, when in contact with other atoms. From these principles we obtain the fundamental types of atomic bonding (Fig. 2.2):

i) Heteropolar or ionic bond (a): The number of valence electrons of the partners adds up to eight. The partner with smaller valency donates its valence electrons to the other partner with higher valence. Both elements attain a noble gas configurations, but the atoms lose their charge neutrality. For instance: \( \text{Na}^+\text{Cl}^- \); the sodium atom donates its only valence electron to the chlorine atom with seven valence electrons. It is also possible that more than two atoms are involved in the formation of a molecule, for instance \( \text{Ca}^{2+} (\text{F}^-)_2 \), where each of the three atoms attains the noble gas configuration.
Fig. 2.1. Diagrammatic illustration of the electronic configuration of the $^{12}\text{C}$ atom after Bohr's atomic model.

(a) heteropolar bond

(b) covalent bond

(α) $\bullet \longrightarrow \bullet$

(β) $\bullet \longrightarrow \bullet$

(γ) $\bullet \longrightarrow \bullet$

(d) van-der-Waals bond

(e) metallic bond

(c) metallic bond

Fig. 2.2. Basic types of chemical bond. When atoms of the same kind are bound covalently, specific arrangements occur.