

Chapter 2

Disorder and glass transition

2.1 Definition of disorder

Disorder is classified by compositional disorder and topological disorder. The former occurs when the constituent atoms A and B in crystalline binary alloys $A_{1-x}B_x$ are randomly substituted into lattice sites, so this is also called substitutional disorder, as shown in Figs. 2.1(a) and (b). The latter disorder is manifested in liquids, as shown in Fig. 2.2, where no translational order exists. The disorder seen in amorphous solids is also of this type.

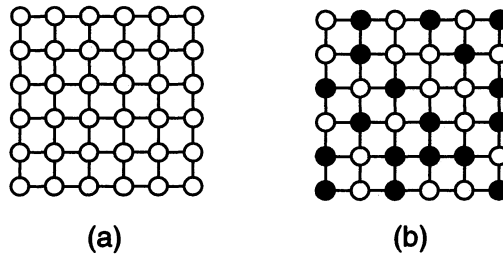


Figure 2.1. (a) A two dimensional crystalline binary array, (b) substitutionally disordered binary array $A_{1-x}B_x$.

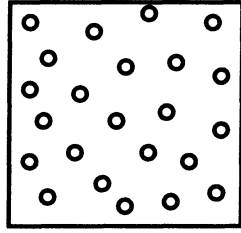


Figure 2.2. Schematic diagram of a model for liquid.

It is well known that there is a translational order in crystalline solids, i.e., a periodic structure. This feature makes the theory dealing with electronic properties of crystalline solids mathematically easy as first demonstrated by Bloch. The Bloch theory is the basis for understanding their electronic properties. On the other hand, the disordered solids provide difficult challenges to theoreticians. For disordered binary alloys, coherent potential approximation (CPA) (for review, see Yonezawa and Morigaki, 1973) has been used as a theoretical means for dealing with their electronic and vibrational properties. In this approximation, the potentials by surrounding atoms for a central atom are treated as an effective media, as shown in Fig. 2.3. A different approach, i.e., the so-called scaling theory (Abrahams, Anderson, Licciardello and Ramakrishnan, 1979) was applied to disordered systems, e.g., impurity systems in heavily doped semiconductors. This theory has successfully accounted for essential features of metal–nonmetal transition in disordered systems, as will be mentioned in Sec. 7.3.

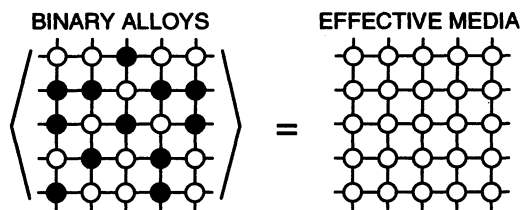


Figure 2.3. Schematic illustration of the effective media for a binary alloy $A_{1-x}B_x$.

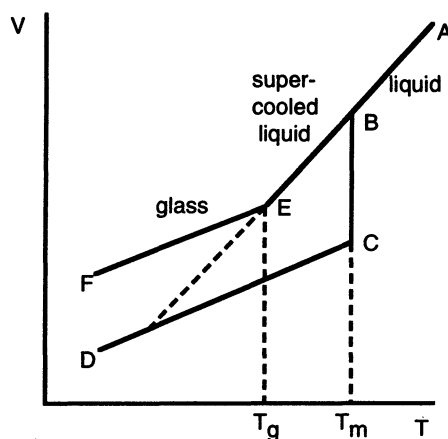


Figure 2.4. Schematic illustration of the volume versus temperature curve. T_g : glass transition temperature, T_m : melting temperature.

In the topological disorder seen in amorphous semiconductors, however, the short-range order is reserved in a similar way to their crystalline counterparts. As will be mentioned in Sec. 5.1, the chemical bonding theory constitutes a convenient approach to understand fundamental properties of amorphous semiconductors.

2.2 Glass transition

When the temperature decreases from their liquid phase, some materials do not crystallize below their melting temperature, but they become a supercooled liquid. As the temperature keeps decreasing, the so-called *glass transition* occurs at a certain temperature, T_g , below which they become glasses. These behaviours are explained by the volume versus temperature curve, as shown in Fig. 2.4. Glasses are typical examples of metastable and non-equilibrium states which are also classified as amorphous materials, as was mentioned in Chapter 1. Not all of amorphous materials, however, become glasses. Glasses exhibit the following feature as an example. Above T_g , viscosity η generally behaves like the following