

performance can be understood and optimized. Section 12.6 describes some of the issues involved in manufacturing modules. To conclude this chapter, Section 12.7 presents some of the directions that we consider important for future progress in the field.

There have been several excellent monographs and review chapters on amorphous silicon and amorphous silicon-based solar cells in recent years. In the body of the chapter, we direct the reader to these works where we feel that they may be useful for expanded or complementary discussion.

12.2 ATOMIC AND ELECTRONIC STRUCTURE OF HYDROGENATED AMORPHOUS SILICON

12.2.1 Atomic Structure

Silicon atoms in amorphous silicon largely retain the same basic structure as that of crystal silicon: each silicon atom is connected by covalent bonds to four other silicon atoms arranged as a tetrahedron. This understanding emerges from measurements of the scattering (“diffraction”) of X rays by the two materials [23] as well as from theoretical and computational studies of the two materials.

If you build a noncrystalline silicon structure with wooden sticks (to represent covalent bonds) and wooden balls drilled with four small holes for the sticks (to represent the silicon atoms), you will have some trouble in making a noncrystalline structure. To avoid a crystalline structure, you will need to bend the sticks. Quite soon, you will have to give up on the fourth stick on some atom, and you will have created an imperfect noncrystalline structure with a “dangling bond.” Your problem is related to tetrahedral bonding: there are too many constraints on the positions of atoms to keep *all* bond lengths and angles reasonably close to the values demanded by silicon’s chemistry in any noncrystalline structure. The same conclusion is reached by mathematical and computational methods [24, 25]. Alloys such as As_2Se_3 , which easily form noncrystalline glasses by cooling from a liquid, have an average number of bonds per atom of about 2.7 or less.

For hydrogenated amorphous silicon (a-Si:H), silicon–hydrogen bonds resolve this structural problem. Several percent of the silicon atoms make covalent bonds with only three silicon neighbors; the fourth valence electron of the silicon bonds to a hydrogen atom. This crucial hydrogen is essentially invisible to X rays, but is quite evident in nondestructive measurements (proton magnetic resonance [26] and infrared spectroscopy [27]) as well as destructive testing (secondary ion mass spectroscopy [28] and hydrogen evolution during annealing [29]).

There are quite a few distinct atomic configurations for the hydrogen in a-Si:H. The two principal “phases” of hydrogen evidenced by proton magnetic resonance are termed the *dilute* and *clustered* phases [26]. In the dilute phase a particular hydrogen atom is about 1 nm away from any other hydrogen atom; in the clustered phase there are two or more hydrogen atoms in close proximity. A computer calculation of a particular instance of this structure [30] is presented in Figure 12.7(a). The densities of hydrogen in each of the individual phases, as well as the total density of hydrogen, depend upon the conditions under which the material is made.