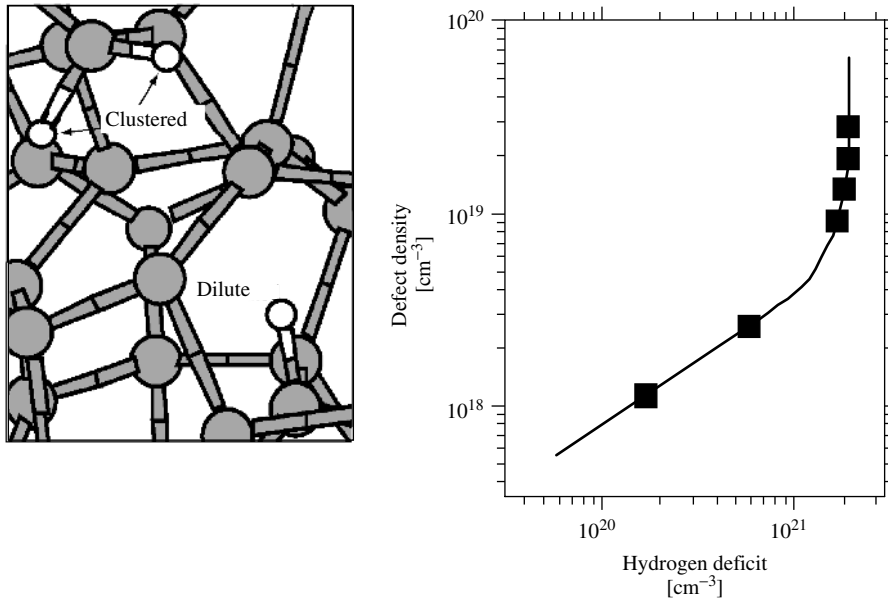

Figure 12.7 (a) Computer model of the chemical bonding of hydrogenated amorphous silicon. The larger, gray spheres indicate Si atoms; the smaller, white spheres indicate hydrogen atoms, which are found in clustered and relatively isolated, dilute-phase configurations as indicated. (b) Correlation of the defect (dangling bond) density in a-Si:H with the density of hydrogen removed from the material by heating (the hydrogen deficit). The data points are derived from deuterium and defect profiles by Jackson *et al.* [31] (350°C deuteration). The curve is a fit to a model proposed by Zafar and Schiff [32]

12.2.2 Defects and Metastability

While the underlying structure illustrated in Figure 12.7 is noncrystalline, it is a chemically ideal structure: each atom forms the normal number of chemical bonds (four for silicon, one for hydrogen). This noncrystalline atomic structure largely determines the overall electronic and optical properties of the material, as we will discuss shortly. However, many electronic properties in a-Si:H are also strongly affected by the gross defects of chemical bonding. The atomic structure of the bonding defects in a-Si:H has been extensively studied using electron spin resonance. A single type of defect, the *D*-center, dominates most measurements in undoped a-Si:H [23]. The *D*-center is generally identified as a silicon dangling bond [33].

A dangling bond may be envisioned using Figure 12.7: just imagine that the hydrogen atom is removed from the dilute-phase site in the lower right-hand corner of the figure, leaving behind a single unbonded electron (the "dangling bond"). This simple picture is consistent with the following observation: the density of dangling bonds increases when hydrogen is removed from a-Si:H by heating. We present a comparison of a model for this relationship together with measurements illustrating the effect in Figure 12.7(b) [31, 32]. Note that the density of dangling bonds is generally much lower than the density of