

the best a-Si:H materials, it is about  $22 \times 10^{-3}$  eV, but increases markedly for amorphous silicon-germanium alloys [42].

Given the presence of exponential bandtails, the very existence of bandedge energy can reasonably be questioned. Remarkably, detailed analysis of drift-mobility measurements supports the concept of a well-defined bandedge [40, 43]. Most workers consider the bandedge to be the energy that separates electron orbitals that are localized (i.e. have well-defined locations in space) from orbitals that are delocalized. The bandedges are correspondingly termed the conduction and valence band *mobility edges* [44].

Unfortunately, for noncrystalline semiconductors there is no single, conclusively established procedure for locating the bandedges within the density-of-states. The band gap is thus difficult to determine without some ambiguity. Since amorphous silicon-based materials with varying band gaps are used in solar cells, it is nonetheless very important to establish conventional procedures for comparing band gaps. By far the most common approach is to analyze measurements of the optical absorption coefficient  $\alpha(h\nu)$  similar to those in Figure 12.2; one typical analysis yields an “optical” or “Tauc” band gap  $E_T$  [45]

$$\alpha(h\nu) = (A/h\nu)(h\nu - E_T)^2 \quad (12.1)$$

The proportionality constant  $A$  incorporates several effects and is not usually studied separately.

The band gap obtained using this procedure is typically about 1.75 eV in a-Si:H, but varies substantially with deposition conditions and alloying with germanium or carbon. A simpler procedure than that of Tauc is to define the band gap to be the photon energy corresponding to a particular optical absorption coefficient  $\alpha$ ; using  $\alpha = 3 \times 10^3/\text{cm}$  yields values (denoted as  $E_{3,5}$ ) similar to the Tauc procedure. Finally, there is undoubtedly a difference between these optical estimates of the band gap and the true, “electrical” band gap  $E_G = E_C - E_V$ . Internal photoemission measurements [46] indicate that the electrical band gap is 50 to 100 meV larger than the Tauc band gap.

### 12.2.5 Defects and Gap States

Between the bandtails lie defect levels; in undoped a-Si:H, these levels appear to be due entirely to the dangling bonds (“ $D$ -centers”) measured by electron spin resonance. For example, infrared absorption at photon energies around 1.2 eV is sensitive to the optical processes that detach an electron from a defect and promote it to the conduction band or that transfer an electron from the valence band to a defect. This infrared signal is visible in Figure 12.2; for samples of varying electronic properties, the infrared absorption coefficient is proportional to the  $D$ -center density over a range of at least a factor of 100 in the density [47].

The next issue to be resolved is the positions of the corresponding levels, as illustrated in Figure 12.9. The  $D$ -center is “amphoteric:” there are three charge states (with  $+e$ ,  $0$ , and  $-e$  charges), leading to two levels (transitions between the  $0/+$  and  $-/0$  charge states). A *rough* guide to level positions estimated under near-dark conditions is the following. The  $(-/0)$  level is about 0.6 eV below  $E_C$  in low defect-density, undoped