13.2.2 Optical Properties

The absorption coefficient α for $CuInSe_2$ is very high, larger than 10^5/cm for 1.4 eV and higher photon energies [40]. In many studies it was found that the fundamental absorption edge is well described by [30]

$$\alpha = A(E - E_g)^2/E \tag{13.1}$$

as for a typical direct band gap semiconductor. The proportionality constant A depends on the density of states associated with the photon absorption. From this relation, a band gap value of $E_g = 1.02 \pm 0.02$ eV is obtained. The temperature dependence follows

$$E_g(T) = E_g(0) - aT^2/(b + T) \tag{13.2}$$

where a and b are constants that vary between different measurements. In general, dE_g/dT is about -2×10^{-4} eV/K [41].

A rather complete picture of the optical properties of $CuInSe_2$ and other Cu-ternary chalcopyrites is given in Reference [42]. Ellipsometric measurements of carefully prepared single-crystal samples were carried out and the dielectric functions were obtained together with the complex refractive index for different polarizations. From these measurements a band gap value for $CuInSe_2$ of 1.04 eV was determined.

A similar study was also made on bulk polycrystalline ingots of Cu(InGa)Se_2 having different compositions from $x \equiv Ga/(Ga + In) = 0$ to 1 [43]. Curves describing the complex refractive index, $n + ik$, for samples with $x = 0$ and 0.2 are reproduced in Figure 13.6. The complex refractive index can be used to calculate other optical parameters like the absorption coefficient

$$\alpha = 4\pi k/\lambda \tag{13.3}$$

In the same work the fundamental transitions for the different compositions were fit to an equation describing the band gap for $CuIn_{1-x}Ga_xSe_2$ as

$$E_g = 1.010 + 0.626x - 0.167x(1 - x) \tag{13.4}$$

In this equation the so-called bowing coefficient is 0.167. A value of 0.21 was obtained by theoretical calculations as compared to values in the range of 0.11 to 0.26 determined in various experiments [44].

13.2.3 Electrical Properties

$CuInSe_2$ with an excess of Cu is always p-type but In-rich films can be made p-type or n-type [45]. By annealing in a selenium overpressure, n-type material can be converted to p-type, and conversely, by annealing in a low selenium pressure, p-type material becomes n-type [46]. It is believed that this affects the concentration of Se vacancies, V_{Se}, which act as compensating donors in p-type films. Device-quality Cu(InGa)Se_2 films, grown with the excess Se available, are p-type with a carrier concentration of about $10^{16}/cm^3$.