

lattice, and casting the crystal structure in terms of a cubic unit cell makes identifying the orientation easier using Miller indices.

3.2.2 Energy Band Structure

Of more consequence to the physics of solar cells, however, is how the periodic crystalline structure of the semiconductor establishes its electronic properties. An electron moving in a semiconductor material is analogous to a particle confined to a three-dimensional box that has a complex interior structure due primarily to the potential fields surrounding the component atom's nucleus and tightly bound core electrons. The dynamic behavior of the electron can be established from the electron wave function, ψ , which is obtained by solving the time-independent Schrödinger equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}[E - U(\vec{r})]\psi = 0 \quad (3.4)$$

where m is electron mass, \hbar is the reduced Planck constant, E is the energy of the electron, and $U(\vec{r})$ is the periodic potential energy inside the semiconductor. Solving this quantum-mechanical equation is beyond the scope of this work, but suffice it to say that the solution defines the band structure (the allowed electron energies and the relationship between the electron's energy and momentum) of the semiconductor and, amazingly, tells us that the quantum mechanically computed motion of the electron in the crystal is, to a good approximation, like that of an electron in free space if its mass, m , is replaced by an effective mass, m^* , in Newton's law of motion from classical mechanics

$$F = m^*a \quad (3.5)$$

where F is the applied force and a is the acceleration of the electron. A simplified energy band structure is illustrated in Figure 3.3. The allowed electron energies are plotted against the crystal momentum, $p = \hbar k$, where k is the wave vector (represented here as a scalar for simplicity) corresponding to the wave function solutions of the Schrödinger equation. Only the energy bands of immediate interest are shown – energy bands below the valence band are presumed to be fully occupied by electrons and those above the conduction band are presumed to be empty. The electron effective mass is thus defined as

$$m^* \equiv \left[\frac{d^2E}{dp^2} \right]^{-1} = \left[\frac{1}{\hbar^2} \frac{d^2E}{dk^2} \right]^{-1} \quad (3.6)$$

Notice that the effective mass is not constant within each band. In addition, near the top of the valence band, the effective mass is actually negative. Electrons (*) fill the states from bottom to top and the states near the top of the valence band are empty (o) due to some electrons being thermally excited into the conduction band. These empty states can conveniently be regarded as positively charged carriers of current called *holes* with a positive effective mass. It is conceptually much easier to deal with a relatively few number of holes that have a positive effective mass since they will behave like classical positively charged particles. The top of the valence band and the bottom of the conduction band are approximately parabolic in shape and therefore the electron effective mass (m_n^*)