2.3.7. Detailed description of the effective mass

2.3.7.1. Introduction

The effective mass of a semiconductor is obtained by fitting the actual *E-k* diagram around the conduction band minimum or the valence band maximum by a paraboloid. While this concept is simple enough, the issue turns out to be substantially more complex due to the multitude and the occasional anisotropy of the minima and maxima. In this section we first describe the different relevant band minima and maxima, present the numeric values for germanium, silicon and gallium arsenide and introduce the effective mass for density of states calculations and the effective mass for conductivity calculations.

Most semiconductors can be described as having one band minimum at k = 0 as well as several equivalent anisotropic band minima at $k \neq 0$. In addition there are three band maxima of interest close to the valence band edge.

2.3.7.2.Band structure of silicon

As an example we consider the band structure of silicon as shown in the figure below:

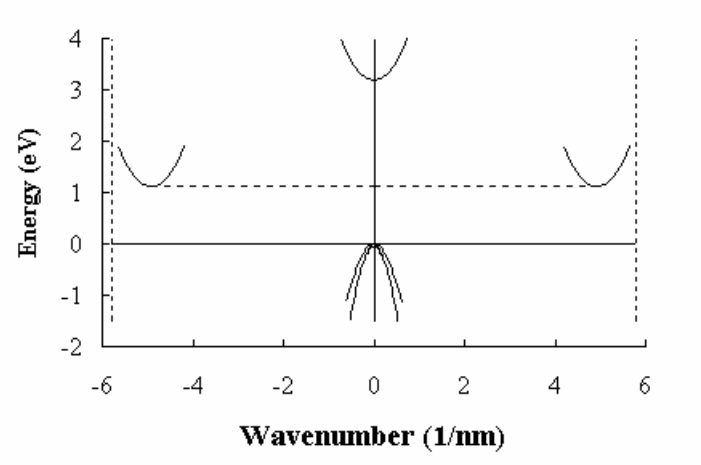

Figure 2.3.12 *E-k* diagram of silicon including the primary band minima and maxima.

Shown is the *E-k* diagram within the first brillouin zone and along the (100) direction. The energy is chosen to be to zero at the edge of the valence band. The lowest band minimum at k = 0 and still above the valence band edge occurs at $E_{c,direct}$ = 3.2 eV. This is not the lowest minimum above the valence band edge since there are also 6 equivalent minima at k = (x,0,0), (-x,0,0), (0,x,0), (0,-x,0), (0,0,x), and (0,0,-x) with x = 5 nm-1. The minimum energy of all these minima equals 1.12 eV = $E_{c,indirect}$. The effective mass of these anisotropic minima is characterized by a longitudinal mass along the corresponding equivalent (100) direction and two

transverse masses in the plane perpendicular to the longitudinal direction. In silicon the longitudinal electron mass is $m_{e,l}^* = 0.98\ m_0$ and the transverse electron masses are $m_{e,t}^* = 0.19\ m_0$, where $m_0 = 9.11 \times 10^{-31}$ kg is the free electron rest mass.

Two of the three band maxima occur at 0 eV. These bands are referred to as the light and heavy hole bands with a light hole mass of $m_{l,h}^* = 0.16\ m_0$ and a heavy hole mass of $m_{hh}^* = 0.46\ m_0$. In addition there is a split-off hole band with its maximum at $E_{v,so} = -0.044$ eV and a split-off hole mass of $m_{h,so}^* = 0.29\ m_0$.

2.3.7.3. Effective mass and energy band minima and maxima of Ge, Si and GaAs

The values of the energy band minima and maxima as well as the effective masses for germanium, silicon and gallium arsenide are listed in the Table 2.3.3:

	Symbol	**Germanium**	**Silicon**	**Gallium Arsenide**
Band minimum at $k = 0$				
Minimum energy	$E_{g,direct}$ (eV)	0.8	3.2	1.424
Effective mass	m_e^*/m_0	0.041	0.2	0.067
Band minimum *not* at $k = 0$				
Minimum energy	$E_{g,indirect}$ (eV)	0.66	1.12	1.734
Longitudinal effective mass	$m_{e,l}^*/m_0$	1.64	0.98	1.98
Transverse effective mass	$m_{e,t}^*/m_0$	0.082	0.19	0.37
Longitudinal direction		(111)	(100)	(111)
Heavy hole valence band maximum at $E = k = 0$				
Effective mass	m_{hh}^*/m_0	0.28	0.49	0.45
Light hole valence band maximum at $k = 0$				
Effective mass	m_{lh}^*/m_0	0.044	0.16	0.082
Split-off hole valence band maximum at $k = 0$				
Split-off band valence band energy	$E_{v,so}$ (eV)	-0.028	-0.044	-0.34
Effective mass	$m_{h,so}^*/m_0$	0.084	0.29	0.154

Table 2.3.3 Properties of band minima and maxima in germanium, silicon and gallium arsenide.

2.3.7.4.Effective mass for density of states calculations

The effective mass for density of states calculations equals the mass which provides the density of states using the expression for one isotropic maximum or minimum or:

$$g_c(E) = \frac{8\pi\sqrt{2}}{h^3} m_e^{3/2} \sqrt{E - E_c} \quad \text{for} \quad E \geq E_c \tag{2.3.12}$$

for the density of states in the conduction band and:

$$g_v(E) = \frac{8\pi\sqrt{2}}{h^3} m_h^{3/2} \sqrt{E_v - E} \quad \text{for} \quad E \leq E_v \tag{2.3.13}$$

for the density of states in the valence band.

for instance for a single band minimum described by a longitudinal mass and two transverse masses the effective mass for density of states calculations is the geometric mean of the three masses. Including the fact that there are several equivalent minima at the same energy one obtains the effective mass for density of states calculations from:

$$m_{e,dos}^* = M_c^{3/2} \sqrt[3]{m_l m_t m_t} \tag{2.3.14}$$

where *Mc* is the number of equivalent band minima. For silicon one obtains:

$$m_{e,dos}^* = M_c^{3/2} \sqrt[3]{m_l m_t m_t} = 6^{3/2} \sqrt[3]{0.89 \times 0.19 \times 0.19} m_0 = 1.08 m_0 \tag{2.3.15}$$

2.3.7.5. Effective mass for conductivity calculations

The effective mass for conductivity calculation is the mass, which is used in conduction related calculations accounting for the detailed structure of the semiconductor. These calculations include mobility and diffusion constant calculations. Another example is the calculation of the shallow impurity levels using a hydrogen-like model.

As the conductivity of a material is inversionally proportional to the effective masses, one finds that the conductivity due to multiple band maxima or minima is proportional to the sum of the inverse of the individual masses, multiplied by the density of carriers in each band, as each maximum or minimum adds to the overall conductivity. For anisotropic minima containing one longitudinal and two transverse effective masses one has to sum over the effective masses in the different minima along the equivalent directions. The resulting effective mass for bands, which have ellipsoidal constant energy surfaces, is given by:

$$m_{e,cond}^* = \frac{3}{\frac{1}{m_l} + \frac{1}{m_t} + \frac{1}{m_t}} \tag{2.3.16}$$

provided the material has an isotropic conductivity as is the case for cubic materials. For instance electrons in the X minima of silicon have an effective conductivity mass given by:

$$m^*_{e,cond} = \frac{3}{\frac{1}{m_l}+\frac{1}{m_t}+\frac{1}{m_t}} = \frac{3}{\frac{1}{0.89}+\frac{1}{0.19}+\frac{1}{0.19}} = 0.26m_0 \qquad (2.3.17)$$

2.3.7.6.Effective mass and energy bandgap of Ge, Si and GaAs

The resulting values are listed in Table 2.3.4. These values correspond very well to those commonly used as listed in Table 2.3.2. The two notable exceptions are the effective masses for holes in silicon. The value on the left is the calculated value, while the value on the right is the generally accepted value in the literature. This is due to the specific shape of the constant energy surfaces. They are not ellipsoids, so that they cannot be properly described with a constant effective mass.

	Symbol	**Germanium**	**Silicon**	**Gallium Arsenide**
Smallest energy bandgap at 300 K	E_g (eV)	0.66	1.12	1.424
Effective mass for density of states calculations				
Electrons	$m_{e^*,dos}/m_0$	0.56	1.08	0.067
Holes	$m_{h^*,dos}/m_0$	0.29	0.57/0.81[1]	0.47
Effective mass for conductivity calculations				
Electrons	$m_{e^*,cond}/m_0$	0.12	0.26	0.067
Holes	$m_{h^*,cond}/m_0$	0.21	0.36/0.386[1]	0.34
Free electron mass	m_0 (kg)	9.11×10^{-31}		

Table 2.3.4 Effective masses for both density of states and conductivity calculations.

[1] Due to the fact that the heavy hole band does not have a spherical symmetry there is a discrepancy between the actual effective mass for density of states and conductivity calculations (number on the right) and the calculated value (number on the left) which is based on spherical constant-energy surfaces. The actual constant-energy surfaces in the heavy hole band are "warped", resembling a cube with rounded corners and dented-in faces.