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ELECTRON DRIFT MOBILITY OF DEGENERATE SEMICONDUCTORS DUE TO IONIZED IMPURITY SCATTERING – PHASE I

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14. ABSTRACT
Study of the electron drift mobility of degenerate semiconductors due to ionized impurity scattering and the electron drift mobility of degenerately doped zinc oxide (ZnO).

15. SUBJECT TERMS
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1. Objective

The objectives for Phase I was to derive analytical expressions for the electron mobility of degenerate semiconductors dominated by ionized impurities, including non-parabolic conduction bands, wave function admixture, Rode-Cetnar screening, impurity compensation, and multiply ionized impurities. Also to compare calculated numerical results to results for classical parabolic bands and Thomas-Fermi screening.

2. Motivation

Classical theoretical treatments of the electron mobility of degenerate semiconductors based on parabolic conduction bands and Thomas-Fermi screening are significantly in error, by about fifty to one-hundred percent, in comparison to experiments.[1] In order to explain experimental results with accuracy within a few percent, it is necessary to incorporate non-parabolicity of the conduction band into the theory. However, when the conduction band is non-parabolic, the electron wave functions are necessarily a mixture of s and p wave functions. Since the s and p wave functions are orthogonal, the electron scattering is weakened, as shown below.

The usual method of treating the screening of ionized impurities is by use of the Thomas-Fermi equation. However, this equation applies only to parabolic conduction bands, which is not accurate for degenerate semiconductors. In recent work, non-parabolic bands have been accounted for by the Rode-Cetnar treatment of screening and this work is incorporated herein.[2]

Since electron mobility at low temperatures is determined predominantly by ionized- impurity scattering when the semiconductor is heavily (i.e. degenerately) doped, it is necessary to treat only ionized-impurity scattering. Thus, other types of electron scattering may be ignored, including lattice vibrations such as piezoelectric and acoustic phonons, and optical and inter-valley phonons, as well as surface scattering, grain boundaries, and scattering by other types of defects.

3. Analysis

In general, whether or not degeneracy prevails, electron drift mobility μ_d is given by the perturbation function g of the electron probability distribution under the influence of a weak electric field of strength F. In the following, the electron wave-vector is k and the equilibrium (Fermi-Dirac) probability distribution function is f. In the present work, g is determined entirely by electron scattering due to ionized impurities and, hence, electron mobility is denoted by μ_{ii} to signify the ionized-impurity mechanism. From Rode, including non-parabolic conduction band, the electron drift mobility is given by[1]

$$\mu_d = \frac{\hbar}{3m} \cdot \frac{\int k^3 (g/Fd)\, dk}{\int k^2 f\, dk} \tag{1}$$

The free-electron mass is m, d accounts for changes in effective mass due to non-parabolicity, and the reduced Planck constant is $\hbar$. When only ionized-impurity scattering is considered, the perturbation g is given by

$$g = -(eF/\hbar\nu_{ii}) \cdot \partial f/\partial k \tag{2}$$

The magnitude of the electron charge is e and the electron scattering rate due to ionized impurities is ν_{ii}. The electron drift mobility due to ionized-impurity scattering is thus given as

$$\mu_{ii} = -\frac{e}{3m} \cdot \frac{\int (k^3/\nu_{ii} d)(\partial f/\partial k)\, dk}{\int k^2 f\, dk} \tag{3}$$

The electron scattering rate due to ionized-impurities is[1]

$$\nu_{ii} = \frac{e^4 N m d}{8\pi\varepsilon_s^2 \hbar^3 k^3} \cdot [D \cdot \ln(1 + 4k^2/\beta^2) - B] \tag{4}$$

where

$$D = 1 + (2\beta^2 c^2/k^2) + (3\beta^4 c^4/4k^4) \tag{5}$$

and

$$B = [4k^2/\beta^2 + 8(1 + 2k^2/\beta^2)c^2 + 6(1 + \beta^2/2k^2 - 4k^2/3\beta^2)c^4]/(1 + 4k^2/\beta^2) \tag{6}$$

Wave function admixture and conduction band non-parabolicity are accounted for by the c and d quantities, where c is the fraction of p compared to s wave functions.[1]

$$c^2 = 1/2 - 1/2\sqrt{1 + 2\hbar^2 k^2 (m/m^* - 1)/mE_g} \tag{7}$$

$$1/d = 1 + (m/m^* - 1)/\sqrt{1 + 2\hbar^2 k^2 (m/m^* - 1)/mE_g} \tag{8}$$

The concentration of ionized scattering centers (impurities) is N and $1/\beta$ is the exponential screening length of the Coulomb potential surrounding the scattering centers. The effective mass m^* is given by the band curvature at the bottom of the conduction band. The effective mass energy gap is E_g.

Combining the above equations, the electron mobility due to ionized-impurities is

$$\mu_{ii} = -\frac{8\pi\varepsilon_s^2\hbar^3}{3e^3 N m^2} \cdot \frac{\int (k^6/d^2)\cdot(\partial f/\partial k)/[D\ln(1+4k^2/\beta^2) - B]dk}{\int k^2 f\, dk} \tag{9}$$

In general, the Fermi-Dirac probability distribution function f is a function of electron energy E and Fermi Level E_F.

$$f = \frac{1}{1 + e^{(E-E_F)/\kappa T}} \tag{10}$$

$$\frac{\partial f}{\partial k} = \frac{\partial f}{\partial E}\cdot\frac{\partial E}{\partial k} = -\frac{e^{(E-E_F)/\kappa T}/\kappa T}{(1+e^{(E-E_F)/\kappa T})^2}\cdot\frac{\hbar^2 k}{md} \tag{11}$$

or

$$\frac{\partial f}{\partial k} = -\frac{\hbar^2 k}{md\kappa T}\cdot f(1-f) \tag{12}$$

Thus, eqs. (9) and (12) give

$$\mu_{ii} = \frac{8\pi\varepsilon_s^2\hbar^5}{3e^3 m^3 N\kappa T} \cdot \frac{\int (k^7/d^3) f(1-f)/[D\cdot\ln(1+4k^2/\beta^2) - B]dk}{\int k^2 f\, dk} \tag{13}$$

For the degenerate case where the Fermi Level E_F greatly exceeds the thermal energy κT, the product *f(1-f)* approaches the behavior of a Dirac Delta Function centered about the momentum at the Fermi Level k_F, and eq. (13) can be written as

$$\mu_{ii} = \frac{8\pi\varepsilon_s^2\hbar^5 k_F^5}{3e^3 m^3 N\kappa T} \cdot \frac{1/d_F^3}{D_F \cdot \ln(1+4k_F^2/\beta_F^2) - B_F} \cdot \frac{\int k^2 f(1-f)\,dk}{\int k^2 f\,dk} \tag{14}$$

The quantities d, D, and B, when evaluated at k_F, are termed d_F, D_F, and B_F. Likewise, the reciprocal of the screening length β_F is β evaluated at k_F. From the Appendix, β_F can be expressed in terms of the Fermi Level.

$$\beta_F^2 = \frac{e^2(2m)^{3/2}}{2\pi^2\varepsilon_s\hbar^3} \cdot \left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F+E_g)}\right]^{1/2} \times \left[1 - \frac{(m/m^* - 1)E_g/2}{\sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F+E_g)}}\right] \tag{15}$$

The Fermi Level is given in the Appendix in terms of the free-electron concentration.

$$E_F = \frac{(3\pi^2 n)^{2/3}\hbar^2}{2m} - \frac{E_g}{2}\left[1 - \sqrt{1 + 2\hbar^2(3\pi^2 n)^{2/3}(m/m^* - 1)/mE_g}\right] \tag{16}$$

In general, the free-electron concentration is

$$n = \int (k^2/\pi^2) f\,dk \tag{17}$$

For degenerate conditions, n is denoted by n_F.

$$n_F = k_F^3/3\pi^2 \tag{18}$$

Therefore, given $n = n_F$, one can calculate E_F and k_F from eqs. (16) and (18); β_F can be calculated from eq. (15); c_F, d_F, D_F and B_F can be calculated from eqs. (5) to (8); and mobility can be calculated as follows. Using the expression in the Appendix for the inverse screening length squared β_F^2 in the degenerate limit,

$$\mu_{ii} = \frac{8\pi\varepsilon_s^2\hbar^5 k_F^5}{3e^5 m^3 d_F^3 n_F N\kappa T} \cdot \frac{\varepsilon_s \kappa T \beta_F^2}{D_F \cdot \ln(1+4k_F^2/\beta_F^2) - B_F} \tag{19}$$

Finally, we have

$$\mu_{ii} = \frac{8\pi\varepsilon_s^3\hbar^5 k_F^5 \beta_F^2}{3e^5 m^3 d_F^3 n_F N[D_F \cdot \ln(1+4k_F^2/\beta_F^2) - B_F]}$$
$$\mu_{ii} = \frac{8\pi^3\varepsilon_s^3\hbar^5 k_F^2 \beta_F^2}{e^5 m^3 d_F^3 N[D_F \cdot \ln(1+4k_F^2/\beta_F^2) - B_F]} \quad (20)$$

As expected, mobility is independent of temperature under degenerate conditions.

Therefore, given the static dielectric constant, the effective mass, the energy gap, and the free-electron and impurity concentrations, the mobility due to ionized impurities can be calculated analytically from eq. (20). The concentration of ionized scattering centers N may comprise *a)* singly ionized donors, *b)* singly ionized acceptors, and *c)* doubly ionized acceptors with respective concentrations N_d, N_a, and N_{aa}. The scattering strength of an impurity is proportional to the square of its charge so, according to Look and Leedy,[3]

$$N = N_d + N_a + 4N_{aa} \quad (21)$$

Results for ZnO are shown in next section.

4. Results

Let K = 8.12, Eg = 3.43 eV, nF = N, and m*/m = 0.34 appropriate to uncompensated ZnO and calculate the electron mobility from eq. (20). See Figure 1.

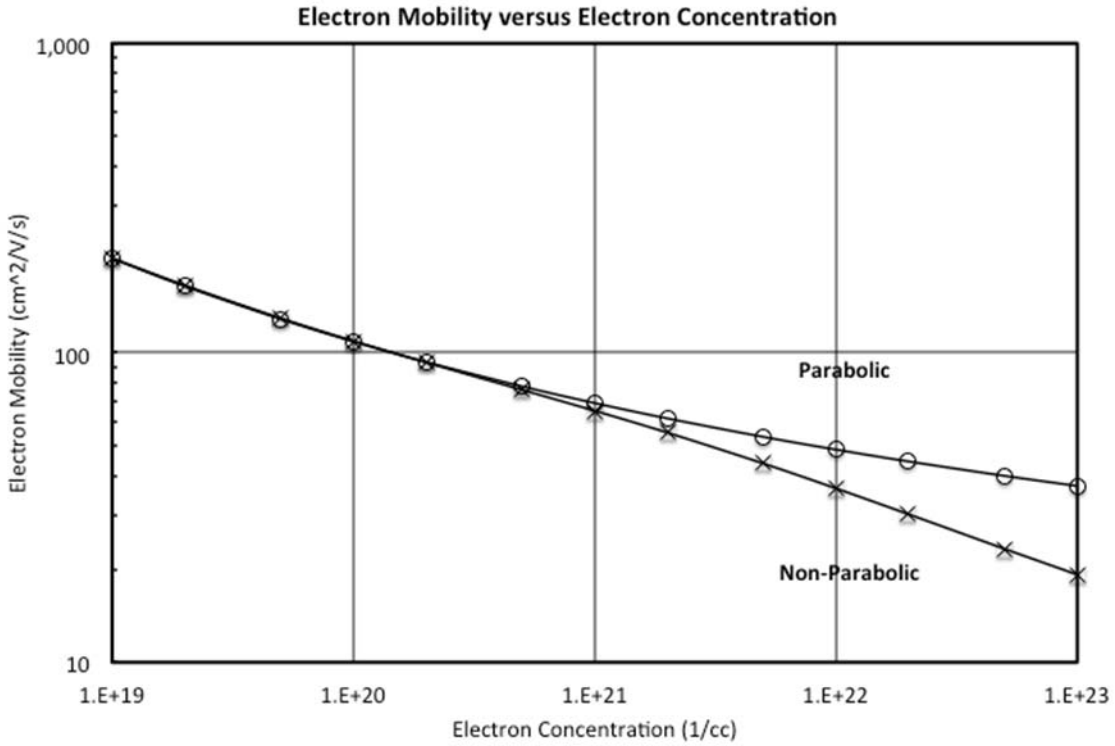

Figure 1: Electron Mobility versus Carrier Concentration is shown for Conditions of High Degeneracy

The mobility decreases slowly with increasing carrier concentration.

The difference between results for parabolic and non-parabolic conduction bands becomes quite large for the higher electron concentrations: 33 percent at 10^{22}/cc and 93 percent at 10^{23}/cc. Part of the difference is due to wave function admixture, given by the quantity c^2 in eq. (7). Figure 2 shows c^2 versus carrier concentration. Above 10^{21}/cc, the proportion of p wave functions becomes significant.

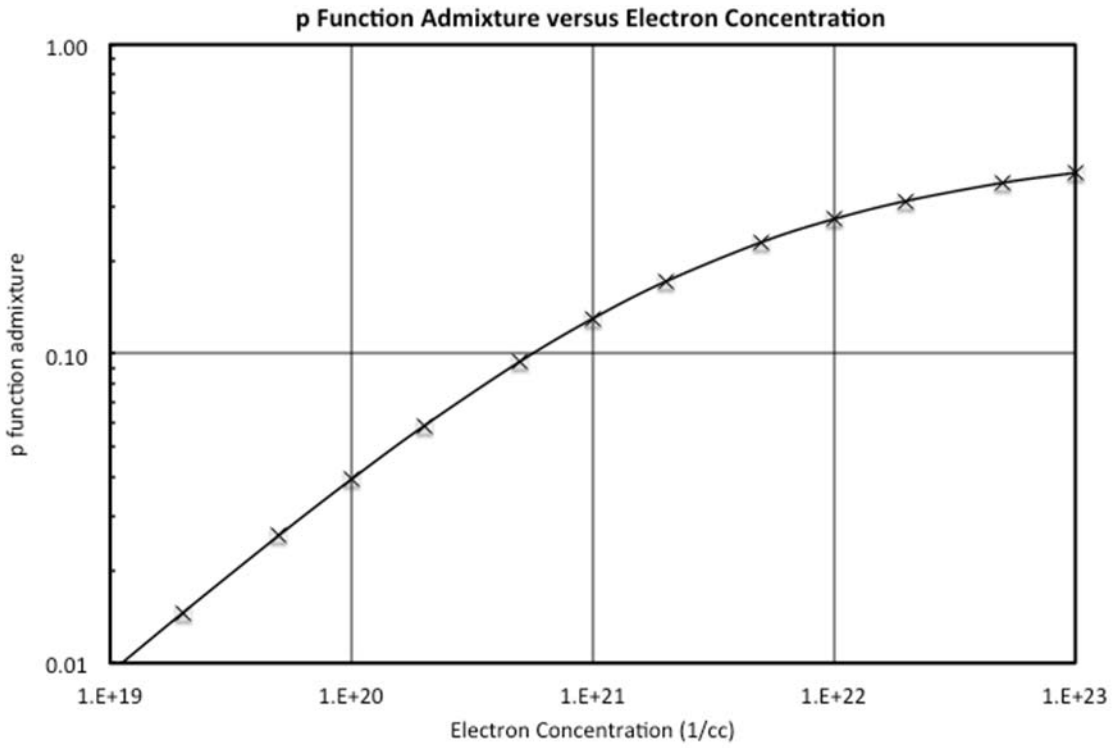

Figure 2: Admixture of p Wave Function versus Carrier Concentration
The ratio of p to s functions becomes significant above 10^{21}/cc carrier concentration.

The importance of accounting for non-parabolic conduction bands is given by *d* in eq. (8). For the case of a parabolic band, *d* is equal to the relative effective mass, but *d* increases significantly for non-parabolic bands at large carrier concentrations as shown in Figure 3. For small electron concentrations where non-parabolicity is unimportant, d is equal to the relative effective mass 0.34. Increase of effective mass, proportional to d, becomes significant above 10^{21}/cc carrier concentration.

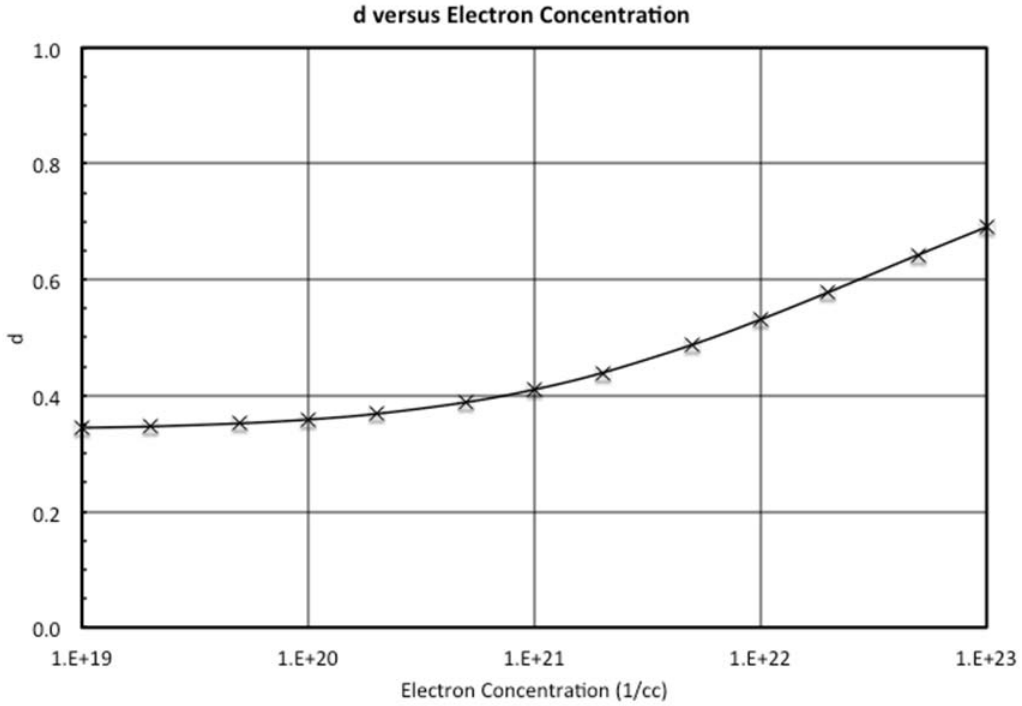

Figure 3: Effective Mass indicated by d versus Carrier Concentration begins at m*/m = 0.34

The screening length is likewise significantly affected by non-parabolicity as shown in Figure 4.

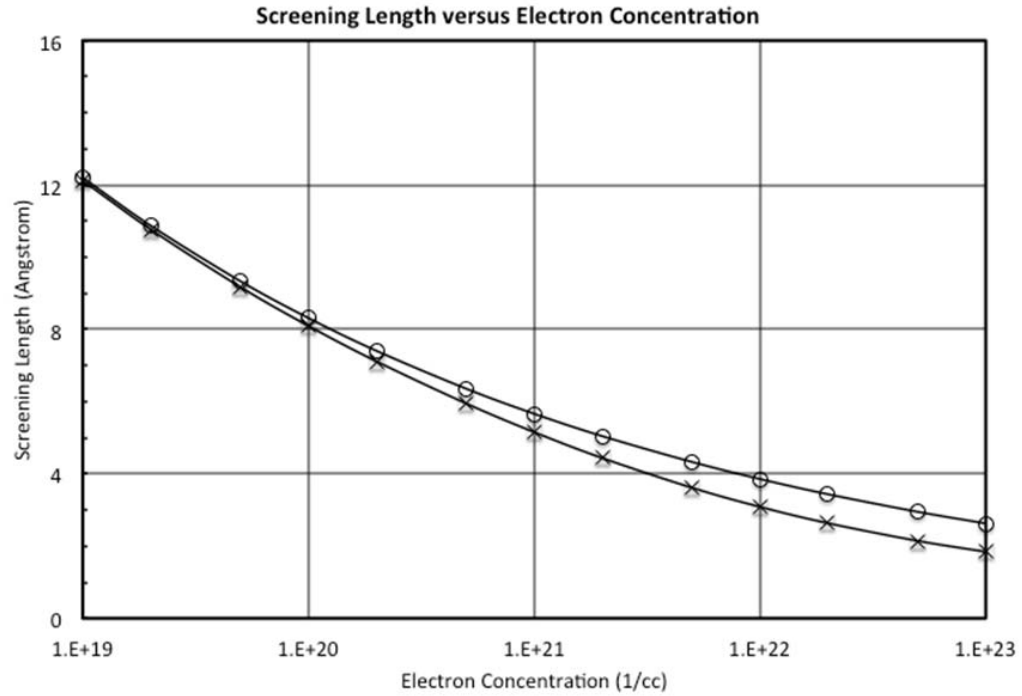

Figure 4: Screening Length versus Carrier Concentration
For non-parabolic bands, screening becomes much stronger above 10^{21}/cc carrier concentration (lower curve).

As a final example, consider the experimental work on ZnO reported by Look *et al*.[4] Set the room-temperature value of K = 8.12, E_g = 3.43 eV, and m* = 0.34m. Look and Leedy have shown the existence of doubly ionized compensating acceptors in this case, with ionized donor concentration N_d = 1.45E21/cc, singly ionized acceptor concentration N_a = zero and doubly ionized acceptor concentration N_{aa} = 1.71E20/cc. Space-charge neutrality requires that the free-electron concentration n = N_d -2N_{aa} = 1.11E21/cc and the scattering concentration $N = N_d + 4N_{aa}$ = 2.13E21/cc. Under these conditions, the effective mass at the Fermi Level as given by d is 0.41m, compared to 0.34m for E = 0. Calculation using eq. (20) gives the mobility equal to 33.0, whereas experiment[4] gives 31.7 cm^2/V-s, agreeing within 4%. The value K = 8.12 should perhaps be decreased about 3% due to the reduced temperature (T = 20K) used in the experiment. A 3% reduction[5] in K gives theoretical mobility equal to 31.7, in perfect agreement with experiment. However, the temperature dependence of the effective mass and the energy gap might also be considered; in addition, other possible types of scattering mentioned at the end of Section 2 may be significant, especially interface scattering.[4]

Nevertheless, it appears to be firmly established that the theoretical treatment of Section 3 is capable of giving agreement between theory and experiment within a few percent, which is one of the major goals of this work. Lastly, it should be said that the fine agreement shown here is a tribute to the high quality of the experimental work cited.

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Appendix: Fermi Level & Ionized-Impurity Screening in Degenerate Semiconductors with Non-Parabolic Energy Bands

The Fermi Level E_F and the inverse screening length β are calculated using non- parabolic Kane bands and Fermi statistics in the degenerate limit, where $E_F/\kappa T >> 1$. Quantities corresponding to degenerate conditions are denoted by subscript F. The unique contribution here is the use of non-parabolic bands.

In general, the free-electron energy, inverse screening length squared, and free-carrier electron concentration are expressed as[1] m is the free-electron mass, ε_s is the static dielectric permittivity, and n_F corresponds to the degenerate limit. The static dielectric permittivity can be expressed as $\varepsilon_s = K\varepsilon_o$ where K is the dielectric constant and ε_o is the free-space permittivity.

$$
\begin{aligned}
E_o &= \frac{\hbar^2 k^2}{2m} \\
\beta^2 &= \frac{e^2}{\varepsilon_s \kappa T} \int \left(\frac{k}{\pi}\right)^2 f(1-f)\,dk \\
n &= \int \left(\frac{k}{\pi}\right)^2 f\,dk \\
n_F &= \frac{k_F^3}{3\pi^2}
\end{aligned}
\tag{A1}
$$

The inverse screening length squared is β_F^2 in the degenerate limit. From eq. (A1)

$$
\begin{aligned}
\beta^2 &= \frac{e^2}{\varepsilon_s \kappa T} \int \left(\frac{k}{\pi}\right)^2 \frac{e^{(E-E_F)/\kappa T}}{(e^{(E-E_F)/\kappa T}+1)^2}\,dk \\
\beta^2 &= \frac{e^2}{\varepsilon_s \kappa T} \int \left(\frac{k}{\pi}\right)^2 \frac{e^{(\varepsilon-\varepsilon_F)}}{(e^{(\varepsilon-\varepsilon_F)}+1)^2}\,dk \\
\beta^2 &= \frac{e^2}{\varepsilon_s \kappa T} \cdot \frac{\partial}{\partial \varepsilon_F} \int \left(\frac{k}{\pi}\right)^2 \frac{dk}{e^{(\varepsilon-\varepsilon_F)}+1} \\
\beta^2 &= \frac{e^2}{\varepsilon_s \kappa T} \cdot \frac{\partial n}{\partial \varepsilon_F} = \frac{e^2}{\varepsilon_s} \cdot \frac{\partial n}{\partial E_F} \\
\beta_F^2 &= \frac{e^2}{\varepsilon_s} \cdot \frac{\partial}{\partial E_F} \frac{k_F^3}{3\pi^2} \\
\beta_F^2 &= \frac{e^2 k_F^2}{\pi^2 \varepsilon_s} \cdot \frac{\partial k_F}{\partial E_F}
\end{aligned}
\tag{A2}
$$

In order to carry out the differentiation in eq. (A2), it is necessary to solve for k_F in terms of the Fermi level EF. For non-parabolic Kane bands,[1,6] the electron kinetic energy E measured upward from the bottom of the conduction band is

$$
\begin{aligned}
&E = E_o - \frac{E_g}{2}\left[1 - \sqrt{1 + 4E_o\left(\frac{m}{m^*} - 1\right)/E_g}\right] \\
&(E - E_o + E_g/2)^2 = E_g^2/4 + E_o E_g(m/m^* - 1) \\
&E_o^2 - 2E_o(E + E_g/2) + (E + E_g/2)^2 = E_g^2/4 + E_o E_g(m/m^* - 1) \\
&E_o^2 + (-2E - 2E_g/2 - E_g m/m^* + E_g) + E^2 + EE_g = 0 \\
&E_o^2 - (2E + E_g m/m^*)E_o + E(E + E_g) = 0 \\
&E_o = E + E_g m/2m^* - \sqrt{(E + E_g m/2m^*)^2 - E(E + E_g)} \\
&\frac{\hbar^2 k_F^2}{2m} = E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)}
\end{aligned}
\tag{A3}
$$

Therefore, the carrier concentration and Fermi level are related as

$$
\begin{aligned}
&k_F^2 = (3\pi^2 n)^{2/3} \\
&(3\pi^2 n)^{2/3} = \frac{2m}{\hbar^2}\left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)}\right] \\
&n = \frac{(2m)^{3/2}}{3\pi^2\hbar^3}\left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)}\right]^{3/2}
\end{aligned}
\tag{A4}
$$

and

$$
\begin{aligned}
&E_F = \frac{\hbar^2(3\pi^2 n)^{2/3}}{2m} - \frac{E_g}{2}\left[1 - \sqrt{1 + \frac{2\hbar^2(3\pi^2 n)^{2/3}}{m}\left(\frac{m}{m^*} - 1\right)/E_g}\right] \\
&E_F = \frac{(3\pi^2 n)^{2/3}\hbar^2}{2m} - \frac{E_g}{2}\left[1 - \sqrt{1 + 2\hbar^2(3\pi^2 n)^{2/3}(1/m^* - 1/m)/E_g}\right]
\end{aligned}
\tag{A5}
$$

(A5)

In general, the inverse screening length from eq. (A2) is,

$$
\beta^2 = \frac{e^2}{\varepsilon_s} \cdot \frac{\partial n}{\partial E_F} \tag{A6}
$$

Under degenerate conditions the inverse screening length is

$$\beta_F^2 = \frac{e^2}{\varepsilon_s} \cdot \frac{\partial n_F}{\partial E_F}, \text{ where}$$

$$\frac{\partial n_F}{\partial E_F} = \frac{(2m)^{3/2}}{3\pi^2\hbar^3} \cdot \frac{3}{2} \cdot \left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)} \right]^{1/2} \times \left[1 - \frac{1}{2} \cdot \frac{2E_F + mE_g/m^* - 2E_F - E_g}{\sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)}} \right]$$

$$\frac{\partial n_F}{\partial E_F} = \frac{(2m)^{3/2}}{2\pi^2\hbar^3} \cdot \left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)} \right]^{1/2} \times \left[1 - \frac{(m/m^* - 1)E_g/2}{\sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)}} \right]$$

$$\beta_F^2 = \frac{e^2(2m)^{3/2}}{2\pi^2\varepsilon_s\hbar^3} \cdot \left[E_F + E_g m/2m^* - \sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)} \right]^{1/2} \times \left[1 - \frac{(m/m^* - 1)E_g/2}{\sqrt{(E_F + E_g m/2m^*)^2 - E_F(E_F + E_g)}} \right] \quad \text{(A7)}$$

This completes the derivation of analytical expressions for the Fermi level and the screening length. The particulars of the semiconductor material are specified by three parameters: the effective mass at the bottom of the conduction band, the energy gap, and the dielectric constant. Therefore, given the free-electron concentration, the Fermi level and the screening length are calculated from eqs. (A5) and (A7).