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# A consistent model for carrier transport in heavily doped semiconductor devices

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**Abstract.** A self-consistent model for describing carrier transport in heavily doped semiconductor devices has been developed. The proposed model allows convenient treatment of non-uniform semiconductors in a manner that is both thermodynamically consistent and consistent with the transport equations, the steady-state continuity equations and the electrostatic potetial with explicit boundary conditions at the contacts. The complex problems are reduced to determining two types of quantities: the reference electrostatic potential and the activity coefficient of the carriers. In order to find the simple working equations for the model, two choices of reference for the electrostatic potential are discussed. The presented transport equations are written in a simple Shockley-like form, in which the effects associated with the non-uniform band structure and the influence of Fermi–Dirac statistics are described by a thermodynamic property, the activity coefficient of the carriers, which is expressed in terms of two band model parameters, the effective band-gap shrinkage, $\Delta E_g$, and the effective asymmetry factor, $A$. In this form they are convenient for use in computer-aided analysis and the design of heavily doped semiconductor devices.

## 1. Introduction

The general analytic characterisation of the carrier transport in heavily doped semiconductor devices is difficult because of the complex heavy-doping effects [1] that must be accounted for. These effects may include the actual band-gap narrowing [2, 3], the carrier degeneracy [4], the influence of the impurity band [5], and the built-in electric field due to a graded doping density [6]. The resulting changes in the energy bands must be considered in order to model p–n junction devices accurately [1, 7, 8, 9]. Transport equations for materials with a position-dependent band structure have been derived by Mock [10], van Overstraeten and co-workers [11], Marshak and van Vliet [12–14] and Lundstrom and co-workers [15]. However, a systematic study (including the choice of the reference states) of a self-consistent solution of transport equations, steady-state continuity equations, Poisson's equation and electrochemical potential equation (irreversible thermodynamics) does not seem to exist in the previous studies.

The electrochemical potential of a given charged species in a phase is generally divided into two terms (as shown in equation (26) below): the first one comes from a chemical contribution and the second an electrical contribution. The chemical contribution is produced by the chemical environment in which the charged species exists, and is usually split into two terms, a composition-independent term (called the reference state chemical potential) and a term which is composition dependent and accounts for the non-ideal behaviour (named the activity coefficient) of the real system. The electrical contribution depends on the electrical condition of the phase and may contain some other potential energy (for example, due to strain) besides electrostatic energy.

In this paper we consider the carrier transport in heavily doped semiconductor devices based on position-dependent band-structure approach. A simple but self-consistent formulation of the thermodynamic quanttities, the transport equations, the steady-state continuity equations and the Poisson's equation with explicit boundary conditions at the contacts is presented. By the proper choice of reference for the electrostatic potential, we develop a simpler and more complete analytic model. The model includes the effects of the modified band structure and the activity coefficient of the carriers which is a useful quantity for describing a system behaviour deviated from its ideality. The heavy-doping effects mentioned above are accounted for in a consistent manner that yields a useful model which can be an effective aid to design and an informative guide to physical and thermodynamic understanding. The results presented here are of great importance both in practical device applications and in pedagogy.

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## 2. Energy bands in heavily doped semiconductors

Figure 1 shows the energy band diagram for a heavily doped semiconductor. The validity of this energy band model has been discussed by Marshak and van Vliet [12]. From figure 1, we have

$$E_L(x) = E_0 - qV(x) \tag{1}$$

$$\chi(x) = E_L(x) - E_C(x) = E_0 - qV(x) - E_C(x) \tag{2}$$

and

$$E_G(x) = E_C(x) - E_V(x) \tag{3}$$

where $E_0$ is the field-free vacuum level, $E_L$ is the local vacuum level, $V$ is the electrostatic potential (neglecting the other potentials), $\chi$ is the electron affinity, $E_G$ is the band-gap energy, $E_C$ is the bottom of the conduction band, $E_V$ is the top of the valence band, and $q$ is the magnitude of the electronic charge.

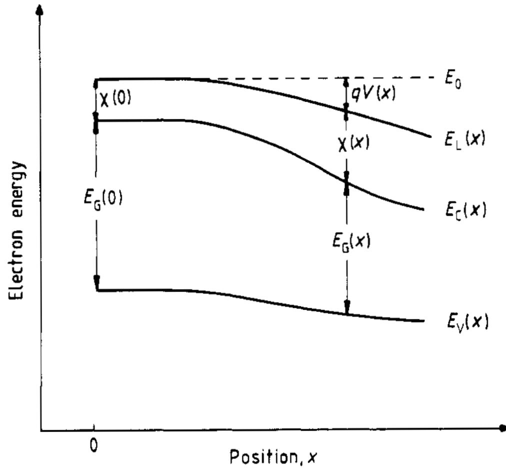


**Figure 1.** The energy bands for an inhomogeneous material

If we assume Fermi–Dirac statistics and write the non-equilibrium carrier densities as

$$\begin{aligned} n(x) &= N_C(x) F_{1/2}(\eta_C(x)) \\ &= n_i(x)\zeta_C(x)\exp[(E_{Fn}(x) - E_I(x))/kT] \end{aligned} \tag{4}$$

and

$$\begin{aligned} p(x) &= N_V(x) F_{1/2}(\eta_V(x)) \\ &= n_i(x)\zeta_V(x)\exp[(E_I(x) - E_{Fp}(x))/kT] \end{aligned} \tag{5}$$

where $E_{Fn}$ and $E_{Fp}$ are the quasi-Fermi levels for electrons and holes, respectively, and

$$n_i(x) = (N_V(x) N_C(x))^{1/2} \exp(-E_G(x)/2kT) \tag{6}$$

is the position-dependent intrinsic carrier concentration. $N_C(x)$ and $N_V(x)$ are effective densities of states in the conduction band and in the valence band, respectively. $\zeta_i(x)$ is the degeneracy effect and is defined by

$$\zeta_i = \frac{F_{1/2}(\eta_i)}{\exp(\eta_i)} \tag{7}$$

and $F_{1/2}$ is the Fermi–Dirac integral of order one-half with

$$\eta_C(x) = \frac{E_{Fn}(x) - E_C(x)}{kT} \tag{8}$$

and

$$\eta_V(x) = \frac{E_V(x) - E_{Fp}(x)}{kT}. \tag{9}$$

After some algebraic manipulation, these parameters can be related to the electrostatic potential as

$$\eta_C(x) = \left[ q(V - \varphi_n) + (\chi(x) - \chi(0)) + \tfrac{1}{2}kT \ln\left(\frac{N_V(0)\exp(-E_G(0)/kT)}{N_C(0)}\right)\right] \Big/ kT \tag{10}$$

and

$$\eta_C(x) = \left[ q(\varphi_p V) + (\chi(x) - \chi(0)) - (E_G(x) - E_G(0)) - \tfrac{1}{2}kT \ln\left(\frac{N_V(0)\exp(E_G(0)/kT)}{N_C(0)}\right)\right] \Big/ kT \tag{11}$$

where

$$\varphi_n(x) = \frac{E_F^0(0) - E_{Fn}(x)}{q} \tag{12}$$

$$\varphi_p(x) = \frac{E_F^0(0) - E_{Fp}(x)}{q} \tag{13}$$

are the quasi-Fermi potentials for the electrons and holes, respectively. It should be noted here that quasi-equilibrium condition is applied at $x = 0$. Thus, by convention, we have $E_{Fp}(0) = E_{Fn}(0) \equiv E_F^0(0)$ (assuming p-type material here).

Using Equations (2)–(6) we obtain the intrinsic energy level

$$E_I(x) = E_0 - \chi(x) - \tfrac{1}{2}E_G(x) + \tfrac{1}{2}kT \ln\left(\frac{N_V(x)}{N_C(x)}\right) - qV(x). \tag{14}$$

It is apparent from (14) that $E_I(x)$ is not, in general, parallel to $V(x)$ as it is in a uniform non-degenerate semiconductor. Indeed, $E_I$ is a purely thermodynamic property of the intrinsic bulk semiconductors as shown by Chang [16]. Thus, one cannot use it to align the energy levels in the energy band diagram.

## 3. Poisson's equation

To obtain the electrostatic potential within a heavily doped semiconductor device we must solve Poisson's equation [17] with appropriate boundary conditions. For convenience, consider a one-dimensional p–n junction with Ohmic contacts at $x = 0$ on the p-side and

$x = W$ on the n-side, and with the junction at $x_j$. The Poisson's equation is given by

$$\frac{d^2V}{dx^2}+\frac{d\ln K}{dx}\frac{dV}{dx}=-\frac{q}{K\varepsilon_0}(p-n+N^+) \quad (15)$$

where $K$ is the dopant density-dependent dielectric constant, $\varepsilon_0$ is the permittivity in vacuum, and $N^+ = N_D^+ - N_A^-$ is the ionised dopant density. The carrier concentrations, p and n, can be expressed in terms of the electrostatic potential. Algebraic manipulation of equations (4), (5), (6) and (14), with quasi-equilibrium condition at $x = 0$ and the reference electrostatic potential

$$V(0)=\frac{kT}{q}\ln\left(\frac{\zeta_V(0)n_i(0)}{N_A(0)}\right)$$

gives the following carrier densities

$$n(x)=n_i(0)\exp\left(\frac{q(V(x)-\varphi_n(x))+A\Delta E_g}{kT}\right) \quad (16)$$

and

$$p(x)=n_i(0)\exp\left(\frac{-q(V(x)-\varphi_p(x))+(1-A)\Delta E_g}{kT}\right) \quad (17)$$

where

$$\Delta E_g=(E_g(0)-E_g(x))+kT\ln\left(\frac{N_C(x)N_V(x)}{N_C(0)N_V(0)}\right)+kT\ln(\zeta_C(x)\zeta_V(x))\equiv\Delta_{BGN}+\Delta_{DOS}+\Delta_{FD} \quad (18)$$

and

$$A=\left[(\chi(x)-\chi(0))+kT\ln\left(\frac{N_C(x)}{N_C(0)}\right)+kT\ln(\zeta_C(x))\right]/\Delta E_g. \quad (19)$$

As shown in figure 1, we choose $x = 0$ as the reference position for the electrostatic potential at which the material is uniform. Also, the actual band-gap narrowing effect ($\Delta_{BGN} = E_G(0) - E_G(x)$) is generally greater than the degeneracy effect ($\Delta_{FD} = kT\ \ln(\zeta_C(x)\zeta_V(x))$). So, both $\Delta E_g$ and $A$ are positive quantities. $\Delta E_g$ is called the effective band-gap shrinkage and accounts for the actual band-gap narrowing effect ($\Delta_{BGN}$), the density-of-state effects ($\Delta_{DOS}$), and the influence of Fermi–Dirac statistics ($\Delta_{FD}$). $A$, called the effective asymmetry factor [18], measures the fraction of the reduction in band gap that occurs in the conduction band, $0 \leqslant A \leqslant 1$. In a lightly doped material with uniform band structure, $\Delta E_g$ and $A$ are zero. These extra terms over conventional results are due to the non-ideal behaviour of the carriers and can be related to the activity coefficients of the carriers [16].

Assuming that the potential of the Ohmic contacts remains in equilibrium, we obtain the electrostatic potential $V(W)$ from (16) as

$$qV(W)=q\varphi_n(W)-A_0(W)\Delta E_{g0}(W)+kT\ln\left(\frac{n_0(W)}{n_i(0)}\right) \quad (20)$$

where subscript 0 represents the equilibrium value. In n-type semiconductors, where $N_A(W) = 0$, $n_0(W) \gg p_0(W)$ and one can neglect $p_0(W)$ and $N_A(W)$ in the charge neutrality condition to yield $n_0(W) \cong N_D(W)$. Also, from (14), $\varphi_n(W)$ is given by

$$q\varphi_n(W)=E_F^p(0)-E_{Fn}(W)=E_F^p(0)-E_F^n(W)=-qV_a \quad (21)$$

where $V_a$ represents the terminal voltage. Again, note that quasi-equilibrium condition at contact $x = W$ gives $E_{Fp}(W) = E_{Fn}(W) \equiv E_F^n(W)$. It is the well known result that the separation of the majority quasi-Fermi levels across the entire device is given by the terminal voltage.

The electrostatic potential difference $V_t$ across the entire device is given by

$$V_t = V(W) - V(0). \quad (22)$$

Substituting (20), (21) and

$$V(0)=\frac{kT}{q}\ln\left(\frac{\zeta_V(0)n_i(0)}{N_A(0)}\right)$$

into (22) gives

$$qV_t=-A_0(W)\Delta E_{g0}(W)+kT\ln\left(\frac{N_D(W)N_A(0)}{n_i^2(0)}\right)-kT\ln(\zeta_V(0))-qV_a. \quad (23)$$

It is also noted that the built-in potential $V_{bi}$ of the junction for the degenerate case is given by [19]

$$qV_{bi}=-A_0(W)\Delta E_{g0}(W)+kT\ln\left(\frac{N_D(W)N_A(0)}{n_i^2(0)}\right)-kT\ln(\zeta_V(0)). \quad (24)$$

Substituting (24) into (23), we have

$$V_t = V_{bi} - V_a. \quad (25)$$

Equation (25) gives the total voltage across the junction from $x = 0$ on the p side to $x = W$ on the n side. In equilibrium $V_a = 0$ and $V_{bi}$ is given by (24), but if an external voltage $V_a$ is applied it changes $V_t$. It is important to note that, for a given bias, $V_t$ becomes smaller as either $A_0(W)$ or $\Delta E_{g0}(W)$ becomes larger. The reference electrostatic potential $V(0)$ and equation (20) can be served as two explicit boundary conditions for solving the Poisson equation.

## 4. A consistent formulation

In this section, equations presented earlier are used to derive the self-consistent results for the band-model

parameters and thermodynamic quantities, for example, the reference state chemical potentials and activity coefficients of the carriers which appear in the electrochemical potentials of the carriers. The electrochemical potential ($\tilde{\mu}_i$), or quasi-Fermi level, of a charged species $i$ in phase $\alpha$ is defined as the sum of its chemical potential and its electric potential energy [20]

$$\tilde{\mu}_i^\alpha = \mu_i^\alpha + z_i q V^\alpha = \mu_i^{*,\alpha} + kT\ln(\gamma_i^\alpha c_i^\alpha) + z_i q V^\alpha \quad (26)$$

where $\mu_i^\alpha$ is the chemical potential, $\mu_i^{*,\alpha}$ is the reference state chemical potential and is a function only of temperature, pressure, and choice of reference state, $\gamma_i^\alpha$ is the activity coefficient, $c_i^\alpha$ is the concentration ($c_i = n$ for electrons; $c_i = p$ for holes), and $z_i$ ($z_i = 1$ for holes; $z_i = -1$ for electrons) is the elemental charge of species $i$. The potential $V^\alpha$ is the electrostatic potential which is obtained through integration of Poisson's equation (15).

For electrons ($i = \text{n}$), equating $\tilde{\mu}_\text{n} = E_\text{Fn}$, we have

$$E_\text{Fn} = \tilde{\mu}_\text{n} = \mu_\text{n}^* + kT\ln(n\gamma_\text{n}) - qV. \quad (27)$$

Here we have dropped the superscripts because (27) holds on either the n-side or p-side. It is clear that we have two reference states in (27), i.e., $\mu_\text{n}^*$ and $qV(0)$. This implies that we have two unknowns and only one equation. To get the consistent results, these two reference states cannot be chosen independently. When one is specified, the other must be fixed. In a similar manner, for holes ($i = \text{p}$), equation $\tilde{\mu}_\text{p} = -E_\text{Fp}$ gives

$$-E_\text{Fp} = \tilde{\mu}_\text{p} = \mu_\text{p}^* + kT\ln(p\gamma_\text{p}) + qV. \quad (28)$$

Note that negative quasi-Fermi energy is used in equation (28). This is because a hole has a charge opposite that of an electron.

Chang [21] has recently addressed the calculation of the reference state chemical potentials and the activity coefficients of the carriers with three different choices of reference for the electrostatic potentials. In the case of

$$qV(0) = kT\ln\left(\frac{\zeta_\text{V}(0)n_\text{i}(0)}{N_\text{A}(0)}\right)$$

the results of his analysis for electrons and holes are

$$\mu_\text{n}^*(T) = E_\text{i}(0) - kT\ln(n_\text{i}(0)) + qV(0) \quad (29)$$

$$\mu_\text{p}^*(T) = -E_\text{i}(0) - kT\ln(n_\text{i}(0)) - qV(0) \quad (30)$$

$$\gamma_\text{n}(T, n, x) = \exp\left(\frac{-A\Delta E_\text{g}}{kT}\right) \quad (31)$$

and

$$\gamma_\text{p}(T, p, x) = \exp\left(\frac{-(1-A)\Delta E_\text{g}}{kT}\right) \quad (32)$$

where $\Delta E_\text{g}$ and $A$ are defined by (18) and (19), respectively. These values combined with (15) and (26) can be used in the self-consistent result calculations. It is seen from figure 1 that the value of the reference electrostatic potential at $x = 0$ can be arbitrarily chosen because the field-free vacuum level $E_0$ is an arbitrary one. The choice of

$$qV(0) = kT\ln\left(\frac{\zeta_\text{V}(0)n_\text{i}(0)}{N_\text{A}(0)}\right)$$

(a particular value), however, results in the simple equations (29) through (32) and also leads to a simple form of Poisson's equation [19]. This choice will be used henceforth.

## 5. Transport equations

The electron and hole current densities under isothermal conditions are given by

$$J_\text{n} = nU_\text{n}\nabla E_\text{Fn} \quad (33)$$

and

$$J_\text{p} = pU_\text{p}\nabla E_\text{Fp} \quad (34)$$

where $U_\text{n}$ and $U_\text{p}$ are the mobilities of electrons and holes, respectively. The validity of these equations for materials with position-dependent band structures has been established by Marshak and van Vliet [12, 22].

If the definition of $E_\text{Fn}$, (27), is used, the gradient of the electron quasi-Fermi level can be expressed as

$$\nabla E_\text{Fn} = -q\nabla V + kT\nabla\ln n + kT\nabla\ln\gamma_\text{n}. \quad (35)$$

Note that $\nabla\mu_\text{n}^*$ is zero because the reference state chemical potential is a function only of temperature, pressure and the choice of the reference state. Substituting (35) into (33) yields

$$J_\text{n} = kTU_\text{n}\nabla n - qnU_\text{n}\nabla V + kTnU_\text{n}\nabla\ln\gamma_\text{n}. \quad (36)$$

Furthermore, substituting (31) into (36), followed by some algebraic manipulation, gives

$$J_\text{n} = kTU_\text{n}\nabla n - qnU_\text{n}\nabla(V + A\Delta E_\text{g}/q). \quad (37)$$

The hole current density is derived in a similar manner. For holes, an expression for the gradient of the quasi-Fermi level can be obtained by using the definition of $E_\text{Fp}$ in (28). The result for $E_\text{Fp}$ is

$$\nabla E_\text{Fp} = -q\nabla V - kT\nabla\ln p - kT\nabla\ln\gamma_\text{p}. \quad (38)$$

Again, we use the fact that $\nabla\mu_\text{p}^* = 0$. Substituting (38) into (34), we obtain

$$J_\text{p} = -kTU_\text{p}\nabla p - qpU_\text{p}\nabla V - kTpU_\text{p}\nabla\ln\gamma_\text{p}. \quad (39)$$

Equation (39) can be rewritten in terms of $\Delta E_\text{g}$ and $A$. Using (32) in the last term of (39) and rearranging yields

$$J_\text{p} = -kTU_\text{p}\nabla p - qpU_\text{p}\nabla\left(V - (1-A)\frac{\Delta E_\text{g}}{q}\right). \quad (40)$$

Equations (37) and (40) or (36) and (39) are convenient to use in semiconductor device analysis. Although these equations are expressed in a simple form, they correctly describe carrier transport in materials with a

position-dependent band structure. The effects of the non-uniform band structure and the carrier degeneracy are described by two parameters, $\Delta E_g$ and $A$, which are expressed in terms of the carrier activity coefficients. The results presented here are identical in form to those derived by Marshak and van Vliet [22]. The treatments, however, are different. These results along with those discussed in [22] would give a good description of the carrier transport in degenerate materials with non-uniform band structure.

## 6. The *pn* product

The carrier concentrations given by equations (16) and (17) can be related to their activity coefficients by (31) and (32) as

$$n(x)=\frac{n_i(0)}{\gamma_n(x)}\exp\left(\frac{q(V(x)-\varphi_n(x))}{kT}\right) \tag{41}$$

and

$$p(x)=\frac{n_i(0)}{\gamma_p(x)}\exp\left(\frac{-q(V(x)-\varphi_p(x))}{kT}\right). \tag{42}$$

It is noted that the pre-exponential factor in equations (41) and (42) has the same value only if band-gap narrowing is symmetric (i.e., $A=\frac{1}{2}$ or $\gamma_n=\gamma_p$), which rarely occurs [23]. Even as the carrier is non-degenerate, asymmetric band-gap narrowing gives different pre-exponential factors in (41) and (42). This is contrary to the results of [8].

From (41) and (42), the *pn* product is then given by

$$p(x)n(x)=\frac{n_i^2(0)}{\gamma_n(x)\gamma_p(x)}\exp\left(\frac{E_{Fn}-E_{Fp}}{kT}\right) \tag{43}$$

where the $\gamma_n\gamma_p$ product, from (31) and (32), is given by

$$\gamma_n(x)\gamma_p(x)=\exp\left(\frac{-\Delta E_g}{kT}\right)$$
$$=\exp\left(\frac{-(\Delta_{BGN}+\Delta_{DOS}+\Delta_{FD})}{kT}\right). \tag{44}$$

We define an effective intrinsic carrier concentration as the *pn* product in equilibrium ($E_{Fn}=E_{Fp}$) [1, 11, 13]; thus

$$p_0n_0\equiv n_{ie}^2(x)=\frac{n_i^2(0)}{\gamma_{n0}\gamma_{p0}}$$
$$=n_i^2(0)\exp\left(\frac{\Delta^0_{BGN}+\Delta^0_{DOS}+\Delta^0_{FD}}{kT}\right) \tag{45}$$

where the subscript zero denotes equilibrium. Substituting (45) into (43) gives the *pn* product for all cases

$$p(x)n(x)=n_{ie}^2(x)\frac{\gamma_{n0}(x)\gamma_{p0}(x)}{\gamma_n(x)\gamma_p(x)}\exp\left(\frac{E_{Fn}-E_{Fp}}{kT}\right). \tag{46}$$

These equations can be simplified for special cases of interest. As an example, for non-degenerate uniform semiconductors ($\gamma_n=\gamma_{n0}=\gamma_p=\gamma_{p0}=1$), equations (41), (42) and (46) reduce to

$$n(x)=n_i(0)\exp\left(\frac{q(V(x)-\varphi_n(x))}{kT}\right) \tag{47}$$

$$p(x)=n_i(0)\exp\left(\frac{-q(V(x)-\varphi_p(x))}{kT}\right) \tag{48}$$

and

$$p(x)n(x)=n_i^2(0)\exp\left(\frac{E_{Fn}-E_{Fp}}{kT}\right). \tag{49}$$

In the case of low-level injecton, i.e. $\gamma_n\simeq\gamma_{n0}$ and $\gamma_p\simeq\gamma_{p0}$ or $\Delta E_g\simeq\Delta E_{g0}$, (46) reduces to

$$p(x)n(x)=n_{ie}^2(x)\exp\left(\frac{E_{Fn}-E_{Fp}}{kT}\right). \tag{50}$$

This result can be used for all practical conditions (even for high-level injection) in Si.

## 7. Discussion

### 7.1. The choice of reference states

The choice of the reference states is quite arbitrary. The proper choice, however, of these reference states can lead to simpler working equations for the problems. For example, we choose $x=x_j^-$ as the reference position for the electrostatic potential at which $qV(x_j)=0$. The results for the carrier concentrations and the potential at the contacts are given by

$$n(x)=n(x_j^-)\exp\left(\frac{q(V(x)-\varphi_n(x))+A\Delta E_g}{kT}\right) \tag{51}$$

$$p(x)=p(x_j^-)$$
$$\times\exp\left(\frac{-q(V(x)-\varphi_p(x))+(1-A)+\Delta E_g}{kT}\right) \tag{52}$$

$$qV(0)=q\varphi_p(0)$$
$$+(1-A_0(0))\Delta E_{g0}(0)-kT\ln\left(\frac{p_0(0)}{p(x_j^-)}\right) \tag{53}$$

and

$$qV(W)=q\varphi_n(W)$$
$$-A_0(W)\Delta E_{g0}(W)+kT\ln\left(\frac{n_0(W)}{n(x_j^-)}\right) \tag{54}$$

where

$$\varphi_n(x)=(E^0_{Fn}(x_j^-)-E_{Fn}(x))/q \tag{55}$$

and

$$\varphi_p(x)=(E^0_{Fp}(x_j^-)-E_{Fp}(x))/q. \tag{56}$$

The parameters $\Delta E_g$ and $A$ in equations (51)–(54) are defined by equations (57) and (58) as

$$\Delta E_g = kT \ln\left(\frac{N_V(x)N_C(x)}{N_V(x_j^-)N_C(x_j^-)}\right) - (E_G(x) - E_G(x_j^-)) + kT\ln\left(\frac{\zeta_C(x)\zeta_V(x)}{\zeta_C(x_j^-)\zeta_V(x_j^-)}\right) \quad (57)$$

and

$$A = \left[(\chi(x) - \chi(x_j^-)) + kT\ln\left(\frac{N_C(x)}{N_C(x_j^-)}\right) + kT\ln\left(\frac{\zeta_C(x)}{\zeta_C(x_j^-)}\right)\right] \Big/ \Delta E_g. \quad (58)$$

Note that the parameters $\Delta E_g$ and $A$ given by (57) and (58) are different from those defined by (18) and (19) due to two different choices of the reference states. It is also noted that the pre-exponential factors in (51) and (52) are different from those given by (16) and (17).

It is clear that the boundary conditions for the integration of Poisson's equation are explicit for the case of

$$qV(0) = kT\ln\left(\frac{\zeta_V(0)n_i(0)}{N_A(0)}\right)$$

(discussed previously), while they are implicit for $qV(x_j^-)=0$ due to the unknown quantities $p(x_j^-)$ and $n(x_j^-)$. Therefore, the numerical computation for solving the Poisson equation is quite straightforward for the former case.

### 7.2. Alternative current equations

In a typical analysis, the electric field is expressed in terms of the electrostatic potential as

$$E = -\nabla V. \quad (59)$$

Using (59) in (36) and (39), we obtain the current equation, which is rewritten in terms of $E$

$$J_n = kTU_n\nabla n + qnU_nE + kTnU_n\nabla\ln\gamma_n \quad (60)$$

and

$$J_n = -kTU_p\nabla p + qpU_pE - kTpU_p\nabla\ln\gamma_p. \quad (61)$$

In this form, only one parameter, i.e. the activity coefficient, is necessary to describe the effect of the non-uniform band structure and the influence of the Fermi–Dirac statistics. The current density, via its dependence on $\gamma_n$ in (60) and $\gamma_p$ in (61), depends not only on the effective band-gap narrowing but also on the effective asymmetry in band-gap narrowing. It is important to note that the diffusivity is not needed to evaluate (60) and (61) because the coefficient in front of the diffusion terms involves only the mobility, which can be obtained from experiment.

### 7.3. Minority-carrier current and concentration

In order to solve for the steady-state minority carrier concentration, for example $p$ in a heavily doped n-type region in low injection, we return to (40). It should be useful to define the effective electric field in analysis as

$$J_p = -kTU_p\nabla p + qpU_pE_p \quad (62)$$

where

$$E_p = -\nabla\left(V - (1-A)\frac{\Delta E_g}{q}\right) = E + \nabla\left((1-A)\frac{\Delta E_g}{q}\right). \quad (63)$$

The 'effective' electric field (electric plus quasi-electric) $E_p$ can be evaluated by equating (62) to zero for thermal equilibrium conditions

$$E_p = \frac{kT}{q}\frac{\nabla p_0}{p_0}. \quad (64)$$

For low-injection conditions, $E_p$ is not altered from its equilibrium value given by (62) [18]. Combining (45) and (64) yields

$$E_p = \nabla\left(\frac{\Delta E_{g0}}{q}\right) - \frac{kT}{q}\frac{\nabla N_D}{N_D}. \quad (65)$$

Here we assume $n_0 \simeq N_D$. Substituting (65) into (62) gives

$$J_p = -kTU_p\nabla p + qpU_p\left[\nabla\left(\frac{\Delta E_{g0}}{q}\right) - \frac{kT}{q}\frac{\nabla N_D}{N_D}\right]. \quad (66)$$

Equation (66) shows that the minority carrier current density is evaluated independently of how $A$ is chosen.

Equation (66) is inserted into the steady-state hole continuity equation:

$$\nabla\cdot J_p + q(R-G) = 0 \quad (67)$$

where $R$, the recombination rate of carriers and $G$, the rate at which they generate, are assumed to be independent of the effective asymmetry factor. When two boundary conditions on $p$ are specified, (67) can be solved for the steady-state hole density. The boundary condition at the contact $W$ can be either a Dirichlet type or a Neumann type. The second boundary condition at the edge of the space charge region follows from the non-equilibrium form of (50)

$$p \cong \frac{n_i^2(0)}{N_D}\exp\left(\frac{\Delta E_{g0}}{kT}\right)\exp\left(\frac{qV_{ja}}{kT}\right) \quad (68)$$

where $V_{ja}$ represents the portion of the applied voltage that appears across the junction. Equation (68) indicates that the relationship between the junction potential and the minority carrier density at the edge of the

space charge region is obtained regardless of the choice of $A$ in the transport equations.

The discussion presented above shows that the carrier concentrations and minority carrier current density of heavily doped semiconductor device are correctly modelled even when the choice for $A$ in (37) and (40) is made arbitrarily. However, the electrostatic potential, built-in potential and chemical potential cannot be evaluated unless $A$ is known. These quantities depend strongly on the $A$-value. These results are also observed when the semiconductor equations for a Gaussian p–n junction are solved numerically [24].

## 8. Conclusions

In this paper we present a self-consistent formulation for the thermodynamic quantities, the transport equations, the steady-state continuity equations and the electrostatic potential with explicit boundary conditions at the contacts. The formulation of the model requires the selection of reference for the electrostatic potential and the evaluation of the activity coefficients of the carriers. Special emphasis has been placed on writing the working equations in a simple form by the proper choice of the reference states. These general transport equations, which are similar to those derived by Marshak and van Vliet [13, 22], were obtained from a simple but general thermodynamic point of view and written in a simple form for use in device analysis. In this form, the effects of the non-uniform band structure and the influence of Fermi–Dirac statistics are described by one thermodynamic quantity, the activity coefficient of the carriers, which is expressed in terms of two energy band model parameters, the effective band-gap shrinkage, $\Delta E_g$, and the effective asymmetry factor, $A$. These parameters correctly account for the changes in the band structure and the carrier degeneracy which occur in regions that are heavily doped. When experimentally measured heavy-doping parameters are used in the simple Shockley-like transport equations, no further correction for degenerate statistics is necessary. Finally, it was shown, in the case of low injection, that the carrier densities and the minority carrier current density in semiconductor devices with quasi-neutral, heavily doped regions, can be modelled accurately, independently of the choice of $A$.

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