

One-Dimensional Corrected Drift-Diffusion Model: McKelvey's Method Extended with Accelerated-Multi-Flux

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Abstract – By introducing accelerated-multi-flux into McKelvey's one-flux method, we have developed a novel macroscopic carrier transport model in one-dimensional steady-state. The developed model, referred to as “Corrected Drift-Diffusion Model”, takes into account both velocity overshoot and ballistic transport of carriers. It is revealed that introducing accelerated-multi-flux under two fundamental hypotheses requires a conventional drift-diffusion model to be corrected only with additional carrier concentration calculation. Numerical calculation for one-dimensional n+n-n+ structure demonstrates that the additional carrier concentration calculation substantially affects self-consistent electrostatics.

I. INTRODUCTION

Drift-diffusion and energy transport models have been used commonly as defacto standard models to describe carrier transport in TCAD [1]. Full-band Monte Carlo simulation for quarter-micron Si-MOSFET's [2] revealed, however, substantial off-equilibrium carrier transport such as carrier velocity overshoot under the high lateral electrostatic fields, indicating a drawback of a drift-diffusion model that originates from constraint on velocity saturation [3, 4]. On the other hand, it was demonstrated that [3-5] an energy transport model overestimates not only the average carrier velocity under the low lateral electrostatic fields, such as at the beginning of the channel [4, 5], but also the ballistic limit current. These two findings [3-5] have required us to establish a macroscopic model advanced suitably for describing highly off-equilibrium, quasi-ballistic carrier transport.

In this report, we develop a novel macroscopic carrier transport model, referred to as “Corrected Drift-Diffusion Model”, that fairly captures the unidirectional carrier velocity under both the high- and low-fields and hence both velocity overshoot and ballistic transport of carriers. Assuming device design of bipolar junction transistors (BJT's) and ultra-thin-body double-gate MOS(MIS)FET's, we restrict ourselves to one-dimensional (1-D) space. In addition, we consider steady-state without recombination-generation of carriers.

In Sec. II, we extend McKelvey's one-flux method, which is identical with a conventional drift-diffusion model in 1-D steady-state [6], by introducing accelerated-multi-flux. In Sec. III, we derive the corrected drift-diffusion model from the extended McKelvey's method, by utilizing a concept of the pseudo carrier concentration [7]. In Sec. IV, we generalize the corrected drift-diffusion model with the spatial distribution of the carrier temperature and with excess scattering of the accelerated-multi-flux. In addition, we reveal two fundamental hypotheses inherent in our model

through the generalization. Section V shows results of numerical calculation. Finally, conclusions of this report are presented in Sec. VI.

II. MCKELVEY'S METHOD EXTENDED WITH ACCELERATED-MULTI-FLUX

In 1-D space on the z-axis, we identify a calculation node where the electrostatic potential Ψ and field E are respectively minimum and 0 with the beginning of the channel z_{\min} [4, 5]. (The suffix **min** indicates the calculation node index.) In addition, expecting $E \leq 0$ for the downward region ($z \geq z_{\min}$), we define accelerated carrier flux starting from every calculation node in that region. Moreover, the velocities of every accelerated carrier flux are assumed to obey the energy conservation law. These definitions are illustrated in Fig. 1.

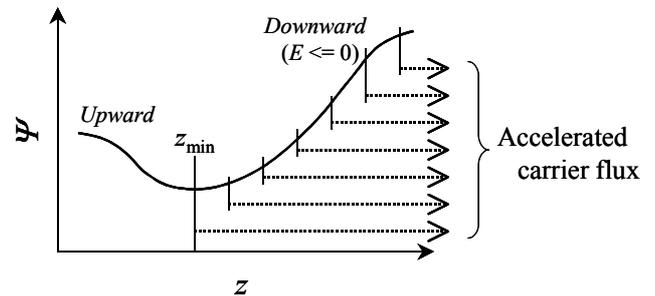


Figure 1: Illustration of the beginning of the channel and accelerated carrier flux starting from every calculation node in the downward region.

Next, we specify details of accelerated carrier flux $J_{d,i+1}^+$ for $z \geq z_i$ ($i \geq \mathbf{min}$) as follows. (The suffix d indicates the downward region.) $J_{d,i+1}^+$ is assumed to be in pre-acceleration for $z_i \leq z \leq z_{i+1}$ and to be accelerated for $z > z_{i+1}$. Pre-acceleration and accelerated carrier flux $J_{d,i+1}^+$ for $z \geq z_i$ is assumed to undergo reflection transition into deceleration carrier flux J_d arising from scattering of $J_{d,i+1}^+$ itself. Pre-acceleration carrier flux $J_{d,i+1}^+$ for $z_i \leq z \leq z_{i+1}$ is assumed to be supplied by reflection transition of deceleration carrier flux J_d arising from its scattering. We note that accelerated carrier flux $J_{d,i+1}^+$ for $z > z_{i+1}$ is not supplied directly by any scattering processes, because acceleration originates from the start of acceleration itself. All kinds of carrier flux are defined in positive [6]. In order to avoid current discontinuity at every calculation node, $J_{d,i+1}^+$ at $z = z_i$ is assumed to be 0. Expecting local thermal equilibrium, the absolute velocities of the pre-acceleration and the deceleration carrier flux are assumed to be the carrier

thermal velocity v_T . These definitions are illustrated in Fig. 2. ξ_d^+ and ξ_d^- appearing in this figure denote the rate coefficients for reflection transition arising from scattering of $J_{d,i+1}^+$ and J_d , respectively [6].

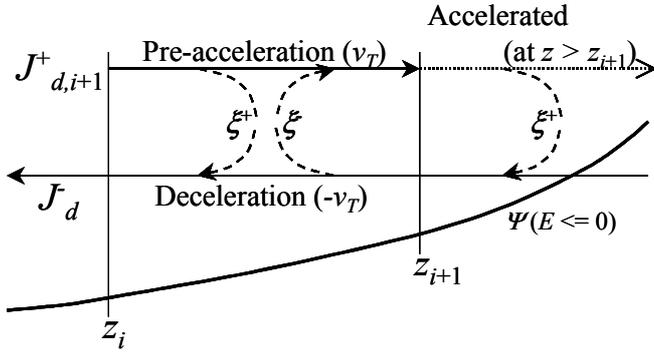


Figure 2: Illustration of carrier flux assumed in the developed model. $J_{d,i+1}^+$ (for $z \geq z_i$) is defined for every i larger than or equal to \min . Each dashed arrow indicates a specific scattering process.

According to the above definitions, one can extend 1-D steady-state McKelvey's one-flux equations [6] with accelerated-multi-flux. The extended McKelvey's equations are summarized in Fig. 3, where accelerated carrier flux $J_{d,\min}^+$ for $z \geq z_{\min}$ is introduced additionally to take into account ballistic carrier flux. $J_{d,\min}^+$ for $z \geq z_{\min}$ is assumed to undergo reflection transition into deceleration carrier flux J_d arising from scattering of $J_{d,\min}^+$ itself. At $z = z_{\min}$, $J_{d,\min}^+$ is identified with deceleration carrier flux in the upward region ($z \leq z_{\min}$), denoted by J_u^- . (The suffix u indicates the upward region.) A similar set of equations can be derived for the upward region. We note that the absolute unidirectional velocity of carrier flux at $z = z_{\min}$ is pinned fairly on v_T , because acceleration based on the energy conservation law is excluded from the position where Ψ is minimum. We also note that at ballistic limit, our extended McKelvey's method corresponds to the ballistic drift-diffusion model already established in Ref. [7].

For $z_i \leq z \leq z_{i+1}$ in downward ($E \leq 0$),

$$\begin{aligned} \frac{dJ_{d,i+1}^+}{dz} &= -\xi_d^+ J_{d,i+1}^+ + \xi_d^- J_d, & J_{d,i+1}^+ : \text{Ordinary + flux with the velocity } \llbracket v_T \rrbracket \\ & & \text{but accelerated at } z > z_{i+1}, \text{ and } J_{d,i+1}^+(z_i) = 0. \\ \frac{dJ_d^-}{dz} &= -\xi_d^+ \left(\sum_{j=\min}^{i+1} J_{d,j}^+ \right) + \xi_d^- J_d, & J_d^- : \text{Ordinary - flux with} \\ & & \text{the velocity } \llbracket -v_T \rrbracket. \\ \frac{dJ_{d,j}^+}{dz} &= -\xi_d^+ J_{d,j}^+, \quad (\min \leq j \leq i) & J_{d,j}^+ : \text{+ flux accelerated from the} \\ & & \text{j-th node with the velocity } v_{d,j}^+ \\ & & = [v_T^2 + 2q\{\Psi(z) - \Psi(z_j)\}/m^*]^{1/2}. \\ \xi_d^+ &= \xi_0, \quad \xi_d^- = \xi_0 - \frac{qE}{k_B T}. \end{aligned}$$

Figure 3: McKelvey's equations extended with accelerated-multi-flux. q denotes the elementary electronic charge, and k_B and T the Boltzmann constant and absolute temperature, respectively. Each equation describes the spatial gradient of specific carrier flux. Each term in right-handed sides corresponds to a specific scattering

process (see Fig. 2). Accelerated carrier flux decays exponentially with respect to z . Equations for ξ_d^+ and ξ_d^- have already been established in Ref. [6].

III. CORRECTED DRIFT-DIFFUSION MODEL AND PSEUDO CARRIER CONCENTRATION

Re-formulating our extended McKelvey's equations shown in Fig. 3 and defining $J_d^+ = \sum_{\min < j \leq i+1} J_{d,j}^+$ for $z_i \leq z \leq z_{i+1}$, a pair of equations identical apparently with original McKelvey's one-flux equations [6] is derived for J_d^+ and J_d^- . The re-formulation and the definition are summarized in Fig. 4.

$$\begin{aligned} \frac{dJ_{d,i+1}^+}{dz} &= -\xi_d^+ J_{d,i+1}^+ + \xi_d^- J_d^-, & (1) \\ \frac{dJ_d^-}{dz} &= -\xi_d^+ \left(\sum_{j=\min}^{i+1} J_{d,j}^+ \right) + \xi_d^- J_d^-, & (2) \\ \frac{dJ_{d,j}^+}{dz} &= -\xi_d^+ J_{d,j}^+, \quad (\min \leq j \leq i) & (3) \end{aligned}$$

$$\left[(1) + \sum_{j=\min}^i (3) \right] \text{ and defining } J_d^+ = \sum_{j=\min}^{i+1} J_{d,j}^+, \quad \begin{cases} \frac{dJ_d^+}{dz} = -\xi_d^+ J_d^+ + \xi_d^- J_d^- \\ \frac{dJ_d^-}{dz} = -\xi_d^+ J_d^+ + \xi_d^- J_d^- \end{cases}$$

Figure 4: Calculation of [(1) + $\Sigma(3)$] and definition of J_d^+ for $z_i \leq z \leq z_{i+1}$, which reduce extended McKelvey's equations into a pair of equations identical apparently with original McKelvey's one-flux equations.

It is well known that [6] in 1-D steady-state, substitution of $J_d^+ - J_d^- = -J/q$ and $J_d^+ + J_d^- = v_T N$ into original McKelvey's one-flux equations leads to conventional drift-diffusion equations for the current density J and the carrier concentration N , including Caughey-Thomas high-field mobility expression [1] with $\beta = 1$. On the other hand, in case of the same substitution into our extended McKelvey's equations, N should not be identified with the carrier concentration but with the pseudo one instead, because J_d^+ includes accelerated carrier flux whose velocity is not v_T . Therefore, we utilize the pseudo carrier concentration N^* instead of N . Consequently, our extended McKelvey's equations are reduced into the above conventional drift-diffusion equations in which the carrier concentration N is converted into the pseudo carrier concentration N^* . We note that a concept of the pseudo carrier concentration has already been established in Ref. [7].

By using the first equation shown in Fig. 5, the pseudo carrier concentration N^* can be transformed easily into the actual one denoted hereafter by n . $J_{d,j}^+(z_i)$ for $\min \leq j \leq i-1$ appearing in this equation is expressed as the second or third equation shown in Fig. 5, because $J_d^+ = [v_T N^* + (-J/q)]/2$, $J_{d,j}^+$ for $z > z_j$ is not supplied directly (see the second paragraph in Sec. II) and decays exponentially (see Fig. 3), and $J_{d,j}^+(z_j) = J_d^+(z_j) - J_d^+(z_{j-1}) \exp[-(z_j - z_{j-1})\xi_{0,j-1/2}]$ for $\min < j$. ($\xi_{0,j-1/2}$ denotes $\xi_d^+ = \xi_0$ for $z_{j-1} \leq z \leq z_j$.) We note that the charge density appearing in Poisson's equation should not be calculated from N^* but n instead.

$$\begin{aligned}
n(z_i) &= N^*(z_i) + \sum_{j=\min}^{i-1} J_{d,j}^+(z_i) \left\{ \frac{1}{v_{d,j}^+(z_i)} - \frac{1}{v_T} \right\}, \quad (\min < i) \\
J_{d,\min}^+(z_i) &= \frac{1}{2} \left[v_T N^*(z_{\min}) + \left(-\frac{J}{q} \right) \right] e^{-\sum_{k=\min}^{i-1} (z_{k+1}-z_k) \xi_{0,k+1/2}}, \\
J_{d,j}^+(z_i) &= \frac{1}{2} \left[v_T N^*(z_j) + \left(-\frac{J}{q} \right) \right. \\
&\quad \left. - \left\{ v_T N^*(z_{j-1}) + \left(-\frac{J}{q} \right) \right\} e^{-(z_j-z_{j-1}) \xi_{0,j-1/2}} \right] e^{-\sum_{k=j}^{i-1} (z_{k+1}-z_k) \xi_{0,k+1/2}}. \quad (\min < j)
\end{aligned}$$

Figure 5: Equations that transform the pseudo carrier concentration N^* into the actual one n . In these equations, the spatial distribution is considered for the transition rate coefficient $\xi_d^+ = \xi_0$. $v_{d,j}^+(z_i)$ denotes the velocity of accelerated carrier flux $J_{d,j}^+(z_i)$ for $\min \leq j \leq i-1$ (see Fig. 3).

IV. GENERALIZATION OF CORRECTED DRIFT-DIFFUSION MODEL AND TWO FUNDAMENTAL HYPOTHESES

Although an isothermal condition is assumed implicitly in Sec. II and Sec. III, the spatial variations for the temperature and thermal velocity of carriers can be evaluated, in principle, by considering the velocity distribution of accelerated-multi-flux and the energy dissipation into the x- and y-directions and into the lattice system owing to scattering processes. We note that under existence of these spatial variations, re-examination of the substitution discussed in Sec. III brings expression of the current density J to be generalized into $J = q\mu EN^* + qD(dN^*/dz) + (qDN^*/v_T)(dv_T/dz)$, where μ and D denote the high-field mobility and the diffusion coefficient, respectively. We also note that the suffix indicating the appropriate calculation node index should be added for v_T in Fig. 3 and Fig. 5. Consequently, one of fundamental hypotheses in this report is transferred from an isothermal condition into that carriers after scattering start moving with their local thermal velocities regardless of their history before scattering. We refer to the transferred fundamental hypothesis as velocity history truncation.

Next, we consider excess scattering owing to carrier acceleration. Our corrected drift-diffusion model derived in Sec. III neglects the excess scattering, because Sec. II assumes reflection transition arising from scattering of accelerated carrier flux to be equal to that for pre-acceleration one in the rate coefficient. Therefore, to take into account the excess scattering, we generalize our model by adding not only slowdown transition of accelerated carrier flux into pre-acceleration one but also dependence of the transition rates on the velocities of accelerated carrier flux. This generalization leads to equations (1'), (2'), and (3') for $z_i \leq z \leq z_{i+1}$ shown in Fig. 6, where ζ and η describe dependence of the reflection and slowdown transition rates on the velocities of accelerated carrier flux, respectively. If ζ and η are respectively $\mathbf{1}$ and $\mathbf{0}$ regardless of the carrier velocities, equations (1'), (2'), and (3') shown in Fig. 6 are reduced into equations (1), (2), and (3) shown in Fig. 4. We note that as far as ζ is $\mathbf{1}$, a pair of equations identical apparently with original McKelvey's one-flux

equations is derived regardless of details of η (see Fig. 6). This fact indicates that if ζ is $\mathbf{1}$ and if η accounts for excess scattering of accelerated carrier flux, our corrected drift-diffusion model is valid. We refer to these two conditions, which provide another fundamental hypothesis in this report, as ζ -priority or reflection transition priority. Under these two conditions, expression of $J_{d,j}^+(z_i)$ for $\min \leq j \leq i-1$ shown in Fig. 5 is generalized into a recursion formula shown in Fig. 7 so as to take into account velocity-dependent slowdown transition. We also note that deviation of ζ from $\mathbf{1}$ clouds relationship between our model and a conventional drift-diffusion one.

$$\frac{dJ_{d,i+1}^+}{dz} = -\xi_d^+ J_{d,i+1}^+ + \xi_d^- J_d^- + \xi_d^+ \left\{ \sum_{j=\min}^i \eta(v_{d,j}^+) J_{d,j}^+ \right\}, \quad (1')$$

$$\frac{dJ_d^-}{dz} = -\xi_d^+ J_{d,i+1}^+ + \xi_d^- J_d^- - \xi_d^+ \left\{ \sum_{j=\min}^i \zeta(v_{d,j}^+) J_{d,j}^+ \right\}, \quad (2')$$

$$\frac{dJ_{d,j}^+}{dz} = -\xi_d^+ \zeta(v_{d,j}^+) J_{d,j}^+ - \xi_d^- \eta(v_{d,j}^+) J_{d,j}^+. \quad (\min \leq j \leq i) \quad (3')$$

$$\begin{aligned}
&\left[(1') + \sum_{j=\min}^i (3') \right] \text{ and defining} \quad \begin{cases} \frac{dJ_d^+}{dz} = -\xi_d^+ J_d^+ + \xi_d^- J_d^-, \\ \frac{dJ_d^-}{dz} = -\xi_d^+ J_d^+ + \xi_d^- J_d^-. \end{cases} \\
&\zeta(v_{d,j}^+) = 1 \text{ and } J_d^+ = \sum_{j=\min}^{i+1} J_{d,j}^+,
\end{aligned}$$

Figure 6: Generalized version of extended McKelvey's equations for $z_i \leq z \leq z_{i+1}$. As far as ζ is $\mathbf{1}$, the same calculation and definition as shown in Fig. 4 also reduce the generalized version into a pair of equations identical apparently with original McKelvey's one-flux equations.

$$\begin{aligned}
J_{d,\min}^+(z_i) &= \frac{1}{2} \left[v_T N^*(z_{\min}) + \left(-\frac{J}{q} \right) \right] \\
&\quad e^{-\sum_{k=\min}^{i-1} (z_{k+1}-z_k) \xi_{0,k+1/2} [1 + \eta\{v_{d,\min}^+(z_{k+1/2})\}]}, \\
J_{d,j}^+(z_i) &= \left[\frac{1}{2} \left\{ v_T N^*(z_j) + \left(-\frac{J}{q} \right) \right\} \right. \\
&\quad \left. - \sum_{l=\min}^{j-1} J_{d,l}^+(z_j) \right] e^{-\sum_{k=j}^{i-1} (z_{k+1}-z_k) \xi_{0,k+1/2} [1 + \eta\{v_{d,j}^+(z_{k+1/2})\}]} \quad (\min < j)
\end{aligned}$$

Figure 7: Generalized expression of accelerated carrier flux $J_{d,j}^+(z_i)$ for $\min \leq j \leq i-1$. ζ is assumed to be $\mathbf{1}$ regardless of the carrier velocities. η is assumed to depend on the velocities of accelerated carrier flux. For a reference, see the second and third equations shown in Fig. 5.

V. NUMERICAL CALCULATION

Assuming 1-D n+-n-n+ structure and an isothermal condition without excess scattering of accelerated carrier flux ($\zeta = \mathbf{1}$ and $\eta = \mathbf{0}$), we carried out numerical calculation for our corrected drift-diffusion model by means of a naive self-consistent loop. For a reference, we also carried out

self-consistent calculation of conventional drift-diffusion and energy transport models [1]. The concentrations of completely-ionized donor impurities in the n+-region and n-region were set as 1×10^{20} and 4×10^{17} $1/\text{cm}^3$, respectively. The low-field mean-free-paths in the both regions were set as 3.22 and 21.7 nm, respectively. We applied a bias difference between input and output ohmic contacts as 1 V. According to Ref. [8], the parameter f_{hf} in an energy transport model was set empirically as 0.1.

We confirmed that when the n-region was 1000 nm in length, self-consistent electrostatics remained almost the same for all the three models (see Fig. 8). On the contrary, when the n-region was 100 nm in length, the three models exhibited the substantially different pictures in self-consistent electrostatics, as shown in Fig. 9. Moreover, Fig. 9 indicates that forming a contrast with remarkable carrier velocity overshoot reproduced by our corrected drift-diffusion model, an energy transport one with $f_{hf} = 0.1$ accelerates carriers only near the beginning of the channel and decelerates those under the increasing fields [9]. This result seems to suggest that the energy transport model underestimates carrier acceleration under the increasing fields and makes carrier deceleration effects owing to the increasing carrier temperatures pronounced.

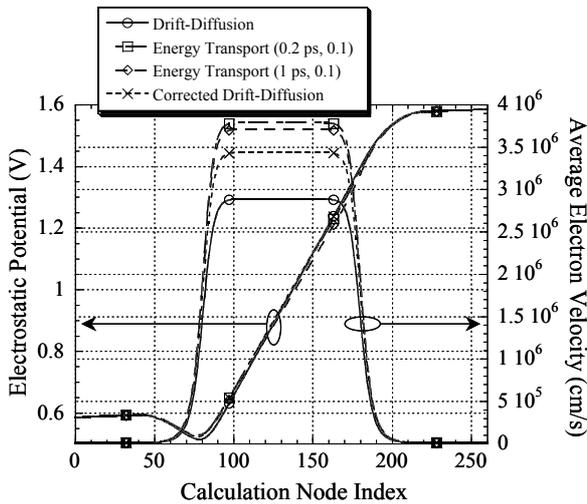


Figure 8: Electrostatic potentials and average electron velocities as a function of the calculation node index. The distance between neighboring calculation nodes was 10 nm and the length of the n-region was 1000 nm. For an energy transport model, the energy relaxation time was set as 0.2 or 1 ps and f_{hf} as 0.1.

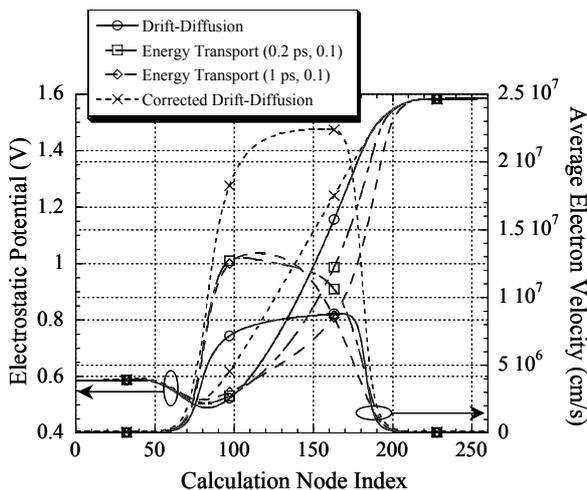


Figure 9: Electrostatic potentials and average electron velocities as a function of the calculation node index. The distance between neighboring calculation nodes was 1 nm and the length of the n-region was 100 nm.

VI. CONCLUSION

By introducing accelerated-multi-flux into McKelvey's one-flux method, we have developed the corrected drift-diffusion model in one-dimensional steady-state. The developed model takes into account not only carrier acceleration owing to the electrostatic fields, namely, carrier velocity overshoot but also the pinning of the absolute unidirectional carrier velocity at the beginning of the channel on its thermal value, namely, ballistic carrier transport limit. Generalization of the developed model reveals two fundamental hypotheses, namely, velocity history truncation and reflection transition priority, which justify the drift-diffusion model corrected only with additional carrier concentration calculation. Self-consistent calculation seems to suggest that description of the carrier velocities utilizing the explicitly introduced accelerated-multi-flux is advantageous to the modeling of highly off-equilibrium quasi-ballistic carrier transport, as against conventional hierarchical moment equations based on an assumption of the diffusion-dominated system with low Knudsen number enough to neglect the convective terms.

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