

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].

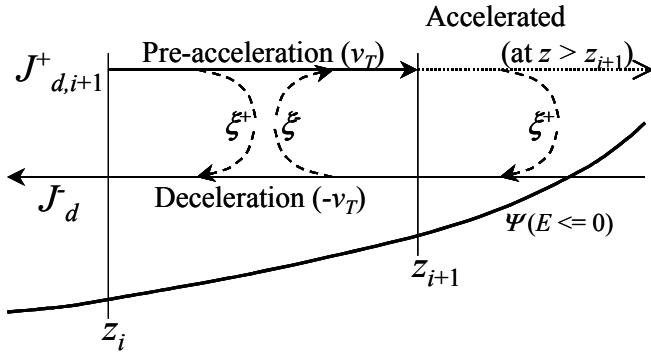


Figure 2: Illustration of carrier flux assumed in the developed model. $J_{d,i+1}^+$ (for $z \geq z_i$) is defined for every i larger than or equal to \min . Each dashed arrow indicates a specific scattering process.

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

