A Fermi-Dirac Statistics Based Quantum Energy Transport Model for High Mobility MOSFETs

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Abstract. In this paper, a Fermi-Dirac statistics based quantum energy transport (FDQET) model is developed for numerical simulations of high mobility MOSFETs. The QET model allows simulations of carrier transport including quantum confinement and hot carrier effects. Fermi-Dirac statistics are further considered for the analysis of device characteristics with high degeneracy material such as In0.53Ga0.47As. Numerical stability and convergence are achieved by developing an iterative solution method used when Fermi-Dirac statistics are modeled. Numerical results for Si, Ge and In0.53Ga0.47As bulk n-MOSFETs are presented. The FDQET model allows us to evaluate the device characteristics with high degeneracy material such as In0.53Ga0.47As.

Keywords: Quantum energy transport model, Fermi-Dirac statistics, semiconductor device simulation, InGaAs

1. Introduction

The performance of semiconductor devices primarily relies on carrier transport properties in the short channels. As pointed out in [1], new channel materials are needed to achieve high performance and low power CMOS devices. For this reason, the numerical simulation of quantum hydrodynamics in semiconductors is a major concern to understand the quantum effects and hot carrier effects in scaled devices. The quantum hydrodynamic (QHD) model is derived by Gardner [2] from a moment expansion of the Wigner-Boltzmann equation adding a collision term. The quantum energy transport (QET) model is derived by a diffusion approximation of the QHD models. It is shown in [3] that the QET model allows simulations of carrier transport including quantum confinement and hot carrier effects. Due to a smaller density of states and a stronger degeneracy of Ge and In0.53Ga0.47As compared with Si, Fermi-Dirac statistics should be considered in the transport model for future CMOS devices. A number of authors have focused on numerical simulations under Fermi-Dirac statistics, using Ensemble Monte Carlo simulation [4], multi-subband Monte Carlo simulation [5, 6],
In this paper, we newly develop a Fermi-Dirac statistics based QET (FDQET) model. Numerical stability and convergence are achieved by developing an iterative solution method with a relaxation method. Numerical results of Si, Ge and In$_{0.53}$Ga$_{0.47}$As n-MOSFETs are demonstrated.

The paper is organized as follows: In Section 2, we describe a Fermi-Dirac statistics based four-moments QET model. An iterative solution method for the FDQET model is developed in Section 3. Section 4 discusses numerical results of Si, Ge and In$_{0.53}$Ga$_{0.47}$As MOSFETs obtained under Boltzmann and Fermi-Dirac statistics. Section 5 concludes this paper.

2. Four-moments quantum energy transport model

2.1. A Boltzmann statistics based QET model

For the simulations of quantum confinement transport with hot carrier effects in scaled MOSFETs, we develop a four-moments quantum energy transport (QET) model based on Boltzmann statistics in [3]. This model is viewed as one of the hierarchy of the quantum hydrodynamic models [2]. Fig.1 shows a hierarchy of carrier transport models. In analogy to the classical hydrodynamic model, the quantum hydrodynamic (QHD) model is derived from a Chapman-Enskog expansion of the Wigner-Boltzmann equation. The QET and quantum drift diffusion (QDD) models are further derived by using a diffusion scaling of the QHD model. For classical hydrodynamic simulations, the closure relation based on the four-moments of the Boltzmann equation has been discussed in [9, 10, 11], and a four-moments energy transport (ET) model [12] has been developed for simulations of thin body MOSFETs.

In [3], the four-moments QET model is developed from four moments equations with quantum corrections to the stress tensor $P_{ij}$ [13] and the energy density $W$ [14], which are given by

$$P_{ij} = -nkT_n\delta_{ij} + \frac{\hbar^2}{12m}n\frac{\partial^2}{\partial x_i \partial x_j} \log n + O(\hbar^4),$$

$$W = \frac{1}{2}mv^2 + \frac{3}{2}nkT_n - \frac{\hbar^2}{24m}n\frac{\partial^2}{\partial x_k^2} \log n + O(\hbar^4),$$

where $n$, $T_n$ and $v$ are the electron density, electron temperature, and electron velocity, respectively. $k$, $\hbar$, and $m$ are the Boltzmann’s constant, Plank’s constant, and effective mass. In this case, the parabolic band is assumed. The quantum potential

$$\gamma_n = \frac{\hbar^2}{6mq} \frac{1}{\sqrt{n}} \frac{\partial^2}{\partial x_j^2} \sqrt{n}$$

(3)
is derived from $O(h^2)$ corrections to the stress tensor $P_{ij}$. This term is included in the current continuity equation as

$$\frac{1}{q} \text{div} J_n = 0, \quad (4)$$

$$J_n = q\mu_n(\nabla(n\frac{kT_n}{q}) - n\nabla(\varphi + \gamma_n)), \quad (5)$$

where $q$ and $\mu_n$ are the electronic charge and electron mobility. $\varphi$ is the electrostatic potential. From (3), the quantum potential equation is described as

$$2b_n\nabla^2 n + \nabla \cdot (n\nabla E_n) = 0, \quad (6)$$

where $b_n = \frac{g^2}{\tau_{sp}}$. The root-density under Boltzmann statistics is written as $\rho_n = \sqrt{n} = \sqrt{n_nexp(u_n)}$ by a variable $u_n = \frac{q}{kT_n} (\frac{\varphi + \gamma_n - \varphi_n}{2})$, where $\varphi_n$ is the quasi-Fermi-level. As shown in [15], (6) is replaced by

$$b_n \nabla \cdot (\rho_n \nabla u_n) - \frac{kT_n}{q} \rho_n u_n = -\frac{\rho_n}{2} (\varphi - \varphi_n). \quad (7)$$

If the variable $u_n$ is uniformly bounded, the electron density is maintained to be positive. This approach provides numerical advantages for developing an iterative solution method of the QET model [3] as well as the QDD model [15, 16].

The fourth moment of the Wigner-Boltzmann equation is given by

$$\nabla \cdot (nR) - n(WI + U) \cdot F_E = -\frac{qS}{\mu_s}, \quad (8)$$

Figure 1: A hierarchy of transport models.
where the fourth moment tensor is specified by the classical form as

$$ R = \frac{5}{2} k^2 T_n^2 I. \quad (9) $$

Using closure (9), we have the same form as that of the classical model [9] for an expression of the energy flow

$$ S_n = \frac{\mu_s}{\mu_n} (W I + n U) \cdot \mathbf{v} + \frac{\mu_s}{q} ((w I + U) \cdot \nabla \cdot (n U) - \nabla \cdot \left( \frac{5}{2} nk^2 T_n^2 I \right)), \quad (10) $$

where $I$ is the identity tensor. By assuming a parabolic band, we give the closure relation for $U$ as

$$ U_{ij} = m v_i v_j - \frac{P_{ij}}{n}, \quad (11) $$

The first term of (10) is the drift contributions and the second term of (10) is the diffusive contributions to the energy flow which includes the classical form of $R$. In the four-moments QET model, the quantum corrections to the energy density $W$ and stress tensor $P_{ij}$ are included in the drift contributions to the energy flow $S_n$ and neglected in the diffusive contributions. The energy balance equation then becomes

$$ \nabla \cdot S_n = -J_n \cdot \nabla \varphi - \frac{3}{2} k n T_n - T_L, \quad (12) $$

$$ S_n = -\frac{\mu_s}{\mu_n} \frac{5 k T_n}{2 q} - \frac{h^2}{24m q} \Delta \log n - \gamma_n J_n - \frac{\mu_s}{\mu_n} \frac{5}{2} \left( \frac{k}{q} \right)^2 q n T_n \nabla T_n, \quad (13) $$

where $T_L$ and $\tau_{\omega}$ are the lattice temperature and the energy relaxation time.

### 2.2. A Fermi-Dirac statistics based QET model

Numerical implementation of Fermi-Dirac statistics is discussed in [15] for the QDD model. The electron density $n$ is approximated by introducing the band parameter $\omega_n$ as

$$ n = n_i \exp(\frac{q}{k T_n}(\varphi + \gamma_n + \omega_n - \varphi_n)), \quad (14) $$

where $\varphi_n$ is the quasi-Fermi-level. The band parameter $\omega_n$ is determined as

$$ \omega_n = \frac{k T_n}{q} \left( \log(\frac{n}{N_c}) - G_{\frac{1}{2}} \left( \frac{n}{N_c} \right) \right), \quad (15) $$

where $N_c$ is the density of states in the conduction band, and $G_{\frac{1}{2}}$ is the inverse Fermi function of order 1/2. A convenient fit for numerical implementation is given in [17].

By employing the expression (14) in the QET model, we obtain the current density

$$ J_n = q \mu_n \nabla \left( n \frac{k T_n}{q} \right) - n \nabla (\varphi + \gamma_n + \omega_n)). \quad (16) $$
Using (14), we can also employ an exponential transformation of a variable \( \rho_n = \sqrt{n} = \sqrt{\frac{q}{kT}}(\varphi_n + \omega_n + \varphi_n^2) \). For Fermi-Dirac statistics, (6) is replaced by the equivalent form

\[
b_n \nabla \cdot (\rho_n \nabla u_n) - \frac{kT_n}{q} \rho_n u_n = -\frac{\rho_n}{2}(\varphi + \omega_n - \varphi_n).
\]

(17)

For the case of electrons, the four-moments QET model based on Fermi-Dirac statistics is described as follows:

\[
\epsilon \Delta \varphi = q(n - p - C_{imp}),
\]

(18)

\[
\frac{1}{q} \text{div} J_n = 0,
\]

(19)

\[
J_n = q\mu_n(\nabla(n\frac{kT_n}{q}) - n\nabla(\varphi + \omega_n + \gamma_n)),
\]

(20)

\[
b_n \nabla \cdot (\rho_n \nabla u_n) - \frac{kT_n}{q} \rho_n u_n = -\frac{\rho_n}{2}(\varphi + \omega_n - \varphi_n),
\]

(21)

\[
\nabla \cdot S_n = -J_n \cdot \nabla \varphi - \frac{3}{2} \frac{k}{\tau_e} n T_n - T_L
\]

(22)

\[
S_n = -\frac{\mu_s}{\mu_n} \frac{5}{2} \frac{kT_n}{q} - \frac{h^2}{24mq} \Delta \log n - \gamma_n J_n - \frac{\mu_s}{\mu_n} \frac{5}{2} \frac{k}{q} \mu_n n T_n \nabla T_n
\]

(23)

where \( p, \epsilon \) and \( C_{imp} \) are the hole density, the permittivity of semiconductor, and the ionized impurity density, respectively. The ratio \( \mu_n/\mu_s \) selected here is 0.8 [8].

The system (18)-(23) are solved in the bounded domain \( \Omega \). The boundary \( \partial \Omega \) of the domain \( \Omega \) splits into two disjoint part \( \Gamma_D \) and \( \Gamma_N \). The contacts of semiconductor devices are modeled by the boundary conditions on \( \Gamma_D \), which fulfill charge neutrality and thermal equilibrium. We further assume that no quantum effects occur at the contacts. Here, the boundary conditions are given as follows:

\[
\varphi = \varphi_b + \varphi_{app}, \quad n = n_D, \quad u_n = u_D, \quad T_n = T_L \quad \text{on} \quad \Gamma_D,
\]

(24)

\[
\nabla \varphi \cdot \nu = \nabla u_n \cdot \nu = \nabla S_n \cdot \nu = 0 \quad \text{on} \quad \Gamma_N,
\]

(25)

where \( \varphi_b \) is a built-in potential and \( \varphi_{app} \) is an applied bias voltage. It should be noted that the Dirichlet boundary conditions of the FDQET model are different from that of the Boltzmann statistics based QET (BQET) model. The built-in potential and \( u_D \) are given by the band parameter \( \omega_n \) as follows:

\[
\varphi_b = \frac{kT_n}{q} \log(n_{\text{ni}}/n) - \omega_n
\]

(26)

\[
u_D = \left\{ \begin{array}{ll}
(q(\varphi_b + \omega_n))/(2kT_L) \quad \text{on the contacts}, \\
u_0 \quad \text{at the interface},
\end{array} \right.
\]

(27)

where \( u_0 \) is a small positive constant.
2.3. Mobility model

For the energy dependence of the mobility, we apply the model of the Baccarani et al. [18],

$$\frac{\mu_n(T_n)}{\mu_{LF}} = \frac{T_L}{T_n}. \quad (28)$$

To account for the mobility reduction due to ionized impurity scattering, we use the formula of Caughey and Thomas[19] for the low-field mobility $$\mu_{LF}$$ in this work:

$$\mu_{LF} = \mu_{min} + \frac{\mu_L - \mu_{min}}{1 + \left(\frac{T}{C_{ref}}\right)\alpha}. \quad (29)$$

The model parameter values [20, 21] are summarized in Table 1. The effects of interface traps and surface roughness scattering are not included in the mobility model.

2.4. I-V characteristics and temperature distribution

Fig. 2 shows a comparison of $$I_D-V_D$$ characteristics of a 25nm Si bulk n-MOSFET for $$V_g=0.8V$$. The results are calculated by the FDQET model with (28) and low-field mobility, respectively. We obtain the saturated drain current when using the temperature dependent

| Material   | $$\mu_L$$ (cm$$^2$/Vs) | $$\mu_{min}$$ (cm$$^2$/Vs) | $$C_{ref}$$ | $$\alpha$$ |
|------------|-------------------------|-----------------------------|-------------|------------|
| Si         | 1400[20]                | 80                          | 1.12e17     | 0.72       |
| Ge         | 3900[20]                | 850                         | 2.6e17      | 0.56       |
| In$_{0.53}$Ga$_{0.47}$As | 14000[21] | 300[21]                     | 1.3e17[21]  | 0.48[21]   |

Figure 2: Comparison of the $$I_D-V_D$$ characteristics of a 25nm Si bulk n-MOSFET with low-field mobility and Baccarani’s mobility model.
Figure 3: Comparison of the $I_d - V_G$ characteristics of a 25nm bulk Si n-MOSFET between the FDQET and FDET models.

Figure 4: Lateral profiles of electron temperature distributions calculated by the FDQET and FDET models at $V_g = 0.8V$ and $V_d = 0.8V$.

mobility model. We also plot the $I_D-V_D$ characteristics calculated by the BQET model with (28). It is shown that the drain current calculated by the FDQET model is slightly lower than that calculated by the BQET model. This result is consistent with that in [5].

In Fig. 3, we compare the $I_D-V_G$ characteristics at $V_d=0.05$ and 0.8V. The results are compared between the FDQET and Fermi-Dirac based classical ET (FDET) models. As the FDQET model includes the quantum effect, the SS and DIBL are increased from 81mV/dec to 89mV/dec and from 56mV/V to 86mV/V, respectively. The channel broadening effect increases the SS and DIBL. The threshold voltage is increased due to the quantum confinement effects in the channel, in this case by about 90mV. Fig. 4 shows lateral profiles of electron temperature calculated by the FDQET and FDET models at $V_g=0.8V$ and $V_d=0.8V$. 
The device has the gate length of 25nm. At the same gate voltage, the FDQET model exhibits a sharper distribution of electron temperature at the lateral direction, when compared to that calculated by the FDET model. This difference is caused by the threshold voltage shift due to the quantum confinement in the channel, as shown in Fig. 3.

3. Iterative solution method

As mentioned in our previous work [3], we also consider the conservation of the total energy flow \( H = S_n + \varphi J_n \). In case of Fermi-Dirac statistics, the current density \( J_n \) and energy flow \( S_n \) can be written in the same form as

\[
\nabla \cdot F = \nabla \cdot (C(\nabla \xi - \frac{q}{kT_n} \xi \nabla (\varphi + \gamma_n + \omega_n))),
\]

where \( F \) is the flux. The variable \( \xi \) and constant \( C \) are defined as \( \xi = n \frac{kT_n}{q} = n \eta \) and \( C = q\mu_n \) in the current density \( J_n \) and \( \xi = n(\frac{kT_n}{q})^2 = n \eta^2 \) and \( C = -\frac{q}{2} q\mu_n \) in the energy flow \( S_n \). By projecting (30) onto a grid line and using the variable \( g = \int_{x_i}^{x} \frac{kT_n}{q} \nabla (\varphi + \gamma_n + \omega_n) \), a one-dimensional self-adjoint form is obtained as

\[
\frac{d}{dx} F = \frac{d}{dx} (Ce^\theta \frac{d}{dx} (e^{-\eta x})).
\]

In order to mention the iterative solution method for the FDQET model, we discuss an iterative solution method for the Fermi-Dirac based QDD (FDQDD) model. As shown in [15], the FDQDD model for the case of electrons is described as follows:

\[
\epsilon \Delta \varphi = q(n - p - C_{imp}),
\]
\[
\frac{1}{q^2} \text{div} J_n = 0,
\]
\[
J_n = q\mu_n e^\varphi \nabla (e^{-\eta x} n),
\]
\[
b_n \nabla \cdot (\rho_n \nabla u_n) - \frac{kT_n}{q} \rho_n u_n = -\frac{\rho_n}{2} (\varphi + \omega_n - \varphi_n).
\]

The electron temperature \( T_n \) is equal to \( T_L \) in the FDQDD model. An iterative solution method for the FDQDD model is developed by constructing an extended Gummel map [22] with a set of unknown variables (\( \varphi, u_n, n \)) as follows:

- For \( j = 1, \ldots, j_{\text{max}} \) (\( j \) is the outer iteration counter)

  \textbf{(A1)} Let \( \varphi^j \) and \( n^j \) are given, solve the nonlinear Poisson equation with respect to the electrostatic potential \( \varphi^{j+1} \). (18) is linearized using a Newton method. Then the linearized equation becomes

\[
\epsilon \Delta \varphi^{j+1} - \frac{q^2}{k} (\frac{n^j}{T_n} + \frac{P}{T_p}) \varphi^{j+1} = q(n^j - p^j - C) - \frac{q^2}{k} (\frac{n^j}{T_n} + \frac{P}{T_p}) \varphi^j.
\]
(A2) Let $\phi^{j+1}, \rho_n^j, \omega_n^j,$ and $\varphi_n^j$ are given, solve the potential $u_n^{j+1}$:

$$b_n \nabla \cdot (\rho_n^j \nabla u_n^{j+1}) - \eta \rho_n^j u_n^{j+1} = -\frac{\rho_n^j}{2} (\varphi_n^{j+1} + \omega_n^j - \varphi_n^j).$$  \hspace{2cm} (37)

(A3) Set: $\gamma_n^{j+1} = 2 \eta u_n^{j+1} + \varphi_n^j - \varphi^{j+1} - \omega_n^j$.

(A4) For $k = 1, \ldots, k_{\text{max}}$ ($k$ is the inner iteration counter)

\begin{itemize}
  \item [(B1)] Let $\phi^{j+1}, \gamma_n^{j+1},$ and $\omega_n^k$ are given, solve the electron density $n^{k+1}$:

\end{itemize}

$$\frac{1}{q} \text{div} J_n = 0,$$

$$J_n = q \mu_n e^\varphi (\varepsilon - g_n^{j+1} \eta).$$  \hspace{2cm} (39)

(B2) Set: $\omega_n^{k+1} = \frac{kT_{n+1}}{q} (\log(n_{n+1}^{k+1} N_n) - G_j \frac{n_{n+1}^{k+1}}{N_n})$

(B3) If the stopping criterion is satisfied, set: $n^{j+1} = n^{k+1}, \omega_n^{j+1} = \omega_n^{k+1}, \varphi_n^{j+1} = -\eta \log \frac{n_{n+1}^{j+1}}{n_n^j} + \varphi_n^j + \gamma_n^{j+1} + \omega_n^j$. and proceed to step (A5).

else: set: $\omega_n^{k+1} = \omega_n^k + \alpha (\omega_n^{k+1} - \omega_n^k)$ and return to step (B1).

(A5) If the stopping criterion is not satisfied, return to step (A1).

An iterative solution method, which consists of the inner (loop B) and outer (loop A) iteration loops, is developed, as shown in Fig. 5 (a). The algorithm using the variable $u_n$ in (35) ensures the positivity of the root-density of electrons without introducing damping parameters as pointed out in [15]. We can further enhance the numerical stability of the loop B by introducing an under relaxation method with a parameter $\alpha$, $0 < \alpha < 1$:

$$\omega_n^{k+1} = \omega_n^k + \alpha (\omega_n^{k+1} - \omega_n^k).$$  \hspace{2cm} (40)

The relaxation parameter $\alpha = 0.2$ for Si and Ge n-MOSFETs and $\alpha = 0.01$ for $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ n-MOSFET are used in this work.

We extend a Gummel map developed in the FDQDD model to an iterative solution method for the FDQET model. The iterative solution method for the FDQET model with a set of unknown variables ($\varphi$, $u_n$, $n$, $T_n$) is developed as follows:

- For $j = 1, \ldots, j_{\text{max}}$ ($j$ is the iteration counter)

\begin{itemize}
  \item [(A1)] Let $\phi^j, n^j, T_n^j$ are given, solve the nonlinear Poisson equation with respect to the electrostatic potential $\phi^{j+1}$:

$$\varepsilon \Delta \phi^{j+1} - \frac{q^2}{k} \left( \frac{n^j}{T_n^j} + \frac{P}{T_p} \right) \phi^{j+1} = q(n^j - p^j - C) - \frac{q^2}{k} \left( \frac{n^j}{T_n^j} + \frac{P}{T_p} \right) \phi^j.$$  \hspace{2cm} (41)

  \item [(A2)] Let $\phi^{j+1}, \rho_n^j, \omega_n^j, \varphi_n^j, T_n^j$ are given, solve the potential $u_n^{j+1}$:

$$b_n \nabla \cdot (\rho_n^j \nabla u_n^{j+1}) - \eta \rho_n^j u_n^{j+1} = -\frac{\rho_n^j}{2} (\varphi_n^{j+1} + \omega_n^j - \varphi_n^j).$$  \hspace{2cm} (42)

\end{itemize}
(A3) Set: \( \gamma^{j+1}_n = 2\eta^j u^{j+1}_n + \varphi_n^j - \varphi^{j+1} - \omega_n^j \).

(A4) For \( k = 1, \ldots, k_{\text{max}} \) (\( k \) is the iteration counter)

(B1) For \( l = 1, \ldots, m_{\text{max}} \) (\( m \) is the iteration counter)

(C1) Let \( \varphi^{j+1}_n, \gamma^{j+1}_n, \omega^k_n \), and \( T^m_n \) are given, solve the electron density \( n^{m+1} \):

\[
\frac{1}{q} \text{div}J_n = 0, \quad J_n = q\mu_ne^\varphi(e^{-qT^{m+1}n^{m+1}},) \tag{43}\]

\[
\n^{m+1} = -J_n \cdot \nabla(\varphi^{j+1} + \frac{\mu_e}{\mu_n}(\gamma^{j+1}_n + b_n \Delta u^{j+1}_n) + \frac{3}{2} \frac{k^{m+1}T^{m+1}}{\tau_e}. \tag{44}\]

\[
S_n = -\frac{5}{2} q\mu_ne^\varphi(e^{-qT^{m+1}n^{m+1}}(\eta^{m+1})^2). \tag{45}\]

(C3) If the stopping criterion is satisfied, set: \( n^{k+1} = n^{m+1}, T^{k+1}_n = T^{m+1}_n \) and proceed to step (B2)

else: set: \( T^{m+1}_n = T^n_n + \beta(T^{m+1}_n - T^n_n) \) and return to step (C1).

(B2) Set: \( \omega^{k+1}_n = \frac{kT^{k+1}_n}{\eta}(\log(\frac{n^{k+1}_n}{N_i}) - G_1(\frac{n^{k+1}_n}{N_i})) \)

(B3) If the stopping criterion is satisfied, set: \( n^{j+1}_n = n^{k+1}_n, \omega^{j+1}_n = \omega^{k+1}_n \), \( T^{j+1}_n = T^{k+1}_n, \varphi^{j+1}_n = -\eta^{j+1}_n \log(\frac{n^{j+1}_n}{N_i}) + \varphi^{j+1}_n + \gamma^{j+1}_n + \omega^{j+1}_n \). and proceed to step (A5).

else: set: \( \omega^{k+1}_n = \omega^{k}_n + \alpha(\omega^{k+1}_n - \omega^{k}_n) \) and return to step (B1).

(A5) If the stopping criterion is not satisfied, return to step (A1).

An iterative solution method, which consists of the triple iteration loops (loop A, B, and C), is developed, as shown in Fig. 5 (b). The Gummel iteration is applied in each inner loops. We introduce an additional inner loop (loop C) to solve the current continuity and energy balance equations. In order to enhance numerical stability of the loop C, we also introduce an under relaxation method with a parameter \( \beta, 0 < \beta < 1 \):

\[
T^{m+1}_n = T^n_n + \beta(T^{m+1}_n - T^n_n). \tag{47}\]

The relaxation parameter \( \beta = 0.2 \) is used for all devices. The convergence behaviors for each iteration loops in the FDQET model are shown in Fig. 6. The convergence analysis of the numerical method is performed with numerical experiment on a two dimensional bulk
Figure 5: Iterative solution methods for (a) the FDQDD model and (b) the FDQET model.

Figure 6: Convergence behaviors of electron temperature, band parameter $\omega_n$, and electrostatic potential vs. number of iterations.
n-MOSFET. For the electrostatic potential and the band parameter $\omega_n$, the error is estimated as follows:

$$
||\varphi|| = \max_{i,j} |\varphi_{ij}^{k+1} - \varphi_{ij}^k|, 
$$

(48)

$$
||\omega_n|| = \max_{i,j} |\omega_{nj}^{k+1} - \omega_{nj}^k|.
$$

(49)

The iteration loops A and B are stopped when the values of (48) and (49) are less than $10^{-3}$. The relative error for the electron temperature is estimated as

$$
||T|| = \max_{i,j} \frac{|T_{nj}^{m+1} - T_{nj}^m|}{|T_{nj}^m|}. 
$$

(50)

The iteration loop C is stopped when the value of (50) is less than $10^{-3}$. The error estimates are obtained in the first iteration of Gummel map at the bias condition $V_g = 0.4V$ and $V_d = 0.3 \rightarrow 0.4V$. It is clearly show that the error decreases as the number of Gummel iterations increases in each loops, respectively.

4. Numerical results

The schematic views of simulated devices are shown in Fig. 7. Si, Ge, and In$_{0.53}$Ga$_{0.47}$As bulk n-MOSFETs with high-k/metal gates are examined. 7708 grids are used for simulations. Selected material parameters are listed in Table 2. The relative dielectric permittivity considered here is 22, and the value is known as "HfO$_2". The equivalent oxide thickness (EOT) is 0.7nm. The threshold voltage of all devices is obtained by adjustment of the gate work function, which are selected for each semiconductor material to meet a common threshold voltage of 0.2V. The gate length of simulated devices is 70nm. The S/D doping is $N_{SD} = 1.0 \times 10^{20} cm^{-3}$ for Si and Ge n-MOSFETs. Since activated donor concentrations larger than $2.0 \times 10^{19} cm^{-3}$ cannot be obtained in In$_{0.53}$Ga$_{0.47}$As n-MOSFETs [23], we adopt $N_{SD} = 2.0 \times 10^{19} cm^{-3}$ for an In$_{0.53}$Ga$_{0.47}$As n-MOSFET. We further assume channel dopings of $2.0 \times 10^{18} cm^{-3}$ for bulk n-MOSFETs.

Figure 7: Schematic views of the simulated 70nm Bulk n-MOSFET.
Figs. 8 (a)-(c) show electron density distributions perpendicular to the interface calculated by the BQET and FDQET models for 70nm Si, Ge, and In$_{0.53}$Ga$_{0.47}$As bulk n-MOSFETs at the center of the channel. The simulations are done at $V_g=0.5V$ and $V_d=0.05V$. It is clearly show that the inversion layer electrons calculated by the BQET and FDQET models are almost identical for Si and Ge n-MOSFETs. The inversion layer electron for In$_{0.53}$Ga$_{0.47}$As n-MOSFET calculated by the FDQET model is lower than that calculated by the BQET model due to the smaller $N_c$ and the stronger carrier degeneracy of In$_{0.53}$Ga$_{0.47}$As. This result in the significant decrease of the on current calculated by the FDQET model in In$_{0.53}$Ga$_{0.47}$As n-MOSFET.

Figs. 9, 10, and 11 show comparisons of $I_D-V_G$ characteristics of the BQET and FDQET models for 70nm Si, Ge, and In$_{0.53}$Ga$_{0.47}$As bulk n-MOSFETs with logarithmic and linear scales. The simulations are done at $V_d=0.05V$. In the subthreshold region, $I_D-V_G$ characteristics between two models are almost identical in all devices and hence the subthreshold slopes evaluated by the BQET and FDQET models are almost identical. Even in saturated region, both models show the almost identical drain current characteristics for the Si n-MOSFET. Because of the smaller $N_c$ and the stronger carrier degeneracy of Ge and In$_{0.53}$Ga$_{0.47}$As, the drain currents calculated by the FDQET model is lower than that calculated by the BQET model in Ge and In$_{0.53}$Ga$_{0.47}$As n-MOSFETs. It is shown that the linear and saturated drain currents are significantly decreased in In$_{0.53}$Ga$_{0.47}$As n-MOSFETs.

| semiconductor | Si  | Ge  | In$_{0.53}$Ga$_{0.47}$As |
|---------------|-----|-----|-------------------------|
| $E_G$(eV)     | 1.12[24] | 0.66[24] | 0.73[24] |
| $\varepsilon\varepsilon_0$ | 11.7[24] | 16.0[24] | 14.0[24] |
| $m_{eff}/m_0$ | 0.26[25] | 0.12[25] | 0.048[24] |
| $n_i$(cm$^{-3}$) | $1.08 \times 10^{10}[25]$ | $1.64 \times 10^{13}[25]$ | $9.0 \times 10^{11}[26]$ |
| $v_{saf}$(cm/s) | $1.0 \times 10^7[27]$ | $0.7 \times 10^7[27]$ | $0.75 \times 10^7[27]$ |
| $N_c$(cm$^{-3}$) | 2.86e19[25] | 1.05e19[25] | 2.64e17 |
| $N_{SD}$(cm$^{-3}$) | $1.0 \times 10^{20}$ | $1.0 \times 10^{20}$ | $2.0 \times 10^{19}[23]$ |
Figure 8: Electron density distributions perpendicular to the interface calculated by the BQET and FDQET models for 70nm (a) Si, (b) Ge, and (c) In$_{0.53}$Ga$_{0.47}$As bulk n-MOSFETs at the center of the channel. V$_{g}$=0.5V, V$_{d}$=0.05V.

Figure 9: Comparisons of the $I_D - V_G$ characteristics of Boltzmann statistics based QET model and Fermi-Dirac based QET model for a 70nm bulk Si n-MOSFET with (a) logarithmic and (b) linear scales.
Figure 10: Comparisons of the $I_D - V_G$ characteristics of Boltzmann statistics based QET model and Fermi-Dirac based QET model for a 70nm bulk Ge n-MOSFET with (a) logarithmic and (b) linear scales.

Figure 11: Comparisons of the $I_D - V_G$ characteristics of Boltzmann statistics based QET model and Fermi-Dirac based QET model for a 70nm bulk In$_{0.53}$Ga$_{0.47}$As n-MOSFET with (a) logarithmic and (b) linear scales.
5. Conclusion

A Fermi-Dirac statistics based four-moments quantum energy transport model has been developed for high mobility MOSFETs. Numerical stability and convergence are achieved by developing an iterative solution method with an under relaxation method used when Fermi-Dirac statistics are modeled. The iterative solution method for the FDQET model results in an extended version of a Gummel solution method developed for the FDQDD model, which consists of the triple iteration loops. The drain current of In$_{0.53}$Ga$_{0.47}$As bulk n-MOSFETs calculated by the FDQET model is much lower than that calculated by the BQET model due to a smaller density of states and stronger degeneracy of In$_{0.53}$Ga$_{0.47}$As. The FDQET model allows us to evaluate the device characteristics with high degeneracy material such as In$_{0.53}$Ga$_{0.47}$As.

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