A New Hydrodynamic Model for High Energy Tail Electrons

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I. Introduction - The hydrodynamic model has been widely used to obtain the carrier density and average carrier velocity and temperature(T_{n1}) in semiconductor devices. Additionally the model is used to determine the 'high energy tail electrons(n_2)' contributing to the impact ionization and the injection current into the gate oxide assuming a Boltzmann distribution [1]. Often this approach overestimates the energy tail density and cannot predict the carriers in the region with high density of cold electrons [2]. In order to deal with these tail electrons properly, we first introduce a set of transport equations from the moment method of the BTE [3] for the electrons having energy higher than a threshold energy of interest ($\mathcal{E}_1$). The model is introduced and preliminary results applied to one and two dimensional devices will be presented.

II. Formulation of the Transport Equations for $\mathcal{E} \geq \mathcal{E}_1$ - The 0th, 1st, 2nd, and 3rd moment equations for the carriers with energy $\mathcal{E} \geq \mathcal{E}_1$ can be obtained in the same manner as that used for the conventional hydrodynamic equations except the integration is performed only in the region for $\mathcal{E} \geq \mathcal{E}_1$ as given below:

$$0th\,Moment\;:\; -\frac{q|\vec{E}|}{4\pi^3\hbar}N_0 - \frac{1}{q}\vec{\nabla}\cdot\vec{J_{n2}} = C_{n2} \quad (1)$$

$$1st\,Moment\;:\; q\mu_{n2}(\frac{N_1}{4\pi^3} + n_2)\vec{E} + \mu_{n2}\vec{\nabla}(n_2 k_B T_{n2}) = \vec{J_{n2}} = \mu_{n2}C_{\vec{p}2} \quad (2)$$

$$2nd\,Moment\;:\; -\frac{q|\vec{E}|}{4\pi^3\hbar}N_0\mathcal{E}_1 - \vec{E}\cdot\vec{J_{n2}} + \vec{\nabla}\cdot\vec{S_{n2}} = C_{w2} \quad (3)$$

$$3rd\,Moment\;:\; -\frac{5}{2}k_B T_{n2}\frac{\vec{J^*_{n2}}}{q} - \frac{5}{2}\sigma^*_{n2}(\frac{k_B}{q})^2 T_{n2}\vec{\nabla}T_{n2}. = \vec{S_{n2}} = -\frac{1}{q}\mu_{s2}C_{\mathcal{E}\vec{p}2}. \quad (4)$$

Here, C_x terms represent the increase of each quantity in the tail region due to the scattering events and

$N_0 \equiv |\oint_{\mathcal{E}=\mathcal{E}_1} f d\vec{\sigma_k}\cdot\hat{z}|$, $\quad N_1 \equiv \oint_{\mathcal{E}=\mathcal{E}_1} f k_z d\vec{\sigma_k}\cdot\hat{z}$,

$n_2 \equiv \int_{\mathcal{E}\geq\mathcal{E}_1} f d^3\vec{k}/4\pi^3$, $\quad \vec{J_{n2}} \equiv -qn_2 <\vec{v}>_2$, $\quad k_B T_{n2} \equiv m^* <v_z^2>_2$, $\quad \vec{S_{n2}} \equiv n_2 <\mathcal{E}\vec{v}>_2$,

($<\phi>_2$ means $\int_{\mathcal{E}\geq\mathcal{E}_1} f\phi d^3\vec{k}/\int_{\mathcal{E}\geq\mathcal{E}_1} f d^3\vec{k}$)

$\vec{J^*_{n2}}$ and σ^*_{n2} are modified quantities of $\vec{J_{n2}}$ and $\sigma_{n2} \equiv q\mu_{n2}n_2$, respectively, in order to treat the truncation of higher order moments, the contribution of N_0 and N_1, and the difference between μ_{n2} and μ_{s2} [4]. Eq. (1) - (4) are the conservation laws for carrier, momentum, energy, and energy flux, respectively. Most of the expressions are similar to the conventional formulation except for the terms including N_0 and N_1 which arise from the integration of the momentum gradient term of the BTE by parts. The terms including N_0 and N_1 in Eq. (1) - (4) represent the increased values of carrier, momentum, energy, and energy flux due to the flux of carriers from the zone1($\mathcal{E} < \mathcal{E}_1$) to zone2(the tail region). It can be verified after lengthy derivation that

$$\frac{q|\vec{E}|}{\hbar}\frac{N_0}{4\pi^3} = q|\vec{E}|f(\mathcal{E}_1)g(\mathcal{E}_1)u(\mathcal{E}_1), \qquad \frac{N_1}{4\pi^3} = m^*(\mathcal{E}_1) <v_z^2>_{\mathcal{E}_1} f(\mathcal{E}_1)g(\mathcal{E}_1) \quad (5)$$

where $u(\mathcal{E}_1)$ and $<v_z^2>_{\mathcal{E}_1}$ are the average of carrier velocity and v_z^2, respectively, for carriers having a fixed energy $\mathcal{E}_1$. In order to check the validity of above formulation we have performed the Monte Carlo simulation for uniform bulk silicon and compared the RHS and LHS of Eq. (1) - (4), while varying $\mathcal{E}_1$, with N_0 and N_1 represented by Eq. (5). Although only one case for $|\vec{E}| = 1\times10^5 V/cm$ is shown in Fig.1, similar agreement is obtained for $|\vec{E}|$ up to $5\times10^5 V/cm$.

Having the moment equations for the carriers in the zone2, we model each term in Eq.(1) - (4) in order to incorporate the formulations in the numerical simulator. In fact, several approaches can be taken for the physical modeling, especially for terms including N_0, N_1, and scattering related terms C_x's. We adopted the conventional relaxation approximation for C_x terms and expressed the N_0 and N_1 terms as follows:

$$\frac{q|\vec{E}|}{4\pi^3\hbar}N_0 = \gamma_0\frac{1}{q}\vec{J_{n1}}\cdot\vec{E}, \qquad \frac{N_1}{4\pi^3} = \gamma_1 n_2 \quad (6)$$

where γ_0 and γ_1 are model parameters and can be represented as a function of T_{n1} and T_{n2}, respectively, from the MC simulations. Also relaxation times for each moment are determined from the MC results.

III. Results and Discussion - Eq. (1) - (4) comprise the continuity equations for n_2 and T_{n2}. Since n_2 is much smaller than total electron concentration for most cases of interest, the results obtained from the conventional hydrodynamic equations can be considered as solution for the zone1(n_1 and T_{n1}). Also the solution of Eq. (1) - (4) can be performed as a post processing after n_1 and T_{n1}, and field distribution are obtained. For the discretization of the current and energy flux equations we use an improved discretization scheme based on the temperature dependent carrier density [5]. In this work, we set $\mathcal{E}_1$(border between the zone1 and zone2) to 1.5 eV. The simulated results obtained for bulk silicon, 1 dimensional N-I-N diode(channel length of 0.4 micron), and conventional NMOSFET(channel length of 0.8 micron) are shown in Fig.2, 3, and 4, respectively. Also in the figures are the data for n_2 from the result of uniform MC simulation for corresponding field intensity in the device and the data obtained using the Boltzmann distribution and n_1 and T_{n1} from the conventional hydrodynamic model. The 'tail temperature' defined as $3/2k_BT_{n2}-\mathcal{E}_1$ and T_{n1} is also compared. In Fig. 2, where the bulk silicon data are shown, the agreement with the MC results is excellent saying our new model reproduces the MC results well in the uniform case. In Fig. 3 and 4, agreement with the MC results in the channel region are reasonable whereas the prediction of the Boltzmann distribution overestimates the tail electrons. Also it is exciting to see that we were able to obtain the existence of 'hot' tail electrons in N^+ region by our model, which would be buried in the cold electrons sea and cannot be predicted by the uniform MC and the conventional hydrodynamic model. Calibration of the models by comparison with the full MC device simulation is needed and will be a subject of further study.

IV. Conclusion - We have proposed the hydrodynamic equations for high energy tail electrons and shown that

the model can predict the tail electrons in the channel and the n+ region. After the refinement of the model parameters using full Monte Carlo simulation, the hydrodynamic formulation will be a good tool to predict the impact ionization and gate injection .

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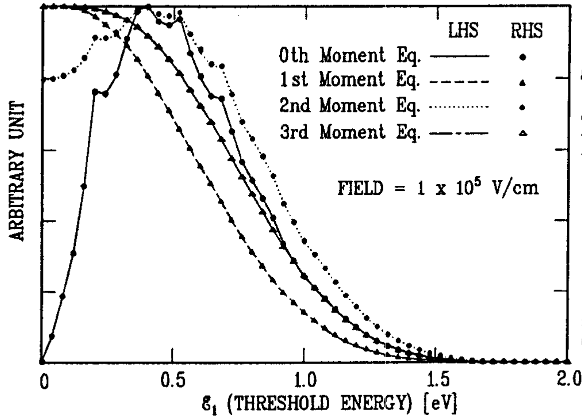


Fig.1 Comparison of LHS and RHS in 0th, 1st, 2nd, and 3rd moment equations for each $\mathcal{E}_1$ from the data of Monte Carlo simulation for DC and uniform case, $|\vec{E}| = 1 \times 10^5 V/cm$.

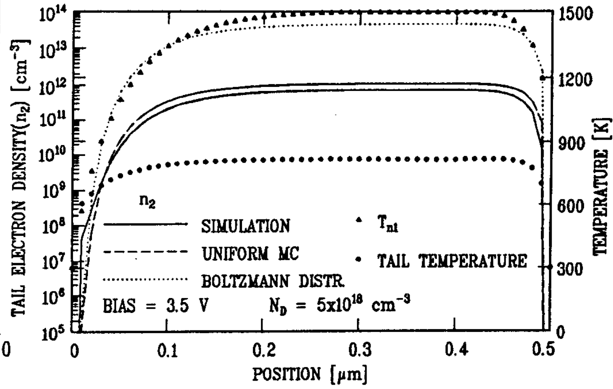
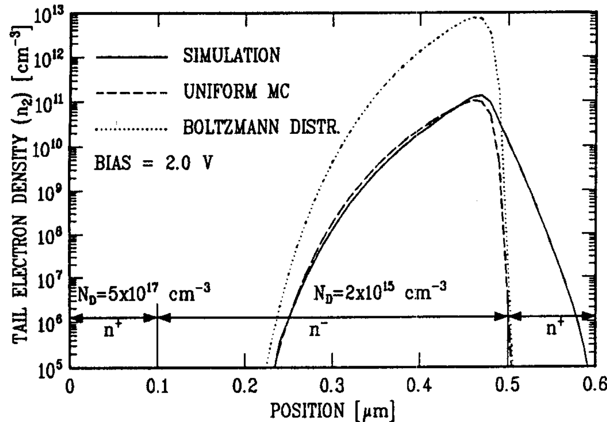
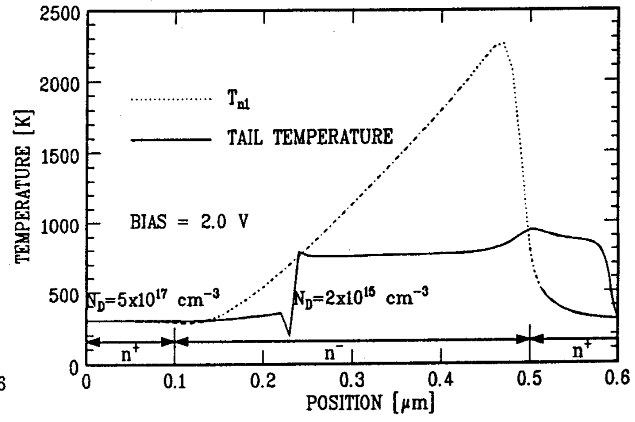


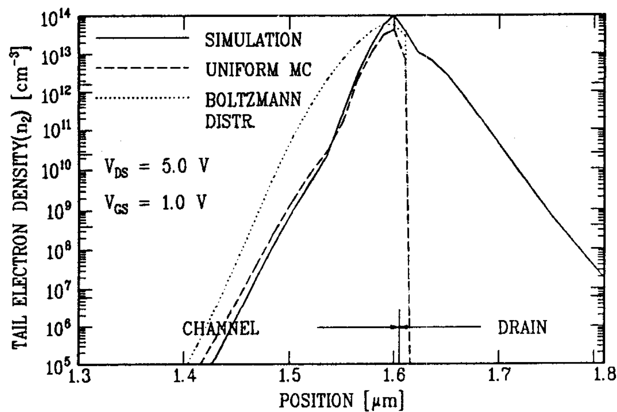
Fig.2 Simulated results for bulk silicon.

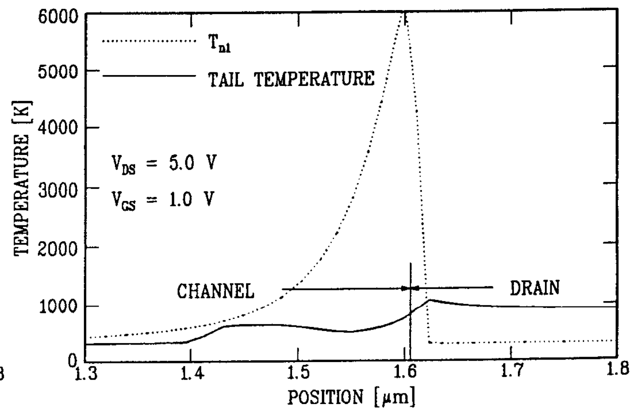




(a) (b)

Fig.3 Simulated results for 1-dim. N-I-N diode. (a) Tail electron density (b) Temperatures.





(a) (b)

Fig.4 Simulated results for the surface of conventional NMOSFET. (a) Tail electron density (b) Temperatures.