SIMULATION OF BAND-STRUCTURE DEPENDENT TRANSPORT AND IMPACT IONIZATION IN SEMICONDUCTOR P-N JUNCTIONS USING AN IMPROVED MULTIVALLEY HYDRODYNAMIC MODEL

Mohammad. HAMZA, H. MOREL and J. P. CHANTE
mhs@isi-soft.com

INSA LYON, LCPA, BAT. 401, 69621 VILLEURBANNE, FRANCE.

Abstract: An improved multivalley hydrodynamic model (HDM) including realistic band structure effects and impact ionization is developed. Unlike the recently-proposed HDM by Thoma et al [1] for nonparabolic band structures, our model minimizes the number of relaxation times and includes impact ionization. Furthermore, the intervalley transitions of hot carriers are considered. Also, the momentum relaxation times are finally eliminated from the set of hydrodynamic equations (HDE's). Instead, the carrier mobility is selfconsistently derived from the HDE's themselves. On the basis of this model, the HDE's are solved in the p-i-n diode over a large scale of reverse bias voltages (up to the avalanche breakdown). The results of simulation are compared with those we previously presented [2] using the classical HDE's with constant carrier effective mass. It's shown that the inclusion of the realistic band structure results in smaller, and hence more realistic, breakdown voltages.

I- INTRODUCTION

It is well known that the concept of the effective mass breaks down at high carrier energies when the external forces are strong enough to preclude interband transitions. So far, the impact ionization mechanism, which naturally encounters interband transitions, was either neglected [1] or considered with a constant carrier effective mass [3]-[4] in the HDM. According to the Monte-Carlo simulation results of Tang and Hess [5], the inclusion of the second conduction band of Si and the L-minimum of the first one is necessary for an accurate simulation of the high-field transport and impact ionization phenomena in silicon devices. In fact, even with the inclusion of a nonparabolicity factor in the E(k) relation, the dynamics of energy exchange between valleys is not properly taken into account when using a single-valley description [6]. On the other hand, the simultaneous presence of many groups of charge carriers (i.e. many valleys) with significantly unequal carrier energies needs to a large number of relaxation times particularly if the band structure of each valley is considered. In addition, we must admit that the validity of the relaxation time approximation becomes questionable near avalanche breakdown zone where the deviation from the equilibrium is more pronounced.

In order to reduce the complexity of the HDM while maintaining its ability to rigorously simulate high-field transport phenomena, we try to minimize the number of the relaxation times. We do so by suppressing the least significant intervalley relaxation times and expressing some of the intravalley relaxation times selfconsistently as functions of the average carrier energy. We also redefine the carrier temperature tensor in such the manner that it satisfies the themodynamic definition and keeps the number of relaxation times as minimum as possible.
II- THE HYDRODYNAMIC MODEL.

II A. Basic Assumptions.
A1) The high-field transport of charge carriers can be described within the framework of Boltzmann transport equation (BTE).
A2) The carrier effective mass concept holds as long as intervalley and interband transitions are not concerned. The local effects of the energy band structure $E_i(k)$, where $E_i$ is the carrier energy and $k$ is the carrier wave vector, is taken into account using what we'll call "the piecewise effective mass approximation". For each valley, we define an inverse apparent mass tensor $\mathcal{M}_i^{-1}$ as follows:

$$\mathcal{M}_i^{-1} = \langle \mathcal{M}_i^{-1} \rangle = \langle (\mathbf{F} \cdot \nabla_k) E_i(k)/\hbar^2 \rangle_i$$

where $\mathbf{F}$ is the external force vector, $\hbar$ is Planck’s constant divided by $2\pi$, $\mathcal{M}_i^*$ is the conventional microscopic effective mass and the angular brackets $\langle \rangle_i$ represent the statistical average over the momentum distribution function of the $i$th valley. This approach assumes that intervalley and interband transitions are instantaneous. So, the intervalley and interband transfers, which are frequently associated with a high energy exchange, can change the carrier mass without violating the effective mass concept. The valleys are given analytic expressions whose parameters can be fixed by best fitting the density of states taken from band structure calculations [7]. Over each valley, $\mathcal{M}_i^{-1}$ is assumed as a weak function of space and time. This assumption is more general than to assume a central valley with an average effective mass that varies little with space and time. In fact, even if $\mathcal{M}_i^{-1}$ is considered as a scalar quantity, the anisotropy is still partly conserved because $\mathcal{M}_i^{-1}$ can change from one valley to another.
A3) The correlation between the electron and hole distribution functions is neglected as long as the net recombination and the generation by impact ionisation are not concerned. Also, the carrier-carrier interactions are ignored (i.e. the Maxwellianization relaxation times are infinite).
A4) We assume also that the intervalley scattering randomizes momentum so that no momentum transfers from a certain valley to another. So, the intervalley momentum relaxation times are infinite.
A) The energy relaxation time is assumed to be a function of the carrier mean energy and so the impact ionization rate.

II B. Definition of the Carrier Temperature Tensor
For a given valley we define the carrier temperature as follows

$$\mathcal{M}_i^{-1} \frac{k_B}{T} = \langle (\boldsymbol{u}_g i - \langle \boldsymbol{u}_g i \rangle) \otimes (\boldsymbol{u}_g i - \langle \boldsymbol{u}_g i \rangle) \rangle_i$$

where $\boldsymbol{u}_g i = \nabla_k E_i(k)/\hbar$ is the carrier group velocity in $i$th valley and $\otimes$ denotes the tensor product (circle-cross product). The total pressure tensor $(n k_B T)$, where $n$ and $T$ are the total carrier density and temperature respectively, can be obtained by summing the local pressures $(n_i k_B T_i)$ of all valleys. This definition has the merit that it results in carrier temperature values which are very close to those calculated by Monte-Carlo (MC) simulation in the bulk (where $3/2 k_B T = \langle E \rangle$). In fact, if the drift-energy term is extracted from the MC carrier energy, the discrepancy between $T$ and the trace of $T$ (the sum of diagonal terms) becomes in
the order of 2-3% over a large scale of electric fields. Fig. 1 depicts the Monte-Carlo temperature ($T^{MC}$), the trace of $T$ as well as the classical hydrodynamic temperature defined by $<E> = 3/2 k_BT + 1/2 m_d^* \langle u_{gi}^2 \rangle$ where $m_d^*$ is the density effective mass at the bottom of main conduction band. According to this feature one can immediately establish a relation between $T_i$ and $<E_i>$ without need to specify additional relaxation times as Thoma et al did.

\[ M_{i-1}^{-1} <E_i> = M_i^{-1} k_B T_i + (1/2) \langle u_{gi}^2 \rangle \langle u_{gi} \rangle \]  

(II-2b)

II C. Conservation Equations.

The BTE in the ith valley can be written as

\[ \partial_t f_i + \mathbf{u}_{gi} \cdot \nabla f_i + (\mathbf{F}/h) \cdot \nabla_k f_i = (\partial f_i/\partial t)_c \]  

(II-3)

where $f_i = f_i (k_i, r, t)$ is the distribution function in the ith valley and $(\partial f_i/\partial t)_c$ is the total change happening in $f_i$ due to the intravalley and intervalley collisions. Let's denote the statistical average of any microscopic quantity $\psi_i(k)$ which is defined in the ith valley by $<\psi_i>$. The semiclassical conservation equation of $\psi_i$ can be written as follows

\[ \partial_t n_i <\psi_i> + n_i <(\mathbf{F} \cdot \nabla) \psi_i > + \nabla_i (n_i <\mathbf{u}_{gi} \psi_i >) = n_i (\partial <\psi_i>/\partial t)_c + <\psi_i> (\partial n_i/\partial t)_c \]  

(II-4)

where $n_i = \int z f_i d^3 k_i$ is the carrier average density, $z = (2\pi)^{-3}$ is the density of states in the volume $d^3 k_i$ and $n_i <\psi_i> = \int z \psi_i f_i d^3 k_i$. The set of carrier density-, momentum- and energy-conservation equations in a certain valley can be obtained by substituting $\psi_i(k) = 1, \mathbf{u}_{gi}(k)$ and $E_i(k)$ respectively. In order to close the system of HDE's, we'll write down a fourth conservation equation for the energy flux density $S_i = n_i <E_i \mathbf{u}_{gi}>$. We'll consider the carrier energy $E_i$ and its mean value $w_i$ as scalar quantities. Hence the energy flux $S_i$ will be considered as a vector quantity. Table I shows the different terms resulting from these substitutions. As shown in Table I, all the dyadic products which appear in the RHS of the HDE's can be simplified in terms of the basic average quantities (i.e. $n_i, v_i, w_i$ and $T_i$) and the inverse apparent mass $M_i^{-1}$. The indicated products are exact but the terms $<(\mathbf{F} \cdot \nabla)^{-1} E_i>$ and $\nabla_i (n_i <E_i \mathbf{u}_{gi} \otimes \mathbf{u}_{gi}>)$ need some simplifying assumptions. The adopted assumptions should be compatible with the chosen $E_i(k)$ relations or models. These models must compromise between the simplicity and the validity at high carrier energy. Actually, one can find in the literature, at least for Si conduction bands, such simple and accurate models for carrier energies up to 3 eV (e.g. [7]). For instance, let's consider the second conduction band of Si and the L-valley of the first one. We'll call the two lowest valleys of these two conduction bands the X- and X2-valley. Actually X- and X2-valleys intersect at the X point where the energy is 0.1eV. Also, the minimum of the L-valley of the first conduction band is about 1 eV above the X-minimum. So, it seems very important to consider them during the study of high-field transport and the avalanche breakdown by impact ionization. The conservation equations of X-valley of the lowest conduction band can be written as follows where all variables have the same meaning as above and the suffix x replaces the index i

\[ \partial_t n_x - \nabla_i (n_x v_x) = (\partial n_x/\partial t)_c \]  

(II-6a)

\[ n_x v_x + n_x \mu_x \left[ e M_x^{-1} \right] (v_x) = -n_x \mu_x F + k_B \mu_x \nabla_i (n_x T_x) \]  

(II-.6b)
\[ \partial_t (n_x w_x) + \nabla S_x = n_x F. v_x + (\partial n_x / \partial t)_c w_x + n_x (\partial w_x / \partial t)_c \]  
(II-6.c)

\[ \partial_t S_x + \nabla (n_x < E_x u_{gx} \otimes u_{gx}> ) = n_x F. < M^*_E x + u_{gx} \otimes u_{gx}> + (\partial S_x / \partial t)_c \]  
(II-6.d)

Here \( \mu_x \) is the carrier mobility and \( F = -e E \) where \( E \) is the electric field and \( e \) is the electron charge. Also the carrier and energy collision rates are expressed in terms of the local generation-recombination rates \( (G_i - R_i) \) and the mutual density and energy exchange rates between the X-valley and the X1- and L-valleys as follows:

\[ (\partial n_x / \partial t)_c = G_x - R_x + (\partial n_x / \partial t)_{X-X1} + (\partial n_x / \partial t)_{X-L} \]  
(II-7.a)

\[ (\partial \omega_x / \partial t)_c = (\omega_x - \omega_o) / \tau_{Exx} + (\partial \omega_x / \partial t)_{X-X1} + (\partial \omega_x / \partial t)_{X-L} \]  
(II-7.b)

where \( \omega_o \) is the carrier energy at equilibrium and \( \tau_{Exx} \) is the intravalley energy relaxation time in the X-valley (will be considered as a scalar quantity). Note that charge carriers in a certain valley cannot exchange density but can exchange energy by the emission and absorption of phonons. Similar systems of conservation equations can be written for other considered electron and hole valleys. In this study we consider three electron valleys (X-, X2- and L-valleys for electrons. At this points of symmetry all equivalent valleys are averaged. Also we consider one hole valley at \( \Gamma \) averaging heavy and light holes. The overall system of conservation equations must be solved with Poisson's equation:

\[ \nabla \cdot (\varepsilon \nabla \phi) = -e (p - n + D_{op} - N_F) \]  
(II-8)

where \( eN_F \) is the fixed charge density at the interface of the semiconductor, \( D_{op} = N_{D^+} - N_{A^-} \) is the net concentration of ionized impurities in the semiconductor bulk and \( \varepsilon \) is semiconductor permittivity. Also the electron and hole concentrations \( (n, p) \) are the sum of individual concentrations in all considered valleys (i.e., \( n = n_x + n_{x2} + n_L \), \( p = p_{\Gamma} \)).

## II D. System Closure.

One can simplify the 4th conservation equation (II-6.d) by assuming that the symmetric part of the distribution function is nearly isotropic and dominates the perturbation. This approximation is quite crude but it admits to close the system of HDE’s. Then one can express the energy flux in the ith valley \( S_i \) as follows:

\[ S_i = Q_i + (5/2) n_i v_i \mu_{isi} [\mu_i]^{-1} \cdot k_B T_i \]  
(II-9a)

\[ Q_i = - (5/2) (k_B / e)^2 e n_i \mu_{isi} T_i \cdot (\nabla T_i) \]  
(II-9b)

with

\[ (\mu_{isi} = e \tau_{isi} k_B / e) \]  
(II-9c)

where \( \mu_{isi} = e \tau_{isi} k_B / e \) is "energy flux mobility" and \( \tau_{isi} \) is energy flux relaxation time due the intravalley collisions. Equation (II-7d) resembles the usual heat flux expression that one can obtain by substituting the carrier thermal conductivity from the the Wiedmann-Franz relation \( (k_i = (5/2) (k_B / e)^2 e n_i \mu_i T_i) \) into the Fourier phenomenological relation \( Q_i = -k_i (\nabla T_i) \).
However, we propose here a more accurate approach which consists in expressing the dyadic products in (II-6.d) as follows:

\[
\mathbf{F} \langle \mathbf{E}_i \mathbf{u}_{gi} \otimes \mathbf{u}_{gi} \rangle = \mathbf{F} \langle (3 \alpha_i/2) \mathbf{u}_{gi} \otimes \mathbf{u}_{gi} \rangle + \langle \mathbf{u}_{gi} \otimes \mathbf{u}_{gi} \rangle
\]

(II-10.a)

and

\[
\langle \mathbf{E}_i \mathbf{u}_{gi} \otimes \mathbf{u}_{gi} \rangle = (5 \beta_i/2) \langle \mathbf{u}_{gi} \otimes \mathbf{u}_{gi} \rangle \cdot \langle \mathbf{u}_{gi} \otimes \mathbf{u}_{gi} \rangle
\]

(II-10.b)

where \( \alpha_i = (3 \alpha_i' + 2)/5 \) is a factor expressing the mean anisotropy of the ith-valley. Also \( \beta_i \) is a correction factor representing the mean deviation of the energy distribution function from the Maxwell-Boltzmann distribution at equilibrium. We duly note that the dot product of two tensors (contraction product) is another tensor of the same order. The above correction parameters, \( \alpha_i \) and \( \beta_i \), can be determined from the MC simulation with realistic band structure. For the matter of simplicity we'll assume here a mean value for them over all considered valleys. According to the MC simulation in a central nonparabolic conduction valley [1], [8] one can consider the parameter \( \alpha_i \) to be one for electric fields up to 200 kV/cm (if the anisotropy is negligible) and \( \beta_i \) can be expressed as follows on the basis of our definition (II-10.b):

\[
\beta_x = \frac{6.464}{\omega_x} \left[ 1 + \left( \frac{Dop}{N_{r b 1}} \right)^{1/2} \right] + \frac{0.9775}{\left[ 1 + \left( \frac{Dop}{N_{r b 2}} \right)^{1/2} \right]}
\]

(II-10.c)

where \( \omega_x \) in electron volts and \( N_{r b 1}, b_1, b_2 \) are constants. When \( \omega_1 = 0.15 \text{ eV} \) and \( Dop = 10^{19} \text{ cm}^{-3} \) one can use these values : \( N_r = 10^{21} \text{ cm}^{-3} \), \( b_1 = 0.192 \), \( b_2 = 0.372 \). The impact of this correction parameter on the energy and heat fluxes can be evaluated by comparing (II-9) with the following more general expressions for mean-energy and carrier-heat fluxes:

\[
\mathbf{S}_i = \mathbf{H}_i + (5 \alpha_i/2) n_i \mathbf{v}_i \left( \mathbf{\mu}_{gi} \mathbf{[\mathbf{\mu}_{gi}]^{-1}} k_B T_i \right)
\]

(II-11a)

(II-11b)

where

\[
k_i' = -\frac{5}{2} \left( \frac{k_B}{e} \right)^2 \left( e n_i \mu_{si} \right)
\]

(II-11c)

And

\[
k_i'' = k_i'' = -\frac{5}{2} \left( \frac{k_B}{e} \right)^2 \left( e n_i \mu_{si} \right) \left( \beta_i - 1 \right) T_i
\]

(II-11d)

Equation (II-11.b) predicts that the carrier heat flux is not strictly proportional to the carrier-temperature gradient where carrier density changes abruptly. So, the classical model of the carrier heat flux (i.e. \( Q_i \) expression) doesn't take into account the heat flux component due to non homogeneous carrier distribution (carrier density diffusion) which is particularly important around semiconductor junctions and interfaces. In fact, the direct solution of the BTE around silicon grain boundaries has shown that the carrier heat flux is not directly proportional to the carrier-temperature gradient due to this phenomenon [9]. However, even in the semiconductor regions where the carrier gradient is not dominant, the usual Fourier phenomenological expression doesn't hold because \( \beta_i \) is not equal to one particularly at high carrier energy ( \( \beta_i \approx 1.25 \text{ at } \zeta = 240 \text{ kV/cm} \)). In order to estimate the error committed when
using the usual heat flux expression (II-9.b) we can match $Q_i$ and $H_i$ expressions to obtain the following correction factor for $Q_i$

$$
\gamma_i = \frac{5}{2} \mu_s i \mu_i \left( \beta_i + \langle \beta_i \rangle - 1 \right) \left[ 1 + \left\{ \frac{T_i}{\nabla . T_i} \nabla n_i \right\} \right]^{\beta_i - 1} \left( \nabla T_i / \nabla . T_i \right)
$$

(II-12)

This scalar factor, which is called the Lorentz number, must replace the constant $(5/2)$ in (II-9.b) or $(5/2 + r)$ in the usual Wiedmann-Franz relation [10] in order to take into account the deviation of the energy distribution function (DF) at high energies from the Boltzmann-Maxwell one. Fig. 1 depicts the variation of $\gamma_i$ as a function of doping and mean electron energy when the electron-density gradient is negligible, or more precisely when $\nabla n / n \ll \left| \text{tr } (T) / \nabla . T \right|$. As shown in this figure the carrier-heat-flux expression (II-9.b), which is currently used in almost all the hydrodynamic simulators, under-estimates the actual electron heat flux by a factor of 3 when $\omega_n$ is about 0.5eV and this factor increases monotonically with the electron mean energy.

### II E. Collision Terms

All the collision rates (including the generation term) in the RHS of (II-7) can be calculated in terms of the intervalley collision probabilities and the carrier distribution function in the valley. As the distribution functions in the different valleys are not generally Maxwellian at high carrier energies, these terms are usually modeled by additional relaxation times. The detailed expressions of intervalley and intravalley relaxation parameters can be found in [6] where the authors use the concept of macro kinetic distribution function to calculate these rates. In all cases, as the number of considered valleys increases, the number of these relaxation times increases and the calculation of their energy dependence by empirical formula or from MC simulation at static field conditions becomes doubtful particularly at very high carrier energies. In the next section we show how to get rid of the momentum and energy-flux relaxation times.

### II F. Carrier Mobility

It is obvious from the set of hydrodynamic equations in a certain valley (II-6) that the momentum relaxation times are finally eliminated. This is done by selfconsistently deriving an analytical expression for the carrier mobility from the HDE’s themselves. Similarly, the energy flux relaxation times can be replaced by "energy-flux mobility" terms. Our procedure consists in expressing the collision terms $(\partial \langle v_i g_i \rangle / \partial \alpha)_c$ and $(\partial \langle E_i v_i g_i \rangle / \partial \alpha)_c$ in terms of $(\partial \omega_i / \partial \alpha)_c$. For instance, the carrier mobility at high carrier energy is defined as follows [12]:

$$
\mu_{iW} = -e \frac{M_i^{-1} v_i^2}{[v_i \cdot (\partial \n_i / \partial \alpha)_c]^T}
$$

(II-13a)

where $v_i^2$ is a diagonal scalar matrix and the brackets $[ . ]^T$ denotes the tensor of the internal dot product. Then the momentum collision term $(\partial v_i / \partial i)_c$ is replaced in terms of $(\partial \omega_i / \partial \alpha)_c$ using the following relation which can be derived from the conservation equations

$$
[v_i (\partial \n_i / \partial \alpha)_c]^T = \beta_i^{-1} (\partial \omega_i / \partial \alpha)_c
$$

(II-13b)
Substituting (II-13.b) into (II-13.a) we can obtain the following relation of the bulk mobility 
\[ \mu_i = \mu_{io} / \mu_{iw} \]
where \( \mu_{io} \) is the low-field carrier mobility in the ith valley

\[ \mu_i = \frac{\mu_{io}}{1 + \eta_i \left( w_i - w_o \right)} \quad \eta_i \approx \frac{\mu_{io}}{e v_i^2 \tau_{Eii}(w_i)} \]  

(II-13c)

where \( \eta \) is unity tensor and \( \mu_{io} \) is carrier drift mobility at low field (or low energy). Similarly, one can eliminate the entravalley energy flux relaxation times \( \tau_{sii} \) and express analytically the "energy flux mobility" \( \mu_{sii} \) as a function of the carrier mean energy [12]

\[ \mu_{sii} = \frac{\mu_{sio}}{1 + \zeta_i \left( w_i - w_o \right)} \quad \zeta_i \approx \frac{5}{2} \frac{n_i w_i \mu_{sio}}{e v_i \tau_{Eii}} \]  

(II-13d)

where \( \mu_{sio} \) is the energy flux mobility at low energy and can be determined by the same methods we use to get the carrier drift mobility at low field (i.e., \( \mu_{io} \)).

II G. The Impact Ionization Model

The form of the local generation rate is given by

\[ G_i = \left( \frac{n_i}{\tau_{in}} \right) + \left( \frac{p_i}{\tau_{ip}} \right) \]  

(II-14a)

where \( 1/\tau_{in}(w_i) \) and \( 1/\tau_{ip}(w_i) \) are the electron and hole average ionisation rates. The carrier generation rates \( 1/\tau_{in,p} \) is related to the usual ionisation coefficients \( \alpha_i \) through the carrier mean velocity \( v_i \). For instance, the electron ionisation coefficient is given by:

\[ \alpha_n \left( w_n \right) = \left( \tau_{in} v_n \right)^{-1} = \lambda_n^{-1} \exp \left( - \frac{E_n^{f_n}}{w_n - w_o} \right) \]  

(II-14b)

where \( \lambda_n \) and \( E_n^{f_n} = E_n^{f_{no}} \left( \tau_{wn} v_n / \lambda_n \right) \) are the carrier mean free path and effective ionization energy respectively. These parameters depend on the carrier energy and the valley index (i.e. the band structure). The carrier mean free path can be modeled by matching the hot-carrier energy DF with the lucky electron model (see Goldsman et al [13]). Also the energy relaxation time can be simply modeled, with a good agreement with MC results, as follows

\[ \tau_{wn}(w_n) = \tau_{wno} m_d^* M_n^{-1}(w_n) \]  

(II-14c)

where \( \tau_{wno} \) is intravalley relaxation time at the bottom of the conduction band and can be taken as a constant at room temperature (0.3 -0.5 ps). Once the energy dependences of \( \lambda_{n,p} \) and \( \tau_{wn,p} \) are known, no specific fitting is required as each parameter corresponds to a physical quantity whose order of magnitude is a physical characteristic of the semiconductor material. Moreover, the above impact ionization model can be considered as a generalization of the currently-used one in the classical hydrodynamic simulators. In fact, one of the pitfalls
of the classical HDM impact ionization models is that they result in abnormally high breakdown voltages. This problem was attributed to the thermal diffusion currents [14]. However, as we'll see in the next section that the new impact ionization model (II-14.b) for nonparabolic band structures results in lower breakdown voltages and hence it corrects the errors of the classical model. More theoretical details about the new mobility and impact ionization models will be soon published.

III- SIMULATION AND RESULTS.

On the basis of this model, we have simulated the bipolar transport of both electrons and holes in a reverse-biased p-i-n diode. Actually, this model is integrated in the two-dimensional hydrodynamic simulator SIMULADD-2HD [15]. The discretization scheme that we previously proposed [2] has been successfully used for the new system of hydrodynamic equations by assuming that the norm of the ratio \( \left( \nabla n_i / n_i \right) / \left( T_i / \nabla T_i \right) \), that appear in the heat flux expression, changes little between mesh nodes. The results of simulation are compared with those we obtained by the classical single-valley HDE's with constant carrier effective mass [2]. In the medium biasing range, the carrier velocity increases and the carrier density decreases in the central space-charge region in a more pronounced manner. Surprisingly, the electric field distribution is persistently unchanged in this range (the same as that obtained by the drift-diffusion model DDM). Other significant results exist near and at the avalanche zone. The inclusion of the band structure results in more electrons at high energies (i.e. in the negative space-charge region just after the phonon-collision-limited region). However, this large number of electrons doesn't imply a much higher generation rate by impact ionization because of the competition of the phonon collisions which still exist (but not dominant) in this region. The generation rate contours in the two cases are shown in Fig. 3. Also Fig. 4 depicts the final current-voltage characteristics of the reverse-biased p-i-n diode. As shown, the J-V characteristics are more soft and the breakdown voltage is smaller than that we obtained by the classical HDM. This is due to the saturation of \( \gamma_n \) and \( \lambda_n \) at high carrier energy while \( \tau_{wn} \) continues to decrease when carrier energy increases (band-structure effect). So the inclusion of the realistic band structure increases the impact ionization rate. Consequently it results in smaller breakdown voltages which agree with the results we obtain by fitting the Chynoweth model with experimental results (i.e., the DDM results).

IV- CONCLUSIONS

In this paper an improved multivalley band-structure dependent HDM is developed. In this model the number of energy-dependent relaxation times is minimized. In fact our model can be contracted to a single-valley non parabolic model containing only one energy-dependent relaxation time, namely, the entravalley energy relaxation time. The very interesting feature of our model is, however, that the band structure effects are implicit in this single parameter. So, the classical hydrodynamic simulators can be easily upgraded to include nonparabolicity effects by simply adopting the ensemble of our physical parameters which are expressed in terms of this relaxation time. We've also suggested a new method to improve the closure of the hydrodynamic system. Using this model, we've studied the influence of the band structure on the hot-carrier transport and impact ionization phenomena in the p-i-n diode. The results of simulation are compared with those obtained by the classical hydrodynamic and drift-diffusion models. The breakdown voltage obtained by the new band-structure-dependent hydrodynamic model is found to be smaller than its value obtained with a constant effective mass and hence more close to the experimentally-fitted DDM results.
REFERENCES
Table 1. Macroscopic averages that appear in the LHS of (II-4)

<table>
<thead>
<tr>
<th>$\psi_i(k) &lt;\psi_i&gt;$</th>
<th>$&lt;(\mathbf{F}. \nabla_k)\psi_i &gt; / h$</th>
<th>$\nabla.(n_i &lt;\mathbf{u}_{gi}\psi_i&gt;)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1$</td>
<td>$1$</td>
<td>$0$</td>
</tr>
<tr>
<td>$\mathbf{u}_{gi}$</td>
<td>$\mathbf{v}_i$</td>
<td>$\mathbf{F} : \mathcal{M}_i^{-1}$</td>
</tr>
<tr>
<td>$E_i$</td>
<td>$\omega_i$</td>
<td>$\mathbf{F}.\mathbf{v}_i$</td>
</tr>
<tr>
<td>$E_i \mathbf{u}_{gi} S_i/n_i$</td>
<td>$&lt;\mathbf{F}. \mathcal{M}<em>i^{-1}E_i + \mathbf{F} \mathbf{u}</em>{gi} \otimes \mathbf{u}_{gi}&gt;$</td>
<td>$\nabla.(n_i &lt;E_i \mathbf{u}_{gi}&gt;)$</td>
</tr>
</tbody>
</table>

Fig. 1. Monte-Carlo and hydrodynamic carrier temperatures vs. electric field.

Fig. 2. Lorentz number of electrons in homogeneous Silicon vs. normalized electron energy.

(a) (b)

Fig. 3. Impact ionisation rate (pairs/cm$^3$ sec) contours in the pin diode near breakdown as obtained by the classic HDM (a) and the present model (b).
Fig. 4. The reverse J-V C/Cs of the p-i-n diode as obtained by the DDM, the classic HDM and the present model.