A Comparison Between Hydrodynamic and Monte Carlo Model Characteristics of $n^+\!-\!i(n)\!-\!n^+$ Diode Based on InP Material

H. Arabshahi

Abstract— We performed a two-dimensional ensemble Monte Carlo simulation of a $n^+\!-\!i(n)\!-\!n^+$ diode based on InP material in comparison with hydrodynamic model. Scattering processes taken into account are polar optical phonon scattering, acoustic phonon scattering, piezoelectric scattering, intervalley phonon scattering, nonpolar optical phonon scattering and the ionized impurity scattering. The carrier transport phenomena in the submicron sized device is illustrated by the distribution of over 100000 particles in two dimensional device structure. Channel electrons can reach velocities that largely exceed the saturation velocity (velocity overshoot). Such effect guarantees very fast transit times in submicron structures. The electric field is determined self-consistently from the Poisson equation. Numerical results are presented by two models. Based on these data, the excellent agreement of the hydrodynamic approach with Monte Carlo simulations is discussed.

Index Terms— Ensemble Monte Carlo; Hydrodynamic; polar optical phonons.

I. INTRODUCTION

InP has long been considered promising material for electronic and optoelectronic device applications [1-3]. While initial efforts to study this material was hindered by growth difficulties, recent improvements in the material quality have made possible the realization of a number of InP-based devices. In particular, lasers [4], transistors and photodetectors [5] have been fabricated with these materials. These developments have fueled considerable interest in the GaN material. In order to analyze and improve the design of InP-based devices, an understanding of the electron transport that occurs within these materials is necessary. While electron transport in bulk InP has been extensively examined [6-7], the sensitivity of these results to variations in the material parameters has yet to be considered. The diode is one of the most favored devices in the construction of large scale integrated circuits because of its simplicity of construction, the comparative lack of dopant diffusion problems and the resultant high packing densities possible. Whilst the preferred semiconductor is still silicon, industry is now tooling up for wide band gap semiconductors like GaN or SiC production, which offers high electron mobility and hence the prospect of greater frequency operating rates. InP offers the prospect of mobilities comparable to GaAs and is increasingly being developed for the construction of optical switches. Other authors have also pointed out the potential importance of InP and a few simple devices have been simulated [6]. InP has unfortunately proved to be a difficult material to work with in practice and very little experimental work has been done because of technical problems in forming Schottky contacts with sufficiently high barrier potentials [7-8]. Nevertheless some experimental work has been done on other types of InP field effect transistor, most notably MISFETs [9-10], and there is every reason to be optimistic that some form of heterojunction under the gate may well overcome the problem of the low barrier. In this paper we show that, if the aforementioned problems can be overcome, InP shows every indication that it will fulfill its promise as a useful material. However, simulations for higher anode voltages are needed in view of the situation in practical devices where engineering problems call for anode voltages of no less than about the Schottky barrier height or the p-n junction barrier height. The boundary conditions are important as they have significant influence on the space-charge-limited current flow which become dominant in submicron devices. In recent years, various theoretical approaches have been developed and used to calculate electronic transport characteristics in semiconductor devices. Among these methods the hydrodynamic approach, which combines the simplicity of the drift-diffusion model with the possibility of accounting for non-local effects, such as velocity overshoot, has emerged as a very reliable technique [8]. In general, the hydrodynamic description is based on velocity and energy conservation equations which are derived from the Boltzmann kinetic equation. However, such a derivation implies the introduction of several assumptions to close the system of conservation equations and, as a consequence, there exists a certain degree of freedom in the choice of the parameters to be used. The aim of this paper is to apply the hydrodynamic model to the case of submicron $n^+\!-\!i(n)\!-\!n^+$ InP structures. The comparison between

Manuscript received January 15, 2012. (This work was supported in part by the Department of Physics, Payame Noor University, Tehran, Iran.)

H. Arabshahi, Department of Physics, Payame Noor University, Tehran, Iran. e-mail: arabshahi@um.ac.ir.
the hydrodynamic model and a Monte Carlo simulation is taken as a validating proof of the hydrodynamic model. In particular, an original decomposition procedure involving the velocity and energy profiles in terms of field, convective and diffusive components has enabled us to carry out a detailed interpretation of electron transport in submicron n⁺-i(n)-n⁺ diode.

II. SIMULATION METHOD

For a one-dimensional geometry, the hydrodynamic approach model equations consist of the continuity equation

\[ \frac{\partial n}{\partial t} + \nabla \cdot j = 0 \]  

(1)

for negligible charge carrier generation and recombination, the momentum balance equation given by

\[ \frac{\partial p}{\partial t} + (\nabla p) \cdot v + (p \nabla) \cdot v = -enE - \nabla (nkT) - \frac{p}{\tau_p} \]  

(2)

or alternatively (only for x-component)

\[ \frac{[m'(\varepsilon')n_{v_x}]}{\partial t} + \nabla [m'(\varepsilon')n_{v_x}v_x] = -qnE_x - \frac{\partial (nkT)}{\partial x} - \frac{m'(\varepsilon')n_{v_x}}{\tau_p(t')} \]  

(3)

and the energy balance equation is

\[ \frac{\partial \varepsilon}{\partial t} + \nabla (\varepsilon v) = -qnE - \nabla (nkT) - \nabla (-k\nabla T) - \frac{\varepsilon - 3/2nkT}{\tau_s(\varepsilon')} \]  

(4)

where \( n, \varepsilon (\varepsilon' = \varepsilon/n) \), and \( v \) are the electron density, the electron energy density (average electron energy) and the electron drift velocity, respectively. \( v_x \) is the x-component of the electron drift velocity and \( p=m^*nv \) is the momentum density. Corresponding equations are valid for the y and z components. \( T \) is the electron temperature and \( \varepsilon' = 3/2kT \) is the average thermal equilibrium energy of electrons, where \( T_l \) is the lattice temperature. The electronic current density \( j \) inside the active device is \( j = nev \), so the total current density is

\[ j = -nev + \varepsilon_0 \varepsilon_r \frac{\partial E}{\partial t} \]  

(5)

The momentum relaxation time \( \tau_p(\varepsilon') \) is related to the mobility of the electrons via \( \mu(\varepsilon') = e/m^*(\varepsilon') \tau_p(\varepsilon') \), and the energy relaxation time \( \tau_{\varepsilon}(\varepsilon') \) describes the exchange of energy between the heated electron gas and the lattice. \( \tau_p \) and \( \tau_{\varepsilon} \) and the effective electron mass \( m^* \) are assumed to be functions of the mean electron energy. The hydrodynamic equations, together with Poisson's equation

\[ \Delta \phi = \nabla E = -\frac{\varepsilon}{\varepsilon_0 \varepsilon_r} (N_0^+ - n) \]  

(6)

form a complete set of equations that can be used to solve for the electron density, velocity, energy and electric field for given boundary conditions.

The hydrodynamic model based on equations 1-4 has an evident advantage in that it gives the possibility of verifying directly the assumptions used to close the system of conservation equations. Indeed, the spatial profiles of both velocity and energy can be directly calculated with the Monte Carlo simulation for the structure investigated and compared with those which can be deduced from the hydrodynamic calculations.

Self-consistent Monte Carlo simulation was performed using an analytical band structure model consisting of three non-parabolic ellipsoidal valleys [9-10]. The scattering mechanisms considered in the model are acoustic, polar optical, ionized impurity, piezoelectric and nonequivalent intervalley scattering. The nonequivalent intervalley scattering is between the \( \Gamma, X \) and \( L \). Acoustic and piezoelectric scattering are assumed elastic and the absorption and emission rates are combined under the equipartition approximation, which is valid for lattice temperatures above 77 K. Elastic ionized impurity scattering is described using the screened Coulomb potential of the Brooks-Herring model. The band structure and material parameters necessary for calculating the scattering probabilities used in the present Monte Carlo simulation are given in table 1. Steady-state results of high field transport studies have been obtained for lattice temperatures up to 300 K, in order to gain some insight into the hot carrier transport and the energy distribution function that would be generated in the gate-drain region of a power field effect transistor. The overall diode length which is used in both hydrodynamic and Monte Carlo models is 0.6 \( \mu \)m in the x-direction. A lightly doped active layer (n-layer) is sandwiched between cathode and anode layers, which are abruptly doped with a donor density of \( 10^{23} \text{ m}^{-3} \). The length of the active layer is 0.15 \( \mu \)m. Approximately \( 10^8 \) particles are used in the simulation and calculations are performed at room temperature. The applied anode voltage \( V_a \) is varied between 0 and 2.5 V to investigate the effects of field variations on the transport properties. This range of voltages is large enough that velocity overshoot and intervalley transfer effects occur.

III. RESULTS

The electron density and electric field profiles calculated with the hydrodynamic and Monte Carlo models are presented in figures 1a and 1b, respectively. An excellent agreement between the results of the two approaches is found. By comparing the value of the electron density through the device, we conclude that the electrons diffuse from the cathode and anode into the active layer and are accelerated towards the anode by the field. The resulting space charge causes the departure from a uniform electric field clearly apparent in figure 1b.
It is apparent from figure 1b that both hydrodynamic and Monte Carlo models show that essentially all the potential is dropped in the active layer. However, as a result of the inhomogeneous space charge the field does vary substantially with position, resulting a maximum magnitude near the anode. As the next step, figures 2a and 2b give the comparison between the hydrodynamic and Monte Carlo calculations for the velocity and energy profiles. Even in this case a good agreement between the two approaches is achieved. Figure 2a shows that the average drift velocity in the active layer has a maximum value of about \(2.25 \times 10^5 \text{ m s}^{-1}\) at 300 K. The plot of average electron kinetic energy across the device (figure 2b) provides further information on the dynamics. The electrons reach an average energy between 0.12 and 0.14 eV near the anode region and the more energetic electrons in the distribution have sufficient energy to transfer to the upper valleys.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>InP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band-gap (eV)</td>
<td>1.34</td>
</tr>
<tr>
<td>Electron effective mass (m*)</td>
<td>0.082</td>
</tr>
<tr>
<td>Nonparabolicity (eV⁻¹)</td>
<td>0.61</td>
</tr>
<tr>
<td>Static relative permittivity (\varepsilon_0)</td>
<td>12.61</td>
</tr>
<tr>
<td>Optical relative permittivity (\varepsilon_c)</td>
<td>9.61</td>
</tr>
<tr>
<td>Density (kgm⁻³)</td>
<td>4810</td>
</tr>
<tr>
<td>Sound velocity (ms⁻¹)</td>
<td>5130</td>
</tr>
<tr>
<td>Deformation potential (eV)</td>
<td>5</td>
</tr>
<tr>
<td>Piezoelectric constant (Cm⁻²)</td>
<td>0.03</td>
</tr>
<tr>
<td>Optical phonon energy (eV)</td>
<td>0.042</td>
</tr>
</tbody>
</table>

Table 1. Important parameters used in our calculations for InP material [7-9].

![Fig. 1](image1.png)  
**Fig. 1.** Spatial profiles of electron density and electric field calculated with Monte Carlo and hydrodynamic approaches for the 0.6 \(\mu\)m InP \(n^+-(n)-(n^+\) diode with doping levels \(n=10^{21}\) m⁻³ and \(n^+=10^{24}\) m⁻³. The applied anode voltage is varied between 0 to 2.5 V and the results are at room temperature.

![Fig. 2](image2.png)  
**Fig. 2.** Spatial profiles of (a) drift velocity and (b) electron average energy calculated with Monte Carlo and
hydrodynamic approaches for the 0.6 µm InP n⁺-i(n)-n⁺ diode with doping levels n=10^{21} m^{-3} and n⁺=10^{24} m^{-3}. The applied anode voltage is varied between 0 to 2.5 V and the results are at room temperature.

IV. Conclusion

An ensemble Monte Carlo simulation has been carried out to simulate the electron transport in n⁺-i(n)-n⁺ InP diode at 300 K in comparison with hydrodynamic approach. Our hydrodynamic model has been validated by comparison with a Monte Carlo particle simulator. An original decomposition of electron velocity and energy profiles in terms of field, convective and diffusive contributions has evidenced their importance and their mutual balancing near the homo-junctions. The electrons injected from the cathode initially travel quasi-ballistically but there is substantial transfer to the upper satellite valleys as the anode is approached, resulting in a reduced average electron velocity in that region.

REFERENCES


Hadi Arabshahi received the B. Sc degree in physics from the Ferdowsi University of Mashhad, Iran, in 1992 and the Ph. D. degree in computational physics from Durham University, United Kingdom, in 2002. He has published over 150 peer-reviewed journal papers and contributed to more than 80 conference papers and presentations. His research activities include semiconductor device simulations, high field transport properties in bulk and devices, transient relaxation in materials and devices, simulation of optoelectronic devices, electronics properties of low-dimensional and curved nanostructures and quantum information.