Steady-State and Transient Electron Transport within bulk InAs$_x$P$_{1-x}$, InAs and InP using A Semi-classical Three-Valley Monte Carlo Simulation Analysis

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Abstract

We study how electrons, initially in thermal equilibrium, drift under the action of an applied electric field within bulk zincblende InAs$_x$P$_{1-x}$, InAs and InP. Calculations are made using a non-parabolic effective mass energy band model, Monte Carlo simulation that includes all of the major scattering mechanisms. The band parameters used in the simulation are extracted from optimized pseudopotential band calculations to ensure excellent agreement with experimental information and ab-initio band models. The effects of alloy scattering on the electron transport physics are examined. For all materials, it is found that electron velocity overshoot only occurs when the electric field is increased to a value above a certain critical field, unique to each material. This critical field is strongly dependent on the material parameters. Transient velocity overshoot has also been simulated, with the sudden application of fields up to 1600 kVm$^{-1}$, appropriate to the gate-drain fields expected within an operational field effect transistor. The electron drift velocity relaxes to the saturation value of about $1.5 \times 10^5$ ms$^{-1}$ within 4 ps, for all crystal structures. The steady-state and transient velocity overshoot characteristics are in fair agreement with other recent calculations.

Key words: Non-parabolic; pseudopotential; alloy scattering; velocity overshoot; critical field.

Introduction

InP and InAs offer the prospect of mobilities comparable to GaAs and are increasingly being developed for the construction of optical switches and optoelectronic devices. While GaAs has been extensively studied [1-3], InAs and InP and alloy constructed from them like InAs$_x$P$_{1-x}$, have yet to examined to the same extent. Alloys of InAs and InP have unfortunately proved to be a difficult material to work with in practice and very little experimental work on InAs$_x$P$_{1-x}$ material and devices have been done because of technical problems in forming Schottky contacts with sufficiently high barrier potentials. Nevertheless some experimental work has been done on
other types of InAs and InP field-effect transistor, most notably MISFETs [4-5], 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.

Improved electron transport properties are one of the main targets in the ongoing study of binary and ternary InP, InAs and InAs$_x$P$_{1-x}$ materials. The Monte Carlo technique has proved valuable for studying non-equilibrium carrier transport in a range of semiconductor materials and devices [6-7]. However, carrier transport modeling of InP and InAs materials has only recently begun to receive sustained attention, now that the growth of compounds and alloys is able to produce valuable material for the electronics industry. In this communication we present Monte Carlo calculations of steady-state and transient electron transport conditions in InP, InAs and InAs$_x$P$_{1-x}$. We demonstrate the effect of injection energy and electric field on the transient electron transport. The differences in transport properties are analyzed in terms of important material parameters.

Our current approach employs a one-dimensional ensemble Monte Carlo technique to investigate steady-state and transient electron transport in InP, InAs and InAs$_x$P$_{1-x}$. However, the momentum space treatment is three dimensional, and the scattering events consider all three dimensions. Specifically, our model includes the three lowest valleys of the conduction band with non-parabolicity. This article is organized as follows.

Details of the conduction band parameters and the Monte Carlo simulation are presented in section 2, and the results of steady-state and transient transport simulations are discussed in section 3.

**Model details**

Our ensemble Monte Carlo simulations of electron transport in zincblende InP, InAs and InAs$_x$P$_{1-x}$ are similar to those of Arabshahi et al [8-9]. As indicated earlier, a three-valley model for the conduction band is employed.

In order to calculate the electron drift velocity for large electric fields, consideration of conduction band satellite valleys is necessary. The first-principles band structure of zincblende InAs, InP and InAs$_x$P$_{1-x}$ predicts a direct band gap located at the $\Gamma$ point and lowest energy conduction band satellite valleys at the $X$ point and at the $L$ point. In our Monte Carlo simulation, the $\Gamma$ valley, the three equivalent $X$ valleys, the four equivalent $L$ valleys, are represented by ellipsoidal, nonparabolic dispersion relationships of the following form [10-12]

$$E(k)[1 + \alpha_i E(k)] = \frac{\hbar^2 k^2}{2m^*}$$

where $m^*$ is effective mass at the band edge and $\alpha_i$ is the non-parabolicity coefficient of the $i$-th valley given by Kane model [13] as

$$\alpha_i = \frac{1}{E_g} \left[ 1 - \frac{2m^*}{m_0} \right] \left[ 1 - \frac{E_g \Delta}{3(E_g + \Delta)(E_g + 2\Delta/3)} \right]$$

where $E_g$ is the band-gap energy and $\Delta$ is the spin-orbit splitting.

We assume that all donors are ionized and that the free-electron concentration is equal to the
dopant concentration. For each simulation, the motion of ten thousand electron particles are examined, the temperature being set to 300 K, and the doping concentration being set to $10^{17}$ cm$^{-3}$.

In the case of the ellipsoidal, non-parabolic conduction valley model, the usual Herring-Vogt transformation matrices are used to map carrier momenta into spherical valleys when particles are drifted or scattered. Electrons in bulk material suffer intravalley scattering by polar optical, non-polar optical and acoustic phonons scattering, intervalley phonons, and ionised impurity scattering.

Acoustic scattering is assumed elastic and the absorption and emission rates are combined under the equipartition approximation, which is valid for lattice temperatures above 77 K. Elastic ionised impurity scattering is described using the screened Coulomb potential of the Brooks-Herring model. Band edge energies, effective masses and non-parabolicities are derived from empirical pseudopotential calculations. Important parameters used throughout the simulations are listed in tables 1-2.

<table>
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<tr>
<th></th>
<th>InAs</th>
<th>InP</th>
<th>InAs$<em>{0.2}$P$</em>{0.8}$</th>
<th>InAs$<em>{0.8}$P$</em>{0.2}$</th>
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<td>4810</td>
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<tr>
<td>$m_{\Gamma}$</td>
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<td>12.4</td>
<td>12.84</td>
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<tr>
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<tr>
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<td>8.3</td>
<td>7.62</td>
<td>5.58</td>
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<td>$\Gamma-L$</td>
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Table 1: Valley parameter selections for InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ [3-5]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>InAs</th>
<th>InP</th>
<th>InAs$<em>{0.2}$P$</em>{0.8}$</th>
<th>InAs$<em>{0.8}$P$</em>{0.2}$</th>
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<td>Longitudinal sound velocity $v_s$ (ms$^{-1}$)</td>
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<td>5300</td>
<td>5096</td>
<td>4484</td>
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<tr>
<td>Low-frequency dielectric constant $\varepsilon_s$</td>
<td>14.6</td>
<td>12.4</td>
<td>12.84</td>
<td>14.16</td>
</tr>
<tr>
<td>High-frequency dielectric constant $\varepsilon_{\infty}$</td>
<td>12.25</td>
<td>9.55</td>
<td>10.09</td>
<td>11.71</td>
</tr>
<tr>
<td>Acoustic deformation potential $D$(eV)</td>
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<td>8.3</td>
<td>7.62</td>
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<tr>
<td>Polar optical phonon energy (eV)</td>
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Table 2: Material parameter selections for InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ [3-5]

**Results**
Figure 1 shows the simulated velocity-field characteristics of zincblende InAs, InP, InAs$_{0.2}$P$_{0.8}$, and InAs$_{0.8}$P$_{0.2}$ semiconductors at 300 K, with a background doping concentration of $10^{17} \text{ cm}^{-3}$, and with the electric field applied along one of the cubic axes. The simulations suggest that the peak drift velocity for zincblende InAs is $3.4 \times 10^5 \text{ ms}^{-1}$, while that for InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ are about $\sim 2.3 \times 10^5 \text{ ms}^{-1}$, $2.5 \times 10^5 \text{ ms}^{-1}$ and $3.2 \times 10^5 \text{ ms}^{-1}$, respectively. At higher electric fields, intervalley optical phonon emission dominates, causing the drift velocity to saturate at around $1.5 \times 10^5 \text{ ms}^{-1}$ for all materials.

![Figure 1: Calculated steady-state electron drift velocity in bulk zincblende InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ using non-parabolic band models at room temperature](image)

The calculated drift velocities apparent from figure 1 are fractionally lower than those that have been calculated by Adachi et al. [14-16], who assumed an effective mass in the upper valleys equal to the free electron mass. The threshold field for the onset of significant scattering into satellite conduction band valleys is a function of the intervalley separation and the density of electronic states in the satellite valleys. The valley occupancies for the $\Gamma$, $X$ and $L$ valleys are illustrated in figure 2 and show that the inclusion of the satellite valleys in the simulation is important. Significant intervalley scattering into the satellite valleys occurs for fields above the threshold field for each material. This is important because electrons which are near a valley minimum have small kinetic energies and are therefore strongly scattered. It is apparent that intervalley transfer is substantially larger in InAs over the range of applied electric fields shown, due to the combined effect of a lower $\Gamma$ effective mass, lower satellite valley separation energy, and slightly lower phonon scattering rate within the $\Gamma$ valley.

We have also examined transient electron transport in bulk InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ semiconductors. The transient response of electrons in these materials are compared in figure 3 for fields up to 1600 kVm$^{-1}$ strengths. In InAs, we find very little or no overshoot occurs below the threshold field of $400 \text{ kVm}^{-1}$. As the electric field strength is increased to a value above the threshold field, overshoot begins to occur. As the field strength is increased further, both the peak
overshoot velocity increases and the time for overshoot relaxation decreases.

Figure 2: Fractional occupation of the central $\Gamma$ and satellite valleys of zincblende InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ as a function of applied electric field using the non-parabolic band model at room temperature

In InAs, the velocity overshoot initially increases more rapidly with increasing electric field due to the lower $\Gamma$ valley effective mass. For example, at 1600 kV/m$^{-1}$, the maximum overshoot velocity for InAs is about $8 \times 10^5$ ms$^{-1}$, whereas for InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ it is about $4 \times 10^5$ ms$^{-1}$, $5 \times 10^5$ ms$^{-1}$ and $7 \times 10^5$ ms$^{-1}$, respectively. It is found also that for the same value of the electric field above the threshold value, the electron drift velocity is always smaller in InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ than in InAs.
Figure 3: A comparison of the velocity overshoot effect exhibited by InAs, InP, InAs₀.₂P₀.₈ and InAs₀.₈P₀.₂ semiconductors as calculated by our Monte Carlo simulation. The donor concentration is 10^{17} \text{ cm}^{-3} and the temperature is 300 K

Figure 4 shows average velocity of electrons in InAs, InP, InAs₀.₂P₀.₈ and InAs₀.₈P₀.₂ as a function of distance. We note that for the applied field selections 400 to 1600 kV/m the average electron velocity reaches steady-state very quickly, with little or no velocity overshoot. In contrast, for applied electric field selections above 400 kV/m, significant velocity overshoot occurs. It is suggested that in InAs₀.₂P₀.₈ and InAs₀.₈P₀.₂ 400 kV/m is a critical field for the onset of velocity overshoot.
overshoot. As mentioned above, 400 kVm\(^{-1}\) also corresponds to the peak in the velocity-field characteristic associated with InAs\(_{0.2}\)P\(_{0.8}\). Steady-state Monte Carlo simulations suggest that this is the point at which significant upper valley occupation begins to occur, as shown in figure 2. This suggests that velocity overshoot is related to the transfer of electrons to the upper valleys. To optimize device performance, we have to minimize the transit time over a given distance.

![Graphs showing drift velocity vs. distance for different fields in InAs and InP.](image)

**Figure 4:** A comparison of the average electron velocity as a function of the displacement for various applied fields in InAs, InP, InAs\(_{0.2}\)P\(_{0.8}\) and InAs\(_{0.8}\)P\(_{0.2}\) semiconductors. In all cases, we have assumed an initial zero field distribution, a crystal temperature of 300 K and a doping concentration of 10\(^{17}\) cm\(^{-3}\).

From figure 5, it can be seen that there is tradeoff between the peak overshoot velocity and the distance taken to achieve steady-state. In particular, when the applied electric field is set to 1600 kVm\(^{-1}\) the peak overshoot velocity of InAs\(_{0.8}\)P\(_{0.2}\) is 7.8×10\(^5\) ms\(^{-1}\), while the corresponding steady-
state drift velocity, $1.5 \times 10^5 \text{ ms}^{-1}$, is achieved after just 0.2 $\mu$m.

However, for an applied field of 400 kVm$^{-1}$, just above the critical field, the peak overshoot velocity is only $4 \times 10^5 \text{ ms}^{-1}$, and it takes longer, about 0.8 $\mu$m, to achieve the corresponding steady-state drift velocity, $3 \times 10^5 \text{ ms}^{-1}$. Similar results are noted for InAs$_{0.2}$P$_{0.8}$, as is seen in figure 5. In particular, the critical field denoting the onset of velocity overshoot coincides, almost exactly, with the field at which the peak drift velocity in the steady-state velocity field characteristic is found, i.e., 200 kVm$^{-1}$ for InAs and 800 kVm$^{-1}$ for InP. The correspondence between the critical field at which the onset of velocity overshoot effects occur and the peak in the steady-state velocity field characteristic appears to be valid for the case of other III-V semiconductors as well.

![Figure 5: Comparison of the valley occupancies as a function of applied electric field in InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ for $\Gamma$, $X$ and $L$ valleys at room temperature.](attachment:figure5.png)

**Conclusion**

Electron transport at 300 K in bulk zincblende InAs, InP, InAs$_{0.2}$P$_{0.8}$ and InAs$_{0.8}$P$_{0.2}$ have been simulated using an ensemble Monte Carlo simulation. Using valley models to describe the
electronic bandstructure, calculated velocity-field characteristics are in fair agreement with other calculations. Saturation drift velocities $\sim 1.5 \times 10^5$ ms$^{-1}$ match recent measurements on low-doped bulk samples. The velocity-field characteristics of the materials show similar trends, reflecting the fact that all the semiconductors have satellite valley effective densities of states several times greater than the central $\Gamma$ valley. However, the peak velocity in InAs$_{0.2}$P$_{0.8}$ occurs at a field $\sim 700$ kVm$^{-1}$, 2 times larger than for InAs$_{0.8}$P$_{0.2}$. This is a consequence of the large $\Gamma$ valley effective mass in InAs$_{0.2}$P$_{0.8}$ structure. This reduced valley effective mass in InAs$_{0.8}$P$_{0.2}$ permits substantial population of the upper valleys and velocity saturation at far lower electron temperatures than in InP.

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References