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Hot electron effects on the operation of potential well barrier diodes

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Abstract: A study has just been carried out on hot electron effects in GaAs/$Al_{0.3}Ga_{0.7}As$ potential well barrier (PWB) diodes using both Monte Carlo (MC) and drift-diffusion (DD) models of charge transport. We show the operation and behaviour of the diode in terms of electric field, mean electron velocity and potential, mean energy of electrons and Γ-valley population. The MC model predicts lower currents flowing through the diode due to back scattering at anode (collector) and carrier heating at higher bias. At a bias of 1.0 V, the current density obtained from experimental result, MC and DD simulation models are 1.35, 1.12 and 1.77 $\mu A/\mu m^2$ respectively. The reduction in current over conventional model, is compensated to a certain extent because less charge settles in the potential well and so the barrier is slightly reduced. The DD model results in higher currents under the same bias and conditions. However, at very low bias specifically, up to 0.3 V without any carrier heating effects, the DD and MC models look pretty similar as experimental results. The significant differences observed in the *I–V* characteristics of the DD and MC models at higher biases confirm the importance of energy transport when considering these devices.

Key words: Monte Carlo model; back scattering; carrier heating; electron energy; non-stationary fields

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1. Introduction

Potential well barrier (PWB) diodes are non-linear two-terminal diodes with current flow controlled by the barrier formed by a potential well between two intrinsic regions[1]. Just like the planar doped barrier (PDB) diodes[2, 3] with similar design structure and operation as the PWB diodes, the ability to control the barrier height and diode asymmetry independently offers a huge advantage for potential applications in mixers and detectors at microwave frequencies[4]. The PDBs were first introduced by Malik *et al.*[2] and has been an alternative for several applications for which Schottky barriers are used but for which contact stability and ability to redesign the barrier height are of extreme significance. The PDB diode uses a fixed positively doped sheet charge placed between two intrinsic regions which depletes completely to form a barrier when subjected to DC bias. Both the PDB and PWB diodes alternatively has the capability of recreating potential barriers similar to the hybrid planar-doped potential-well barrier[5] and heterostructure barrier varactor (HBV) diodes[6], which gives it an edge over the Schottky barriers with a metal semiconductor junction. The PWB and PDB diodes on the other hand offers the possibility of a tractable barrier height that could be tailored to achieve zero bias detection. Due to the similarity in the principle of operation of a PWB and PDB diodes and also, because it was found that considering hot electron effects was important in these devices at very high electric fields[7–9], it becomes imperative to consider hot electron effects in the PWB diode. Previous papers have investigated the operation of potential well barrier diode using drift-diffusion models[5, 10, 11], with the MC model treated in Ref. [12] though, no energy transport or heating effects were considered. In this paper we will discuss how, whilst the basic semiconductor theory sufficiently describes the behaviour of these diodes, a more advanced treatment of the diode is needed to understand some observed currents and details of carrier dynamics in the device. This is important because at high bias operation of similar devices, there is a transition from barrier controlled non-ohmic transport to the hot electron dominated current as demonstrated in the planar doped barrier and Schottky barrier diodes[13–15] though, some important differences exist which will be shown in this paper. A Monte Carlo model was used to study this device which allows the effect of carrier heating and non-stationary dynamics, which were not included in the conventional DD models[1, 5] reported previously to be taken into account. We have compared the *I–V* characteristics produced from the MC and DD simulation models with experimental results. The Monte Carlo simulation shows significant differences in *I–V* characteristics when compared with drift-diffusion model particularly at biases more than 0.5 V though, but with better agreement with experiment at nearly all biases. Also by simulating the diode with different applied biases, we demonstrate how the electron mean kinetic energy, average velocity of electrons and the Γ-valley occupation across the diode varies with increasing bias. We will also elucidate why the *I–V* characteristics obtained from both the MC and DD models differ significantly at higher applied voltages.

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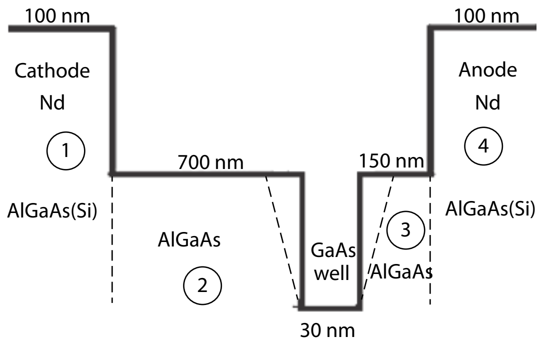

Fig. 1. The epitaxial structure of the potential well barrier diode showing all the design parameters.

2. Experiment

The experimental set up and procedures have been reported in Refs. [1, 10] though, a summary of the experiments will be described in this paper too. We consider importantly the layer design and growth process to realize diodes with low voltage detection capability. The epitaxial structure of the devices used for this investigation was a GaAs/AlGaAs heterostructure as shown in Fig. 1. This structure contains doped n^+ regions of $Al_{0.3}Ga_{0.7}As(Si)$, 100 nm long and doping concentration of 4.10×10^{24} m^{-3} on both diode terminals (labels 1 and 4) which interact with the ohmic contacts. Labels 2 and 3 represent the left and right intrinsic regions of $Al_{0.3}Ga_{0.7}As$ with lengths 7000 and 1500 Å respectively, while a GaAs well of width 300 Å was inserted between the two intrinsic regions. The experiment was done under tight control required over the thickness and composition of each epitaxial layer and performed in a RIBER V90H reactor on n^+ GaAs substrates. Circular diode with diameter 50 μm was fabricated using i-line optical lithography in a standard wet etched process. The front and back contacts, consisting of 50 nm AuGe/13 nm Ni/200 nm Au were thermally evaporated and annealed providing a very low contact resistance. This was followed by an ortho-phosphoric based etch to produce self-aligned mesas to a depth of 1.5 μm using the top contact metal as a mask. Measurements of device were carried out on-wafer using a probe station at room temperature. The device *I*–*V* characteristics were measured using an Agilent (keysight) B1500A Semiconductor Device Analyser from –3 to 2 V.

3. The Monte Carlo model

The Monte Carlo model used here was initially developed to study the transport formalism in semiconductor devices and has been used extensively to study operation of the Gunn diodes[16–18]. The carrier free flights duration between successive collisions and the scattering events involved are selected stochastically in accordance with the given transition probabilities describing the microscopic processes. The conduction band is approximated by nonparabolic multivalley (Γ–L–X) bands, using the dispersion relation[19]. The scattering mechanism involved in this model include inter-valley, acoustic and polar optical phonon scattering with the polar optical scattering dominating scattering mechanism at high fields and in this case, at a bias of 2 V with corresponding higher electric field. Impurity scattering is neglected in the model since there is no doping across the entire active region (intrinsic region) of the diode. Material parameters used in the simulation for GaAs and AlGaAs are taken

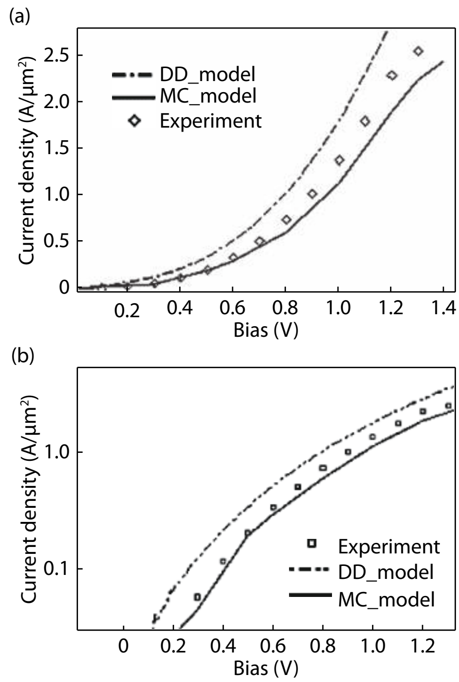

Fig. 2. Comparison of the experimental results (diamond), the drift-diffusion (broken line) and Monte Carlo (solid line) simulation models. Result shows that the MC model has better agreement with the experimental results than the DD model lower bias (a) linear (b) logarithmic plots.

from the experimental results[1]. The simulation of the individual particle trajectories follow the extensively used procedures of Monte Carlo simulation[19–21], with the generation of a sequence of free flights terminated by scattering event such as phonons. A constant lattice temperature of 300 K was used throughout the study in both the MC and DD models. The MC simulation was allowed to run over 80 000 iterations for a time duration of 50 ps for each time step using ~50000 particles. We used a constant step discretization to track the time evolution of electron distribution and also to determine the position of electrons at a given time. The electron densities are computed and Poisson equation is solved self-consistently using the successive over relaxation (SOR) to obtain the electric fields. The Monte Carlo method used in this paper is similar to those covered in the literature as are flow charts for the MC code[22–24]. This diode structure was simulated earlier by the DD model and reported in Refs. [1, 10] with the contacting layers being 0.10 μm thick. The electron concentration in the n^+ region was fixed at a doping level of 4.10×10^{24} m^{-3} throughout the entire simulation. Also for simplicity, the ohmic contacts have been treated ideally in these models. With the left and right intrinsic length maintained at 0.7 and 0.15 μm respectively for the two models with no fitting to achieve good agreement with the experimental device, we simulated the structure with a GaAs band offset of 0.25 eV.

4. Results and discussion

4.1. Comparison of diode *I*–*V* characteristics using experimental results, MC and DD models.

Fig 2 shows the comparison of the *I*–*V* characteristics of the PWB diode using the Monte Carlo (solid line), drift-diffusion (dotted line) models and the experimental data (dia-

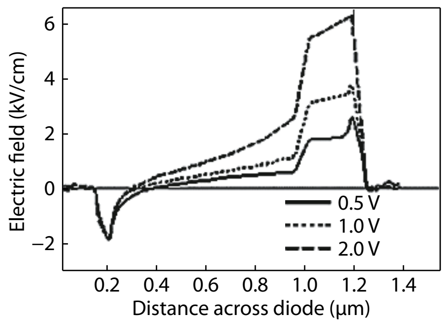

Fig. 3. Behaviour of effective (including the band offset) electric field for various operating bias across the diode.

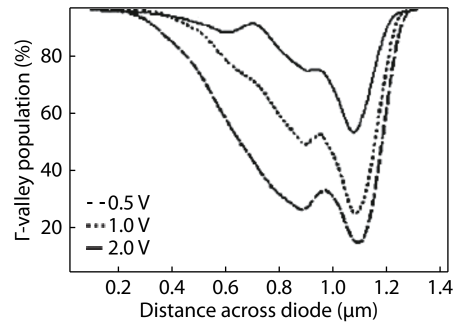

Fig. 4. Effect of varying electric field on the population of electron across the diode. The result shows that there are more electrons in the diode operating at a lower field (bias of 0.5 V).

mond) for the same nominal structure. Both models seem to agree with each other fairly well at low currents, especially up to a bias of 0.3 V but give quite different results at higher currents. This is obviously due to decreases in carrier mobility since carrier heating effect dominates the device by the large electric fields. Though sensitivity to variation in parameters was investigated in Ref. [10] and it was only with fitting to parameters that the DD simulation model agreed well with experimental *I*–*V* characteristics as reported in Ref. [10].

However, for the same nominal values of parameters as the experimental device, we observed that there is a better agreement with the MC model especially at current densities more than 0.5 μA/m^2 (though noise in the MC model makes determining currents below 0.3 V difficult) but the DD simulation model significantly overestimates the current for biases above 0.3 V since the DD treats electron mobility of carriers as being in equilibrium with the field at a constant temperature. Also, in the DD models, the electron gas is assumed to be in thermal equilibrium with the lattice temperature. In the presence of a strong electric field however, electrons gain energy from the field and the temperature of the electron gas is increased further. Thus, electron transport is influenced by pressure gradient rather than just density gradient since the pressure of electron gas is proportional to nk_BT_n[25]. This effect is demonstrated in Fig. 2 where the MC model and experimental results are similar except that the current density at a bias of 0.8 V becomes lower when hot carrier behaviour takes effect. For example, at a voltage of 1.0 V the current density obtained from the experimental result, MC and DD simulation models are 1.35, 1.12 and 1.77 μA/μm^2 respectively.

The differences between the MC and DD models are primarily due to reduction in carrier mobility in the MC model as a result of carrier heating in the active region of diode by large electric fields as suggested by Ref. [7] for PDB's. The lowering of the current density due to carrier heating is also caused by back scattering of hot electrons in the anode (collector) region of the diode which also decreases the net current over the barrier in the MC model as in Ref. [7]. Carrier heating occurs in the PWB diode due to energy exchanges that occur between the electrons and lattice due to phonons especially, when the electric field is so high enough to exceed velocity saturation[26, 27]. At low bias, the rate of energy exchange equals zero and carriers are in thermal equilibrium with the lattice. However, at high bias, the carriers gain so much energy and losing it to lattice through phonons. Due to such high field, the energy possessed by carriers are certainly above acoustic phonons though, mitigated by optical phonons. These carriers then acquire effective electron temperature (T_e); which is higher and different from lattice temperature.

However, unlike in a PDB, there would seem to be a small reduction in the potential barrier in the PWB diode due to a reduction of carriers in the well because of higher temperatures. This to a certain extent mitigates the differences in current between the two models that would be expected in a PDB.

4.2. Influence of bias on the electric field

Fig. 3 shows the variation of the effective electric field with applied bias as simulated by the MC model.

The large electric field changes rapidly over the length of the device as the applied bias increases thus, creating nonlocal and hot carrier effect which dominates the performance of the device. There is however a sudden rise in the effective field at the right edge of the potential well at a position of 1 μm across the diodes as the field receives a boost due to the high energy acquired in the potential well.

4.3. Electron population in the Γ-valley

As shown in Fig. 4, the population of the electrons across the diode varies with changes in the applied bias. As electric field increases across the diode due to increases in the applied bias, this significantly increases the speed of electrons in the lower valley as electrons get heated up and become more excited. As a result, electrons gain significant energy even beyond acoustic phonon thus, intervalley transfer rapidly increases and the gamma valley population reduces significantly with such high electric field. Fig. 4 shows decreases in the percentage of charge in the Γ-valley across the diode. For example at a distance of 1.08 μm (to the right of the diode), the estimated percentage population of electrons at this position for 0.5, 1.0 and 2.0 V respectively are 52.4%, 24.47% and 14.06%. Also in the well at a position between 0.98 and 1.01 μm, the respective estimated percentage of electrons in the gamma valley for biases of 0.5, 1.0 and 2.0 V is 74.12%, 50.04% and 32.5 %.

4.4. Comparison of the mean electron velocity

The velocity of electrons is one of the most important parameter used for characterizing the microscopic quality of semiconductors[28]. As shown in Fig. 5, the effective velocity of the electrons for all biases is in equilibrium with the electric field and there is little sign of ballistic overshoot which would also impact the current. The velocity rises gradually across the diode at all biases. For a bias of 0.5 V, the velocity of the electrons gradually increases to peak at a position of

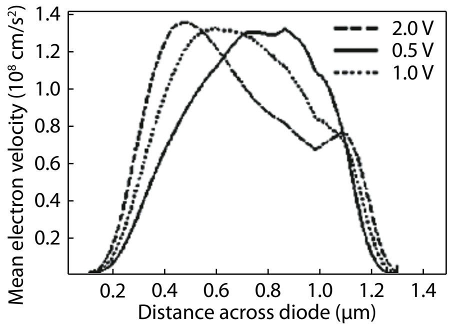

Fig. 5. Electron velocity as a function of positon across the diode under influence of non-stationary field. Results shows little differences in the maximum velocity for the three biases: 0.5, 1.0 and 2.0 V. The velocity drops faster across the diode for diode operating at 2.0 V.

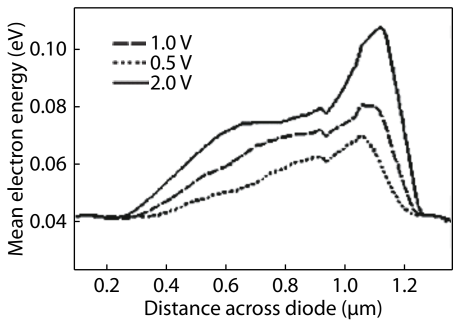

Fig. 6. Average electron energy as function of position across diode for several bias. The mean energy of electrons increases considerably with the bias.

~ 0.75 μm and begins to decay at a position of ~ 0.95 μm after position of the well. For the bias of 2.0 V, the velocity of electrons increases rapidly and reaches a peak at a position of ~ 0.42 μm and decays quickly across the diode as the field increases.

This shows how the electrons at higher bias across the diode saturate faster compared to electrons at lower bias. The most important point we wish to stress here is that, a higher bias results to higher electric field and this initially increases the mobility of the electrons in the device. There is therefore a tendency of achieving a high frequency with PWB diodes operating with high electric field though, frequency operation not considered here in this study.

4.5. Effect of bias on the mean electron energy

Fig. 6 shows that the electrons across the diode get hotter as the bias increases and causes the average kinetic energy to increase. The results shown in Fig. 6 are similar in form to those observed in Ref. [7] for PDB's. For a bias of 0.5 V, the diode maintained a nearly constant energy of approximately 0.041 eV up to a distance of 0.35 μm. Thus, the average kinetic energy starts increasing steadily until it reaches a maximum value of 0.068 eV at position of 1.0 μm across the diode.

For the bias of 2.0 V the electron energy rises steadily from a position of 0.25 μm up to 0.078 eV at the edge of the well. The kinetic energy abruptly increases to 0.11 eV where it reaches a peak in the right intrinsic region (at position of 1.12 μm across diode). For an applied bias of 1.0 V, the mean kinetic energy lies intermediate between the kinetic energy of applied bias of 0.5 and 2.0 V. The average kinetic energy of electrons at this bias increases steadily from position of 0.32 μm and peaks at position of 1.09 μm with a value of 0.08 eV. This result shows that at a higher applied bias, more inter-valley scattering from the Γ–valley to the composite heavy valleys occurs hence, causing greater hot electron effects in the diode compared to lower biases. The average kinetic energy across the diode reflects the applied bias and is similar in form to a PDB[8].

5. Conclusion

In conclusion, the application of Monte Carlo model in the study of hot carrier effects in PWB diodes provides a good understanding of interior carrier transport of these devices and also gives a better description and a quantitative analysis of high and low current operation in these diodes. The *I–V* characteristics values produced by the Monte Carlo model are lower than those predicted by DD models and in better agreement with the experimental results due to reduction in the mobility of carriers because of hot carrier effects. Results of the *I–V* characteristics of the conventional DD models demonstrate the limitation of the model to predicting some of the important diode's attributes. Also, the MC model was used to investigate the behavior of the PWB diode to changes in operating bias in terms of the mean kinetic energy of electrons, average electron velocity, population of charge across device and electric field distribution across diode active region thus, demonstrating the importance of the hot carrier model in the diode analysis. There are of course uncertainties in the epitaxial structure and fabrication of these devices which make the experimental results uncertain and hence any conclusions that we can draw. However, the consistently better agreement between experiment and the MC model which includes hot carrier effects over the DD model which did not include such effects, provides compelling evidence for the importance of hot electron effects in these devices.

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