Investigating the role of band offset on the property and operation of the potential well barrier diodes

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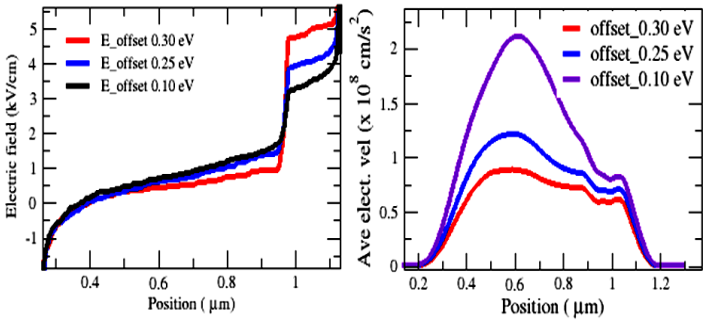
The impact of grading the GaAs/AlGaAs interface on carrier dynamics in a Potential Well Barrier (PWB) diode has been explored and demonstrated in this paper. Three heterostructures in the GaAs/AlGaAs system namely $GaAs/Al_{0.2}Ga_{0.8}As$, $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ with corresponding band offsets of 0.1, 0.25 and 0.30 eV respectively were investigated using the drift-diffusion (DD) and Monte Carlo (MC) models. The behaviour of the diodes with different band offsets were compared in terms of mean electron velocity, mean electron energy and density of charge along the intrinsic regions and in the potential well. The MC simulation model enables the effect of space-charge injection and carrier heating which were not included in previous study of these structures be treated quantitatively. Significant differences exist in the behaviour of the three heterojunctions as this impacts the curvature coefficient and ideality factor of diode. Both the ideality factor and curvature coefficient reflect the magnitude of band offset of the heterojunctions (interface).



1 Introduction Previous study reported in [1-4] shows that the potential well barrier (PWB) diode could be optimized for potential applications in mixers and detectors. With similar operation and structure to the planar-doped potential-well barrier (PPB) [1] and the planar doped barrier (PDB) [5, 6] diodes, there is ease to which barrier height could be controlled and adjusted (during wafer fabrication process) for zero bias detection and with prospects of improved reverse bias operation [1]. It is possible to grade the $GaAs/AlGaAs$ system in a variety of ways that diode structures be achievable with various percentage compositions of Al and Ga to form a heterojunction and hence varying conduction band offset whilst achieving the same function. The heterostructure could generally be written as $GaAs/Al_xGa_{1-x}As$, with x representing the composition of Al atoms in the material. This introduces some variations in property and performance of diode operating under same bias and conditions. For example, the $GaAs/AlGaAs$ system could be graded to $GaAs/Al_{0.2}Ga_{0.8}As$, $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ corresponding to band offset of $0.10, 0.25$ and $0.30\ eV$ [7]. This certainly will affect electron density, mean velocity, average carrier energy transiting along intrinsic layers and in the potential well. We will simulate the PWB $GaAs/AlGaAs$ system using three different heterostructures with band offsets $0.10, 0.25$ and $0.30\ eV$ and show, how the property and also operation of diode could be affected in terms of the charge along intrinsic regions and in the potential well. We will also elucidate why the average velocity of electrons and effective carrier energy in PWB diode structure varies with the band offset.

2 Experiments The experimental set up was fully described and reported in [1, 3] however, a brief description will be given here in this paper. The epitaxial structure of the PWB diode was grown using i-line optical lithography in a standard wet etch process and results measured at $300K$. The front and back contacts which consisted of $50\mu m\ AuGe/13\ nm\ Ni/200nm\ Au$ were thermally evaporated and annealed to provide low contact resistance of less than $0.2\ \Omega mm$. An orthophosphoric based etch was used to produce self-aligned mesas to a depth of $1.5\ \mu m$ using the top contact metal as mask. A RIBER V90H reactor was used to provide tight control over the thickness and composition of each epitaxial layers. Diode I-V characteristics were measured using an Agilent (Keysight) B1500A Semiconductor Device Analyzer ranging from $-3\ to\ 2\ V$ [2]. As shown in Fig. 1, labels 1 and 4 are doped n^{++} regions of $AlGaAs(Si)$ while labels 2 and 3 are the undoped regions of $AlGaAs$. The experiment described here was carried out for $GaAs/Al_{0.3}Ga_{0.7}As$ with band offset of $0.25\ eV$ only. All the other results for the $GaAs/Al_{0.2}Ga_{0.8}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ heterostructures were obtained by simulating an equivalent PWB diode with design parameters as in the experiment.

3 The Monte Carlo model To achieve the purpose of this study, we simulated PWB diode structures with band offsets: $0.10, 0.25$ and $0.3\ eV$ corresponding to $GaAs/Al_{0.2}Ga_{0.8}As$, $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$, and compare their mean electron densities, velocities and average kinetic energies.

Our MC model was used to allow the quantitative discussion of carrier heating effect which could not be accounted for by DD models in the previous study. The MC model has been successfully used to investigate the planar Gunn diodes [8-10] and recently the PWB diode. The model incorporates the $\Gamma - L - X$ valleys of the conduction band and also include the effect of non-parabolicity. Scattering mechanism used in the model are intervalley, acoustic and polar optical phonon scatterings. Impurity scattering are neglected in the model because the active region of diode is purely intrinsic and also, the width of potential well is quite small compared to mean free path of electrons for impurity scattering to occur. We use a constant discretization time step which helps to determine the exact position of electron distribution at a particular time. This scheme allows us to track time evolution of electron distribution as well as determine the points of all sample electrons across the diode. Electron densities were calculated at each mesh point as a function of time and space coordinates. The Poisson solver was used with successive over relaxation process to obtain electric field at mesh points. A constant lattice temperature of $300K$ was used throughout the study in both MC and DD models. The MC simulation was allowed to run over 40000 iterations at $50ps$ for each time step. The simulation also ran for ~ 50000 particles; transient behavior at the beginning of simulation were over within range of $100 - 150$ time steps. The simulation reaches stability and was averaged to give current density for every bias. These structures were simulated with layers of $AlGaAs(Si)$ $0.25\ \mu m$ long each doped to concentration of $4.10 \times 10^{24}\ m^{-3}$. With the left and right intrinsic length maintained at 0.7 and $0.15\ \mu m$ respectively, we simulated the structures over a well thickness of 300Å.

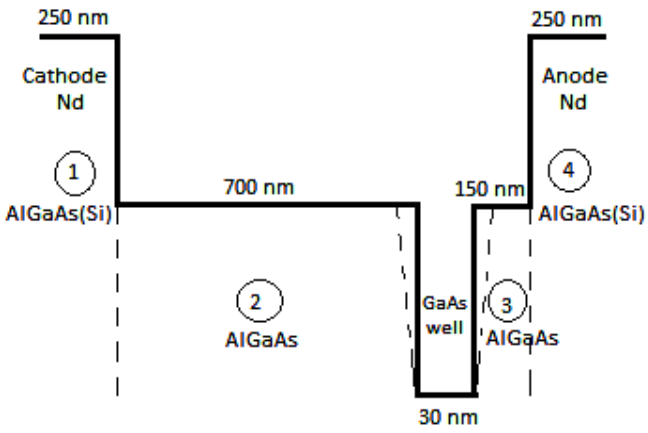


Figure 1 Equivalent device structure showing dimensions and doping profile

4 Analysis and discussion of results

4.1 Comparison of the experiment and simulations Figure 2 shows the I-V characteristics of experimental results of the MC and DD models using same nominal values (that is, without fittings) as in the experiment. As mentioned earlier, we carried out experiments for the $GaAs/Al_{0.3}Ga_{0.7}As$ heterostructure, with band offset of $0.25\ eV$ only and we may also compare just the I-V characteristics of $GaAs/Al_{0.3}Ga_{0.7}As$ with our models. There is a better agreement between the MC and experimental results especially at lower current densities except at bias of $0.7\ V$ and higher where carrier heating effect begins to impact diode ideal performance. The lowering of the current densities in MC model at this bias is due to carrier heating and scattering of electrons in the

diode. The DD model however results in higher currents under same bias and conditions due to its steady state nature as effect of scattering is not taken into account. The DD models overestimates the current densities for all the biases. The significant differences in the MC and DD models demonstrate the importance of including hot carrier transport models in analysis of submicron devices.

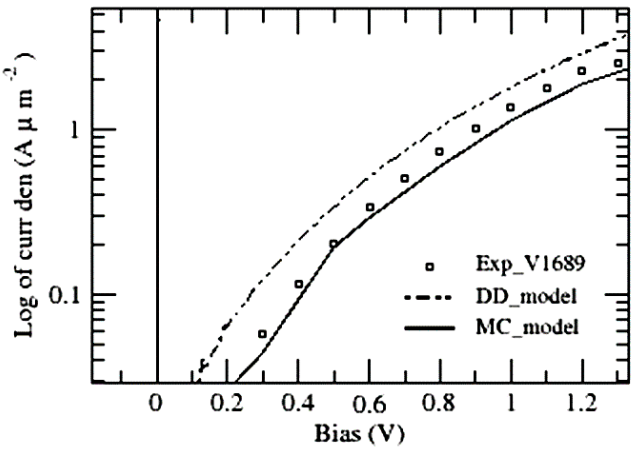


Figure 2 Comparison between the I-V characteristics of experimental results, DD and MC models

4.2 Electric field distribution across each diode The electric fields of the diodes are as presented in Fig. 3 as estimated from the Montel Carlo model. The field in the $GaAs/Al_{0.2}Ga_{0.8}As$ increases rapidly and is higher than both the $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ with the latter having the least electric field up to position of $0.95\ \mu m$ across the diode. This is because in this region as mentioned above, there is less charge in the structure with x composition of 0.4 thus, producing a very low field which is almost constant. The electric field tends to increase as the x composition decreases in this region especially in the Γ-valley. This has influence on the velocity and the average kinetic energy of electrons. Beyond this region however, there is abrupt rise in the electric field in structures with higher *Al* composition. Beyond the position of $0.95\ \mu m$ across the diode, the charge in the well builds up with increasing x composition. This accounts for the abrupt rise in the electric field at this position as shown in Fig 3.

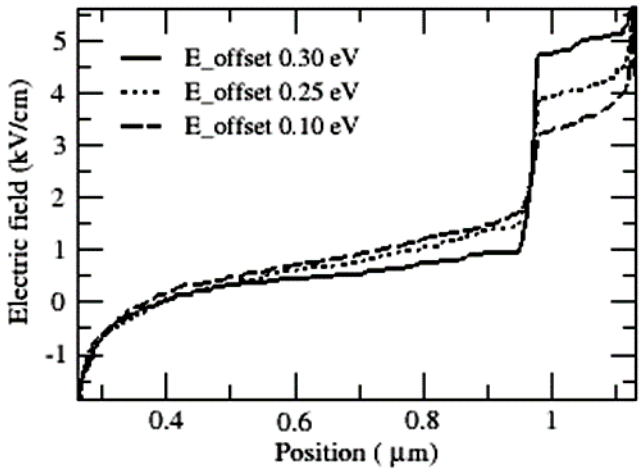


Figure 3 Comparison of the electric field distribution across active region of diode for various compositions of x in $GaAs/Al_xGa_{1-x}As$ across diode.

4.3 Electron distribution along intrinsic regions Figure 4 shows the distribution of electron densities along intrinsic regions as a function of position at $0.1\ V$ for conduction band offsets of $0.10, 0.25$ and $0.3\ eV$ corresponding to $GaAs/Al_{0.2}Ga_{0.8}As$ $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ as simulated using the DD model.

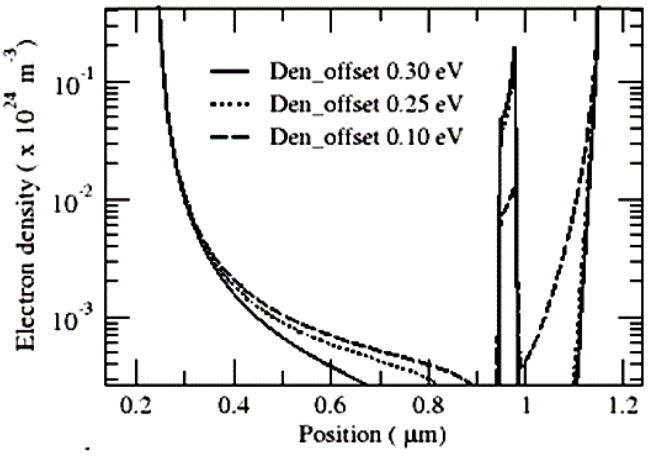


Figure 4 Distribution of charge density in the undoped layers of PWB diodes as a function of position at a bias of 0.1 V for diodes with conduction band offsets of 0.1, 0.25 and 0.30 *eV* corresponding to compositions x of 0.2, 0.3 and 0.4

There is redistribution of mobile electrons in undoped layers with changes in band offset, which probably results in band offset dependence of barrier height. We observed that lower conduction band offset results in higher charge

density distribution along the diode's active (intrinsic) region. As shown in Fig. 4, diode with conduction band offset of $0.10\ eV$ has more charge along this region compared to diode with band offset of 0.25 and 0.30 eV. For example, the electron density for band offsets of $0.10, 0.25$ and $0.3\ eV$ at $0.6\ \mu m$ across the device were respectively obtained as 8.68×10^{20}, 3.35×10^{20} and 2.24×10^{20}. This shows a drop in electron densities as band offset increases.

4.4 Comparison of the electron velocity The velocity of electrons is one of the most important parameter used for characterizing the microscopic quality of semiconductors [11]. Figure 5 shows the mean electron velocity for the three diodes with different compositions of Al and Ga in the alloy. The Monte Carlo results shows that there is high intervalley scattering in the downhill region which causes a reduction in speed of electrons across the device and this randomizes electron distribution in k-space. The severity of the scattering increases as the density of states increases. As estimated from the Monte Carlo simulations, the highest electron velocity was achievable in gamma valley ($\Gamma - valley$) for diodes with band offset of 0.10 eV at position of 0.60 µm with an estimated velocity of $2.06 \times 10^8\ cms^{-1}$ compared to diodes with band offset of $0.25\ eV$ and 0.30 eV with estimated velocities of $1.20 \times 10^8\ cms^{-1}$ and $0.88 \times 10^8\ cms^{-1}$ respectively at same position.

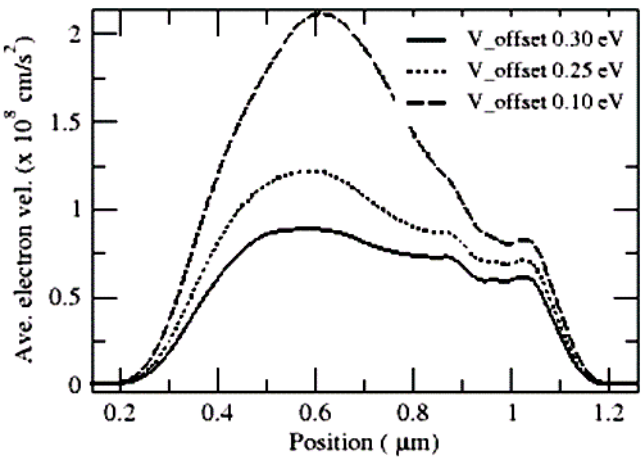


Figure 5 Electron velocity of the PWB diode for band offset of $0.05, 0.10$ and $0.25\ eV$ simulated at a bias of $1.0\ V$ and temperature of $300K$.

The velocity was observed to reduce as band offset increases. High drift velocity is very important in submicron devices such as PWB diode at high electric field as this may offer some improvement in frequency operation of the diode though [12].

There are two reasons for the behavior of electron velocities in this manner. First as shown earlier in Fig 3, the electric field is not the same for all the devices thus, the velocity of electrons across the active region of each diode reflects the value of the electric field. For example, the electric across $GaAs/Al_{0.2}Ga_{0.8}As$ is higher and as such has a higher electron mobility across the active region of diode compared to the other heterostructures, with that of $GaAs/Al_{0.4}Ga_{0.6}As$ being the least. The behaviour of electrons mobility across these structures with respect to the x % composition in the material agrees with the experimental results studied in [13] for $GaAs/Al_xGa_{1-x}As$. This is as a result of the increases in the effective masses of devices as x composition incresases. Thus, as shown in Fig 5, as the composition of Al in the material increases, the mobility of electrons decreases.

4.5 Comparison of the average electron energy of PWB structures Figure 6 shows the Monte Carlo simulations result of the average kinetic energy of electrons across the diodes as a function of position. The carrier energy increases with decrease in band offset; this is because more electrons undergo scattering as the velocity of electrons increases thus, causing hot electron effects in the diode.

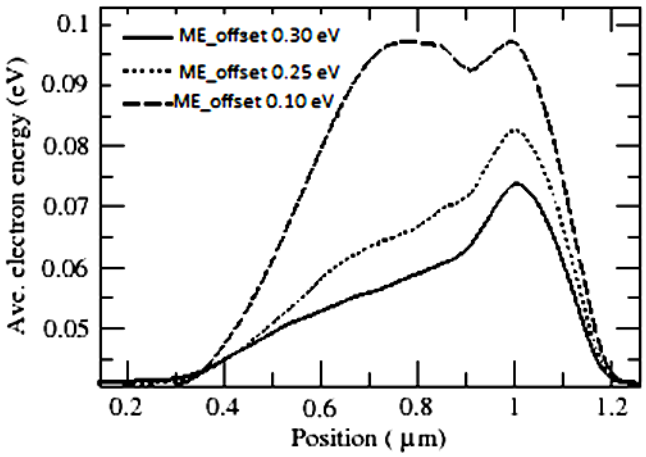


Figure 6 Average electron energy as a function of position (distance) across the diode.

There is a higher increase in the average kinetic energy of the electrons in $GaAs/Al_{0.2}Ga_{0.8}As$ than $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ as shown in Fig. 6. The estimated corresponding carrier energy for diodes with interfaces $GaAs/Al_{0.2}Ga_{0.8}As$, $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ for applied

bias of $1.0\,V$ is 0.098 *eV*, 0.082 *eV* and 0.074 *eV* respectively at position of 1.0 μm across the diode.

4.6 Density of electrons in the potential well at $1.0\,V$ The results of the Monte Carlo simulations shows that the densities of electrons in potential well depends on the well thickness as illustrated in Fig 7. The thicker the well, the more charge accumulates to form a bigger barrier [3]. Under same operating conditions, we observed that the diode with band offset of 0.30 *eV* corresponding to $GaAs/Al_{0.4}Ga_{0.6}As$ accumulates more charge in the well and as such would have a higher potential barrier compared to diodes with band offset of 0.25 and 0.10 *eV* as barrier height depends on amount of charge in the well.

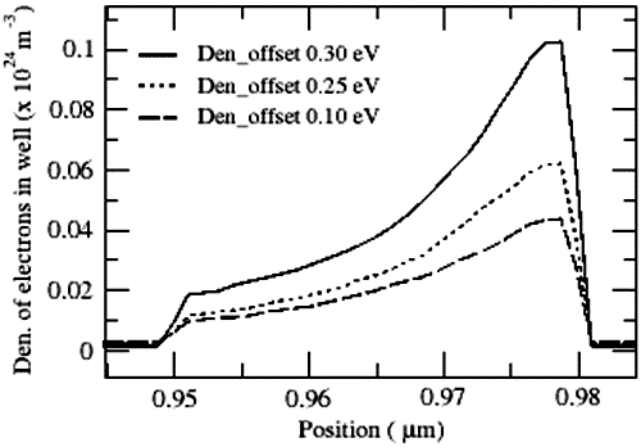


Figure 7 Comparison of the electron density in potential well of PWB diode for three different heterojunctions.

This is as a result of low mobility of electrons across the diode for the case of band offset of 0.30 eV and hence, the electrons did not acquire sufficient energy to jump over the well thus, creating a higher electron density in the well. For the diode with band offset of 0.10 eV, electrons gain higher drift speed with sufficient energy to jump out of the potential well hence, creating small charge density in the well with a smaller potential barrier.

4.7 DC characteristics consideration of the PWB structures We estimated the junction resistance, $R_j = 1/(dI/dV)$ and curvature coefficient, $\gamma = (d^2I/dV^2)/(dI/dV)$ as a measure of diode's performance [14]. The junction resistance of all diodes looks pretty similar with value of ≈2.2 kΩ though, the curvature coefficients differ. The curvature coefficient estimated for $GaAs/Al_{0.2}Ga_{0.8}As$, $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ for bias of 0.30 V were respectively $3.51, 6.02$ and $14.13\,V^{-1}$. This result is much less compared to estimated ideal Schottky barrier curvature coefficient $q/KT \approx 38.6V^{-1}$. It is clear here that the curvature coefficient reflects values of band offset of the heterojunctions. Another important dc quantity we consider is ideality factor as it also impacts the responsivity of diode. The ideality factor of diode with structure $GaAs/Al_{0.2}Ga_{0.8}As$ at 0.1 V was estimated to be 3.24 while that of $GaAs/Al_{0.3}Ga_{0.7}As$ and $GaAs/Al_{0.4}Ga_{0.6}As$ at same bias was obtained to be 3.85 and 4.39 respectively. The ideality factor of the diodes increases with increase in band offset at the heterojunctions.

5. Conclusions The work described in this paper demonstrates a good knowledge and understanding of carrier transport through heterojunctions of the PWB diode. The distribution of electrons across the diode varies depending on the grading of Al and Ga in the $GaAs/AlGaAs$ system. There are variations in the mean velocity of electrons, population of carriers across the diode and effective electron temperature. This shows significant effect on diode performance. More importantly is the estimated curvature and ideality of the three heterojunctions which both reflects the value of conduction band offset. The curvature coefficient estimated for diodes with these heterojunctions are small though, could be improved upon for the optimized diode. We also observed that diode with smaller band offset (in this case $GaAs/Al_{0.2}Ga_{0.8}As$) are suitable where speed and high frequency application are of utmost importance since they have smaller potential barrier and hence turns on quickly compared to diodes with larger band offsets.

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