High-mobility heterostructures based on InAs and InSb: A Monte Carlo study

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In this work, by means of Monte Carlo simulations, two different narrow band gap semiconductors, InAs and InSb, and their associated heterostructures, AlSb/InAs and AlInSb/InSb, have been studied. The parameters for the bulk simulations have been optimized in order to correctly reproduce the experimental mobility values. For the correct simulation of the heterostructures, roughness scattering has been included in the model, and its strength has been adjusted to achieve a good agreement with the experimentally measured mobility.

I. INTRODUCTION

In “traditional” high electron mobility transistors (HEMTs), the highest cutoff frequencies have been achieved by using high In content (up to 70%) InGaAs channels (with an AlInAs barrier). In the past years, semiconductors with narrower band gap have been used for the channel of HEMTs in order to achieve much higher electron mobilities (thanks to a lower effective mass). Heterostructures with narrow band gap semiconductors such as AlSb/InAs and AlInSb/InSb (so-called Sb-based heterojunctions) have thus become a great option for improving the performance of HEMTs in high-speed, low-noise, and low-power applications and so increase their possibilities of being used for military and space applications with ultra low-power requirements. Even if Sb-based 2-dimensional electron gas channels suffer from a degradation due to the roughness of the heterojunction (mainly due to the nonmaturity of the technology and the presence of defects), both InAs and InSb channels provide much higher values of mobility than those obtained in the fastest InP based heterojunctions.

In Sb-based HEMTs, due to the extremely high mobility of narrow band gap semiconductors, electron transport can easily become ballistic (or at least quasiballistic) when the gate length is reduced to submicron length. Under these conditions, the classic drift-diffusion or hydrodynamic models, traditionally used for device simulation and design, are not valid anymore. The most adequate technique is the Monte Carlo (MC) method, able to account for ballistic transport and provide not only static results but also the dynamic and noise behavior of the devices. MC simulations are an exceptionally useful tool for the optimization of the transistors from a physical point of view, taking as a basis the knowledge of the internal microscopic processes.

A first step for the MC simulation of Sb-HEMTs is the adequate simulation of bulk InAs and InSb and their corresponding heterojunctions. However, in spite of increasing efforts being dedicated to the improvement of the fabrication of Sb-based HEMTs, few studies based on detailed microscopic simulations have been published, and the numerous parameters needed for the MC simulations are not well established at all. Therefore, not only a thorough bibliographic search is necessary, but also a process of fine adjustment of the individual parameters is needed in order to verify their influence and obtain satisfactory values for them. As the technology for the fabrication Sb-based heterostructures is far from being advanced, a key parameter for reproducing the properties of electron transport in the channel is the amount of roughness scattering.

The aim of this work is the study of the transport properties in bulk InSb, InAs, and their associated heterostructures by means of the accurate adaptation of MC simulators. A key parameter for the simulation of the heterostructures is the roughness of the interface. The choice of the value of the roughness parameter that provides a good agreement with the experimental results will give us important information about the ideality of the interfaces and will pave the way for the MC study of advanced Sb-HEMTs.

This article is organized as follows. In Sec. II the parameters for the simulation of bulk semiconductors are presented, and the electron transport in bulk InAs, InSb, AlSb, and Al0.15In0.85Sb is studied. Then, in Sec. III, AlSb/InAs and Al0.15In0.85Sb/InSb heterostructures are simulated. The involved parameters are fine tuned by adjusting the strength of roughness scattering, thus allowing obtaining a good agreement with experimental mobilities of real samples. Finally, in Sec. IV, the main conclusions of this work are drawn.

II. BULK SEMICONDUCTORS

The first step for the simulation of devices based in narrow band gap semiconductors is to define correct parameters for the MC models of bulk materials and their corresponding heterostructures. For this sake, a thorough bibliographic study has been performed. Since the interest on these high-mobility semiconductors is recent and the technology not
Acoustic def. pot. /H20849

semiconductors. Indeed, impact ionization appears for elec-

ionization mechanisms have been implemented in the model

single particle MC simulator26,27 properly adapted to be used

0.395 eV, somewhat larger than that of InSb

Intervalley def. pot. /H20849

Effective mass (m^2/m_0) 0.014 0.220 0.130 0.023 0.29 0.64 0.14 0.70 0.53
No parabolicity coef. (eV^{-1}) 5.72 5.72 5.72 1.39 0.54 0.90 5.72 5.72 5.72
Energy from Γ valley (eV) 0.0 0.76 0.46 0.0 1.1 1.6 0.0 −0.09 −0.68
Acoustic def. pot. (eV) 5.96 5.96 5.96 5.93 7.23 9.02 2.20 2.20 2.20
Optic def. pot. (eV) 0.0 2.5 0.0 0.0 2.3 0.0 0.0 1.0 0.0
Intervalley def. pot. (10^{10} eV/m)
from Γ to 0.0 5.0 5.0 0.0 5.6 6.3 0.0 1.0 1.0
from L to 5.0 5.0 10.0 5.6 6.3 5.6 1.0 1.0 1.0
from X to 5.0 10.0 5.0 6.3 5.6 3.4 1.0 1.0 1.0
Intervalley phonon energy (meV)
from Γ to 0.0 19.9 19.9 0.0 17.4 19.2 0.0 36.0 36.0
from L to 19.9 19.9 19.9 17.4 19.2 17.4 36.0 36.0 36.0
from X to 19.9 19.9 19.9 19.2 17.4 19.3 36.0 36.0 36.0

TABLE I. Bulk semiconductor parameters.

Symbol  InSb  InAs  AlSb

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>InSb</th>
<th>InAs</th>
<th>AlSb</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (Kg/m^3)</td>
<td></td>
<td>5790</td>
<td>5667</td>
<td>4260</td>
</tr>
<tr>
<td>Sound velocity (m/s)</td>
<td></td>
<td>4060</td>
<td>4282</td>
<td>4250</td>
</tr>
<tr>
<td>Static dielectric constant</td>
<td></td>
<td>15.68</td>
<td>12.25</td>
<td>10.24</td>
</tr>
<tr>
<td>Optic dielectric constant</td>
<td></td>
<td>17.65</td>
<td>15.15</td>
<td>12.04</td>
</tr>
<tr>
<td>Band gap (eV)</td>
<td></td>
<td>0.18</td>
<td>0.354</td>
<td>1.615</td>
</tr>
<tr>
<td>Lattice parameter (Å)</td>
<td></td>
<td>6.479</td>
<td>6.058</td>
<td>6.135</td>
</tr>
<tr>
<td>Optical phonon energy (eV)</td>
<td></td>
<td>24.4</td>
<td>30.0</td>
<td>36.0</td>
</tr>
</tbody>
</table>

Typically, big discrepancies are found when looking for simulation parameters. This is especially critical for MC simulations, where not only macroscopic parameters are necessary but also those related to scattering rates. Therefore, to correctly choose the values better reproducing the experimental results, the bibliographic revision15–25 has been followed by the fine adjustment of the MC simulation parameters.

In the simulations, in addition to the narrow band gap semiconductors, InAs and InSb, the materials commonly used to form the heterostructure barrier, AlSb and Al_{0.15}In_{0.85}Sb, respectively, need also to be considered. Table I shows the MC simulation parameters used for InSb, InAs, and AlSb. For all of them three nonparabolic spherical valleys (Γ, L, and X) are considered to form the conduction band in the model. As can be observed, both InSb and InAs have a narrow direct band gap with very small electron effective masses in the bottom of Γ valley (0.014 and 0.023, respectively). On the other hand, AlSb has a wide indirect band gap with the lowest valley placed in the Δ direction, exhibiting a high effective mass (0.14). We will also call it X valley even if it is not exactly placed on the X point. In the case of Al_{0.15}In_{0.85}Sb (used as barrier material for InSb), the simulation parameters have been obtained by linear interpolation between those of InSb and AlSb, providing a direct band gap semiconductor with m_{L}=0.033 and a band gap of 0.395 eV, somewhat larger than that of InSb (0.18 eV).

Simulation parameters have been adjusted by means of a single particle MC simulator26,27 properly adapted to be used for narrow band gap semiconductors. For example, impact ionization mechanisms have been implemented in the model since they may play a very important role in this kind of semiconductors. Indeed, impact ionization appears for electron energies lower than those necessary for intervalley transfer, thus practically avoiding the saturation of the I-V curves of devices fabricated with narrow band gap semiconductors.4,6–8 Impact ionization has been introduced in our single particle MC by means of the Keldysh expression, the probability per unit time of having an impact ionization event being \( \frac{dE}{dt} = \frac{S}{E} \left( \frac{E-E_{th}}{E_{th}} \right)^{2} \) for \( E > E_{th} \) and 0 otherwise,19,28,29 with \( E \) the electron energy and \( E_{th} \) a threshold energy (\( E_{th} = 1.08 E_{gap}^{12} \) \( E_{gap} \) being the energy gap of the semiconductor). Since the value of the proportionality factor of impact ionization \( S \) is not known, three values have been considered in the simulations (\( S = 0, 0.5 \times 10^{12}, \) and \( 1 \times 10^{12} \) s^{-1}) in order to analyze the relevance of this process.

The velocity-field curves obtained for undoped InAs, InSb, AlSb, and Al_{0.15}In_{0.85}Sb are shown in Fig. 1(a). As observed in the figure, InAs and InSb offer not only remarkably high mobilities (\( \mu_{1} = 28000 \text{ cm}^{2}/\text{V s} \)) but also very large peak velocities. However, while the values of mobility do not depend on the amount of impact ionization processes, the values of the peak velocity do so. The maximum velocity increases with higher \( S \) since Γ valley population is raised by the more frequent impact ionization events [Fig. 1(b)]. Also, as a consequence of a higher impact ionization probability, the maximum electron velocity is shifted to higher electric fields. The problem is that no complete experimental data of velocity-field characteristics exist for these materials so that the correct value for \( S \) cannot be exactly estimated.

Regarding the materials for the heterostructure barriers, the electron mobility of AlSb is really small,
InSb leads to the use of AlSb gap semiconductor with similar lattice constant to that of low electric field together with very high mobility and peak electron velocity at this value of $x$. InSb/InAs heterojunction, an extremely large conduction band offset constant. In the case of the AlSb/InAs heterojunction, an and InSb channels, respectively, due to their similar lattice constant. In our simulations we have used three different values, of impact ionization probability. The negative charge that appears at the semiconductor-air interface is accounted for in the simulation by means of a fixed surface charge density $\sigma$. Since the value of $\sigma$ is not known because it depends on the fabrication process, in our simulations we have used three different values, $\sigma=0$, $-2\times10^{12}$, and $-4\times10^{12}$ cm$^{-2}$.

The main characteristics of AlSb/InAs and Al$_{0.15}$In$_{0.85}$Sb heterostructures have been compared by using a 2D MC simulator self-consistently coupled with a 2D Poisson solver, adequately modified to correctly model such heterostructures. For example, a correct injection at the contacts, where the channel transport can easily become ballistic (or at least quasiballistic), is essential for an accurate simulation. In order to adequately inject (and extract) electrons into the channel, the simulated electrodes are placed vertically extending across the heterolayer. Usually, the profiles of potential assigned to these electrodes and concentration to be injected correspond to those that would appear along the heterostructure if real top electrodes were used, previously calculated from an initial simulation at equilibrium with contacts at the top. However, the very large conduction band offset at the AlSb/InAs heterostructure makes difficult the obtention of the correct injection profile since the carrier interchange between the $\delta$-doping region and the channel is blocked. In such a situation, the injection conditions fix the electron distribution within the device and top-contact simulation becomes useless to obtain correct injection profiles. In order to correctly set the injection conditions, we have initially performed a self-consistent Schrödinger–Poisson simulation, which indicates a complete electron confinement in the channel. This result allows restricting the injection to the channel. Once this is known, to achieve consistent injection conditions, the initial top-contact simulation used for calculating the injection profiles has been modified by using lateral contacts whose injection conditions are iteratively updated with the values obtained at the center of the 

\[ \Delta E = 0.18 \text{ eV}^{10} \]

so that the sheet electron concentration in the channel is much lower than in the AlSb/InAs heterojunction.\(^8\)

In order to perform a proper comparison, the same geometry has been used for both heterojunctions (Fig. 2): a buffer of wide band gap material of 800 nm followed by a narrow band gap channel of 15 nm and a 25 nm thick wide band gap barrier material. Electrons are introduced by a $\delta$-doping of $\delta=5\times10^{12}$ cm$^{-2}$, 10 nm far from the channel. The negative charge that appears at the semiconductor-air interface is accounted for in the simulation by means of a fixed surface charge density $\sigma$. Since the value of $\sigma$ is not known because it depends on the fabrication process, in our simulations we have used three different values, $\sigma=0$, $-2\times10^{12}$, and $-4\times10^{12}$ cm$^{-2}$.

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sample until reaching convergence. The update is made every 5 ps (50 000 iterations of 0.1 fs). After around ten iterations the profiles converge, thus providing the correct injection conditions. In the case of the Al$_{0.15}$In$_{0.85}$Sb/InSb heterostructure, the conduction band offset is smaller, allowing carrier interchange between the barrier and the channel, and thus being possible to obtain the correct injection profiles with the standard top-contact simulation.

Once the problems related to electron injection have been solved, MC simulations provide the conduction band and concentration profiles shown in Figs. 3 and 4 for both heterojunctions, calculated for the three values of surface charge considered. As observed, the attractive force of the δ-doping layer (counteracted in part by the top surface charge) increases the electron concentration near the upper heterojunction. In AlSb/InAs, due to the total confinement of electrons in the channel, the sheet electron density in the channel, $n_S$, decreases as $\sigma$ becomes more negative, following the charge neutrality condition $n_S = \delta + \sigma$. In the case of the Al$_{0.15}$In$_{0.85}$Sb/InSb heterostructure, not all the electrons are confined in the channel so that $n_{S\text{tot}} = n_S + n_{S\text{b}} = \delta + \sigma$, with $n_{S\text{b}}$ being the sheet electron density of electrons in the barrier layer. Both $n_S$ and $n_{S\text{b}}$ decrease when $\sigma$ is more negative, but $n_{S\text{b}}$ is reduced to a higher extent so that the percentage of electrons in the channel increases [the dependences of $n_S$ and $n_{S\text{b}}$ with $-\sigma$ are shown in the inset of Fig. 4(b)].

The mobilities of the two heterostructures have been obtained by first calculating the resistance of samples with increasing length and then determining the square resistance of the heterojunctions, $R_{\square}$ (Ref. 34) (it is just the slope of the resistance versus length plot). Then the mobility is extracted from the simple formula $\mu = 1/qn_S\sigma\mu^*$. The mobility obtained for the AlSb/InAs heterojunction as a function of $n_S$ is shown in Fig. 5. Values exceeding 60 000 cm$^2$/V s have been obtained, much higher than bulk mobility, and increasing with $n_S$. This dependence is expected due to the effect of degeneracy, which reduces the number of scattering mechanisms. The mobilities obtained with MC simulations are also much higher than those measured experimentally. The complete confinement of electrons in the channel allows directly comparing our results with the experimental Hall measurements in Refs. 4, 7, and 35–37. In order to reduce the mobility and correctly reproduce the experimental results, the effect of interface roughness in the heterojunctions has been introduced in our 2D MC simulator. There are detailed models of roughness scattering, which consider the dependence of the probability on the electron wave vector. In our case, as first approximation we have implemented a more simple global model in which a given fraction of electron reflections at the heterojunction is treated as diffusive (instead of specular). Every time an electron reaches the surface, the diffusive or specular character of the...
reflection is determined by means of a random number. Surface roughness has been considered in both heterojunctions of the channel. Previous works on AlSb/InAs quantum wells without δ-doped layer indicate that the strongest relevance of heterojunction roughness lies on the bottom interface. On the contrary, in our case, the δ-doped layer increases carrier concentration near the top heterojunction, and the surface roughness scattering with this interface becomes critical. Two cases have been simulated, 1% and 2% of diffusive scatterings associated to the heterojunction roughness. In Fig. 6 this mobility is plotted versus \( \sigma \). Surprisingly, for the lower values of \( \sigma \) (0 and \( -2 \times 10^{12} \text{ cm}^{-2} \)), when the population of the Al\(_{0.15}\)In\(_{0.85}\)Sb barrier is higher, the channel mobility takes values much lower than that of bulk InSb. We attribute these low values to noncompletely correct injection conditions, leading to anomalous current loops near the contacts, which affect the values of the extracted resistances (mainly for the shortest samples). For the highest value of \( \sigma \), when fewer electrons are present in the Al\(_{0.15}\)In\(_{0.85}\)Sb barrier, these current loops are almost inexistent, and the calculated value of the mobility is much more reliable, around 79,000 cm\(^2\)/Vs (higher than that of bulk material, as expected). The problems associated to current loops originated by contact injection when there is a significant electron concentration in the barrier layer are not of worrying importance since in practice, the heterolayer is designed to avoid that parasitic channel.

The previous results confirm that the design of the Al\(_{0.15}\)In\(_{0.85}\)Sb/InAs heterostructure is not adequate, leading to the presence of a significant parasitic channel caused by a too high δ-doping. Therefore, this heterostructure must be optimized. In order to compare our simulations with one of the few experimental data available, \( \sigma \)-doping plane has been moved closer to the (20 nm thick) channel, with just 5 nm of separation, and the charge density has been decreased to a value of \( \delta=1 \times 10^{12} \text{ cm}^{-2} \). Figure 7 shows the concentration profile of this heterostructure when considering \( \sigma=-0.1 \times 10^{12} \text{ cm}^{-2} \) (value that provides the best agreement with the experimental \( n_S \)). In this case many of the electrons (63%) are confined in the channel, where the mobility is around \( \mu=76,000 \text{ cm}^2/\text{V s} \), similar to that obtained in the nonoptimized heterostructure for the highest value of \( \sigma \) (Fig. 6). To correctly reproduce the experimental results of Hall mobility (\( \mu_H=23,800 \text{ cm}^2/\text{V s} \)), the percentage of diffusive scatterings associated to the heterojunction roughness must be increased to 7%, possibly indicating that the quality of the (novel) technological process used to fabricate the sample is poorer than in the case of InAs heterojunctions.

**IV. CONCLUSIONS**

Bulk InAs and InSb and their respective heterostructures, AlSb/InAs and Al\(_{0.15}\)In\(_{0.85}\)Sb/InSb, have been studied by means of MC simulations as a first step for the design and optimization on Sb-based HEMTs. Appropriate values for the simulation parameters of the involved semiconductors have been obtained. Experimental bulk mobilities have been reproduced by simulations (\( \mu=28,000 \text{ cm}^2/\text{V s} \) for InAs and \( \mu=67,000 \text{ cm}^2/\text{V s} \) for InSb). The transport properties of the heterostructures have been properly simulated and the
experimental mobilities reproduced by adequately adjusting the amount of roughness scattering at the heterojunction, showing that the technological quality of the InSb interface must still be much improved.

We have confirmed that the large conduction band offset of the AlSb/InAs heterostructure allows a complete confinement of carriers in the channel, thus becoming an attractive option for a new generation of ultrafast HEMTs. Instead, high performance metal-oxide-semiconductor-HEMTs (MOS-HEMTs) could be fabricated by depositing an adequate insulator on the top of the InSb channel.

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33Simulator created by O. Schuler and D. Théron.