The characterization of the hole transport in Sb based strained quantum wells

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Abstract. Compressively strained InSb structures aimed for p-channel heterostructure field effect transistors (HFETs) are analysed in order to maximise their hole mobility. We optimise the heterostructure by the change of the material composition, thickness of the layers and position of δ-doping. The splitting of light and heavy hole bands in compressively strained channels are calculated by nextnano$^3$ software as a function of material mole fraction and quantum well thickness. The 8 × 8 k.p method is used for the determination of corresponding hole eigenvalues. The strained layer bandstructure calculation is carried out with Quantumwise ATK for the Kohn-Sham DFT using double-zeta polarised basis set orbitals as well.

1. Introduction and Motivation

III-V Heterostructure Field Effect Transistors (HFETs) are very promising candidates for future high-performance, low-power digital applications [1, 2] possibly replacing a strained Si transistors. The development of appropriate p-type MOSFET transistor compatible with III-V technology would be advantageous for a possible co-integration of high mobility III-V channels into the CMOS Si architecture even alternative Ge solutions exist [3].

While the electron mobility in III-Vs is larger than in Si, the increase in the hole mobility by strain is crucial for the development of the p-type channel HFETs. A small band gap and high mobility of InSb seems to be right candidate for this purpose. Successful realisation of HFETs with InSb resp. GaSb ultrathin strained layers has been reported recently [4], [5].

2. Structure

In Fig. 1 we show a structure of QWFET under study. We assume a bottom barrier of Al$_x$In$_{1-x}$Sb, then a narrow bandgap p-channel of InSb and a top barrier of Al$_x$In$_{1-x}$Sb with the same mole fraction of x$_{Al}$ as at the bottom layer. In the top barrier, we consider a δ-doped layer with a doping concentration of 2x10$^{12}$ cm$^{-2}$ and assume a Fermi-level pinning of 0.55 eV on the top barrier which will induce a band bending.
Figure 1. Layer structure of the InSb QWFET:
Thickness of top barrier is 13 nm. δ-doping is placed with a nominal 2x10^12 (cm^-2). A spacer between δ-doping and quantum well is 5 nm thick. Quantum well thickness was changed in the interval from 5 to 15 nm. A thickness of the bottom barrier is 25 nm.

3. Simulations
We employ a single band and 8 × 8 k.p method to calculate a band profile and carrier density using nextnano^3 [6] simulation tool within a self-consistent solution. A hole density along the InSb QWFET is shown in Fig. 2.

Figure 2. The band gap of calculated structure.

Figure 3. Detail of wavefunctions calculated by k.p method.

Wavefunctions in the quantum well of the QWFET transistor are shown in Fig. 3 in a simplified way. We have changed the hole sheet density in the quantum well by varying the δ-doping concentration assuming the carbon dopant with an activation energy of 27 meV.

3.1. Bulk dispersion
We have considered various aluminium contents for Al_xIn_{1-x}Sb substrate is order to find the optimal strain conditions. Fig. 4 shows the calculated energy dispersion in two k-space directions: [001] and [011] respectively. Three bands are depicted; heavy holes (HH), light holes (LH) and spin-orbit split-off holes (SO). In this figure, we compare an unstrained 5 nm thick layer of InSb (bold curves) with a strained layer of InSb grow on Al_xIn_{1-x}Sb substrate assuming x=0.3.

The valence band splits off in the Al_{0.3}In_{0.7}Sb barriers due to the strain. The difference of HH and LH at k=0 is 0.121 eV. The difference will reduce to only 0.063eV when x=0.15. As we increase the strain in InSb layer, the effective mass of holes decreases which is very beneficial for the improvement in the hole mobility.

3.2. Effective mass calculation
The InSb strained layer bandstructure calculation is carried out using Quantumwise ATK simulation software. We have employed the Kohn-Sham Density Function Theory (DFT)
approach using double-zeta polarised basis set orbitals. We have used the both DFT models: Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). LDA underestimates the bandgap of the semiconductors and narrow bandgap materials as InSb are found to be metallic within LDA. On the other hand, GGA gives higher bandgap values for InSb then those tabulated. We have used a bulk model with the compressive strain in the \(x-y\) plane. Two lattice vectors in this plane were reduced thus a face-centered cubic lattice was transformed to face-centered orthorombic. A Fig. 5 illustrates the change of the carrier effective masses in InSb under applied strain for LDA (a) and GGA (b) approximations.

\[ m^* = \hbar^2 \left[ \frac{\partial^2 E}{\partial k^2} \right]^{-1}. \]

The analogous values LH\(_X\) and LH\(_L\) are calculated for the light hole band. The average values for LH and HH effective masses are indicated as HH\(_{av}\) and LH\(_{av}\). H\(_{av}\) is an average value of HH\(_{av}\) and LH\(_{av}\).

### 3.3. Hole mobility calculation

Finally, we have calculated a carrier mobility \(\mu\) in a quantum well of \(p\)-type FET transistor. We can assume that a two dimensional hole gas (2DHG) occurs in the quantum well since the layer thickness of InSb is 5 nm. We employ an simple approach of the calculation of hole mobility that includes different scattering mechanisms [7]. We have taken into account the acoustic phonon scattering, the polar optical phonon scattering and the ionised impurity scattering. The carrier
mobility is calculated from the expression \( \mu = \frac{e}{\tau_m^*} \) where \( \tau \) is the scattering time associated with the included scattering process. A total carrier mobility is calculated according to Mathieson’s rule. A detailed description of single scattering mechanisms can be found in [7].

### 3.4. Simulation parameters

Parameters that we used in simulation are summarised in Tab. 1. Even the most of these material parameters are well known and described in literature, some of them are less accurate, e.g., an acoustic deformation potential. We have used a value of 7.2 eV instead of a value 30 eV that have been quoted in past. The value of 7.2 eV is in a very good agreement with the experimental data. The problem with the acoustic deformation potential is discussed in [7].

| Name                              | Value  |
|-----------------------------------|--------|
| bandgap at \( \Gamma \) (eV)     | 0.1737 |
| lattice constant (nm)             | 0.64794|
| LO phonon energy (eV)             | 22.0   |
| static dielectric const (\( \epsilon \)) | 17.5 |
| acoustic deformation potential (eV) | 7.2   |
| optical dielectric const (\( \epsilon \)) | 15.68 |
| sound velocity (m.s\(^{-1}\))    | 3.7    |
| hole effective mass HH (\( m_0 \)) | 0.405  |
| hole effective mass LH (\( m_0 \)) | 0.016  |

We carried out an extensive study of an effective mass of the hole in dependence on the strain. The results of this study are depicted on Fig. 5. In Tab. 1 we quote a unstrained bulk case for InSb.

### 4. Conclusion

We have simulated effective masses and mobilities for the case of thin, 5 nm InSb quantum well embedded into \( \text{Al}_x\text{In}_{1-x}\text{Sb} \) layer which is incorporated into a heterostructure \( p\text{-FET} \).

When we have increased a doping concentration from 1 to \( 3\times 10^{12} \text{cm}^{-2} \), we have achieved a different integrated hole sheet density in the quantum well. The sheet density increased from \( 0.2\times 10^{12} \) to \( 1.4\times 10^{12} \text{cm}^{-2} \), respectively. We have also carried intensive study by changing material and structure parameters to gain a higher mobility in the quantum well. For example, we have increased the spacer between the \( \delta \)-doping position and the quantum well and we broadened the thickness of the quantum well. The carrier mobility has increased more than by factor of two reaching 1085 cm\(^2\)/Vs which is close to measured results from literature [4].

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