Optoelectronic properties of InAs/GaSb superlattices with asymmetric interfaces

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Abstract. In this work the optoelectronic properties of InAs/GaSb superlattices are investigated. The \( k\)-\( p\) method and four-band Kane model were used to calculate the electronic states in the structure at 0K. Superlattices with different period thickness and two types of interfaces were considered. In the calculations strain and nonparabolicity effects were taken into account. Transition energies and the corresponding cut-off wavelengths were determined.

1. Introduction
InAs/GaSb superlattices (SLs) are type-II heterostructures, which are very useful for optoelectronic applications. Their properties may be modelled with the use of the \( k\)-\( p\) method and the multi-band Kane model [1, 2, 3].
The structures are usually grown on GaSb substrates. Because of the lattice mismatch between InAs and GaSb the strain built-in the superlattice should be taken into account. In this work the strain was considered within the framework of the Bir-Pikus theory [4].
InAs/GaSb superlattices are non-common atom structures in which the symmetry is broken at the interfaces between the SL layers [5, 6]. This causes the heavy and light holes wavefunctions to mix, even in the centre of the Brillouin zone (BZ). During the growth by molecular beam epitaxy two types of interfaces may be formed in such structures, i.e. “InSb-like” and “GaAs-like” ones. Each of the interfaces has different properties and causes the coupling of holes minibands with different strength [5, 2, 6, 7, 8]. In this work SL structures with every second interface (IF) formed by In-Sb bonds were considered.
The superlattice bandgap, determined as the separation of the lowest conduction miniband and the highest miniband in the valence band, depends on the thickness of the SL layers. However, it also depends on the number and the thickness of “InSb-like” IFs in the structure [2, 6, 7].

2. Method
The electronic states in \((\text{InAs})_m/(\text{GaSb})_n\) superlattices were calculated with the use of the \( k\)-\( p\) method and the four-band Kane model. The method allows one to find the SL band structure in the neighbourhood of the BZ centre. The four-band Kane model describes the lowest miniband in the conduction band (CB) and the three minibands in the valence band.
The Schrödinger equation which was solved to find the electronic states in the structure takes the form \[1, 2\]:

\[
\begin{bmatrix}
E_C + A & -\sqrt{3}U & \sqrt{2}U & U \\
-\sqrt{3}U^* & E_V - P - Q & S + i\delta(z) & 1/\sqrt{2}S + \sqrt{2}T \delta(z) \\
\sqrt{2}U & S - i\delta(z) & E_V - P + Q & \sqrt{2}Q - i\sqrt{2}Q_{kz} \\
U & 1/\sqrt{2}S^* + \sqrt{2}T \delta(z) & \sqrt{2}Q - i\sqrt{2}Q_{kz} & E_V - P - \Delta
\end{bmatrix}
\begin{bmatrix}
\psi_{CB}(z) \\
\psi_{HH}(z) \\
\psi_{LH}(z) \\
\psi_{SO}(z)
\end{bmatrix}
= E
\begin{bmatrix}
\psi_{CB}(z) \\
\psi_{HH}(z) \\
\psi_{LH}(z) \\
\psi_{SO}(z)
\end{bmatrix}
\tag{1}
\]

The four component \(\psi_{CB}, \psi_{HH}, \psi_{LH}, \psi_{SO}\) envelope function describes the electron and hole states in the respective minibands. The model allows one to consider the biaxial strain which is built-in the SL. In the present work this was done with the use of the Bir-Pikus deformation potentials which are included in the Hamiltonian in the terms on the diagonal. The off-diagonal blocks of the Hamiltonian account for the nonparabolicity effects which are the consequence of the narrow InAs bandgap.

The model also considers the HH and LH wavefunctions mixing at the interfaces of the structure. The strength of coupling of heavy and light hole minibands is expressed by the parameter \(T\). The value of \(T\) depends on the type of the IF in the structure [5, 2, 8].

The effective masses of electrons (\(m_{el}\)), heavy holes (\(m_{HH}\)), light holes (\(m_{LH}\)) and the holes in the SO miniband (\(m_{SO}\)) depend on the coordinate \(z\). In the simulations all these masses take different values in InAs and GaSb SL layers. The values of \(m_{HH}, m_{LH}\) and \(m_{SO}\) are described with the help of the Luttinger parameters. The spatially dependent effective mass of electron reflects also the nonparabolicity effect which is caused by the interaction between the valence band and the conduction band in the superlattice [1, 2].

\[1, 2\]

3. Results

Calculations were performed for \((\text{InAs})_m/\text{(GaSb)}_n\) superlattice structures with InAs and GaSb layers of equal thickness. Simulations were done for superlattices grown on (100) oriented GaSb substrates. Structures with 30 periods were considered. The electronic states were calculated at 0K and the material parameters were assumed to be as those reported in ref. [2]. A band offset energy equal to 140meV was taken into account.

Equation (1) was solved using the finite difference method. The calculations were done with the discretization mesh in which every two neighbouring nodes were separated by one monolayer (ML). Simulations were performed for the superlattices with asymmetric interfaces. For the interfaces formed by In-Sb bonds the coupling Hamiltonian \(H_{xy}\), which determines the parameter \(T\), was assumed to be 580meV [5, 2]. All interfaces in the structure were 1ML thick.

In the simulations the electrons and holes envelope functions were calculated in the respective minibands. Probability densities obtained for \((\text{InAs})_{30}\)/\((\text{GaSb})_{30}\) SL structure are shown in Fig.1. The graph presents \(|\psi_{CB1}|^2\) and \(|\psi_{HH1}|^2\) together with the potential energy describing the bottom edge of the conduction band \(E_C\) and the top edge of the valence band \(E_V\) (see Eq.(1)). Results of calculations were obtained for the SL structure in which every second interface was formed by In-Sb bonds. It can be observed that the type of the interface is quite important for the heavy hole envelope function and it is not very significant for the electron probability density. Such effect is the result of the interaction between heavy and light holes states at the interfaces in the structure.

Interband transition energies (see Fig.2a) and the corresponding cut-off wavelengths (see Fig.2b) were calculated for \((\text{InAs})_m/\text{(GaSb)}_m\) SLs with \(m\) equal to 5, 8, 10 and 12 MLs thick. The results show that the cut-off wavelength rises with the thickness of the SL period. This corresponds well with the experimental observation described by Rodrigues et al. in ref. [9]. In that work \((\text{InAs})_m/\text{(GaSb)}_m\) SLs with \(m\) equal to 5, 8, 10 and
15 MLs were investigated. The PL spectra recorded at 80K show that the cut-off wavelength of such structures varies from 3.9μm ($E_{HH1-CB1}=319\text{meV}$) to 8.4μm ($E_{HH1-CB1}=147\text{meV}$). Our calculations show that the absorption edge of the SL structure with $m=8\text{ML}$ is observed at the energy $E_{HH1-CB1}=278\text{meV}$ (see Fig.2a) and it corresponds to $\lambda_{\text{cut-off}}=4.46\mu\text{m}$ (see Fig.2b). These values are in a good agreement with the absorption edge reported by E. Plis et al. in ref. [10]. The absorbance and PL spectra of (InAs)$_{8\text{ML}}$/GaSb$_{8\text{ML}}$ SL structure (measured at 72K) show that the cut-off of such a superlattice is equal to 4.27μm. The wavelength corresponds to the transition energy of 290.4meV. It’s worth to be noted that the change of the temperature from 0 to 72K will cause the rise of the transition energy by about 6meV and simultaneously the cut-off wavelength will decrease by about 0.1μm. This signifies that the values calculated numerically and determined in the experiment are even closer. Additionally, calculations performed with the use of the pseudopotential method allowed to find almost the same value of $\lambda_{\text{cut-off}}$ as that determined in the experiment mentioned above [10].

**Figure 1.** Square of the absolute value of the electrons and heavy holes envelope functions in (InAs)$_{8\text{ML}}$/GaSb$_{8\text{ML}}$x30 SL structure. $|\psi_{\text{CB1}}|^2$ and $|\psi_{\text{HH1}}|^2$ are presented together with the potential energy describing the bottom of the conduction band $E_C$ and the top edge of the valence band $E_V$. Results of simulations were obtained for the asymmetric SL structure in which every second interface is formed by In-Sb bonds. Calculations were done at 0K and considered the superlattice grown on GaSb substrate.

**Figure 2.** a) Interband transition energy and b) the corresponding cut-off wavelength calculated for (InAs)$_m$/GaSb$_m$x30 superlattices with asymmetric interfaces. Simulations were done for structures in which every second interface is formed by In-Sb bonds. Superlattices grown on GaSb substrates were considered. The analysis was done at 0K.
4. Conclusion
In this work \((\text{InAs})_m/(\text{GaSb})_m\times30\) superlattices with asymmetric interfaces were investigated. Structures with every second IF formed by In-Sb bonds were considered. Interband transition energy and the cut-off wavelength were determined for the superlattices with InAs and GaSb layers 8, 10 and 12 MLs thick.

The results of calculations are in a good agreement with the experimental observations [10, 9] and with the results of simulations undertaken using other models and methods [9, 10, 6, 8]. The bandgap of the SL structures decreases with the thickness of the SL period. The cut-off wavelength calculated for a \((\text{InAs})_{8\text{ML}}/(\text{GaSb})_{8\text{ML}}\) periodic structure is equal to 4.46\(\mu\text{m}\). This value corresponds well with the absorption edge (4.27\(\mu\text{m}\)) determined for the SL structure on the basis of the absorbance and PL spectra measurements [10].

Calculations performed within the present work brings us closer to the numerical characterization of the optoelectronic properties of the strain balanced InAs/GaSb superlattices in which two types of IFs with different thicknesses are contained in the structure.

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5. References
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