Carrier localization and miniband modeling of InAs/GaSb based type-II superlattice infrared detectors

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Abstract

Microscopic features of carrier localization, minibands, and spectral currents of InAs/GaSb based type-II superlattice (T2SL) mid-infrared detector structures are studied and investigated in detail. In the presence of momentum and phase-relaxed elastic scattering processes, we show that a self-consistent non-equilibrium Green’s function method within the effective mass approximation can be an effective tool to fairly predict the miniband and spectral transport properties and their dependence on the design parameters such as layer thickness, superlattice periods, temperature, and built-in potential. To benchmark this model, we first evaluate the band properties of an infinite T2SL with periodic boundary conditions, employing the envelope function approximation with a finite-difference discretization within the perturbative eight-band k.p framework. The strong dependence of the constituent material layer thicknesses on the band-edge positions and effective masses, offers a primary guideline to design performance-specific detectors for a wide range of operation. Moving forward, we demonstrate that using a finite T2SL structure in the Green’s function framework, one can estimate the bandgap, band-offsets, density of states and spatial overlap which comply well with the k.p results and the experimental data. Finally, the superiority of this method is illustrated via a reasonable estimation of the band alignments in barrier-based multi-color non-periodic complex T2SL structures. This study, therefore, provides deep physical insights into the carrier confinements in broken-gap heterostructures and sets a perfect stage to perform transport calculations in a full-quantum picture.

Keywords: quantum transport, type II superlattice detectors, carrier localization, miniband, k.p, non-equilibrium Green’s function

(Some figures may appear in colour only in the online journal)

1. Introduction

Type-II superlattices (T2SL) made of InAs/(In,Ga)Sb [1] have found immense applications in the field of infrared (IR) detectors [2, 3] and focal plane arrays (FPAs) [4, 5] for defense, space, and biomedical applications over the conventional mercury cadmium telluride (MCT) [6], quantum-well (QW) [7], and quantum dot (QD) [8, 9] technologies due of their fine bandgap tuning, flexible band alignment, moderate dark current, suppressed Auger recombination, high quantum efficiency and established III-V growth technology [10–12]. The excellent band-tunability features of highly lattice-matched 6.1 Å family of III-V compound semiconductors [13] enabled in covering a wide range of infrared spectrum spanning from mid-infrared 3–5 µm (MWIR) to long-infrared 8–15 µm.
(LWIR). The research in this field has evolved rapidly over the last few years and has taken a giant leap after the discovery of barrier-based (nBn [11, 15], pBp [16], XBn [17], CBIRD [18], pBiBn [19] etc), complex (M [20], N [21], W [22] structures) and cascaded SL [23] architectures which made detectors to operate at higher operating temperatures and at higher efficiencies.

The key factors in designing detectors using quantum confined SL structures for a specific range of wavelength are the right choice of the constituent materials, their arrangements and the tuning of the growth parameters to have a precise control over their thicknesses. Moreover, in T2SL, a special care must be taken owing to their broken-gap band alignment to achieve adequate absorption. The band properties exhibited by T2SL are primarily dependent on the design parameters which led several groups to study their electronic band structure using different approaches like the k.p [24–27], empirical tight-binding [28, 29], pseudopotential [30], and density functional theory [31]. However, consolidated studies on the variation of the key band parameters regulated by the layer thicknesses for a wide range of operation are still scarce in the literature.

In this work, the k.p approach with the envelope function approximation (EFA) is chosen over other methods to calculate the electronic structure due to its higher accuracy in predicting the SL bandgap and excellent handling of interface [32] to balance the strain effects. The discretization of the envelope functions along the out-of-plane direction is incorporated through the finite difference method (FDM) [26, 33, 34] for its simplicity and accuracy around the high-symmetry point over other techniques like the Fourier transform method (FTM) [35] and the finite element method (FEM) [36], etc. A proper treatment of the interface is taken by adopting the operator-ordered interface matrix [25, 26] approach along with the inclusion of a separate interfacial layer within the unit cell. From the design point of view, our results primarily put emphasis on the variations of the miniband positions and the density of states (DOS) effective masses with respect to the layer thicknesses.

While the bandgap and miniband widths determine the spectral transport properties [56–58] of a finite T2SL structure. In the presence of momentum and phase-breaking elastic scattering processes [37–39, 59, 60], the NEGF results for a finite structure evidence a close agreement with the k.p results of an infinite SL. A systematic study on the DOS, carrier localization and spectral current is also presented for a qualitative understanding of the non-trivial roles played by the thickness parameters, built-in potential and temperature in tailoring the spatial separation of carrier confinement and coupling of periods. The applicability of this method is further shown to extract adequate information about the band alignment properties of the multi–band unipolar or bipolar barrier-based complex T2SL structures of varying SL configurations with broken periodicity. Finally, employing a simple interface modeling technique, we demonstrate that the bandgap of such structures can also be predicted using the NEGF method within an acceptable range which was overestimated earlier in the absence of interface modeling.

The rest of the paper is organized as follows. In section 2, we briefly outline the k.p and NEGF based theoretical models respectively used to calculate the band structure and miniband characteristics. We discuss the results in section 3 which is divided into two subsections, namely, section 3.1 for k.p results and section 3.2 for NEGF results. We conclude this paper in section 4.

2. Theory and model

2.1. k.p method

The k.p perturbation theory is one of the widely studied methods for implementing the electronic band structure of the III-V and II-VI group of compound materials and their hetero-structures. The supremacy of this method in computing bandgap and oscillator strengths has proven its immense capabilities in studying the optoelectronic devices [24–27]. Extensive research has been carried out in understanding the oscillator strengths in order to compute the absorption rate of T2SL based infrared photodetectors [24, 27, 61].

In this paper, a comprehensive formulation of the k.p Hamiltonian of InAs/GaSb superlattice has been presented. Initially, a Hamiltonian for the bulk material is implemented based on the Kane’s model and its extension to the Lowdin’s Perturbation theory for degenerate bands [62]. Spin-orbit interactions are also taken into account for the triply degenerate valance bands. The interpolation of the same method to complex hetero-structures like superlattices, quantum wells etc is done using the EFA technique [63]. Within the EFA theory, the superlattice wavefunctions, \(\Psi_n(z)\), are expressed in terms of the slowly varying envelope functions, \(F(z)\), along the growth direction (here, z-direction) in the orbital basis states \(u_{\beta}(z)\) [63] and are given by

\[
\Psi_n(z) = \sum_j F_j(z) u_{\beta}(z).
\]
These envelope functions are subject to periodic boundary conditions. For a given SL with \( N_z \) grid points having a period of thickness \( d \), one can write
\[
F_j^\dagger(k_j, z_0) = e^{-ik_f d} F_j^\dagger(k_j, z_N), \\
F_j(k_j, z_{N+1}) = e^{ik_f d} F_j(k_j, z_1),
\]
where \( k_f \) is the transverse momentum and \( q \) is the Bloch vector of \( F(z) \) that spans the Brillouin zone (BZ). The spatial dependence of the material properties along the growth direction results in recognizing the quantum number \( k_f \) as differential operators rather than constants which necessitates the implementation of an operator-ordering technique in order to maintain the hermiticity of the overall Hamiltonian [64]. One of the most widely studied operator-ordering methods uses the symmetrization technique which does not accurately estimate the inter-band coupling in the case of heavy hole bands unlike Burt-Foreman’s proposed method of non-symmetry [65]. Since the material properties repeat periodically along the [001] crystalline plane, the quantum number \( k_z \) is modified to a differential operator as \(-i \frac{\partial}{\partial z}\). The resultant Hamiltonian of the SL consisting of differential terms up to 2nd order, is expressed as a sum of three matrices \( H^{(0)}, H^{(1)} \) and \( H^{(2)} \), given by \( H(k_z, k_f) = H^{(0)} + H^{(1)} \), \( H^{(1)} \) consists of \( H^{(0)} \) and \( H^{(2)} \) terms. Hence, a finite difference discretization technique [33] is employed here in converting the coupled differential equations into a set of algebraic equations that can be solved numerically to find the envelope functions.

In semiconductor superlattices having abrupt and non-symmetric interfaces, the interface region plays a crucial role in obtaining accurate bandgaps [66]. To model the interface, a thin layer of InSb is intentionally inserted (figure 1) at the junction of InAs and GaSb in order to compensate the strain effects arising due to the lattice mismatched InAs layers on GaSb substrate. Hence, in the formulation presented in this paper, both operator ordering and interface Hamiltonian (\( H_{IP} \)), given by
\[
H_{IP} = \sum_{z_i} \delta(z - z_i)\begin{bmatrix} D_S & 0 & \pi_{i,x} \\ 0 & D_X & \pi_{i,\alpha} \\ \pi_{i,\beta} & 0 & D_Z \end{bmatrix},
\]
have been considered [25, 26, 67]. Here, the interface parameters \( \alpha \) and \( \beta \) have been set to 0.2 eVÅ and the diagonal fitting parameters \( D_S, D_X, D_Z \) are respectively taken as 3 eVÅ, 1.3 eVÅ and 1.1 eVÅ [24]. The original \( k \cdot p \) Hamiltonian \( H(k_x, k_y) \) considered in this work, is formed in terms of the standard \( F, G, H \) parameters [68].

### 2.2. NEGF method

The quantum mechanical properties of a low-dimensional device connected to several macroscopic contacts and subject to different scattering phenomena can be attributed by the retarded Green’s function \( G^R \) with the proper description of different self-energies \( \Sigma \). For the given SL structures as shown in figure 5, \( G^R \) along the direction of longitudinal energy \( E \) is defined as
\[
G^R_{bs}(z, z', E) = \left[ E+I-H_b-U_b-\sum_j \Sigma_{bs}^j(E) - \Sigma_{sb}^j(E) \right]^{-1},
\]
where \( b \) is the band index, \( z, z' \) are the position indexes, \( E^\pm = E \pm i\eta^\pm \) where \( \eta^\pm \) is a small positive number, \( I \) is the Identity matrix, \( H \) is the real space 1-D tight-binding Hamiltonian of the SL. \( U \) is the potential profile ideally obtained from the self-consistent NEGF-Poisson solver, \( \Sigma \) is the self-energy of the \( j \)th contact (where \( j \in \{L, R\} \)). \( \Sigma \) is the scattering self-energy. The active SL region is modeled using the nearest neighbor tight-binding Hamiltonian \( H \) with decoupled single-band effective mass approximation. At zero transverse momentum \( k_z = 0 \), the elements of the \( \sqrt{z} \)th row of \( H \) are given by \( H_{i,j} = \frac{\Delta z}{\sqrt{z}} \left( \frac{1}{m_{i+1} + m_{i}} - \frac{1}{m_{i} + m_{i-1}} \right), H_{i,i+1} = \frac{\Delta z}{\sqrt{z}} \left( \frac{1}{m_{i+1} + m_{i}} + \frac{1}{m_{i+1} + m_{i}} \right) \). The local density of states (LDOS) at an energy \( E \) is given by the diagonal elements of the spectral function, defined as
\[
A_b(z, z', E) = i \left[ G_b(z, z', E) - G^R_{bs}(z, z', E) \right].
\]

The self-energies of the semi-infinite contacts for a given band are calculated from the out of plane contact dispersion relations [37]. The imaginary part of \( \Sigma \) quantifies the broadening function as \( \Gamma^C = i(\Sigma^C - \Sigma^C) \). In the absence of scattering, the transmission function between the two contacts for any band \( b \) is given by
\[
T_{b}(E) = Re[Tr(\Gamma_{1,b}^C G^R_{2,b} G^C_{2,b} G^R_{2,b})].
\]

It is also important to include the scattering effects via additional self energies [37]. Since, the predominant scattering mechanisms in SL devices at moderate temperatures and zero/low electric field are mostly elastic in nature, we introduce non-coherent elastic dephasing models [37, 69] in our simulation, which in effect include fluctuating local scattering responsible for momentum and phase relaxation. In the scattering picture, \( \Sigma^S \) can be calculated self-consistently from the knowledge of the correlation functions of the electrons (\( G^P \))
and holes \((G^2)\). These correlation functions are evaluated from the total in \((\Sigma^{in})\) and out-scattering \((\Sigma^{out})\) self-energies of the device and are expressed as

\[
G^2(E) = G(E)\Sigma^{in}(E)G^\dagger(E),
\]

\[
G^2(E) = G(E)\Sigma^{out}(E)G^\dagger(E),
\]

(7)

where \(\Sigma^{in}(E) = \sum_{j=L,R} \Gamma_j^S(E)f_j(E - \mu_j) + \Sigma^{in}\) and \(\Sigma^{out}(E) = \sum_{j=L,R} \Gamma_j^S(E)(1 - f_j(E - \mu_j)) + \Sigma^{out}\). Here, \(f_j(E - \mu_j)\) is the equilibrium Fermi function of the \(j\)th contact having electro-chemical potential \(\mu_j\) and \(\Sigma^{in(out)}\) is the in (out) scattering functions for the scattering event \(S\). Within the elastic limit of dephasing [38, 39, 59, 60], \(\Sigma^{in(out)}\) simply becomes proportional to \(G^{0}\) with a scaling factor of \(D_0\), defined via the strength of scattering which in our simulation is assumed to be energy independent and is set equal to \(10^{-5}\) eV². Having obtained \(\Sigma^{in(out)}\), one can evaluate \(\Sigma^S\) as \(\Sigma^S(E) = \hat{\epsilon}(\Sigma^S(E)) * (\delta(E) + \frac{\Sigma^S}{\Gamma})\), where * denotes convolution and \(\hat{\epsilon}(\Sigma^S(E)) = -\frac{1}{2} (\Sigma^{in} + \Sigma^{out})\). After calculating the correlation functions self-consistently with the scattering functions, one can express the spectral current flowing from point \(z_j\) to \(z_{j+1}\) as [37]

\[
I^{p}_{\text{el}(bh)}(E) = \frac{iq}{\pi\hbar} \left[ H_{j+1}G^{(p)}_{j+1,j}(E) - H_jG^{(p)}_{j,j+1}(E) \right].
\]

(8)

3. Results and discussion

3.1. \(k.p\) results

The InAs/GaSb superlattice is distinguished by a broken-gap type-II band alignment with non-common atomic arrangements that exhibit completely different properties when compared with the bulk counterparts. Therefore, the appropriate values of the temperature dependent valence band offsets (VBOs) are important to model such non-common atomic structures as they are highly susceptible to the hetero-interface imperfections. It is already demonstrated in several earlier works that the interface region can ideally be of InSb or GaAs (or their higher order compounds) type based on the growth conditions [28, 32]. However, in most of the cases, InSb is the preferred choice as far as the accurate band modeling is concerned [67].

At first, we calculate the electronic band structure of a 8 ML/8 ML InAs/GaSb MWIR SL at a temperature of \(T = 77 K\) using the eight band \(k.p\) method discussed earlier. The above configurations corresponds to the thicknesses of InAs \((t_{InAs})\) and GaSb \((t_{GaSb})\) layers to be roughly about 2.4 nm each. In our simulation, we assume a fixed layer thickness \((t_{In})\) of 0.5 ML which is symmetric with respect to the junction. Although a few previous studies considered the interface thickness to be somewhere between 0.5 and 1 ML or within and around 10% of the InAs layer thickness [24, 67], it should be kept in mind that the InSb interface cannot be so thick such that it forms a quantum-well region at the junction of the two constituent SL materials or cannot be so thin such that it fails to capture and compensate the strain effects. Thus, a unit cell of the periodic structure as shown in figure 1 is

formed with the arrangement \(\{\text{InSb}(t_{In}/2)-\text{InAs}(t_{InAs} - t_{In})-\text{InSb}(t_{In})-\text{GaSb}(t_{GaSb} - t_{GaSb})-\text{InSb}(t_{In}/2)\}\) which corresponds to the period of thickness \(d = t_{InAs} + t_{GaSb}\). The values of the parameters used in the \(k.p\) calculation are summarized in table 1. The calculated dispersion results along the in-plane (\(E-k_{\parallel}\)) and out-of-plane (\(E-k_{\perp}\)) directions are respectively plotted in figures 2(a) and 2(b) within the first BZ. The obtained value of bandgap \((E_g)\) at \(77 K\) for the given configuration is 0.27 eV which corresponds to a cut-off wavelength of 4.59 µm that matches fairly well with the experimental bandgap values obtained in the range of 0.269–0.275 eV [70]. Figure 2(a) clearly suggests that there is a signature of spin-splitting along the in-plane direction and such a splitting is caused due to

| Parameters                  | InAs | GaSb | InSb |
|-----------------------------|------|------|------|
| Lattice constant (Å)        | 6.0584 | 6.0959 | 6.4794 |
| Energy band gap at 0 K (eV) | 0.418 | 0.814 | 0.24 |
| Varshini Parameter \(\alpha\) (meV K\(^{-1}\)) | 0.276 | 0.417 | 0.320 |
| Varshini Parameter \(\beta\) [K] | 93 | 140 | 70 |
| Effective mass electron \((m^*\text{e})\) | 0.022 | 0.0412 | 0.0135 |
| Luttinger parameter \(\gamma_1\) | 19.4 | 11.84 | 32.4 |
| Luttinger parameter \(\gamma_2\) | 8.545 | 4.25 | 13.3 |
| Luttinger parameter \(\gamma_3\) | 9.17 | 5.01 | 15.15 |
| Interband mixing parameter \(Ep (eV)\) | 21.5 | 22.4 | 23.3 |
| Spin orbit splitting (SO) (eV) | 0.38 | 0.76 | 0.81 |
| Valence band offset (VBO) (eV) | −0.56 | 0.0 | 0.03 |

Figure 2. Electronic band structure of (8 ML/8 ML) InAs/GaSb based T2SL at \(T = 77 K\) using \(8 \times 8\) \(k.p\) technique: (a) In-plane and (b) out-of-plane dispersion in the first Brillouin zone using periodic boundary condition of the given T2SL (period = 16 ML) with InSb interface of 0.5 ML. Calculated bandgap \(E_g = 0.27\) eV perfectly matches with the measured experimental value. The band curvatures at the high symmetry Γ point \((k = 0)\) indicates the low electron effective mass and very high heavy hole effective mass along the out-of-plane direction.
the inclusion of the interface Hamiltonian (H$_{IF}$) matrix in the overall system Hamiltonian. The effect of H$_{IF}$ is more pronounced away from the Brillouin zone center since it induces a finite shift in the maximum energy corresponding to each spin bands, especially the valence minibands. The conduction band (C$_t$) electrons exhibit a strong dispersion along both the parallel and perpendicular directions which point towards a lower electron effective mass (m$_e^*$) and a higher group velocity in either directions. On the other hand, the first heavy hole subband (HH$_1$) remains almost dispersionless along the perpendicular direction while showing a steady dispersion in the parallel plane. This suggests that the heavy holes are strongly localized along the transport direction and conduct only against a strong field.

The wavelength range of the photo-response spectra of a material ideally depends on its bandgap and the band widths. In periodic infinite SL structures, the thicknesses of the constituent materials and the nature of interface play a vital role in determining the subband properties. Therefore, it is necessary to investigate the effect of varying t$_{InAs}$ and t$_{GaSb}$ on the bandgap and the relative band edge values. Figure 3(a) shows the variation of E$_g$ as a function of both t$_{InAs}$ and t$_{GaSb}$ in a 2D color plot. The conduction band minima (CB$_{min}$) and the heavy hole valence band maxima (HH$_{max}$) with respect to the zero energy reference are also plotted respectively in figures 3(b) and (c) with respect to the same parameters. Both t$_{InAs}$ and t$_{GaSb}$ are varied from 8 to 16 ML and the resultant bandgap spans in the range of 0.08–0.348 eV which corresponds to 3.5–15 μm cut-off wavelength range that roughly covers the MWIR and LWIR range. One must notice that both E$_g$ and CB$_{min}$ exhibit similar patterns and are quite sensitive to the variations of both t$_{InAs}$ and t$_{GaSb}$. Since the InAs layers confine electrons and act as a potential well, an increase in t$_{InAs}$ results in a steady lowering of CB$_{min}$ towards the InAs conduction band edge. On the other hand, GaSb layers isolate the overlap of electrons between the adjacent InAs layers and act as a barrier for them. This results in a rise of CB$_{min}$ with increasing t$_{GaSb}$. In contrast to the above picture, HH$_{max}$ slowly moves closer to the valence band maxima of GaSb with the rise of t$_{GaSb}$ and remains nearly invariant with t$_{InAs}$ due to the strong localization of heavy holes in GaSb layers. This study encompasses a key aspect of band-engineering of T2SL structures for a wide infrared range and can be further utilized to design T2SL-based unipolar or bipolar barrier layers.

The carrier transport properties in a superlattice structure in the form of miniband or hopping transport are strongly governed by the quantum mechanical tunneling of carriers through the adjacent material layers. Since the tunneling probability has an exponential dependence on the carrier effective masses, the calculation of effective mass as a function of the layer thicknesses holds much significance. In InAs/GaSb SL, effective masses are less influenced by the interaction between the valence and conduction bands as they mainly depend on the electron (hole) wave function overlap between the adjacent material layers. Since the tunneling probability in 2D color plots: effective mass of (a) electron (m$_e^*$) and (b) hole (m$_h^*$) are plotted as functions of t$_{InAs}$ and t$_{GaSb}$ (in ML). m$_e^*$ rises sharply with the increase of t$_{GaSb}$ and reduces marginally with increasing t$_{InAs}$. On the other hand, an increase in both t$_{InAs}$ and t$_{GaSb}$ leads to the rise of m$_h^*$.
and \( m^*_h \) with respect to \( t_{\text{InAs}} \) and \( t_{\text{GaSb}} \). It can be seen that for the 8 ML/8 ML configuration, \( m^*_e = 0.0245 \) which is closer to that of the bulk InAs value and \( m^*_h = 0.16 \), way lesser than both bulk InAs and GaSb. However, due to the strong out-of-plane heavy hole confinement, \( m^*_h \) comes in the range of tens. One must notice that \( m^*_e \) increases sharply with \( t_{\text{GaSb}} \) due to the suppression of carrier overlap between adjacent InAs layers and falls marginally with \( t_{\text{InAs}} \), thereby maximizing at lower \( t_{\text{InAs}} \) and higher \( t_{\text{GaSb}} \) values. On the other hand, \( m^*_h \) rises with both \( t_{\text{InAs}} \) and \( t_{\text{GaSb}} \) due to its identical values in both the materials. This study thus offers an engineering guideline to have a reasonable estimate about the range of dark current, noise level and quantum efficiency while designing T2SL detectors.

### 3.2. NEGF results

Having obtained the band structure, we now shift our attention towards examining the miniband, carrier localization and spectral current properties of a finite-sized T2SL structure both in the position and energy space using the NEGF approach. To model a T2SL structure using single-band NEGF, we first assume that the atoms of the constituting materials are arranged in an one-dimensional chain along the \( z \)-axis with nearest-neighbour interaction as shown in figure 5. The interatomic coupling parameters between the two adjacent atoms are denoted as \( \tau_{\text{In}} \) and \( \tau_{\text{GaSb}} \) respectively for InAs and GaSb, and the coupling parameter between the two atoms on the opposite sides of the interface is given by \( \tau_{\text{InGaSb}} \). These values are calculated from the parabolic dispersion relations of the individual bulk materials in terms of their effective masses. The material parameters used in the NEGF simulation are summarized in table 2. Based on the interfacial arrangement of atoms, we consider two different configuration schemes, namely, (a) No-interface atoms and (b) Common-interface atoms, respectively shown in figures 5(a) and (b). In the following, we discuss both the configurations and present a comparative study of the simulated results.

#### Table 2. Material parameters used in the NEGF simulation [24, 71].

| Parameters                  | InAs   | GaSb   |
|-----------------------------|--------|--------|
| Electron effective mass \( m^*_e \) | 0.023  | 0.041  |
| Heavy hole effective mass \( m^*_h \) | 0.41   | 0.4    |
| VBO (eV) @77 K              | −0.56  | 0      |
| VBO (eV) @300 K             | −0.50  | 0      |

#### Figure 5. 1D schematic of T2SL unit cell: Nearest-neighbour 1D atomic chain representation of a T2SL unit cell having (a) no-interface atom, and (b) common-interface atom. The green atoms, forming the interface are modeled with GaAs material parameters.

#### Figure 6. Transmission function and Local density of states: (a) electron and heavy hole transmission probabilities of a ten period 8 ML/8 ML T2SL plotted with respect to the energy along with the energy flat band diagram. The only conduction miniband \( (C_1) \) shows a sparse band-spectrum due to the low \( m^*_e \), however the high \( m^*_h \) leads to a formation of two dense heavy hole minibands \( (HH_1, HH_2) \) and the absence of interface layer naturally overestimates the bandgap. (b) 2D color plot of the local density of states (LDOS) shown with respect to the position and energy space indicates the inter-layer transition due to spatial separation of electron and hole confinements which leads to a maximum optical absorption around the interface.

#### Figure 3.2.1. No-interface atoms. In this scheme, the interface is assumed to be abrupt between the InAs and GaSb layers and there is no separate interfacial layer of atoms. For such an arrangement of a ten period 8 ML/8 ML superlattice, at first, we calculate the electron and heavy hole transmission probabilities in the ballistic limit [41–44], given by equation (6) at 77 K and plot them in figure 6(a) along with the energy flat band diagram. The conduction and valence band edges of the two contact regions are intentionally terminated to their respective lowest and highest values to get perfect transmission peaks. One can notice from figure 6(a) that the electrons, owing to their lower effective mass, exhibit a sparse transmission spectra \( (C_1) \) where the number of transmission peaks equals the number of SL periods considered, indicating the number of bound eigen states inside the band. The heavy holes, on the other hand, due to their large effective mass, form two sharp and dense transmission channels \( (HH_1, HH_2) \) inside the valence band with the same number of allowed bound states. The LDOS, given by equation (5), of the aforementioned structure as shown in figure 6(b), exhibits the localization profile of the carriers in \( HH_1 \) and \( HH_2 \) bands which clearly indicates the spatial separation of the electron and hole confinements respectively in InAs and GaSb layers. The finite overlap between them around the interface determines the strength of absorption. The delocalization of conduction band electron wave functions between the neighbouring InAs layers also
points towards a possible formation of spatially continuous miniband. However, the strongly localized heavy holes in the GaSb layers do not allow to form the same. The bandgap of the given structure is calculated from the difference between the bottom of C1 and the top of HH1 which in this case comes out to be 0.315 eV. It is quite evident that the overestimation of the bandgap happens due to the absence of an interfacial layer, in compliance with the \( k.p \) calculation. The correct value of bandgap can be obtained through an interface modeling and will be shown later using the common-interface model. However, one can gain deeper physical insights into the spatial as well as spectral properties of the individual bands using this simple model as elaborated in the following.

To investigate the spatial confinement and interband overlap properties of the carriers, we incorporate the effects scattering processes through the dephasing model as discussed in section 2.2. These processes are inherently present in any nano-structured device at finite temperatures and can be generally attributed to the class of near-elastic scattering events such as the interaction between the electrons and low-energy acoustic phonons or the surface/interface scattering mechanisms, especially at low fields. In setting up the simulation, we further consider that the left and right contacts are respectively of GaSb and InAs type which make them carrier-selective in the microscopic picture, one must note that unlike the other methods \([36, 56]\), the wave functions do not peak at the center of the lattice, rather they spread evenly over the entire structure owing to the re-distribution of the allowed states arising due to the dephasing effects. The beauty of this method lies in the practical consideration of multiple momentum and phase-breaking processes occurring inside the system which tend to smear out the LDOS both in the real and energy space that give rise to a finite broadening in the energy spectrum. This helps manifesting a more realistic picture of the carrier localization and band properties which could not be observed in the ballistic case due to the spatial and spectral randomness and the discrete nature of the LDOS. The strength of absorption, on the other hand, being primarily governed by the amount of interband overlap of the electron and hole states, becomes a strong function of the layer thicknesses. Therefore, the spatial product of \( \tilde{A}_c \) and \( \tilde{A}_v \) as plotted with respect to position in figure 7(b), plays a major role in the present context. One notices that the overlap peaks right at the interfaces and falls sharply away from it. This suggests that the maximum amount of absorption takes place at the junctions of the two material layers and one should prefer to have thin layer T2SL structures to maximize the absorption. However, this enhances the possibility of recombination too which can severely degrade the detector performance. This study, therefore, provides significant information on the design strategies to achieve an optimum trade-off between the absorption and recombination factors.

In quantum confined heterostructures, the knowledge of 1-D DOS (\( \mathcal{D}_{1D} \)) becomes indispensable in determining the carrier concentrations and their vertical transport properties. This quantity can be calculated from the out-of-plane dispersion (\( \varepsilon_n(q) \)) relation obtained from the \( k.p \) results with periodic boundary conditions and is given by \( \mathcal{D}_{1D}(E) = \frac{\pi}{2} \sum_{q} \left( \frac{2\varepsilon_n(q)}{\Delta E} \right)^{-1} \mathcal{D}_{1D}(q) \) \([58]\). Using this relation, in figure 8, we plot the conduction band 1D-DOS, calculated from the dispersion profile depicted in figure 2(b), as a function of energy. The sharp features at the two ends arising from the flat dispersion at
the corners and the center of the first BZ, indicate the two edges of the miniband which also provide an estimate of the bandwidth. We further show that using only a finite structure in the NEGF approach, the 1D-DOS at zero transverse momentum can also be evaluated by integrating the LDOS over the entire finite SL structure, given by \( D_{1D}(E) = \frac{1}{2\pi} \int dz A(z, \vec{k}_0) = 0 \), where \( L_z \) denotes the length of the structure. For comparison, we display the 1D-DOS profiles obtained from NEGF for different number of SL periods in figure 8 alongside the \( k, \vec{p} \) result. The plots show a fair amount of agreement between the 1D-DOS derived from the finite and infinite structure in terms of the bandwidth and shape except for some dissimilarities in the magnitude and symmetry. However, one must notice that as we increase the number of periods, these discrepancies start to disappear, resulting in a more accurate 1D-DOS profile inside the band.

In order to understand the physical properties of carrier localization and the miniband formation, and their dependency on the layer thicknesses, we display the LDOS profile of two different SL configurations, 8 ML/8 ML and 12 ML/12 ML, respectively in figures 9(a) and (b) under flat-band conditions and in figures 9(c) and (d) under a finite built-in potential of 0.2 eV. These figures collectively depict some interesting signatures of the T2SL band properties. As the layer width increases, the miniband widths converge at a rapid rate along with the reduction of bandgap and more number of subbands appear inside the band. The LDOS of the 8 ML/8 ML structure, under both the flat-band and built-in potential, reveals the strong delocalization of the electronic states and the formation of the conduction miniband. However, with the increasing layer thicknesses, these states start to localize more and more in the InAs layers resulting in a weaker coupling of periods which ceases the possibility of miniband formation as visible from the LDOS of the 12 ML/12 ML structure. Specifically, the thickness of the electron blocking GaSb layers play the key role here in tailoring the strength of coupling and the amount of delocalization. On the other hand, the heavy hole states in all these cases remain strongly localized in the GaSb layers which suggests that the vertical transport of heavy holes in the MWIR range and at moderate temperatures is mostly governed by the phonon and defect-states assisted hopping transport between the localized states. This study, therefore, helps to find out the critical thicknesses of the layers that distinguishes the mode of carrier transport and determines the spectral properties.

A more detailed picture of the carrier transport through the miniband states inside the band can be obtained from the spectral current properties of electrons and holes over the entire structure. In the dephasing model, the current flowing between any two adjacent atoms at a particular energy, given by equation (8), is plotted for the 8 ML/8 ML structure at two different operating temperatures of 77 K and 300 K, respectively in figures 10(a) and (b). For a qualitative discussion, the spectral currents \( I_{sp}^p \) and \( I_{sp}^h \) are shown with respect to position and energy at (a) 77 K and (b) 300 K. Raising the temperature leads to an increasing population of the miniband states resulting in a significant current flowing through them.
left GaSb contact. On the other hand, at a higher temperature of 300 K, both these states are largely populated with carriers and conduct significantly with a broader spectral profile of current. This can be easily verified from figure 10(b) where the electrons and heavy holes exhibit a clear signature of miniband transport through the extended Bloch states, although the coupling of periods is still weak in the heavy hole band. Under finite built-in potential, the current spectrum can become much more broadened with the inclusion of inelastic scattering events such as electron-optical phonon interaction.

The applicability of this method is further extended towards a comprehensive understanding of the barrier-based complex detector structures. The family of next-generation high performance detectors is characterized by their high temperature operation and multi-color detection. This necessitates the integration of multiple absorber regions along with the inclusion of unipolar or bipolar carrier blocking barrier layers in a single device. In T2SL based structures, all these layers can be realized by varying the SL configurations using different shutter sequences in the growth chamber. In order to understand the different band alignments in such complex structures, one needs to separately evaluate the band properties of each SL region assuming perfect periodicity and combine them together for comparison. However, the NEGF method reveals its supremacy in obtaining the band profiles of such complex structures in an integrated simulation approach even when the SL periodicity is lifted. In doing so, we consider a T2SL structure that contains two absorber regions and one unipolar electron blocking barrier layer. The two absorber regions are configured using a 10 ML/10 ML and 12 ML/12 ML T2SL and the barrier region is configured using a 8 ML/8 ML structure. The LDOS profile of the given structure is displayed in figure 11. For the sake of reduced computational complexity, we have only considered three periods for each of these layers while ideally the number can be stretched further. The composite band diagram of this structure is shown in a blue dotted line which is drawn on the bottom of the conduction miniband and the top of the first heavy hole band. The two absorber regions clearly reveal different bandgaps which indicate dual-color detection under different biasing condition. The barrier layer, on the other hand, shows a higher value of bandgap and a large conduction band offset while depicting a negligible valence band offset in compliance with the requirement of unipolar electron blocking layer. The minute differences between the heavy hole states in different regions both in the energy and position space can also be clearly observed. This study is thus extremely fruitful for a qualitative understanding of the band profiles and localization in any complex SL structures with broken-periodicity which eventually justifies the effectiveness of the method adopted.

3.2.2. Common-interface atoms. The study, so far, was aimed to build an adequate understanding of the band and transport properties in a qualitative manner. However, the bandgap, being overestimated earlier, should be predicted accurately for a given T2SL structure in order to get the right absorption wavelength. From our earlier discussion, we understand that the appropriate modeling of the interface can give rise to correct bandgap values. Several earlier works were dedicated to achieve bandgap values within the acceptable limit of errors through interface engineering [67, 72]. This work, too, adopts a simple interface modeling approach by inserting different atoms common to either side of the interface as shown in figure 5(b). Unlike the $k.p$ method, we consider that the interface atoms only change the inter-atomic coupling parameters and do not form a separate material layer. In our simulation, we assume that the interface atoms are of GaAs type and the coupling parameters around the interface are accordingly calculated from GaAs effective masses ($m_e^* = 0.067m_0$, $m_h^* = 0.4m_0$). For the earlier 8 ML/8 ML structure at 77 K, the bandgap using this model is calculated as 0.278 eV which matches reasonably well with the $k.p$ results and the experimental data. However, due to the large electron effective mass of GaAs, the conduction miniband width reduces substantially. A comparative study of the bandgap ($E_g$) and the conduction miniband width $\Delta_C1$ of the 8 ML/8 ML structure obtained from both these methods and experiments is presented in table 3. To validate this model for bandgap estimation, we further simulate other structures and compare them in table 4 with the $k.p$ and the available experimental data in the literature. While the bandgap matches well in the common-interface atom model, the no-interface model fairly estimates the bandwidth which improves further with the increasing number of SL periods. In future outlook, we believe that a rigorous multi-band tight-binding modeling in the NEGF formalism can lead to even more accurate results in terms of both the miniband and carrier transport properties.


| Configurations | InAs/GaSb | k.p    | NEGFI | NEGFI | Experimental Result |
|----------------|-----------|--------|-------|-------|---------------------|
| 7 ML/8 ML      | 0.305     | 0.36   | 0.31  | 0.3   |
| 8 ML/8 ML      | 0.27      | 0.315  | 0.278 | 0.269–0.277          |
| 10 ML/10 ML    | 0.225     | 0.25   | 0.215 | 0.22–0.23            |
| 8 ML/12 ML     | 0.315     | 0.33   | 0.285 | 0.304–0.308          |

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### Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.
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