Photo-excited carrier density in short-period InAs/GaSb

type-II superlattice

Fan LI¹, Wen XU², Yan-li SHI¹ ¹Kunming Institute of Physics, Kunming 650223, P.R.China ² Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China

ABSTRACT

We present a systematic theoretical study on optical properties of short-period InAs/GaSb type-II superlattices (SLs) which can serve for Mid-Infrared (MIR) detection. From the energy dispersion relation for the electron derived from using the standard Kronig-Penney model we calculate the electron-minibands structure in InAs layer and the hole-minibands structure in GaSb layer of such SLs. The obtained band-gap energies are in line with those realized experimentally. On the basis of the mass-balances equations derived from the Boltzmann equation, at the same time considering the polarization direction of the infrared irradiation vertical to the growth direction of the material, we develop an approach to calculate the Fermi level and photo-excited carrier density in the corresponding SL systems. The dependence of photo-conductivity in InAs/GaSb type-II SLs on temperature and well-widths are examined. This study is pertinent to the application of InAs/GaSb type-II SLs as uncooled MIR photodetectors.

Key words: Type-II superlattice (SL), Miniband, Bandgap, Photo-excited carrier density

1. INTRODUCTION

In contrast to conventional semiconductor superlattice (SL) systems in which the conducting electrons and holes are located mainly in the same material layer, the confined electrons and holes in an InAs/GaSb type-II SL are separated spatially in different well layers¹. As a result, in an InAs/GaSb type-II SL the energy-gap between confined electron states in the InAs layer and confined holes states in the GaSb layer can be tuned artificially by simply varying the sample growth parameters such as the widths of the InAs and GaSb well layers. In an undoped InAs/GaSb SL, there are mainly two mechanisms responsible for optical transition via direct electron/hole interactions with the radiation fields. One is to excite electrons in the occupied minibands in the valence-band in one well layer across the forbidden zone into the unoccupied minibands in the conduction at InAs/GaSb interfaces. Another is to excite electrons or holes from occupied minibands to unoccupied minibands in the conduction-band or valence-band in the same well layer that is the intra-layer transition which is similar to that in a conventional SL. These inter-layer and intra-layer optical transition channels can also be controlled by adjusting the SL layer thicknesses. Owing to these unique features, InAs/GaSb-based

Author: Fan Li (1983~), male, master student in Kunming Institute of Physics Corresponding author: Yanli Shi (1969~), female, professor in Kunming Institute of Physics

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type-II SLs have been chosen as material systems for high-speed infrared detection at ambient temperature 2,3 . In particular, it has been proposed in 2004 that short-period InAs/GaSb type-II SLs can be used as uncooled mid-infrared (MIR) photo detectors working at 3-5µm bandwidth for various applications 4 .

It has been realized experimentally⁴ that when the widths of the InAs/GaSb layers in a SL are around 20/25Å, MIR band-gap can be achieved between the highest heavy-hole miniband in the GaSb layer and the lowest electron miniband in the InAs layer. Pronounced signals of the photo-response generated from transition between these two states can also be observed at T=10K⁴. These important experimental findings have shed the lights on the realization of InAs/GaSb type-II SLs as uncooled MIR photo-detectors. In conjunction with this experimental work, a theoretical work has been carried out to calculate the band-gap energies in the corresponding SL systems on the basis of the modified Envelope Function Approximation (EFA)⁴. By including the interface coupling of heavy, light and spin-orbit holes resulting from the in-plane asymmetry at the InAs/GaSb interfaces via the standard 8×8 EFA model⁵, good agreement between experimental and theoretical data for the type-II energy gaps could be reached⁴. It should be noted that the modified EFA model⁴ is a rather complicated theoretical approach which involves heavily the numerical calculations. In the present study we would like to examine if the simplest theoretical approach, such as the popularly used Kronig-Penney model, can be used to calculate the miniband structure of InAs/GaSb type-II SL systems with MIR band-gap energy. One of the major advantages for using simple model to calculate the electronic miniband structure in a SL is that we can use the eigenfunctions and eigenvalues obtained from such a model to calculate more easily and tractably the electronic, transport and optoelectronic properties of the systems. The prime motivation of this study is to develop a simple theoretical approach to study optoelectronic properties of the short-period InAs/GaSb type II SL for the application of infrared detection. In conjunction with the reported experimental findings⁴, in this study we undertake a theoretical investigation to examine the dependence of photo-conductivity in InAs/GaSb type-II SLs on the layer thickness and temperature. We would like to understand more deeply the physical mechanisms behind the application of short-period InAs/GaSb type-II SLs as MIR photo-detectors.



FIG. 1: An InAs/GaSb SL along the grown direction (z-axis). E_A and E_B are respectively the band-gaps for bulk materials InAs and GaSb, L_A and L_B are respectively the well widths for InAs and GaSb layers, and V_s and V_p are respectively the conduction and valence band offsets. The energy E=0 is measured from the bottom of the conduction band in the InAs layer.

The paper is organized as follows. In Section II, we briefly outline the method to calculate electronic miniband structure in a type-II SL using the standard Kronig-Penney model. In Section III, on the basis of the Boltzmann equation we develop a simple approach to calculate the electron and hole's Fermi level and photo-excited carrier density at finite temperature for type-II SLs, The main results obtained from this study are presented and discussed in Section IV and the major conclusions drawn from this study are summarized in Section V.

2. MINI-BAND STRUCTURE

In this study we generalize the standard Kronig-Penney model⁶ for the calculation of the electronic miniband structure of InAs/GaSb type-II SLs. We consider an InAs/GaSb SL in which the growth direction is taken along the z-axis. The diagram of the band alignment along the growth direction for such a SL is illustrated in FIG.1. In an InAs/GaSb type-II SL, the electrons and holes are separated spatially in the InAs and GaSb layers respectively. Here we employ the following notations to describe such a SL structure. L_A and L_B are respectively the InAs and GaSb layer thicknesses, therefore, the periodicity of the SL is $d = L_A + L_B$. m_A and m_B are respectively effective masses for an electron or a hole in the InAs and GaSb layers. V_s (measured from the bottom of the conduction band in the InAs layer) and V_p (measured from the top of the valence band in the GaSb layer) are respectively the conduction and valence band offsets which play the roles as the barriers for confining electrons and holes. In the absence of scattering centers and external fields and neglecting the interactions between electrons and holes in the structure, the electron and hole miniband structures can be solved separately. Firstly, we consider an electron confined within the InAs layers. Under the effective-mass approximation, the Schrödinger equation for an electron in the growth direction is

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(z)}\frac{d\psi(z)}{dz} + V(z)\psi(z) = \varepsilon\psi(z)$$
(1)

where the confining potential energy (see FIG.1) is

$$V(z) = \begin{cases} 0, & -L_A \le z \le 0\\ V_s, & 0 \le z \le L_B \end{cases}$$
(2)

and

$$m(z) = \begin{cases} m_A, & -L_A \le z \le 0\\ m_B, & 0 \le z \le L_B \end{cases}$$
(3)

is the electron effective-mass in different layers. The solution of Eq.(1) must obey the condition of the Bloch periodicity:

$$\psi(z+d) = e^{ik_z d} \psi(z) \tag{4}$$

with $k_z = [-\pi / d, \pi / d]$ being the superlattice wavevector along the growth direction. In the zeroth period, the solution for a bound state $V_s > \varepsilon$ can be written as

$$\psi(z) = \begin{cases} c_1^A e^{ik_A z} + c_2^A e^{-ik_A z}, & -L_A \le z \le 0; \\ c_1^B e^{-k_B z} + c_2^B e^{k_B z}, & 0 \le z \le L_B \end{cases}$$
(5)

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where $k_A = \sqrt{2m_A \varepsilon / \hbar^2}$ and $k_B = \sqrt{2m_B (V_s - \varepsilon) / \hbar^2}$. Using the continuities of $\psi(z)$ as well as the weighted derivative $m^{-1}(z)d\psi(z)/dz$ at the InAs/GaSb interface and the condition of the Bloch periodicity, one obtains a 4×4 matrix,

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ \Lambda & -\Lambda & -i\Gamma & i\Gamma \\ \mu^{-} & \mu^{+} & -\nu^{+} & -\nu^{-} \\ \Lambda\mu^{-} & -\Lambda\mu^{+} & -i\Gamma\nu^{+} & i\Gamma\nu^{-} \end{pmatrix} \begin{pmatrix} c_{1}^{A} \\ c_{2}^{A} \\ c_{1}^{B} \\ c_{2}^{B} \end{pmatrix} = 0$$
(6)

where $\Lambda = k_A/m_A$, $\Gamma = k_B/m_B$, $\mu^{\pm} = e^{i(k_z d \pm k_A L_A)}$ and $\nu^{\pm} = e^{\mp k_B L_B}$. For a nontrivial solution of Eq.(6), the 4×4 determinant of the corresponding matrix must be zero, which results in the Kronig-Penney equation for an electron in a bound state

$$\cos(k_z d) = \frac{1}{2} \left(\beta - \frac{1}{\beta}\right) \sin(k_A L_A) \sinh(k_B L_B) + \cos(k_A L_A) \cosh(k_B L_B) \tag{7}$$

where $\beta = \Gamma / \Lambda$. The corresponding electron wavefunction becomes

$$\psi(z) = A \begin{cases} \cos(k_A z) + \beta F \sin(k_A z), & -L_A \le z \le 0; \\ \cosh(k_B z) + F \sinh(k_B z), & 0 \le z \le L_B \end{cases}$$
(8)

where $F = \frac{\cos(k_A L_A)e^{ik_z d} - \cosh(k_B L_B)}{\beta \sin(k_A L_A)e^{ik_z d} + \sinh(k_B L_B)}$ and A is determined by the normalization condition: $\int_{-L_A}^{L_B} \psi^*(z)\psi(z)dz = 1$.

Using the Kronig-Penney equation given by Eq.(7), the energy for an electron in the n^{th} miniband in the InAs layer, $\mathcal{E}^e = \mathcal{E}_n^e(k_z)$ can be determined and, then from it the corresponding $\psi^e(z) = \psi_{nk_z}^e(z)$ along the growth direction, can be obtained. Using the similar approach the energy, $\mathcal{E}_n^h(k_z)$, and wavefunction, $\psi_{nk_z}^h(z)$, for a hole in the n^{th} miniband in the GaSb layer can also be calculated. Thus, the simple Kronig-Penney model can be used to calculate the electronic miniband structure of a type-II SL.

3. PHOTO-RESPONSE IN A SL

3.1 Energy and wavefunction

In a SL, the wavefunction and energy spectrum for an electron (j=e=2) or a hole (j=h=1) can be written, respectively as

$$\begin{cases} \Psi_{nK}^{j}(R) = e^{ik \cdot r} \psi_{nk_{z}}^{j}(z), \\ E_{n}^{j}(K) = (-1)^{j} \hbar^{2} k^{2} / 2m_{j}^{*} + \varepsilon_{n}^{j}(k_{z}) \end{cases}$$
(9)

R = (r, z) = (x, y, z), and $K = (k, k_z) = (k_x, k_y, k_z)$ with k being the electron/hole wavevector along the xy-plane and k_z the wavevector of the reciprocal space along the growth direction, and m_j^* is the density of states effective mass for an electron or a hole. We now consider an electromagnetic (EM) field, which is polarized linearly along the z-direction, is applied to the SL. Applying the electron and hole wavefunctions and energy spectra given by Eq.(9) into the Fermi's golden rule, the steady-state electronic transition rate induced by direct interactions between electrons/holes and the radiation field is obtained as

$$W_{nn'}^{jj'}(K,K') = \frac{2\pi}{\hbar} \left(\frac{e\hbar F_0 k_x}{2m_j^* \omega} \right)^2 X_{nn'}^{jj'}(k_z) \delta_{K',K} \delta \left(E_n^j(K) - E_{n'}^{j'}(K') \pm \hbar \omega \right)$$
(10)

which measures the probability for scattering of an electron or a hole at a state $|n, K\rangle$ in layer j to a state $|n', K'\rangle$ in layer j' through emission (lower case) or absorption (upper case) of a photon. Here, F_0 and ω are, respectively, the electric field strength and frequency of the EM field, $X_{mn'}^{jj'} = \delta_{n',n}$ for intra-band transition,

and
$$X_{n'n}^{eh}(k_z) = X_{nn'}^{he}(k_z) = \left| \int_{-L_A}^{L_B} dz \psi_{n'k_z}^{e^*}(z) \psi_{nk_z}^{h} \right|^2$$
 for inter-band transition. The term $\delta_{K',K}$ reflects the fact that the

directelectron/hole-photon coupling in a SL does not change the momentum of an electron or a hole.

3.2 Balance-equations

We now consider a dc electric field with a strength F_z is applied along the growth-direction of the SL system. In this study, we employ the semi-classic Boltzmann-equation as the governing transport equation to study the response of the carriers (electrons and holes) in a SL to the applied radiation field and driving electric field. At a degenerate statistics, the steady-state Boltzmann-equation for an electron or a hole take a form Eq.(11). Here, $I^j = -1$ for an electron and $I^j = +1$ for a hole, $g_s = 2$ counts for spin-degeneracy, $F_{nn'}^{jj'}(K, K') = f_n^j(K)[1 - f_{n'}^{j'}(K')]W_{nn'}^{jj'}(K, K')$, $f_n^j(K)$ is the momentum-distribution function for a carrier at a state $|n, K\rangle$ in layer j, and $W_{nn'}^{jj'}(K, K')$ is the steady-state electronic transition rate.

$$I^{j} \frac{eF_{z}}{\hbar} \frac{\partial f_{n}^{j}(K)}{\partial k_{z}} = g_{s} \sum_{j',K',n'} [F_{n'n}^{j'j}(K',K) - F_{nn'}^{jj'}(K,K')]$$
(11)



FIG.2: Dispersion relation of the electron/hole miniband energies, $\mathcal{E}_n^e(k_z) / \mathcal{E}_n^h(k_z)$, for the fixed InAs/GaSb layer widths L_A / L_B as indicated.



FIG.3: Band-gap energies between the bottom of the electron mini-band in the InAs layer and the tops of the two heavy-hole mini-bands in the GaSb layer as a function of InAs layer width L_A at a fixed GaSb layer width L_B =2.40nm. The results are shown for k_z =0.

This equation implies that only the inter-band scattering $(i.e., j \neq j')$ can alter the number of the carries in the system. It also reflects the fact that the change of the electron number in the conduction-band equals to that of the hole number in the valence-band, namely this equation gives the condition of change number conservation in the system. For the case where

$$f_n^j(K) = f_j(E_n^j(K)) \quad \text{with} \quad f_j(x) = [e^{(x - E_F^j)/K_B T} + 1]^{-1}, \text{ Eq. (12) becomes}$$

$$0 = \sum_{k_z, n', n} \Theta(X_0) X_0 X_{nn'}^{eh}(k_z) \{ [1 - f_h(X_2)] f_e(X_1) - (m_e^* / m_h^*)^2 [1 - f_e(X_1)] f_h(X_2) \}$$
(13)

where $X_0 = \hbar \omega + \varepsilon_{n'}^h(k_z) - \varepsilon_n^e(k_z)$,

$$X_{1} = \frac{m_{h}^{*}[\varepsilon_{n'}^{h}(k_{z}) + \hbar\omega] + m_{e}^{*}\varepsilon_{n}^{e}(k_{z})}{m_{e}^{*} + m_{h}^{*}} \text{ and } X_{2} = \frac{m_{e}^{*}[\varepsilon_{n}^{e}(k_{z}) - \hbar\omega] + m_{h}^{*}\varepsilon_{n'}^{h}(k_{z})}{m_{e}^{*} + m_{h}^{*}}$$

In the presence of the radiation, the electron and hole densities are:

$$n_{e} = 2\sum_{K,n} f_{e}(E_{n}^{e}(K)) = \frac{m_{e}^{*}K_{B}T}{\pi\hbar^{2}} \sum_{k_{z},n} \ln\left\{1 + e^{[E_{F}^{e} - \varepsilon_{n}^{e}(k_{z})]/K_{B}T}\right\}$$
(14)

$$n_{h} = 2\sum_{K,n} [1 - f_{e}(E_{n}^{e}(K))] = \frac{m_{h}^{*}K_{B}T}{\pi\hbar^{2}} \sum_{k_{z},n} \ln\left\{1 + e^{[\varepsilon_{n}^{h}(k_{z}) - E_{F}^{h}]/K_{B}T}\right\}$$
(15)

Another fact which is considered in the calculation is the condition of the charge number conservation. For an sample, the carrier density is zero in the absence of the radiation field. When the radiation field is applied, the electron number in the system should equal to the hole number, i.e.

$$n_e = n_h \tag{16}$$





FIG.4: Form factor $X_{n'n}^{he}(k_z)$ induced by electron/hole photon interaction in an InAs/GaSb SL as a function of wavevector k_z for the fixed InAs/GaSb layer widths L_A/L_B as indicated.

FIG.5: Temperature dependence of the Fermi level of electron/hole for fixed InAs/GaSb layer widths L_A/L_B as indicated.

4. NUMERICAL RESULTS AND DISCUSSIONS

4.1 Mini-band structure

In the present work, we employ the simplest approach such as the Kronig-Penney model to calculate the electronic miniband structure of InAs/GaSb type-II SLs. We are interested in short-period SLs which can be used for MIR detection. The ideal case is considered, where the electrons and holes in different layers are well separated, the system is isotropic, and the effects such as the presence of strain, interface coupling of different kinds of holes, etc. are not taken into consideration. We assume that these effects can be incorporated into the material parameters such as the carrier effective masses. We know that the electron effective mass in bulk InAs is $0.038 m_0$ and the heavy-hole effective mass in bulk GaSb is $0.33 m_0$, where m_0 is the vacuum electron mass. It is a fact that the effective masses for an electron and a hole will be enhanced in the presence of quantum confinement in the system. Previous experimental results obtained from cyclotron resonance (CR) measurements have indicated that in short-period InAs/GaSb type-II SLs, the effective electrons in the InAs layer and heavy-holes in the GaSb layer can be enhanced significantly¹¹. The narrower the InAs/GaSb layer thicknesses are, the larger the effective masses for an electron and a hole are. It should be noted that the presence of the strain and carrier coupling at InAs/GaSb interfaces can enhance the confinement of the carriers in the SL. Therefore, these effects can also result in the larger effective masses for different carriers in the SL. In line with experimental findings obtained from the CR measurements¹¹, we take the effective masses for carriers in short-period InAs/GaSb SLs with the well layer widths $L_A \sim 20$ Å and $L_B \sim 25$ Å as: m_e^* (InAs) = $m_A^e = 0.042 m_0$ and m_h^* (InAs) $= m_A^h = 0.41 m_0$, m_e^* (GaSb) $= m_B^e = 0.049 m_0$ and m_h^* (GaSb) $= m_B^h = 0.50 m_0$. In the calculation, we take the conduction-band and valence-band offsets at the InAs/GaSb interfaces to be $V_s = \Delta E_c$ =900meV and $V_n = \Delta E_v = 500 \text{ meV}$ and the conduction-band and valence-band overlap energy is $\Delta = 150 \text{ meV}$. These band parameters have led to the good agreement between experimental and theoretical results in InAs/GaSb type-II quantum well systems¹²

4.2 Photo-excited carriers

We can calculate the $X_{nn'}^{jj'}(k_z) = \left| \int dz \psi_{n'k_z}^{j'*}(z) \psi_{nk_z}^{j-2} \right|$ induced by electron/hole interactions with the radiation field in a SL with the electron and hole wavefunctions obtained from the Kronig-Penney model. This factor determines the strength of the electron/hole photon coupling. In FIG.4 we show $X_{n'n}^{he}(k_z)$ as a function of k_z . Here hh1 \rightarrow e and hh2 \rightarrow e refer to transition channels from the highest (hh1) and second-highest (hh2) hole mini-bands in the GaSb layer to the electron (e) mini-band in the InAs layer.

In an undoped type-II SL, the presence of the radiation field can pump electrons in the valance band in the GaSb layer into the conduction band in the InAs layer. Such process changes Fermi level and induces photo-excited carriers whose transitions contribute mainly to the optical absorption in the SL. In general, the photo-execited carrier density depends on the radiation intensity, frequency and on other scattering and relaxation mechanisms. Because in an InAs/GaSb SL the electron and heavy-hole has different effective mass, the Fermi level of electron and hole are different. Introducing the energy spectrum for an electron or a hole in a SL into the corresponding density-of-states, the Fermi level can be calculated through Eq.(13), Eq.(14), Eq.(15), Eq.(16). In FIG.5 we show the dependence of the Fermi level of electron frequency, the electron Fermi level was significantly increased, while the hole Fermi level did not change significantly. It is because that the big

difference effective mass between electron and hole in InAs/GaSb SL structure. With increasing temperature, the electron Fermi level decreased significantly, while the hole Fermi level increased.

The result obtained from the Kronig-Penney model indicate that in short-period InAs/GaSb SLs with the layer widths $L_A/L_B \sim 20/25$ Å, there is only one electron miniband in the InAs layer and there are two heavy-hole mini-band in the GaSb layer (see FIG.2). Hence, in such SL structures the photo-exceited carrier is achieved mainly via the miniband for $k_z = 0$ in the MIR bandwidth. In FIG.6, we show the dependence of the photo-excited carrier density on temperature in a short-period InAs/GaSb SL with the well widths $L_A/L_B = 2.35/2.40$ nm. The photo-excited carrier density is about $10^{18} \sim 10^{19}$ cm⁻³. With the increase in phon energy, the photo-excited carrier density is increasing. This transition also attributes to the photon energy corresponding cut-off frequency, where the intensity of the photo-excited carrier density becomes low when the radiation photon energy is below this photon energy in a short-period InAs/GaSb SL (see FIG.3). We find this photon energy for $L_A/L_B = 2.35/2.40$ nm at T=77K is about 306meV. We are only interested in medium-wave infrared, we consider the maximum photon energy of transition channels from the highest hole miniband in the GaSb layer to the electron miniband in the InAs layer. It is about 513meV. So we don't calculate the photo-excited carrier density when photon energy is more than 513meV.

The dependence of the photo-excited carrier density on the InAs layer width is shown in FIG.7 at T=77K for a fixed GaSb layer width. As can be seen from FIG.3, because the electron is mainly lacated in the InAs layer, varying the InAs layer width can alter efficiently the bandgap for the type-II optical transitions. With increasing the InAs layer width L_A , the red-shift of the photon energy corresponding cut-off frequency can be observed. And the photo-excited carrier density didn't shift significantly. It is also about $10^{18} \sim 10^{19}$ cm⁻³. This feature is in line with the experimental finding⁴. We find that the photon energy corresponding cut-off frequency for optical absorption is shifted from 390.3meV to 305.2meV as the InAs layer width increases from 1.75nm to 2.35nm when the GaSb layer width is fixed at L_B =2.40nm.



FIG. 6: Temperature dependence of photo-excited carrier density for the fixed InAs/GaSb layer widths L_A/L_B as indicated.



FIG. 7: Photo-excited carrier density at a fixed GaSb layer width L_B and a fixed temperature T for different InAs layer widths as indicated

5. CONCLUSIONS

In this paper, we have conducted a systematic theoretical investigation into optical prperties of short-period InAs/GaSb type-II SL systems. We have demonstrated that a simple Kronig-penney model can be employed to calculate the electronic miniband structure of such SL systems. The presence of the quantum size effects and the interactions among different carries at the interfaces can be in corporated into the carrier effective masses. Based on the Boltzmann equation, a simple theoretical approach has been developed to calculate the photo-excited carrier density in SL systems at a finite temperature. We have examined the dependence of the photo-excited carrier density on temperature and SL layer width. By considering that the presence of the quantum confinement and the interactions among different carriers at the interfaces can result in heavy effective masses for electrons and holes in a short-period InAs/GaSb type-II SL, the Kronig-Penney model can be used to calculate the wavefunctions and energy spectra of the mini-bands for an electron and a hole in the SL. This simple model calculation can reach a good agreement between theoretical results and experimental data. From this calculation, we have found that in short-period InAs/GaSb SLs with the layer widths about 20/25Å, the electron wavefunction overlaps significantly with the hole wavefunctions at the InAs/GaSb layer to the electron mini-band in the InAs layer) can be achieved in such SL structure. The photo-excited carrier density is about 10¹⁸ ~10¹⁹ cm⁻³. It can reach a good agreement with experimental data.

In short-period InAs/GaSb type-II SLs, the photon energy corresponding cut-off frequency of the optical absorption is determined by the fundamental band-gap between the highest heavy-hole miniband in the GaSb layer and the electron miniband in the InAs layer. When the InAs/GaSb layer widths are about 20/25Å, the fundamental band-gap is within the MIR bandwidth.

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