Flexibility of Ga-containing Type-II superlattice for long-wavelength infrared detection

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Abstract
In this paper, the flexibility of long-wavelength Type-II InAs/GaSb superlattice (Ga-containing SL) is explored and investigated from the growth to the device performance. First, several samples with different SL period composition and thickness are grown by molecular beam epitaxy. Nearly strain-compensated SLs on GaSb exhibiting an energy band gap between 105 to 169 meV at 77 K are obtained. Second, from electronic band structure calculation, material parameters are extracted and compared for the different grown SLs. Finally, two p-i-n device structures with different SL periods are grown and their electrical performance compared. Our investigation shows that an alternative SL design could potentially be used to improve the device performance of diffusion-limited devices for long-wavelength infrared detection.

Keywords: InAs/GaSb superlattice, long-wavelength infrared, molecular beam epitaxy, electronic band structure, dark-current, photodiodes

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

1. Introduction
The Type-II InAs/GaSb superlattice (Ga-containing SL) is a material of great interest for infrared imaging as it offers many advantages including a tunable energy band gap in the midwave (MWIR, 3–5\,\mu m) and longwave (LWIR, 8–12\,\mu m) infrared spectral domain, a high absorption coefficient and low tunnelling currents. Recently, the InAs/InAsSb SL (Ga-Free SL) has emerged as an alternative to the Ga-containing SL as longer minority carrier lifetime have been reported [1, 2]. Although significant results have been obtained [3, 4], it is understood that the InAs/GaSb SL remains the material of choice for LWIR detection thanks to better optical and hole transport properties [5, 6]. For this reason, as well as the growing interest in space applications such as Earth Observation missions [7, 8], the research in recent years has mainly been focused on developing InAs/GaSb SL for LWIR detection [9–12].

A variety of engineered heterostructures, also called barrier structures, such as nBn [13], pBp [14], pBn [15], p-\pi-M-n [16], pBiBn [17], CBIRD [18] have been demonstrated. These devices allow for reduction of the dark-current compared to standard p-i-n photodiodes by suppressing the generation–recombination (G–R) current in the absorption region thanks to the insertion of a high band gap material [19]. For all these structures and for most of the LWIR SLs reported in the literature, the absorber layer is made of a SL composed of X monolayers (MLs) of InAs and 7 MLs of GaSb with X varying from 13 to 15 MLs, which exhibits a cut-off wavelength between 9 to 10.8\,\mu m at a temperature of 77\,K. It is somehow surprising to see such a limited choice of the SL composition throughout the literature knowing that the SL offers a great flexibility in the choice of the SL period to target a specific...
cut-off wavelength. Indeed, the energy band gap of the SL can be tuned by varying not just the period thickness but also the average composition, that is to say it depends on the ratio $R$ of the layer thicknesses (with $R = \text{InAs thickness} / \text{GaSb thickness}$ per period). The material properties, i.e. electronic band structure, of the SL are ruled by the ratio $R$ and it has already been proven that it has an influence on the electro-optical properties of midwave SL photodiodes with the same energy band gap [20, 21]. The objective of this work, therefore, is to explore and investigate the period flexibility of Ga-containing SLs for the LWIR spectral range. First, the growth by molecular beam epitaxy (MBE) of various SLs with different ratio $R$ is studied since the lattice mismatch $\Delta a/a$ between the SL layer and GaSb substrate directly depends on the period composition and thickness. To compensate for the tensile strain of the InAs layer on GaSb ($\Delta a/a \approx -0.6\%$), the migration-enhanced epitaxy (MEE) technique was used to grow an intentional InSb layer at the interfaces. The structural and optical properties are then evaluated by means of x-ray diffraction (XRD) and photoluminescence (PL) measurements. Secondly, to gain insight and understanding of the SL material, an 8-band $k\cdot p$ solver is used to calculate the dispersion curve ($E(k)$ plot) of Ga-containing SL. After briefly presenting the method, the $k\cdot p$ modeling is calibrated by comparing the calculated and measured band gap of the grown SLs. The effective mass is then extracted from the electronic band structure and discussed for different SL designs. Finally, two different p-i-n device structures are grown with an active region made of a 14 MLs InAs/7 MLs GaSb SL and a 12 MLs InAs/4 MLs GaSb SL. Both samples show a cut-off wavelength between 10 and 11 $\mu m$ at 77 K. Photodiodes are fabricated, and the electrical performance compared.

2. Growth and material characterization

2.1. Experiment details

All Ga-containing SL structures presented in this paper were grown on a quarter of two-inch p-type (0 0 1)-oriented GaSb substrate in a Veeco Gen 930 MBE reactor equipped with dual filament SUMO Knudsen effusion cells for gallium (Ga) and indium (In) and Mark V valved cracker effusion cells for arsenic (As) and antimony (Sb). The In and Ga growth rates were set to 0.3 and 0.5 ML s$^{-1}$, respectively. The InAs and GaSb layers were grown using a V/III flux ratio calibrated from RHEED oscillations of 1.2 and 2, respectively. The
growth temperature was monitored by pyrometer and thermocouple and, calibrated with the (1 × 3) to (2 × 5) reconstruction transition on the GaSb substrate and buffer surface. Before the growth, the native oxide on the GaSb substrate was first thermally desorbed at 540 °C. The growth temperature was then lowered down to 490 °C for the GaSb buffer layer and to 410 °C for the SL layer.

To compensate for the tensile strain of the InAs layer on GaSb, the SL is grown with an InSb layer intentionally grown by MEE at both interfaces, namely the GaSb-on-InAs and InAs-on-GaSb interfaces. The particularity of the MEE technique is that both group III and V shutters are asynchronously opened in contrast to conventional MBE (shutters synchronously opened) [22, 23]. It has been demonstrated that abrupt interfaces can be obtained by MEE [24, 25] and, in the case of SLs, it has led to a smoother surface with improved optical properties compared to an InSb interface layer grown by MBE [26]. The shutter sequence used for the SL growth is therefore as follows: after the growth of the InAs layer, only the In shutter remains open. It is then closed and, only the Sb shutter is opened for 6 seconds (s) to saturate the In surface with Sb at the GaSb-on-InAs interface. The Ga shutter is then opened to grow the GaSb layer. At the InAs-on-GaSb interface, the Sb shutter remains open for an additional 6 s and, then only the In shutter is opened before growing the InAs layer. Note that the In shutter opening time is the same at both interfaces and depends on the SL period. In this work, it is used to control the thickness of the InSb interface layer. In one SL period, an InSb thickness of approximately 10% of the InAs thickness is required to compensate for the tensile strain of the latter. It is also worth mentioning that all fluxes are kept constant during the entire SL growth.

The samples presented in this paragraph consist of a 45 nm undoped GaSb buffer, followed by 100 pairs of undoped InAs/GaSb SL sandwiched between two AlSb barriers (~20 nm thick). Finally, an undoped GaSb capping layer is grown with a thickness of 4 MLs. The SL periods studied are made of X MLs of InAs and Y MLs of GaSb with X = 10, 12, 14 and Y = 4, 7. For the sake of clarity, we use the notation X/Y SL. The In shutter opening time is set at 1 s, 1.5 s and 2 s for a SL with an InAs layer of 10, 12 and 14 MLs, respectively.

Following the growth, the structural quality of the samples was evaluated using a Bede D1 x-ray diffractometer. To access the optical properties of the SL structures, samples were then loaded in a cryostat equipped with CaF2 windows to carry out PL measurements. The samples were optically excited using a 735 nm laser diode modulated at a frequency of 20 kHz. To collect the signal, a Nicolet iS50R Fourier transform infrared spectrometer equipped with KBr beamsplitter and MCT-A detector was used.

### 2.2. XRD and PL measurements

The XRD spectra of the ω/2θ scan around the GaSb (004) reflection of a 10/4 SL (R = 2.5), 12/4 SL (R = 3), 14/4 SL (R = 3.5) and 14/7 SL (R = 2) are presented in Figure 1. The lattice mismatch $\Delta a/a$ and the full-width at half maximum (FWHM) of the first-order SL satellite peak (SL−1) extracted from the XRD spectra are summarized in Table 1. It can be seen that the 10/4 SL sample is under compressive strain on GaSb with a lattice mismatch of about $\Delta a/a \sim 0.149\%$. Considering that the InSb binary is on compressive strain on GaSb ($\Delta a/a \sim +7.8\%$), this indicates that the total thickness of InSb within the period is too thick to obtain a strain-compensated SL. This result is similar to what have been obtained for mid-wave 7/4 SL with InSb interface grown by MEE [27]. Further adjustment of the In and Sb shutter opening times could be made to reduce the thickness of the InSb interface layers, although it has been shown in [27] that exposing the InAs layer to an Sb incident flux to form an ‘InSb-like’ interface via Sb-for-As exchange suffices to obtain a strain-compensated SL in the case of thinner InAs layer. Nevertheless, when the InAs thickness increases the compressive strain caused by the InSb interface reduces and nearly strain-compensated SLs are
obtained. In addition to having the smallest lattice mismatch (nearly ~0%), the 14/4 SL also has the smallest FWHM (38 arcsec) among the X/4 SLs suggesting that this sample has the best structural quality. When increasing the GaSb thickness to 7 MLs, the FWHM is increased to 58 arcsec for the 14/7 SL. However, both 14/Y SLs are nearly strain-compensated on the substrate and present the lowest FWHMs compared to the other SLs, respectively. Note that for the sake of comparison, the measured energy band gap of the X/4 SLs is represented by the solid lines and the grey area.

3. Electronic band structure calculation

3.1. Method

The 8-band $k$-$\ell$ envelope-function method employed for this work is available in Nextnano software [29] and described in detail in [30]. The interface matrix $H_{IF}$ formulated by P C Klipstein to model the no-atom-in-common InAs/GaSb SL is implemented in the software framework and defined as [31]:

$$H_{IF} = \sum_i \delta (z - z_i) \begin{bmatrix} D_S & 0 & \pi_i \beta \\ 0 & D_K & \pi_i \alpha \\ \pi_i \beta & 0 & D_Z \end{bmatrix}$$

where $i$ is the index of the interface at the position $z_i$ and $\pi_i$ takes a value of −1 or 1 at the InAs-on-GaSb and GaSb-on-InAs interfaces. The interface parameters $\alpha$ and $\beta$ have been fixed to a value of 0.2 eV · Å [32] whereas the $D$ diagonal interface parameters ($D_x, D_y, D_z$), which are equal to zero in the case of a common atom superlattice, are determined in order to obtain a good agreement between the calculated and measured energy band gap of the X/4 and 14/Y SLs at 77 K (figure 2). A strain-compensated SL on GaSb is assumed in our simulation by including the InSb intentional layer at both interfaces and by considering homogenous strain for the strain calculation. As previously mentioned, in one period of SL the total thickness of the InSb layer required is 10% of the InAs thickness. The material parameters for InAs, GaSb and InSb binaries used for the $k$-$\ell$ band structure calculation are given in table 1 of [33].
3.2. Results and discussion

The calculated cut-off wavelength as a function of the measured cut-off wavelength at 77 K is represented in figure 3, along with the ideal prediction line. The $\pm k_BT$ deviation in the predicted $\lambda_c$ is also represented. Note that the $D$ diagonal interface parameters ($D_x$, $D_y$, $D_z$) of equation (1) used are equal to (0.8, 0.3, $-0.3$). We observe a good agreement between the simulation and experiment for all the different SLs with an error in the $\pm k_BT$ deviation range, apart from the 10/4 SL. This can be explained by the fact that the 10/4 SL is under compressive strain on GaSb with a large lattice mismatch as discussed in section 2 while in our simulation we assume a SL layer lattice matched on GaSb. In addition, a slight change in the growth rate during the MBE growth can lead to a slight change in composition and thickness of the SL period compared to the targeted layer thicknesses which we do not take into consideration in our simulation. In addition, the cut-off wavelengths calculated without taking into account the interface matrix $H_{IF}$ and considering neither the $H_{IF}$ nor the InSb layer at the interfaces are also plotted in figure 3 for comparison. We can see that if both the $H_{IF}$ and the InSb interfaces are not considered the model cannot predict the measured cut-off wavelength and underestimates it. This result demonstrates the importance of the interface consideration for band gap calculation of Ga-containing SL.

Following this, the electronic band structure of the $X/4$ SLs and $14/Y$ SLs has been calculated for one in-plane direction in the Brillouin zone $k_{//}$ and in the perpendicular direction $k_\perp$ (figure 4). We can easily see in figure 4 that for the $X/4$ SLs, the bottom of the conduction band is moving down with increasing the InAs thickness. It decreases by 49 meV when the InAs thickness increases from 10 to 14 MLs while the top of the first valence band is moving up by a value of only 15 meV. For thicker GaSb, both conduction and valence bands are moving up by 51 and 35 meV, respectively. These changes impact on the energy band gap value as previously observed experimentally. It seems that the $X/4$ SL band structures are quite similar in contrast to the $14/Y$ SLs that present differences. In particular, the lower valence bands of the 14/4 SL are further removed from the top valence band (corresponding to heavy hole) compared to the 14/7 SL. Using thinner GaSb, one could therefore further minimize/suppress Auger recombination in p-type SLs.
The electron and hole effective masses calculated as subscripts referring to electron and heavy hole, respectively. The electron and hole effective masses calculated as $m_e^*$ and $m_h^*$, with $e$ and $h$ subscripts referring to electron and heavy hole, respectively. The electron and hole effective masses calculated as $m_e^*$ and $m_h^*$ are reported in Table 2. The conduction band is similar for the $X/4$ SLs resulting in similar electron effective mass value, in contrast to $m_h^*$ which is strongly dependent on the InAs thickness. Indeed, the valence band width is reduced due to stronger localization of holes when increasing the InAs well thickness especially in the growth direction which results in larger effective mass in this direction. The localization of carriers is further increased, as suggested by the electron–hole wavefunction values, when increasing the GaSb layer thickness leading to larger effective mass for both electron and hole for the 14/7 SL. From figure 4, it is possible to extract the effective masses at the band edge (second derivative at the Brillouin zone center) in both directions ($m_{e,h,\parallel}^*$ and $m_{e,h,\perp}^*$) with $e$ and $h$ subscripts referring to electron and heavy hole, respectively. The electron and hole effective masses calculated as $m_{e,h}^* = m_{e,h,\parallel}^{2/3} m_{e,h,\perp}^{1/3}$ are reported in Table 2. The conduction band is similar for the $X/4$ SLs resulting in similar electron effective mass value, in contrast to $m_h^*$ which is strongly dependent on the InAs thickness. Indeed, the valence band width is reduced due to stronger localization of holes when increasing the InAs well thickness especially in the growth direction which results in larger effective mass in this direction. The localization of carriers is further increased, as suggested by the electron–hole wavefunction values, when increasing the GaSb layer thickness leading to larger effective mass for both electron and hole for the 14/7 SL. From Table 2, it appears that the effective masses depend mainly on the SL period composition and thickness and slightly on the lattice mismatch of the SLs, respectively. The difference of $\alpha$ values with the ones reported in section 2 is probably due to a slight change in the energy band gap in the growth rate leading to a slight change in the average composition and thickness of the SL period. Nevertheless, the FWHM of SLs is in the same range of about ~50 arcsec for both samples suggesting a good structural quality. PL measurements from 77 K to 160 K have also been performed and the energy band gap is plotted as a function of temperature in Figure 6. Its variation can be fitted using the well-known Varshni equation which depends on the parameters $\alpha$ and $\beta$ and the energy band gap at 0 K ($E_g(0$ K$)$). By fixing $\beta$ to 270 K [35], we found that $E_g(0$ K$)$ is equal to 0.111 and 0.124 eV and, the $\alpha$ parameter is 0.019 and 0.094 meV K$^{-1}$ for the 14/7 SL and 12/4 SL, respectively. The InAs/GaSb SL periods studied are composed of a 14/7 SL and a 12/4 SL.

Material characterizations have first been carried out to evaluate the material quality of the two device structures. From the XRD spectra (not shown here), it appears that both samples are under a slight compressive strain on GaSb with a lattice mismatch of +0.069 and +0.05% for the 14/7 SL and 12/4 SL, respectively. The change of $\Delta a/a$ values with the ones reported in section 2 is probably due to a slight change in the growth rate leading to a slight change in the average composition and thickness of the SL period. Nevertheless, the FWHM of SLs is in the same range of about ~50 arcsec for both samples suggesting a good structural quality. PL measurements from 77 K to 160 K have also been performed and the energy band gap is plotted as a function of temperature in Figure 6. Its variation can be fitted using the well-known Varshni’s equation which depends on the parameters $\alpha$ and $\beta$ and the energy band gap at 0 K ($E_g(0$ K$)$). By fixing $\beta$ to 270 K [35], we found that $E_g(0$ K$)$ is equal to 0.111 and 0.124 eV and, the $\alpha$ parameter is 0.019 and 0.094 meV K$^{-1}$ for the 14/7 SL and 12/4 SL, respectively. In the inset of Figure 6, the PL spectra of both samples at 77 K are represented. The energy band gap of the 12/4 SL (~0.122 eV) is close to the value previously measured while it is lower by 13 meV for the 14/7 SL (~0.110 eV). Again, this could originate from a slight
In figure 8, a good agreement between the simulated (solid line) and measured (symbols) dark-current at a temperature of 150 K for the (a) 14/7 SL and (b) 12/4 SL samples shows different energy band gap as illustrated in figure 6. Therefore, for a fair comparison, we corrected the experimental dark-current by the energy band gap, i.e. we divided the dark-current by \( \exp(-E_g/k_BT) \) which accounts for the diffusion component (table 3). It appears that the 12/4 SL still shows a lower diffusion current by a factor of 0.78 than the 14/7 SL even after correction.

To understand this difference, the dark-current characteristic of both samples has been simulated (figure 8) using the Atlas framework from TCAD Silvaco software. The models and method of simulation are reported elsewhere [36]. We used the measured energy band gap and residual doping concentration of the active region as input of the simulation. It is worth mentioning that from capacitance–voltage measurements at 77 K (not shown here), we extracted a residual doping concentration of around \( 1.4 \times 10^{15} \) cm\(^{-3} \) and \( 1.3 \times 10^{15} \) cm\(^{-3} \) for the 14/7 SL and 12/4 SL, respectively. Note that a serial resistance has also been considered in the simulation that accounts for the sheet and contact resistances, for both samples it has a value of around \( 1.5 \Omega \cdot \text{cm}^2 \). This only has an influence on the calculated dark-current in forward bias. The only fitting parameter of the simulation is the minority carrier lifetime \( \tau \). In figure 8, a good agreement between the simulated and experimental dark-current can be observed at 150 K for positive and reverse biases. The minority lifetime extracted from the simulation is equal to 7.5 and 9.4 ns for the 14/7 SL and 12/4 SL. A relatively longer minority carrier lifetime \( \sim 1.25 \) contributes in part to the lower diffusion current measured for the 12/4 SL device. In addition, these two SLs have different effective masses, so they have different effective density of states in the conduction \( N_c \) and valence \( N_v \) bands. In particular, the 12/4 SL has a lower \( N_c/N_v \) product by a factor of 0.63 than the 14/7 SL thanks to smaller electron and hole effective mass which also contributes to the reduction of the diffusion current. It is interesting to note that if we only account for these ratio values of minority carrier lifetime and \( N_c/N_v \) product, the dark-current ratio should theoretically be even lower than the measured one. This difference can be explained by other contributions not taken into account in this analysis such as surface leakage current or tunnelling current for example.

As intermediate conclusion, due to a weaker localization of carriers, the 12/4 SL has smaller electron and hole effective masses compared to the 14/7 SL resulting in stronger tunnelling contributions in the dark-current at low temperature and a lower diffusion at high temperature. However, the former can be counteracted by using an engineered heterostructure such as pBp or nBp barrier structure which are diffusion-limited whatever the temperature. In addition, the electron–hole wavefunction overlap is enhanced in a 12/4 SL (58%) which could lead to an enhancement of the absorption coefficient, and therefore of the quantum efficiency. The present study demonstrates that the SL design can be used to improve the device performance of diffusion-limited devices. Although, we only showed a slight improvement of the diffusion current by a factor of 0.78 at 150 K with a 12/4 SL, we proposed in [21] to use a 12/2 SL (\( -0.118 \text{eV} \)) as the absorber layer of

### Table 3. Measured and corrected dark-current density at 150 K for the 14/7 SL and 12/4 SL samples.

| Temperature (K) | 14/7 SL \( (A \text{ cm}^{-2}) \) | 12/4 SL \( (A \text{ cm}^{-2}) \) | Dark-current ratio |
|----------------|-----------------|-----------------|----------------|
| Measured at \(-50 \text{ mV}\) | 2.52 | 1.07 | 0.42 |
| Corrected by \( \exp(-E_g/k_BT) \) | 12.5 \times 10^3 | 9.8 \times 10^3 | 0.78 |
a nBp structure to further improve the dark-current. In this case however, the growth and, in particular, the control of the interface quality (intermixing, roughness, etc) may be more challenging.

5. Conclusion

In conclusion, in this paper we investigated the flexibility of Ga-containing SLs. Several SL designs with a different ratio of the layer thicknesses \( R \) ranging from 2 to 3.5 that exhibit an energy band gap varying from 0.105 to 0.169 eV at 77 K have been studied. First, we showed that by growing an intentional InSb interface layer using the MEE technique, nearly strain-compensated SL layers on a GaSb substrate can be obtained. The shutter opening times at the interfaces need to be precisely adjusted depending on the InAs layer thickness. The interface quality may impact on the PL broadening especially for a higher ratio \( R \) where the fraction of the interface layers is comparable to the GaSb thickness. In addition, the maximum PL intensity is strongly correlated to the electron–hole wavefunction overlap value. Second, by using an 8-band \( k \cdot p \) envelope function method that can predict the measured band gap within an error of \( \pm 0.040 \) eV, we calculated and compared the electronic band structure of the grown SLs. The electron effective mass has been found to be in the range of \( (0.015–0.040) m_0 \). We also demonstrated that it mainly depends on the period composition and thickness and less on the energy band gap. In particular, for a thick period with a thick GaSb layer, as is the case for a 14/7 SL, the electron and hole effective masses have been found to be the largest due to a stronger carrier localization. Finally, two different p-i-n device structures with the active region made of a 14/7 SL and 12/4 SL have been grown and photodiodes fabricated. By comparing their electrical performance, we showed that at low temperature the minority carrier lifetime observed in a long-wavelength infrared III–V type-II superlattice comprised of InAs/InAsSb Appl. Phys. Lett. 99 251110

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