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# AlSb and InAs-GaSb layer thickness effect on HH-LH splitting and band gap energies in InAs/AlSb/GaSb type-II superlattices

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*This study is based on the investigation of AlSb layer thickness effect on heavy-hole light-hole (HH-LH) splitting and band gap energies in a recently developed N-structure based on InAs/AlSb/GaSb type II superlattice (T2SL) p-i-n photodetector. First principle calculations were carried out tailoring the band gap and HH-LH splitting energies for two possible interface transition alloys of InSb and AlAs between InAs and AlSb interfaces in the superlattice. Results show that AlSb and InAs-GaSb layer thicknesses enable to control HH-LH splitting energies to desired values for Auger recombination process where AlSb/GaSb total layer thickness is equal to InAs layers for the structures with InSb and AlAs interfaces.*

**Keywords:** InAs/AlSb/GaSb type-II SL structure, HH-LH splitting, N-structure, DFT, layer thickness effect.

## 1. Introduction

Latterly, type-II superlattice (T2SL) infrared photodetectors, which become an alternative technology over mercury cadmium telluride (MCT) and QWIP technologies, have received great attention for civilian, military and medical applications. Band gap and HH-LH splitting energies controlled by varying InAs layer thickness [1], with suppressed Auger recombination rates [2] and reduced interband tunnelling due to higher effective masses of electrons and holes [3] make T2SL a very promising technology for most of the infrared region (3 – 30 μm). In the quest of achieving state of art infrared photodetectors, further improvements such as reducing the dark current level due to generation recombination (G-R) mechanisms and surface conductive channels, are needed. Furthermore, most of the photodetectors in the market requires a high operating temperature that is convenient for many applications. Ability to operate higher operating temperatures (HOT) will reduce cost, volume, weight and power requirements.

Embedding a barrier inside the superlattice period is an efficient way to solve the problems listed above. Many such barriers with intuitive material designs have been proposed such as nBn design [4], PbIbN design [5], CBIRD structure [6] and M structure design [7]. The aim of these designs is to block one type of carrier while allowing other type of carriers. These designs become very successful at increasing BLIP temperature above 100K and drastically reduce dark current. Nguyen *et al.* [7] took the advantage of the close lattice constants of InAs/GaSb SL p-i-n photodiodes and inserted an asymmetric AlSb barrier layer inside the GaSb layer and called it "M" structure. Recently, we have designed a new detector structure called "N" structure where AlSb electron barrier is inserted between InAs and GaSb layers. We have investigated HH-LH splitting and band gap energies by varying InAs and GaSb layer thicknesses [8]. In N structure thermal electrons are blocked to reduce dark current. In fact dark current performance of the N structure at higher temperatures is better than a standard type-II SL pin diode [8,9]. This design also allows to increase detectivity by increasing electron-hole wave functions overlap integral which results from the AlSb barrier pushing the electron and hole wave functions towards the GaSb/InAs layer edges. In other words, hole wave functions are pushed towards to GaSb/InAs interfaces to achieve strong type-II transitions. In a comparison to standard type-II SL, N structure gives 25% higher carriers overlap [9]. Experimental results for N structure were very promising for high temperature focal plane applications (FPA) [8,9].

In this report we investigate AlSb and InAs-GaSb layer thicknesses' effects on HH-LH splitting and band gap energies in InAs/AlSb/GaSb type-II SL structures. The theoretical results are carried out by using first principles' calculations. Two possible interface transition alloys of AlAs and InSb are taken in account between InAs/AlSb interfaces. Promisingly, results show that HH-LH splitting and band gap energies are increased by increasing AlSb layer thickness in InAs/AlSb/GaSb T2SL structure to achieve desired cutoff wavelength.

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## 2. Calculation details

Density functional theory (DFT) [10,11] calculations were performed using the plane wave basis pseudopotential method which was implemented in the ABINIT code [12]. The simulations were carried out using the Fritz-Haber Institute (FHI) type pseudopotentials in which the exchange-correlation energy is evaluated in the local density approximation (LDA), using Perdew-Wang parameterization [13] of Ceperley-Alder electron-gas data [14]. For all structures, the plane-wave energy cutoff of 30 Ha were found to be enough for convergence of all the reported quantities.

While constructing InAs/AlSb/GaSb type-II SL structure, two different transition interfaces of AlAs (InAsAl transition) and InSb (InSbAl transition) can be formed between InAs and AlSb layers, see Figs 1(a) and 1(b). In order to understand the effects of these transition interfaces, AlSb blocking barrier and constituent layer thicknesses we have performed calculations of band gap and HH-LH splitting energies for several configurations of InAs/AlSb/GaSb based T2SL structures. On the other hand, band gap and HH-LH splitting energies are particularly important in the suppression of non-radiative electron-hole recombination in practical detector applications.

We have performed the systematical theoretical calculations on InAs/AlSb/GaSb type-II SL material system in two parts. In the first part, the effect of two possible transition interfaces of InSb and AlAs on band gap energies (Egap) and HH-LH splitting energies is examined by band structure calculations of the $(InAs)_x/(AlSb)_n/(GaSb)_{(x-n)}$ (n = 1 to 5 and $x$ = 3 to 6) superlattices, where the AlSb/GaSb total layer thickness is equal to InAs layers for each transition interface type. Results of the first part of calculations show that $(InAs)_6/(AlSb)_4/(GaSb)_2$ structure gives the highest HH-LH splitting energy for AlAs interface. From this point of view, in the second part of our calculations, we quest for the HH-LH splitting energies from band structure calculations of $(InAs)_x/(AlSb)_4/(GaSb)_x$ ($x = 2-6$) superlattice structures. At this step, the AlSb layer thickness is fixed to 4 ML and we changed the InAs and GaSb layers from $x = 2-6$ to see the effect of InAs and GaSb layer thicknesses.

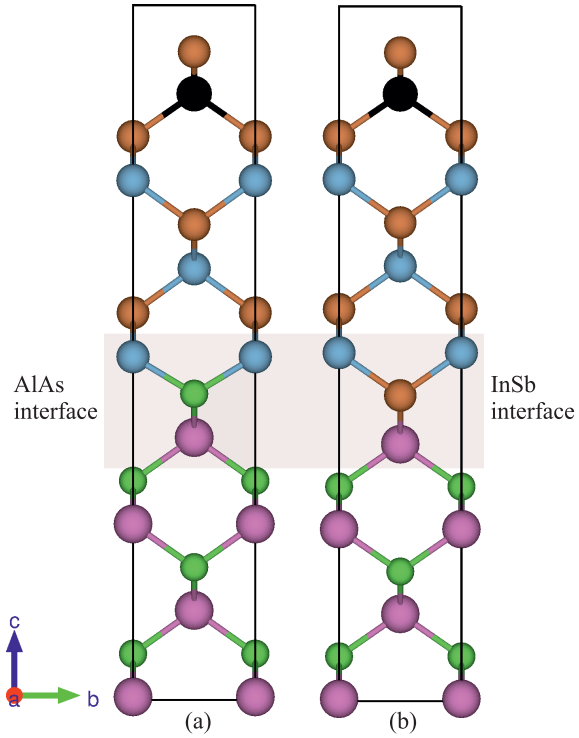


Fig. 1. $(InAs)_4/(AlSb)_3/(GaSb)_1$ structures with (a) AlAs and (b) InSb interfaces. Purple: In, green: As, blue: Al, brown: Sb and black: Ga atoms.

## 3. Results and discussion

As illustrations, calculated band structures of the $(InAs)_4/(AlSb)_3/(GaSb)_1$ superlattices for both AlSb and InSb interface situations are depicted in Figs. 2(a) and 2(b), respectively. Both diagrams have got direct band transitions. While the band gap energy of the structure with AlAs interface is 0.23eV [Fig. 2(a)], it changes to 0.26eV for the structure with InSb interface [Fig. 2(b)]. But HH-LH splitting

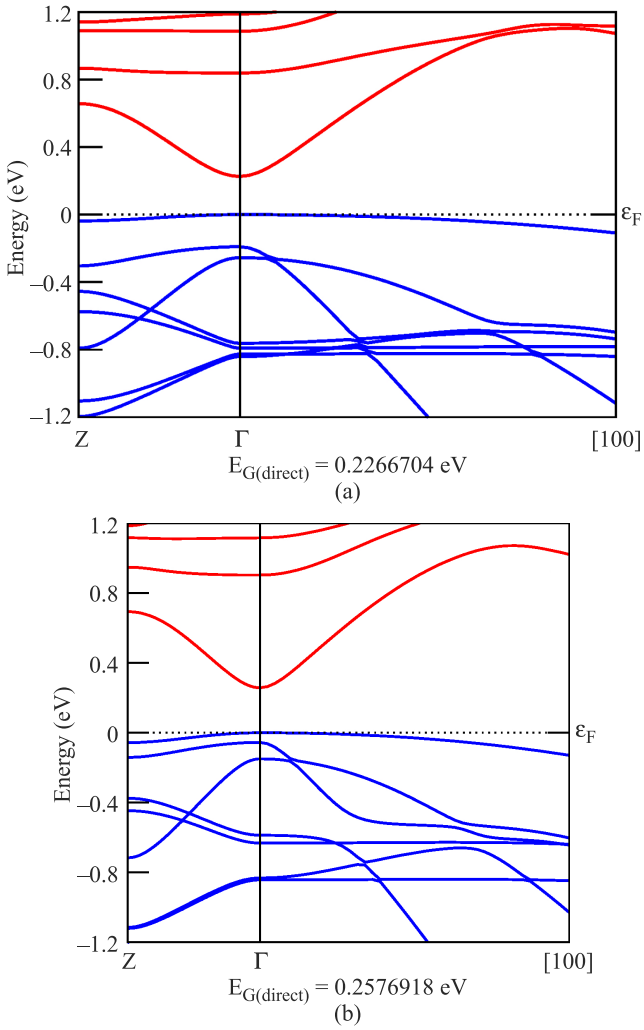


Fig. 2. Band structure of $(InAs)_4/(AlSb)_3/(GaSb)_1$ structures with (a) AlAs and (b) InSb interfaces.

energy for the structure with AlAs interface is higher than that of the structure with InSb interface. For $(InAs)_x/(AlSb)_n/(GaSb)_{(x-n)}$ (n = 1 to 5 and x = 3 to 6) superlattices structure compositions, all $E_{gap}$ and HH-LH splitting energies are extracted from the band calculations. Figure 3 and Figure 4 show the effect of the transition interface types on the band gap and the HH-LH splitting values of superlattice structures under different number of AlSb layers, n respectively. Figures separated from a to d in order to clear out the layer effect. Figure 3 shows the $E_{gap}$ values with increasing number of the AlSb MLs n. Here InAs layers vary 3 MLs [Fig. 3(a)] to 6 MLs [Fig. 3(d)], respectively. $E_{gap}$ values ascend with increasing AlSb layers. But it indicates that there is no prominent difference between the results of two different interfaces. The results of AlSb layer thickness effect on HH-LH splitting energy values of under possible two different interface formations (AlAs and InSb) are also shown in Fig. 4. Results show that HH-LH splitting energies in the structure with AlAs interface are higher than the structure with InSb interface ones for all superlattice types. Each structure has its own maximum value for different AlSb layer thicknesses [Figs. 4 (a) to 4(d)]. This behaviour enables us to construct superlattice structures which have desired HH-LH splitting energies.

In the second part of our calculations we fixed the AlSb layer thickness to 4 ML, then examined the InAs and GaSb layer thickness effect on the band gap and HH-LH splitting energies for $(InAs)_x/(AlSb)_4/(GaSb)_x$ ($x = 2 - 6$) superlattice structures, as illustrated in Fig. 5. Figure 5 (a) denotes the change of the E gap with increasing layer number of InAs and GaSb. One can see that band gap values show exponential decrease according to increasing layer numbers of InAs--GaSb, but when compared to the results of the first step calculations small "*x*" values give much higher band gap energies for fixed AlSb layer thickness. And also there is no significant difference between interface types for band gaps,

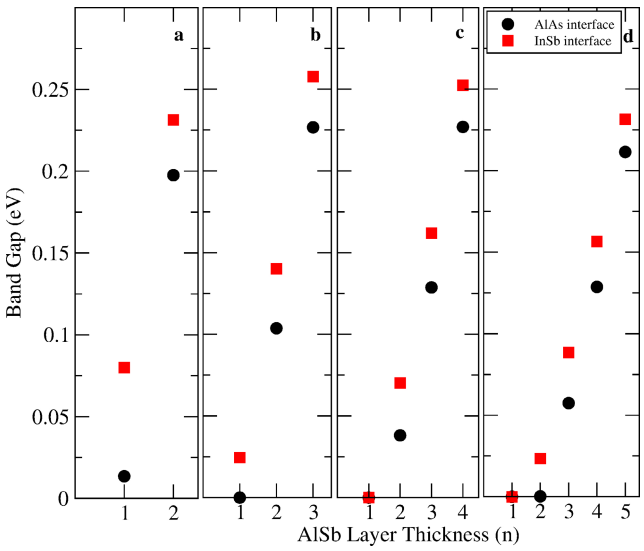


Fig. 3. Band gap energies related with AlSb layer thickness. Circles denote AlAs, squares denote InSb interface.

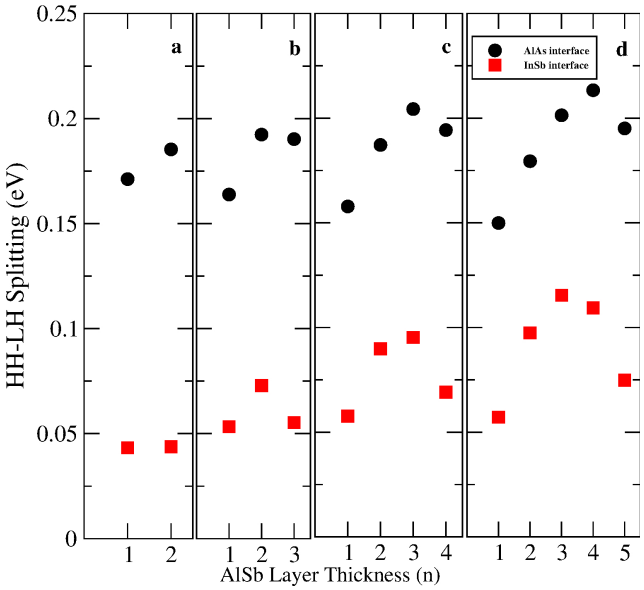


Fig. 4. HH-LH splitting energies related with AlSb layer thickness. Circles denote AlAs, squares denote InSb interface.

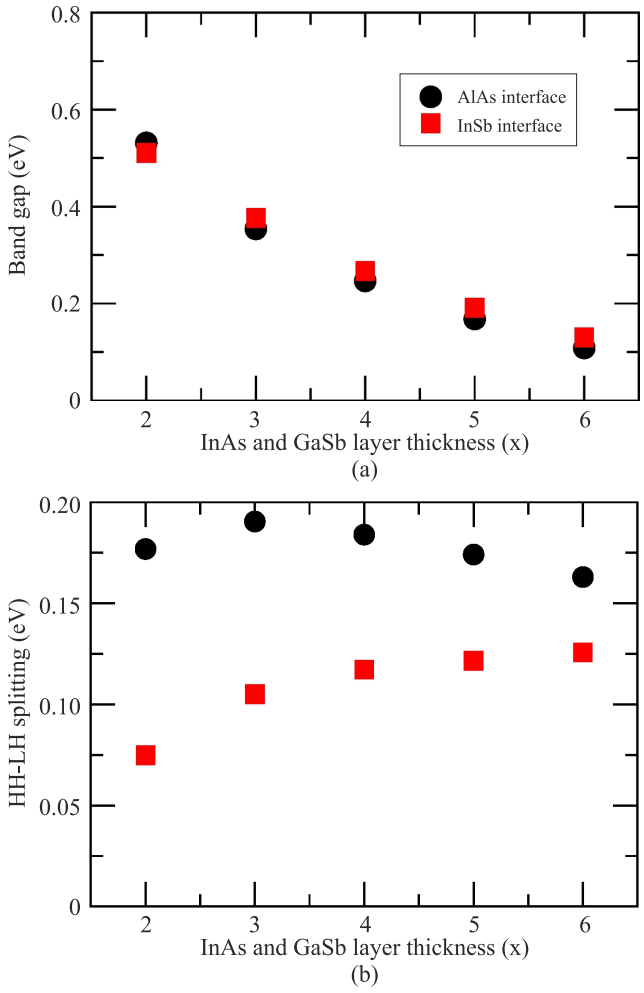


Fig. 5. (a) Band gap and (b) HH-LH splitting energies related with InAs-GaSb layer thickness. Circles denote AlAs, squares denote InSb interface.

 

when the well-known discrepancy of the LDA type pseudopotentials on band gap of semiconductors and insulators is considered. HH-LH splitting for the second part calculations are shown in Fig. 5(b) for both interface types. At the first part of the calculations, energy difference for HH-LH splitting is approximately 0.1 eV for each step of the calculations, but in the second part, energy difference of HH-LH splittings gets closer with increasing thickness of InAs-GaSb layers. On the other hand, the change of the band gap energy with AlSb and InAs-GaSb layer thickness obviously represents the possibility of band gap engineering.

## 4. Conclusions

In summary, our systematical investigations predict that changing the AlSb and InAs-GaSb layer thickness enables us to adjust HH-LH splitting and band gap energies which are important parameters for designing new detector structure to be operated at high temperature applications by suppression of non-radiative recombination such as Auger recombination process. This leads to increasing the optical performance of the T2SL photodetector.

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