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Electronic structure of InAs/GaSb superlattice for the modelling of MWIR pin photodiode

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HIGHLIGHTS

- We present a 18-bands **k.p** method to simulate energies and wavefunctions.
- We study three different type of InAs/GaSb superlattices structures.
- Calculated bandgaps are in good agreement with results for symmetrical superlattice.
- We explain from model the difference of behaviour between the structures.
- We calculate intrinsic carrier concentration and effective mass.

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ABSTRACT

An 18-band **k.p** formalism has been developed to determine the band structure and wavefunctions of InAs/GaSb type II superlattices (T2SL). Bandgap results are in good agreement with measurements for symetrical superlattices. Thus, we are able to calculate intrinsic properties of InAs/GaSb SL as the effective mass, the density of state and the free carrier concentration. Then we compare the modelled and measured electro-optical properties of three different SL structures with a different InAs to GaSb thickness ratio *R* per SL period, but having the same cut-off wavelength of 5 μm at 77 K.

1. Introduction

Type-2 superlattice (T2SL) is now considered as an emerging technology able to satisfy the third generation infrared imagers' requirements [1]. Some very impressive results have been obtained the last past decade by several laboratories but, and although the T2SL is a recent technology compared to the well-established InSb, QWIP and HgCdTe technologies, the devices quite fail reaching the theoretical predicted performances. Consequently, it is necessary to develop an accurate device modelling to analyze first the physical limitations of the T2SL material and devices and then to propose improvements in order to overcome the current performances.

The historical method for heterostructure modelling is the **k.p** method in the envelope function approximation [2] and this approach was employed in the well-known paper of Smith and Mailhot where T2SL structure was first proposed for infrared photodetector [3]. However, as we will discuss further in this paper, the use of **k.p** method has been questioned in the case of T2SL. Therefore other methods have been proposed. The atomistic empirical pseudo-potential (AEPM) method computes energies and wavefunctions by resolving the Bloch equation for each atom. It is an atomistic method quite complicates to implement with a high number of adjustable parameters, but very precise in its description of the structure especially for the interface [4]. Dente and Milton [5] proposed an easier version of AEPM adapted for superlattices, the superlattice empirical pseudopotential (SEPM). This method has less parameters and mostly less adjustable parameter and is easier to implement for equivalent results. Another method is the empirical tight-binding method, where a

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development of the wavefunctions is made on the orbitals of the atoms of the SL [6]. Finally, modified **k.p** method considering asymmetric interface profile has also been proposed to model the T2SL [7–9].

In this paper we present a **k.p** method suitable for the T2SL structures. Our approach is applied to particular quantum structures operating in the midwave infrared (MWIR) domain. With T2SL it is possible to obtain the same bandgap with different periods by changing the thickness ratio between InAs and GaSb in each SL period. Previously, we have fabricated and experimentally characterized three different kinds of structure having the same cut-off wavelength of 5 μm at 77 K [10]. The thickness ratio R between InAs-layer and GaSb-layer in the period is equal to $R = 0.5$ (GaSb-rich), $R = 1$ (symmetric) or $R = 2$ (InAs-rich), and these three isobandgap structures displayed very distinct electro-optical properties, as shown in Fig. 1. These structures are the support of our theoretical investigations and this paper offers a modelling approach to understand the differences between this three T2SL structures.

2. Band structure and wavefunctions modelling: the k.p-method

The **k.p** formalism has been widely used for the description of semiconductor heterostructures [2]. This easy to implement method requires a small number of input parameters that can be obtained from experimental results. Indeed one can obtain the band structure over the whole Brillouin zone by extrapolation from the central energy zone gaps and optical matrix elements. Moreover, results given by this method can be linked to physical mechanisms and thus help for interpretation. In the case of InAs/GaSb T2SL structure, the main particularity of this quantum system is the staggered type-II band alignment of the InAs/GaSb heterostructure where the bottom of the conduction band of InAs is below the top of the valence band of GaSb. So, there is an interaction between near-gap bands of the GaSb layer and higher-lying bands in the InAs layer, as depicted in Fig. 2. As a consequence, traditional **k.p** method tends to overestimate the bandgap energy for InAs/GaSb T2SL [11]. Indeed, traditional **k.p** method takes into account four bands (eight, if one takes the spin into account) in the modelling: the first conduction band and the first three valence bands (heavy hole, light hole and spin orbit). Consequently, one neglects the interaction between near-gap bands of the GaSb layer and higher-lying bands of the InAs layer.

In this paper we use an 18-band **k.p** method to determine the material properties of InAs/GaSb SL. This model takes into account the (counting spin) six Γ_7–Γ_8 valence bands, the two Γ_6 conduction bands, the six Γ_7–Γ_8 higher lying conduction bands, and four Γ_3 conduction bands [12] as shown in Fig. 2. Thus, we can include the near-gap interactions and have a good modelling of the band structure and wavefunctions of SL structures.

The modelled structure is a periodic SL. Each period consists in one InAs layer and one GaSb layer with an abrupt interface, without any applied electric field.

It is assumed that there is no stress between InAs and GaSb, the lateral lattice parameters are fixed by the substrate. We determine the effect of the strain induced by the GaSb substrate by adding the Pikus–Bir matrix elements to the **k.p** matrix [13].

Finally, the diagonalization of the **k.p** matrix gives the band structure and the wavefunctions of the SL for a given wavevector **k**. Thus, we are able to have the band structure, as seen in Fig. 3, and the wavefunctions over the whole Brillouin zone.

From the band structure of Fig. 3, we are able to obtain the bandgap energy, by taking at $k = 0$ the difference of energy between the highest hole band and the lowest electron band. Fig. 4 presents the bandgap energy as a function of the period thickness in the case of symmetrical structure ($R = 1$) and the black points are measured data. There is a very good agreement between simulation and measurements.

3. Modelling of the intrinsic parameters

3.1. The density of states

The density of states is directly derived from the band structure calculated previously. For a given energy we explore the Brillouin zone in k-space to find equal energies and so sum all the possible states in the band structure. We then obtain the DOS as a function of the energy.

$$\mathrm{DOS}(E) = \sum_k \Delta(E - E_k) \tag{1}$$

DOS of an InAs-rich SL, a GaSb-rich SL and a symmetrical SL are presented in Fig. 5 for the valence bands and in Fig. 6 for the conduction bands.

One can see that there are different behaviours for the different types of T2SL structures. The InAs-rich SL has a DOS shape similar

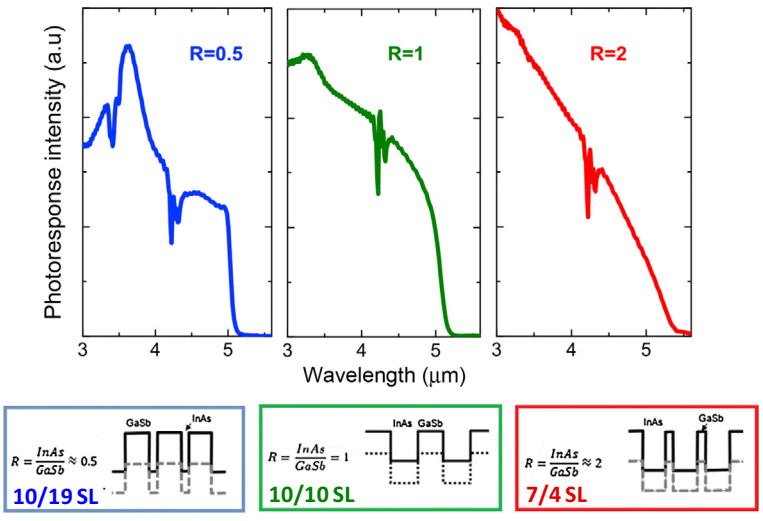

Fig. 1. Photoresponse spectra collected at $T = 77$ K of the three different T2SL structures [10] under theoretical investigation. The first has a 'GaSb-rich' composition, made of 10 monolayers (MLs) InAs/19 MLs GaSb per period, the second is 'symmetric', with the same GaSb and InAs thicknesses (10 MLs), and the last is 'InAs-rich' (7 MLs InAs/4 MLs GaSb).