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Band gap tunability of Type II Antimonide-based superlattices

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Abstract

Current state-of-the art infrared photon detectors based on bulk semiconductors such as InSb or HgCdTe are now relatively mature and have almost attained the theoretical limit of performance. It means, however, that the technology can not be expected to demonstrate revolutionary improvements, in terms of device performances. In contrasts, low dimensional quantum systems such as superlattices, quantum wells, quantum dots, are still the development stage, yet have shown comparable performance to the bulk detector family. Especially for the Type II Antimony-based superlattices, recent years have seen significant improvements in material quality, structural design as well as fabrication techniques which lift the performance of Type II superlattice photodetectors to a new level.

In this talk, we will discuss the advantages of Type II-superlattices, from the physical nature of the material to the practical realisms. We will demonstrate the flexibility in controlling the energy gap and their overall band alignment for the suppression of Auger recombination, as well as to create sophisticated hetero-designs.

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1. Introduction

The 6.1 Angstrom family (Figure 1a) is an important group in the semiconductor technology. It consists of three members that are closely lattice matched to each other: InAs (a = 6.0584 Å), GaSb (a = 6.0959 Å) and AlSb (a = 6.1355 Å). Since GaSb substrates became available, and the growth of III-antimonide semiconductors has become easier to achieve, the 6.1 Å and its compounds have provided enormous flexibility in designing of heterostructures for optical and electronic applications. The advantage of this family is the small lattice mismatch of the constituent materials to GaSb substrates and similar growth windows for the three materials, which enables the growth of high quality materials with a low density of defects and dislocations. The energy gap of the family and related compounds ranging from 0.41 eV (for InAs) to 1.70 eV (for AlSb) is of particular interest for the design of optoelectronic devices in the Short Wavelength Infrared (SWIR) and Mid-Wavelength Infrared (MWIR) regimes. Moreover, a heterojunction formed between InAs and the other two members benefits of the unique features of the Type II band alignments (Figure 1b). On the one hand, the InAs/AlSb interface forms a Type II staggered line up

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where the conduction band of InAs is slightly above the valence band of AlSb. The high energy gap of AlSb leads to an exceptionally large conduction band offset of about 1.45 eV, enabling the realization of very deep quantum wells and very large tunneling barriers. This InAs/AlSb heterostructure has been widely utilized in high frequency field effect transistors (FETs) and resonant interband tunneling diodes (RITDs). On the other hand, the heterojunction between InAs and GaSb leads to the exotic alignment known as the *broken gap* alignment, where the conduction band of InAs is about 0.15 eV lower than the valence band of GaSb. This type of *misaligned* structure is the reason why Type II superlattices have the flexible band gap engineering capability.

2. Physics of Type II superlattice:

The idea of Type II InAs/GaSb superlattice was first proposed by Sai-Halasz and Esaki in the 1970’s. The superlattice is formed by alternating the InAs and GaSb layers over several periods. This creates a one dimensional periodic structure, like the periodic atomic chain in naturally occurring crystals (Figure 2). The Type II broken gap alignment leads to the separation of electrons and holes into the InAs and GaSb layers, respectively. The charge transfer gives rise to a high local electric field and strong interlayer tunneling of carriers without requiring an external bias or external doping. Large period superlattices behave like semimetals but if the superlattice period is shortened, the quantization effects are enhanced causing a transition from a semi-metal to a narrow gap semiconductor.

Rigorous calculations are required to precisely describe the electronic band structure of Type II superlattices. Theoretical methods that have been developed for Type II superlattices include: the k.p based theory, the Empirical Tight Binding Model (ETBM), and the pseudo potential model. Compared to other methods, the ETBM exhibits great advantages with the capability to calculate the band structure in the whole Brillouin zone and to precisely describe the atomic layering to the superlattice, taking into account the growth imperfection. The method is also fast and does not require massive and complex numerical calculation. The calculation results using different techniques can be found in the literature, in this paper, we just describe qualitatively the physics of Type II superlattice and illustrate how one can do the band-structure engineering with this material system.
In Type II superlattice, electrons and holes are spatially confined in the InAs and GaSb layers respectively. The electronic band structure of the superlattice is determined by the energy level of electrons and holes in the quantum wells, and by the interaction between the carriers in adjacent wells. Due to the large effective mass, the energy level of hole is insensitive to the GaSb well width. Moreover, its large effective mass also prevents the hole to tunnel through the InAs barrier. The valence band of Type II superlattice is almost constant; the energy gap is controlled by the conduction band level, via the change in InAs, GaSb layer thicknesses or interface composition.

Effect of the InAs layer

The InAs layer is a quantum well confining the electrons in one period of the superlattice. As an empirical rule, the energy level of a particle is closely inversely proportional to its effective mass and the square of the well width. The conduction band level of Type II superlattice will lower when the InAs layer gets thicker (Figure 2 b and c). For example, a superlattice design aimed for a MWIR cut-off wavelength tends to have thin InAs layer (typically 4-10 Monolayer thick), while a LWIR and VLWIR structure normally has thicker InAs (typically 10-20 Monolayer thick). When the InAs layer is thicker, the energy level will be even lower than the valence band of the GaSb layer. In this case, electrons can directly tunnel from one well to another via the valence band of the GaSb barrier, the superlattice thus becomes a semi-metal.

Effect of the GaSb layer

The GaSb layer acts as a well for holes, but also as the barrier isolating electrons in adjacent InAs wells. Since the effective mass of holes in the valence band is much heavier than that of electrons (about 1 order of magnitude larger than the electron effective mass), the dependence of the energy on the well width becomes much weaker. The energy level of holes with respect to the bottom of the well is normally very small. With a GaSb layer thicker than 1.5 nm (~5 Monolayers), the hole’s energy level is practically unchanged, which means the valence band of superlattices stay constant near the valence band of the GaSb.

However, the GaSb thickness strongly affects the energy gap of the superlattice via the conduction band. Similar to the formation of bulk band structures from discrete atomic levels, the conduction band of the superlattice is the broadening of individual energy levels of electrons in InAs wells due to the “interaction” between wells. In type II superlattice, the “interaction” is dictated by how far the InAs wells are separated from each other, and how high the barrier is which is blocking the electrons. Figure 2 a and b describes qualitatively the broadening of the conduction band as a function of GaSb thickness.

When the GaSb layer is too thick, the “superlattice” is actually a system of non-interacting multi quantum wells. The electron energy level is solely determined by the layer thickness of the InAs wells, and electrons are strictly confined within the wells. When the GaSb thickness is reduced, the electron wavefunctions start overlapping, the electrons start seeing each other, and the single degenerated energy level is split into minibands. The broadening of
The minibands pushes the lowest conduction level downward, closer to the constant valence level. Thus the thinner the GaSb barrier, the more the minibands broaden, and the smaller the energy gap becomes.

Theoretical calculations and experimental measurements have shown that by only changing the layer thicknesses, the energy gap of Type II superlattice can be changed from 40 to 400 mV. Compared with traditional bulk material, Type II superlattice has exhibited great superiority in term of bandgap tunability; however, its immobile valence band shows some limitations in heterostructure designs where a discontinuity in the valence band is desired. In order to overcome these limitations, we have proposed a new variant of Type II superlattice, called M-structure superlattice, which will be shown to have flexible tunability of the valence band.

3. M-structure superlattice: a new type of superlattice with flexible tunability of the valence band

The M-structure superlattice, proposed by 5, is constructed by inserting a thin AlSb barrier in the middle of the GaSb layer of a normal Type-II binary InAs/GaSb superlattice. Figure 3 shows the schematic diagram of the energy band alignment of its constituents. The colored regions represent the prohibited band gap of the structure. This AlSb-containing superlattice is named the M-structure. This stands for the shape of the letter M- of the band alignment of the AlSb/GaSb/InAs/GaSb/AlSb layers. The advantages of M-structure have been described in previous publications 5-8, in this paper, we will focus only on the capability to adjust the valence band level of this new variant of Type II superlattice.

Figure 3: Schematic diagram of M-structure superlattice. Colored regions represent the forbidden bandgap of the materials. The design is named M-structure for the letter-M-shape of the band alignment.

If a thin AlSb layer is inserted in the middle of the GaSb layer, the GaSb quantum well will become a double quantum well with an AlSb barrier. The behavior of holes would be very different because the energy levels couple in pairs. Figure 4 shows the change of hole’s energy levels when we change the thickness of the AlSb barriers, keeping the same InAs and GaSb layer thicknesses. In each small figure, spatial hole density function is sketched for the first four valence bands with a vertical offset equal to the valence band energy at zero wave vector (k=0). The top band corresponds to the effective valence band of the superlattice. As the AlSb layer gets thicker, the first valence band moves downward while the second valence band moves upward due to a weaker interaction between the two wells. At a certain thickness of AlSb, these two bands coincide: \( E_{V1} = E_{V2} \) (at wave vector \( k=0 \)). The double degeneracy of the valence band increases the probability of transition from the valence band to the conduction band at the energy gap level. We also observe the same trend with the third and fourth bands; and even higher order states if the width of GaSb layer is large enough. This coupling of every two adjacent states is actually a corollary of the interaction between holes in the two dependent wells. The two first states in two wells hybridize with each other and create the pair of bonding and anti-bonding states, which become the first and the second levels of the system. Thus, the thicker the barrier is, the smaller the interaction between the two wells. The bonding and anti-bonding levels move closer to each other.
Figure 4- Effect of the AlSb layer thickness on the energy level of holes. As the barrier thickness is increased, the first energy level increases and the energy difference between the first two levels decreases.

Figure 5- Band alignment of a M-structure/Type II Superlattice hetero-interface where the energy gap difference drops mainly in the valence band’s discontinuity.

This simple behavior of the energy levels suggest a technique to engineer the valence band whose results are easy to understand and predict. Figure illustrates a heterojunction between an M-structure superlattice and a traditional superlattice where the energy gap difference drops totally in the valence band discontinuity. The conduction band of the two structures almost perfectly aligns. This type of band alignment has been successfully implanted in a p-π-M-n photodiode architectures and shown one order of magnitude improvement of the electrical performance \(^{6,9}\).
4. Conclusion

Type II Antimonide based superlattice has been shown to have excellent tunability of the conduction band, via the control of constituent layer thicknesses. M-structure superlattice, the new variant of Type II superlattice, exhibited an additional degree of freedom in adjusting the valence band edge of the material, allowing for more flexible hetero-junction designs. These unique properties of Type II superlattice have been widely applied in the infrared detection field, resulting in novel device architectures with very high performance single element detectors and focal plane arrays.