

Interface influence on structural properties of InAs/GaSb type-II superlattices

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Theoretical studies of interface impact on structural properties of InAs/GaSb type-II superlattices were carried out. Multilayer structures used for mid-infrared detection were considered. The superlattices examined consisted of 190 pairs of 9 monolayers (MLs) of InAs and 10 MLs of GaSb. Both types of interfaces, *i.e.*, “GaAs-like” as well as “InSb-like”, were analyzed. The simulations were performed using dynamical theory of diffraction for different thicknesses of interface layers. The lattice mismatch was extracted from X-ray diffraction profiles. The analysis performed shows that the strain-balanced InAs/GaSb superlattice can be optimized by using thin InSb-like or GaAs-like interface layers simultaneously.

Keywords: interface, II type superlattice, InAs/GaSb.

1. Introduction

There is a significant interest in photodetectors operating in mid- and far-infrared range. Most of the fabricated devices utilize HgCdTe and InSb alloys. Detectors based on these materials have good performance, large quantum efficiency and long carrier lifetime. However, these devices have some drawbacks, such as strong dependence of the energy gap on the alloy composition, composition nonuniformity over a large area and large tunnelling current. An alternative to the HgCdTe and InSb alloys is InAs/GaSb material system due to its unique type-II broken gap alignment. This alignment gives a rise to unusual electron properties, such as hybridization of the InAs conduction and GaSb valence band states due to coupling across the interface and spatial separation of electrons and holes. For superlattices (SLs) with a band gap energy in the mid- and far-infrared, the individual layer thicknesses are typically in a range between 5 and 10 monolayers (MLs).

On the other hand, the effective masses in an InAs/GaSb superlattice (SL) are not directly dependent on the band gap energy, as it is in the case of a bulk semiconductor. Compared to the electron effective mass of HgCdTe, the electron effective mass in InAs/GaSb SL is much larger, leading to a reduction in tunneling contributions to

the leakage currents of an infrared photodiode. Also related to the larger effective mass in the SL is a higher matrix element of SL which compensates the smaller optical matrix element of the SL. Additional advantages of SL applications are expected due to smaller Auger recombination rate compared to HgCdTe.

In InAs/GaSb SLs at the transition from InAs to GaSb layer both the group III and the group V elements change and therefore InSb-like as well as GaAs-like interfaces (IFs) can be created. The InSb-like interface introduces compressive strain into the SL, whereas GaAs-like IF induces tensile strain. Therefore, a strain of SL structure can be modified and compensated by using proper sequence of interfaces in device. Due to different physical properties of InSb and GaAs, electronic and optical properties of SLs are strongly affected by the interface bondings [1, 2]. In this paper the effects of thickness for different types of IFs on lattice mismatch in InAs/GaSb SLs are studied.

2. Simulations and results

The analyzed SLs consisted of 10 GaSb MLs/9 InAs MLs pairs repeated 190 times and thin InSb-type or GaAs-type IFs between InAs and GaSb layers. Interfaces were treated in the simulations as additional thin InSb or GaAs layers. Calculations were carried out for a fully strained structure. Theoretical X-ray diffraction profile was calculated utilizing dynamical diffraction theory. For this purpose PANalytical *EPITAXY* software was applied.

The average lattice constant of SL was determined from angular position of 0-th order SL peak in X-ray diffraction pattern. In the calculations the tetragonal deformation and the constant volume of unit cell was assumed. The lattice mismatch was calculated using the following formula:

$$\frac{\Delta a}{a} = \left(\frac{a_{\text{SL}} - a_{\text{SB}}}{a_{\text{SB}}} \right) \times 100\%$$

where a_{SL} is average lattice constant of SL, a_{SB} is lattice constant of substrate and $\Delta a/a$ is lattice mismatch.

Lattice mismatch was analyzed for the following combinations of IFs:

1. All InSb-like or GaAs-like IFs are identical, *i.e.*, of the same type and thickness;
2. InSb-like and GaAs-like IFs coexist in SL.

The results for both groups are as follows.

2.1. All identical InSb-like or GaAs-like IFs

The calculations were performed for two cases. In the first case, only InSb-like IFs at the GaSb on InAs layers were assumed. In the second case, identical InSb-like IFs at the GaSb on InAs layers as well as InAs on GaSb layers were calculated. In both cases, the thicknesses of the IFs varied from 0.5 ML to 3 ML. Similar calculations for

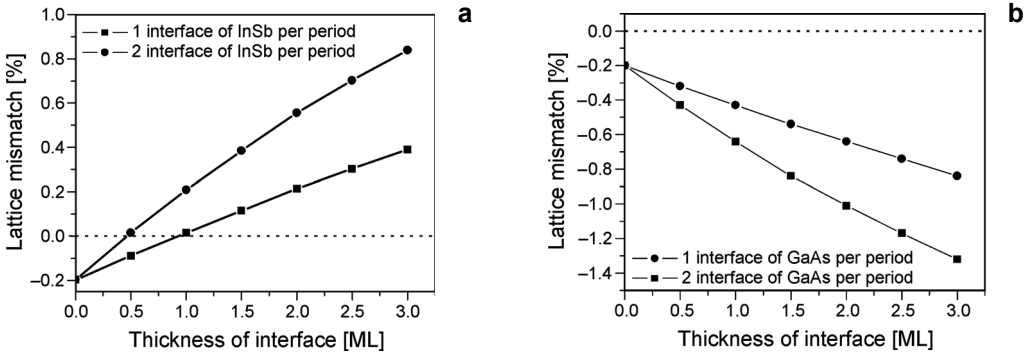


Fig. 1. Lattice mismatch dependence on the thickness of interfaces in InAs/GaSb SLs: InSb-like IFs (a), GaAs-like IFs (b). Dashed lines show lack of lattice mismatch.

the second type, GaAs-like, IFs have been performed. Results of simulations are presented in Fig. 1.

2.2. InSb-like and GaAs-like IFs coexist in the same SL

The influence of InSb-like and GaAs-like IFs existing in the same structure was also investigated. In this case, the structure consisted of 190 periods of 9 ML InAs,

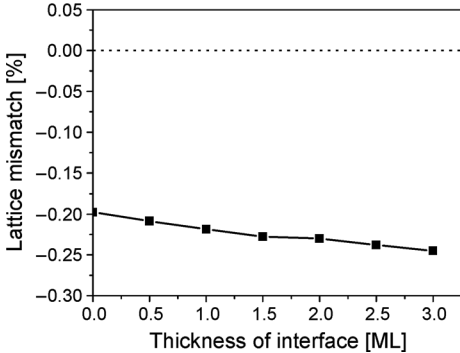


Fig. 2. Lattice mismatch dependence on thickness of InSb-like and GaAs-like IFs existing in the same SL. The amount of MLs in both IFs is identical. Dashed line shows lack of lattice mismatch.

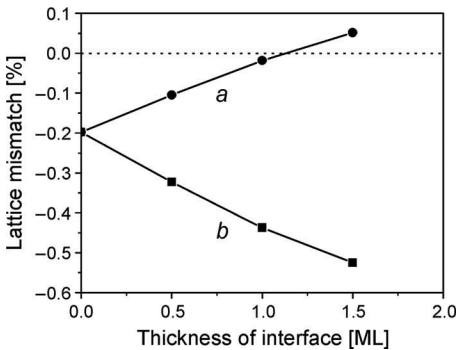


Fig. 3. Lattice mismatch dependence on thickness of n MLs InSb-like IFs and m MLs GaAs-like IFs existing simultaneously in SL; $n = 2m$ (a), $m = 2n$ (b). Dashed line shows lack of lattice mismatch.

m ML GaAs, 10 ML GaSb, n ML InSb each. Three different sequences of IFs were considered:

1. Identical amount of MLs in both IFs, *i.e.*, $n = m$;
2. Amount of MLs in InSb-like IF is two times thicker than in GaAs-like IF, *i.e.*, $n = 2m$;
3. Amount of MLs in GaAs-like IF is two times thicker than in InSb-like IF, *i.e.*, $m = 2n$.

The results obtained for three sequences of IFs are presented in Figs. 2 and 3. The calculations were limited to 3 MLs which is realistic value of interface thickness in InAs/GaSb SLs [3].

3. Discussion

On the basis of the results presented, one can conclude that strain introduced into the InAs/GaSb SL stack can be modified significantly by growing thin IF layers of InSb-like and GaAs-like type. This allows for substantial control of SL stress since interfaces introduce both compressive and tensile strain. From application point of view there is a great demand for completely free-of-stress SLs.

Results of simulations presented in Fig. 1 show that almost negligible strain exists in InAs/GaSb SL when 1 ML thick InSb-like interface per period is applied. The lattice mismatch is the same in SLs when one 1 ML or two 0.5 ML InSb layers are introduced. In this case SLs lattice mismatch $\Delta a/a = +1.5 \times 10^{-4}$. For SLs containing two 1 ML thick interfaces $\Delta a/a = +2.08 \times 10^{-3}$ which is slightly smaller value comparing to $\Delta a/a = +4.1 \times 10^{-3}$ reported by BÜRKLE and FUCHS [4].

It was experimentally observed by HAUGAN *et al.* [5] that SLs degrade with InSb-like IFs thickness beyond 1 ML. Similar observation was reported by RODRIGUEZ *et al.* [3]. They concluded that high quality strain-balanced SL structures of 10 ML InAs/10 ML GaSb could be obtained by inserting an InSb layer of thickness 1 ML and the structural characteristics strongly degrade when the thickness of the InSb IF increases.

Generally, lattice mismatch induced by InSb-like IFs is much smaller comparing to GaAs-like IFs of the same thickness – Fig. 1. It was observed by HERRES *et al.* [6] that the SLs with InSb-like IFs showed superior structural properties and were found to be essentially coherently strained. SLs with GaAs-like IFs, in contrast, showed strain relaxation except for the first 10–20 SL periods closest to the GaSb buffer and the strain profiles were found to depend critically on the InAs layer thickness [6].

Using both types of IFs allows for fabrication of InAs/GaSb SLs with extremely small lattice mismatch of $\Delta a/a = -0.43 \times 10^{-4}$. This can be obtained when 1.5 ML InSb-like and 0.5 ML GaAs-like IFs are applied. It means that in such a case structures are practically free of strain. For SLs containing 2 MLs InSb-like and 1 ML GaAs-like interfaces lattice mismatch increases and $\Delta a/a = -1.8 \times 10^{-4}$ – see Fig. 3.

In practical devices the interface bond plays a key role for the growth of high-quality InAs epilayers on GaSb, while the leading parameter is the growth

temperature. The discrepancies in experimental results concerning IFs may result from different growth temperatures of SLs. The best InAs and GaSb epilayers are grown by molecular beam epitaxy with an InSb-like interface at 400 °C. The InAs/GaSb structures with controlled InSb-like interface monolayer grown at 400 °C allows a layer by layer growth mode [7]. Additionally, the growth of the interface without specific anion intermixing control can result in large and unexpected variability in heterostructures [8]. The use of long group V soaks solely for the purpose of generating a InSb-like or GaAs-like interface does not provide adequate control of interfacial abruptness [9].

4. Conclusions

The theoretical studies of an impact of IFs type and thickness on InAs/GaSb SL lattice mismatch were performed. It was found that small lattice mismatch can be obtained in SL with one per period 1ML thick InSb-like IF. Better lattice matching should be reached when InSb-like and GaAs-like IFs coexist in one period of SLs.

Acknowledgements – This work was partially supported by the Polish Ministry of Science and Higher Education under the project No. PBZ- MNiSW 02/1/2007.

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Received June 19, 2009
in revised form October 1, 2009