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Influence of a strained InAlSb barrier on electron and hole transport in an InSb-based barrier-diode heterostructure

K. A. Savin^{*}, V. S. Krivobok, and S. N. Nikolaev

P. N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, 119991 Russia

^{}E-mail: savinkonstantin93@gmail.com*

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This study presents a simulation of an InSb/InAlSb nBn heterostructure intended for use in mid-wave infrared photodetectors. The influence of the parameters of a strained InAlSb barrier layer on the band profile of the structure and on charge carrier transport is investigated. Particular attention is paid to achieving selective suppression of electron current while maintaining efficient hole transport, which is a key requirement for reducing dark current and increasing the operating temperature of photodetectors. The simulations were performed using the COMSOL Multiphysics software environment. Various barrier-layer designs were analyzed, and the configurations providing the most favorable balance of barrier properties for majority and minority charge carriers were identified. The obtained results can be used in the design of InSb photodetectors based on the nBn architecture for the mid-wave infrared range.

Keywords: IR photodetector, InSb, simulation, COMSOL Multiphysics, molecular beam epitaxy, barrier-diode heterostructures.

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Introduction

Infrared (IR) focal plane arrays are a basic element of modern thermal imaging and thermal radiation detection systems [1]. Increasing requirements for their sensitivity, speed, and energy efficiency make the development of new materials and device architectures for the mid-infrared range urgent.

One of the most common materials for creating mid-IR photodetectors is indium antimonide, a narrow-gap A_3B_5 semiconductor with a bandgap of about 0.23 eV at 80 K [2]. InSb remains one of the most in-demand materials for manufacturing high-speed photodetectors operating in the 3–5 μm range. On this basis, large-format photosensitive arrays have been created, and the development of epitaxial

technologies, in particular molecular beam epitaxy (MBE), has made it possible to improve the structural perfection of layers, reduce background impurity levels, and improve material uniformity [3].

However, the effective operation of InSb photodetectors, typically, requires cooling to cryogenic temperatures, since with increasing operating temperature the dark current sharply increases and the core device characteristics deteriorate [1, 2]. This leads to an increase in the mass, cost, and power consumption of the equipment. Therefore, a key direction in the development of InSb-based IR photodetectors is the creation of devices using barrier-diode heterostructures (nBn) [4]. A selective barrier that blocks the majority charge carriers (electrons) current makes it possible to reduce the dark

current without preventing the free movement of photogenerated holes in the valence band. Thus, an increase in the operating temperature is achieved without a significant deterioration in performance characteristics.

The most common material for the barrier layer of InSb-based structures is InAlSb [5]. This is primarily due to the successful combination of good lattice-parameter matching and a wide bandgap, which makes it possible to form a high potential barrier. This allows electrons to be effectively localized in InSb, reducing their leakage and suppressing parasitic currents, which is especially important for highly sensitive and high-speed devices. In addition, InAlSb provides high heterointerface quality and makes it possible to flexibly control the band structure by changing the layer composition. The study of its characteristics is fundamentally important, since barrier properties – such as the bandgap and band offset heights – largely determine the operating characteristics of the device. At the same time, strained InAlSb barrier layers, despite their practical importance for controlling the band profile and transport properties of the heterostructure, have so far been poorly studied. In this regard, it is of interest to analyze such strained barriers and assess their influence on electron and hole transport in nBn -type structures.

The present work is devoted to the modeling of an InSb/InAlSb heterostructure of the nBn type using the COMSOL Multiphysics software package. The work considers various designs of the InAlSb barrier layer and analyzes their influence on the transport of majority and minority charge carriers. Particular attention is paid to the choice of a barrier configuration that ensures effective suppression of electron transport while maintaining unimpeded hole transport. The obtained results make it possible to determine the optimal design of the barrier layer for application in mid-IR photodetector structures.

Band structure and strain-induced shifts of energy levels in InSb and InAlSb

The barrier-diode structures studied in the present work are traditionally grown by MBE. This is due to the need for precision control of the heteroepitaxial growth parameters that determine the band diagram and transport properties of the

structure. The MBE method provides high accuracy in specifying layer thicknesses, solid solution compositions, and doping profiles, as well as forming sharp and morphologically perfect heterointerfaces. This is especially important for narrow-gap InSb/InAlSb systems, in which even insignificant deviations in composition, barrier layer thickness, or interfacial blurring lead to a noticeable change in potential barrier heights, the position of band edges, and the carrier transport conditions. An additional advantage of MBE is the possibility of controlling the growth of strained and pseudomorphic layers with a reduced density of structural defects, which is fundamentally important for realizing the calculated energy profile of nBn structures and the reproducibility of their electrophysical and photoelectric characteristics.

At the same time, sufficiently thin InAlSb layers grown on InSb are formed in a pseudomorphic state, meaning they retain coherent conjugation with the substrate without the relaxation defect formation. This is due to the small lattice-parameter mismatch and is confirmed by structural data obtained both within the framework of this research direction by our scientific group in [6] for a 70-nm-thick $\text{In}_{0.8}\text{Al}_{0.2}\text{Sb}$ layer, and by independent teams in [5] for a 50-nm-thick graded $\text{In}_{1-x}\text{Al}_x\text{Sb}$ layer (*where* x gradually increased from 0.15 to 0.35). Establishing the pseudomorphic nature of growth is fundamentally important, since it is precisely in this case that the elastically strained state of the barrier layer is realized, which modifies the band structure and the energy profile of the heterosystem.

Further in this work, only fully pseudomorphic InAlSb barrier layers are considered, for which the coherent nature of growth is ensured either by reducing the aluminum content, and consequently, reducing the lattice-parameter mismatch with InSb – or by reducing the layer thickness. Such a limitation makes it possible to analyze heterostructures within the framework of the model of a fully elastically strained barrier model without considering relaxation and the its associated defects.

For a pseudomorphic InAlSb layer on InSb, the condition of equality of lattice parameters

($a_{\parallel} = a_{sub}$) is satisfied. Here $a_{\parallel}$ is the lattice parameter in the interface plane. Then the in-plane strain of the layer is determined by the expression

$$\varepsilon_{\parallel} = (a_{\parallel} - a_{layer}) / a_{layer},$$

where a_{layer} is the lattice parameter of the unstrained layer. The out-of-plane strain, within the framework of the linear theory of elasticity for cubic crystals [7], takes the form

$$\varepsilon_{\perp} = -2(C_{12} / C_{11}) \cdot \varepsilon_{\parallel},$$

where C_{11} and C_{12} are the elastic constants of the layer material. The values of the constants used in the present work, here and below, are taken from source [8]. To describe the elastic properties of the $\text{In}_{1-x}\text{Al}_x\text{Sb}$ solid solution, the elastic constants C_{11} and C_{12} can be estimated using Vegard's rule:

$$C_{11}(\text{In}_{1-x}\text{Al}_x\text{Sb}) = (1-x) \cdot C_{11}(\text{InSb}) + x \cdot C_{11}(\text{AlSb}),$$

$$C_{12}(\text{In}_{1-x}\text{Al}_x\text{Sb}) = (1-x) \cdot C_{12}(\text{InSb}) + x \cdot C_{12}(\text{AlSb}).$$

The presence of pseudomorphic deformation significantly affects the electronic structure of $\text{In}_{1-x}\text{Al}_x\text{Sb}$. In particular, strain leads to a change in the band gap, the splitting of heavy and light hole states, and shift in the effective masses of charge carriers and, accordingly, their mobilities.

The hydrostatic component of strain is determined as the trace of the strain tensor:

$$\varepsilon_h = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = 2\varepsilon_{\parallel} + \varepsilon_{\perp}.$$

In turn, the biaxial shear component of strain, responsible for lifting the degeneracy of the valence band, is given by the expression:

$$\varepsilon_b = \varepsilon_{\perp} - \varepsilon_{\parallel}.$$

To calculate the strain-induced shifts of the band edges, the deformation potentials a_c , a_v , and b are used:

$$\Delta E_c = a_c \cdot \varepsilon_h,$$

$$\Delta E_v(hh) = a_v \cdot \varepsilon_h - b \cdot \varepsilon_b,$$

$$\Delta E_v(lh) = a_v \cdot \varepsilon_h + b \cdot \varepsilon_b.$$

For the $\text{In}_{1-x}\text{Al}_x\text{Sb}$ solid solution, the values of the deformation potentials were determined in a linear approximation with respect to composition:

$$a_c(\text{In}_{1-x}\text{Al}_x\text{Sb}) = (1-x) \cdot a_c(\text{InSb}) + x \cdot a_c(\text{AlSb}),$$

$$a_v(\text{In}_{1-x}\text{Al}_x\text{Sb}) = (1-x) \cdot a_v(\text{InSb}) + x \cdot a_v(\text{AlSb}),$$

$$b(\text{In}_{1-x}\text{Al}_x\text{Sb}) = (1-x) \cdot b(\text{InSb}) + x \cdot b(\text{AlSb}).$$

The absolute positions of the conduction band and valence band edges of the materials relative to vacuum are determined by their χ electron affinity and the band gap E_g . At a temperature of 300 K, for the binary compound InSb the electron affinity is $\chi(\text{InSb}) = 4.59$ eV with a band gap $E_g = 0.17$ eV. For AlSb, the electron affinity is $\chi(\text{AlSb}) = 3.6$ eV with a fundamental band gap $E_g(X) = 1.62$ eV. However, for the $\text{In}_{1-x}\text{Al}_x\text{Sb}$ solid solution, it is necessary to take into account that with increasing Al content, approximately starting from $x \approx 0.45$, a transition from a direct-gap to an indirect-gap structure occurs. Therefore, when analyzing the band diagram, the dependences $E_g(\Gamma)$ and $E_g(X)$ should be considered separately: at small x the conduction band minimum is located at the Γ point, whereas at large x it is at the X point. Since the band gap of AlSb in the Γ valley is about 2.3 eV, to estimate the position of the conduction band level at the Γ point one can take $\chi \approx 2.92$ eV.

For the $\text{In}_{1-x}\text{Al}_x\text{Sb}$ solid solution, the χ dependence on composition in the first approximation can be described by Vegard's law:

$$\chi(\text{In}_{1-x}\text{Al}_x\text{Sb}) = (1-x) \cdot \chi(\text{InSb}) + x \cdot \chi(\text{AlSb}).$$

The influence of strain on electron affinity is due to the strain-induced shift of the conduction band. Under tensile strain, the bottom of the conduction band shifts downward in energy, which leads to an increase in electron affinity by the $\Delta E_c = a_c \cdot \varepsilon_h$ amount.

On the basis of the proposed model, energy diagrams of InSb/InAlSb *nBn* structures were constructed, consisting of an InSb absorbing layer 1 μm thick, two InSb contact layers 200 nm thick each, and an InAlSb barrier layer (see Fig. 1). The thickness of the barrier layer was determined depending on the Al content from the condition of preserving the pseudomorphic state.

The doping impurity concentration (*n*-type) was 10^{16} cm^{-3} in the sensitive layer, $2 \times 10^{16} \text{ cm}^{-3}$ in the upper contact layer, $4 \times 10^{16} \text{ cm}^{-3}$ in the lower contact layer, and 10^{14} cm^{-3} in the barrier layer. The temperature was set equal to 150 K.

Figure 1 shows that for all the considered structures the barrier manifests itself primarily as a jump in the conduction band. With an increase

in Al content from $x = 0.1$ to $x = 0.4$, the height of the electron barrier successively increases. In contrast to the conduction band, the valence band offset changes nonmonotonically and has a substantially smaller magnitude. For structures with $x = 0.1$ and $x = 0.2$, the formation of a potential well for holes is observed. At $x = 0.3$, the value of ΔE_v is close to zero, whereas at $x = 0.4$ a small barrier for holes arises. The nonmonotonic nature of the dependence of ΔE_v (in the inset to Fig. 1) is due to the competition of two factors: an increase in the valence band offset with growing Al content in the barrier layer and the contribution of the biaxial shear component of deformation, which leads to the lifting of the degeneracy of the valence band.

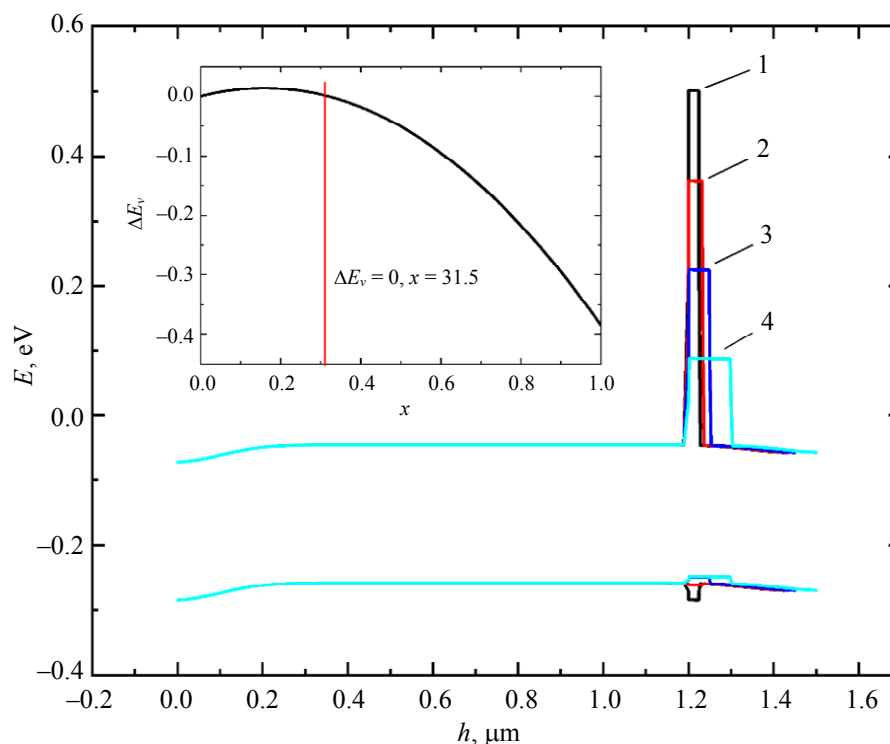


Fig. 1. Energy diagrams of InSb/In_{1-x}Al_xSb *nBn* structures with different barrier layers:

1 – $x = 0.4$, $h = 25 \text{ nm}$; 2 – $x = 0.3$, $h = 33 \text{ nm}$; 3 – $x = 0.2$, $h = 50 \text{ nm}$; 4 – $x = 0.1$, $h = 100 \text{ nm}$.

In the inset – analytically calculated dependence of the valence band offset of strained In_{1-x}Al_xSb on the Al content

For all the studied InSb/In_{1-x}Al_xSb *nBn* heterostructures, the temperature dependences of the electron and hole currents were calculated per pixel with a size of $15 \times 15 \mu\text{m}^2$. The modeling results are presented in Figure 2 for structures with different compositions and thicknesses of the barrier layer. Figure 2 shows that the electron current monotonically increases with temperature for all the considered structures, but its magnitude

depends substantially on the barrier layer parameters. With an increase in the Al content in the barrier, the electron current decreases by several orders of magnitude over the entire studied temperature range. This indicates enhanced barrier suppression of majority carrier transport with increasing barrier height due to the higher x content in the In_{1-x}Al_xSb layer.

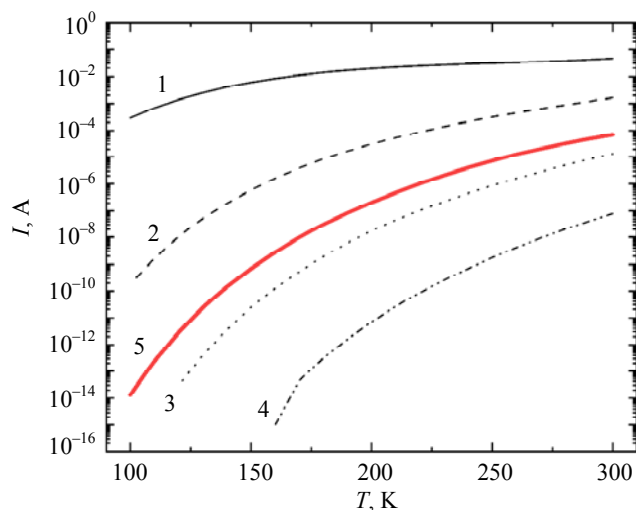


Fig. 2. Temperature dependences of the electron (black) current of InSb/In_{1-x}Al_xSb nBn structures with different barrier layers: 1 – $x = 0.1$, $h = 100$ nm; 2 – $x = 0.2$, $h = 50$ nm; 3 – $x = 0.3$, $h = 33$ nm; 4 – $x = 0.4$, $h = 25$ nm, as well as the common red curve 5 for the hole current of all structures

At the same time, the hole currents for all structures practically coincide, forming a single temperature dependence. Such a weak sensitivity of the hole current to changes in the barrier layer parameters indicates that the transport of minority carriers in the studied nBn structures remains practically unchanged when the composition and thickness of the barrier are varied.

At the same time, for structures with $x = 0.3$ and 0.4 , a transition to the regime $I_e < I_h$ is

observed, indicates the achievement of an effective electron-blocking configuration, making it the most favorable for the practical implementation of nBn devices.

Conclusions

This work investigated the influence of elastic deformation on the energy spectrum of InSb/In_{1-x}Al_xSb heterostructures, and established its role in the formation of band offsets at the heterointerface. It is shown that a change in the composition of the barrier layer leads to a substantial rearrangement of the band diagram, and the specific Al content at which the valence band offset ΔE_v disappears has been determined. The performed modeling of the current characteristics showed that the use of a pseudomorphic barrier layer with $x = 0.3$ – 0.4 makes it possible to effectively suppress the valence band offset, limit the transport of majority charge carriers, and achieve a regime in which the dark current is determined predominantly by the heavy-hole contribution. The obtained results confirm the promise of using pseudomorphic In_{1-x}Al_xSb barriers with increased Al content for optimizing InSb-based nBn structures and reducing the contribution of the electron component to the dark current.

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About the authors

Savin K. A., Candidate of Physical and Mathematical Sciences, Researcher, P. N. Lebedev Physical Institute of the Russian Academy of Sciences (Moscow, 119991, Russia). E-mail: savinkonstantin93@gmail.com SPIN code: 9596-3586, AuthorID: 820563, ORCID 0000-0002-5674-9577, Scopus Author ID 57209027082

Krivobok V. S., Doctor of Physical and Mathematical Sciences, Leading Researcher, P. N. Lebedev Physical Institute of the Russian Academy of Sciences (Moscow, 119991, Russia). E-mail: kolob7040@gmail.com AuthorID: 135304, ORCID 0000-0001-8846-3891, Scopus Author ID 8604415500

Nikolaev S. N., Candidate of Physical and Mathematical Sciences, Senior Researcher, P. N. Lebedev Physical Institute of the Russian Academy of Sciences (Moscow, 119991, Russia). E-mail: nikolaev-s@yandex.ru SPIN code: 6963-3322, AuthorID: 880828, ORCID 0000-0001-6739-7338, Scopus Author ID 16425853400