Enhanced numerical design of two barrier infrared detectors with III-V compounds heterostructures

A. Jóźwikowska[(1)] M. Suligowski[(2),] and K. Jóźwikowski[(2)(3),]
[(1)]Faculty of Applied Informatics and Mathematics, Warsaw University of Life Science SGGW, Nowoursynowska 166 St., 02-787 Warsaw, Poland
[(2)]Institute of Applied Physics, Military University of Technology, 2 Gen. Urbanowicza St., 00-908 Warsaw, Poland,
[(3)]krzysztof.jozwikowski@wat.edu.pl

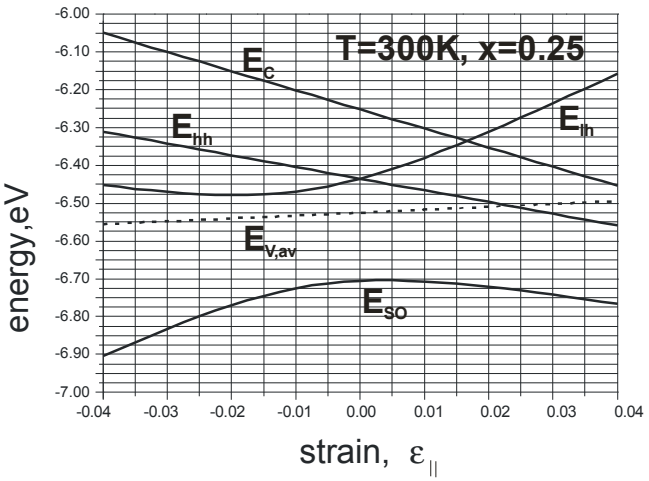
***Abstract*-Using our computer program to iteratively solve the Poisson equation, spatial distribution of energy band edges in III-V heterostructures was calculated. The influence of lattice stress and doping on the energy shift of the edge of the bands was taken into account. It has been shown that the offset can be eliminated in the areas of both barriers in the designed two-barrier detectors.**

I. INTRODUCTION

In Poland in the joint laboratory of the Military University of Technology (MUT) and Vigo System SA, InAsSb hetorostructures grown in MBE processes are intensively developed and investigated [1]. Of particular interest are $InAs_{1-x}Sb_x$ structures with molar compositions x≈0.25 used for the construction of uncooled infrared detectors in the range of 3-5,5 μm . These structures are deposited most often on GaAs or GaSb substrates, however, there is a few percent misfit of lattice constants between the layer and the substrate. The situation is further complicated by the deposition of additional layers acting as energy barriers for electrons or holes [2]. The resulting lattice stresses induce significant lattice strains in the heterostructure. In order to design infrared detectors based on the mentioned heterostructures, we must take into account the effect of these deformations on the physical properties of individual layers. Strains cause a fractional volume change that causes the change in the width of the energy gap. In addition presented shear strains split and line up the valence bands and the indirect conduction bands. Assumption of pseudomorphic interface enables simple determination of strains in the individual layers of the heterostructure. Usually, however, if the layers are not thin enough, the deformations are much smaller than anticipated. The reason for this are misfit dislocations generated in the areas of interfaces. The number of dislocations can be estimated in many cases, although theoretical considerations are rather complicated. Nevertheless, we proposed a theoretical determination of dislocation density from the minimum elastic energy condition. The key to designing two-barrier detectors is to determine, in thermal equilibrium conditions, the spatial distribution of the apex of the valence band and the valley of the conductance band. In III-V compounds, the character of the energy gap may change, depending on the molar composition and temperature. Therefore the minimum of the conduction band with the points Γ, X and L of the Brilouine zone should be taken into account [3].

II. NUMERICAL METHOD AND RESULTS OF CALCULATIONS

Jain and Roulston [4] received an analytic expression of the bandgap-narrowing. Lattice stress has a much greater impact on the shifting of energy bands. Except hydrostatic



strain leading to the band shifts, the shear components of the strain

Fig.1. Effect of strain $\varepsilon_{\|}$ on the position of the edge of E_C band, the averaged valence band edge, $E_{V,av}$ heavy hole band edge, E_{hh}, the light hole band edge, E_{lh} and edge of the split-off spin-orbit band, E_{SO}. Calculations made by us based on the relations obtained in [4] and [5].

can have a profound effect on degenerate bands. They lead to splittings of the valence bands (and of the indirect conduction bands) which are well-described by deformation potential theory, and were discussed by Wan de Walle [5].

In this work we analyze uncooled cylindrical mesa two-barrier detectors with an area of 250.μm^2. The $InAs_{1-x}Sb_x$ epitaxial layer is grown on a 230μm thick GaSb substrate. Absorber with a molar composition x = 0.25 of about 6μm thick is surrounded by two barriers from $AlAs_{1-y}Sb_y$ (y=0.1). Spatial distribution of mole fraction and dopant concentrations in epitaxial layer is shown in Fig.2. The initial values of the

electrical potential are determined from the local condition of electrical neutrality at each point of the structure, assuming that Fermi energy for the whole structure E_F=0.

$$N_D^+(\Psi) + hh(\Psi) + lh(\Psi) - \Gamma n(\Psi) - Xn(\Psi) - Ln(\Psi) - N_A^-(\Psi) = 0 \quad (1)$$

Where $N_D^+, hh, lh, \Gamma n, Xn, Ln$ and N_A^- denote the concentration of ionized donors, heavy holes, electrons in G valley, X valley, L valley and concentration of ionized acceptors, respectively. Then we solve the nonlinear Poisson equation [6] to find the spatial distribution of the edge of the conduction and the valence bands. All shown figures reveal spatial distributions in the epitaxial layer along the axis of symmetry

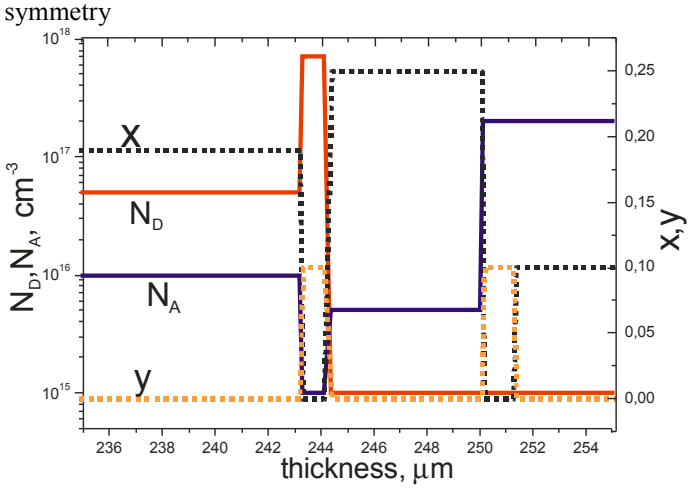


Fig.2. Spatial distribution of donor concentration N_D, Acceptor concentration N_A, and mole fractions x and y in designed epitaxial heterostructure

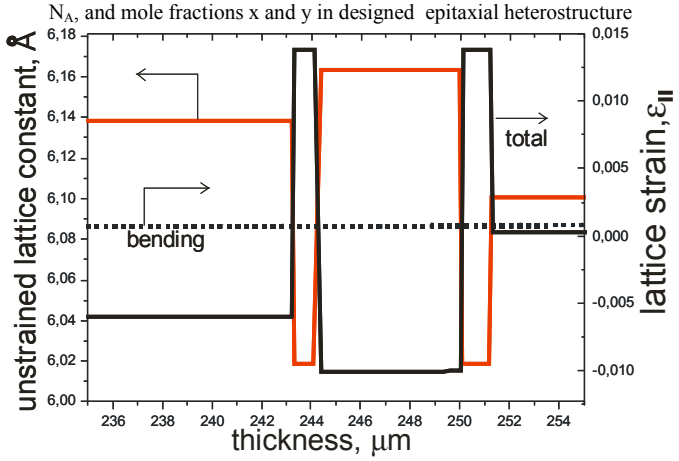


Fig.3. Spatial distribution of unstrained lattice constant and the lattice strain caused by bending (dotted line) and total lattice stain caused by bending and lattice misfit (red line) in layers of epitaxial heterostructure.

The lattice stress is partially relaxed by misfit dislocations that generate in the interfaces between the individual layers. In our work, we have attempted to theoretically estimate dislocation density from the minimum elastic energy condition. Dislocations decreasing the strain as below [7]:

$$\epsilon_{\parallel}^* = \epsilon_{\parallel} - \delta b_1/p, \quad (2)$$

where $b_1 = -bsin\alpha sin\beta$ and b is the Burgers vector, p is the average inter-dislocation distance. For 60° dislocations

$$\alpha = arctg\frac{1}{\sqrt{2}}, \quad \beta = \frac{\pi}{3}. \quad (3)$$

δ takes values 1 or -1, so that $\epsilon_{\parallel}^*$ always takes lower values than $\epsilon_{\parallel}$. b is the magnitude of the Burgers vectors, i.e., the length of a $1/2\langle 1,1,0\rangle$ lattice vector.

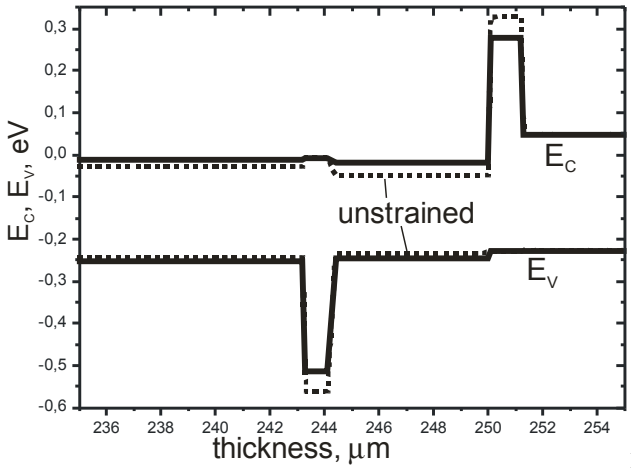


Fig. 4. Spatial distribution of the calculated edge of conduction band E_C and valence band E_V. Doted lines concern structure without the lattice strain. Solid lines are obtained for strained structure.

SUMMARY

In the work, we describe the numerical method of calculating spatial band edge distribution on the example of InAsSb two-barrier detector. The use of barriers with AlAsSb allows practically to erect the offset, which hinders their proper operation. We take into account the influence of the lattice strain on the change in the energetic position of the edge of the bands. Lattice strain caused by lattice misfit in heterostructure has the greatest impact on this phenomenon. The bending of heterostructures and the concentration of dopants has a much smaller effect. We also carried out a theoretical estimation of the density of dislocations in individual interfaces. They cause the reduction of the lattice stresses but introduce additional trap centers decreasing the lifetime of the electric current carriers

ACKNOWLEDGMENT

The work has been undertaken under the financial support of the Polish National Science Centre as research Project No DEC-2016/23/B/ST7/03958.

REFERENCES

[1] E. Gomółka, M. Kopytko, K. Michalczewski, Ł. Kubiszyn, A. Kębłowski, W. Gawron, P. Martyniuk, J. Piotrowski, J. Rutkowski, A. Rogalski, "Electrical and optical performance of mid-wavelength infrared InAsSb heterostructure detectors", *Proc. SPIE* 10433, 104330Y-1 (2017).

[2] P. Klipstein, O. Klin, S. Grossman, N. Snapi, I. Lukomsky, M. Yassen, D. Aronov, E. Berkowitz, A. Glozman, O. Magen, I. Shtrichman, R. Frenkel, E. Weiss, "High operating temperature XBn-InAsSb bariode detectors," Proc. SPIE 8268, Quantum Sensing and Nanophotonic Devices IX, 82680U, 2012

[3] S. Adachi, *Properties of Group- IV, III-V and II-VI Semiconductors* , Wiley Series on Materials for Electronics and Optoelectronic Applications, Wiley & Sons, 2000

[4] S. C. Jain and D. J. Roulston, "A simple expression for band gap narrowing (BGN) in heavily doped Si, Ge, GaAs and Ge_xSi_{1-x} strained layers," Solid-State Electronics Vol. 34 (5), 453, 1991

[5] C. G. Van de Walle, "Band lineups and deformation potentials in the model-solid theory," Phys. Rev. B 39(3) ,p.1871, 1989

[6] A. Jóźwikowska, "Numerical solution of the nonlinear Poisson equation for semiconductor devices by application of a diffusion-equation finite difference scheme", Journal of Applied Physics , 104, 063715, 2008

[7] S. C. Jain, M. Willander, K. Pinardi and H. E. Maes, "A Review of Recent Work on Stresses and Strains in Semiconductor Heterostructures," Physica Scripta. Vol. T69, 65, 1997