Numerical estimation of lattice strain, bending and generation of misfit dislocations in HgCdTe heterostructures grown on GaAs substrate

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***Abstract*- We determined the spatial distribution of lattice strains in the HgCdTe heterostructures grown on GaAs substrate by using our own simulation program. The obtained lattice stresses are greatly relaxed by the misfit dislocations arising in the interfaces. We calculated the minimum elastic energy as a function of the dislocation density in all interfaces. We also estimated the part of dislocation's electrical energy in the total energy balance.**

I. Introduction

We report on our efforts to simulate misfit dislocations in HgCdTe detectors grown on GaAs (100) surface by metal organic chemical vapour deposition (MOCVD). Strong lattice misfit between the GaAs substrate and the CdTe buffer layer is the cause of lattice stresses due to the deformation of the crystal lattice of both materials. Significant relaxation of stress occurs due to the misfit dislocations located mainly in the interface between GaAs and CdTe layers. Dislocations are generated in the form of a grid with the same distance between the dislocation lines lying in the planes of growth. If on the CdTe buffer layer we grow the $Cd_{1-x}Hg_xTe$ hererostructures and the lattice misfit between layers is relatively small, misfit dislocations will also occur in areas where there is a change in molar composition x. These dislocations introduce additional energy states in the energy band gap and they create an additional channel for generation and recombination (G-R) processes known as Shockley-Read-Hall (SHR) mechanism [1]. Thus, if we perform numerical simulations of infrared detectors built of these heterostructures, we should estimate the density of these dislocations to properly calculate of the thermal G-R rates. The rate of SHR processes is influenced by a polarization of the detectors, mainly through the trap assisted tunnelling mechanism (TAT). This effect is noticeable on the current-voltage characteristics of the devices, which confirm that in many cases the dislocation density determines photoelectric parameters of infrared detectors [2].

II. Results and Simulation Procedure

The analysed heterostructure consist of three HgCdTe layers grown by MOCVD method on the GaAs substrate after the CdTe buffer layer. The growth was carried out in a joint laboratory run by VIGO System S.A. and Military University of Technology (MUT). At the bottom was formed a highly doped with iodine ($N_D = 2\times10^{17}$ cm^{-3}), wider-gap ($x = x_{abs} + 0.02$) contact layer with a thickness of 2.10µm. Then, the undoped absorber (with background donor concentration at the level of $N_D = 5\times10^{15}$ cm^{-3}) was grown with a thickness of 5.22µm and composition $x_{abs} = 0.43$. Finally, highly doped with arsenic ($N_A = 2\times10^{17}$ cm^{-3}) contact cap layer with a thickness of 2.11µm and composition $x = x_{abs} + 0.02$ was formed. Thus, we have obtained the P^+nN^+ detection structure (Fig.1).

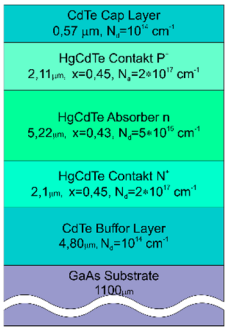

Fig. 1. HgCdTe photodetector P^+nN^+ structure grown on (001) GaAs substrate using the MOCVD method.

The lattice strains are calculated by using our computer program under the assumption that pseudomorphic strains are giving the same value of the lattice constant in the layer's growth plane in all the structure. Then we calculate the bending to determine an additional change in the lattice constant. By calculating the minimum elastic energy caused by the described deformations and dislocations generated in the regions of change in molar x fraction and on the interface between two different dislocations in the structure. In addition, in the energy balance

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we include the energy of the electric field around dislocations and individual interfaces. We determine this field by solving the Poisson equation in a cylindrical region around the dislocation core. Further to determine the spatial distribution of the electric field, we calculate the statistical distribution function of electrons in the dislocation band.

However, this additional energy represents only small fraction of the elastic energy and generates only a little effect on the density of misfit dislocations. Figure 2 shows the spatial distribution of the lattice strain in the GaAs substrate. Pseudomorphic strains (blue line) are constant and assume values slightly above 0.05%. A positive value indicates that they are stretching strains.

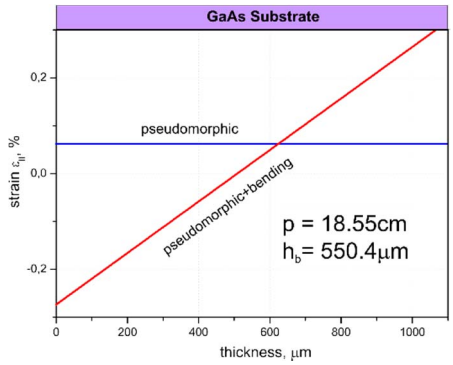

Fig. 2. Distribution of strains ε‖ in a GaAs substrate with a thickness of 1100µm. Blue line refers to the pseudomorphic strains. Red line refers strains with additional bending of the structure.

The bending of the structure is necessary to achieve the equilibrium of moments of internal forces but causes deformation. As Fig. 2 shows, the bottom layer of the substrate is compressive, while the top layer is stretched (red line). At distance h_b= 550.4µm from the bottom, there is a neutral point, not deformed by bending. The bending radius is 18.55cm. Pseudomorphic strains in the epitaxial layer (Fig. 3) are compressive (above 12%). The bending of the structure slightly reduces strain by a fraction of a percent (red line).

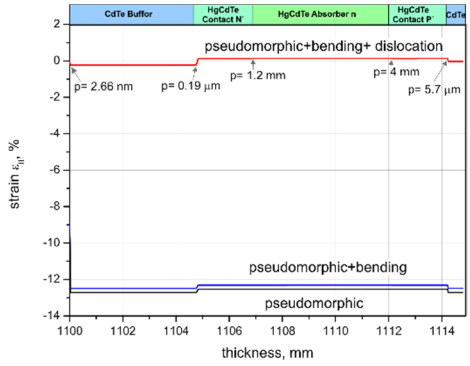

Fig. 3. Spatial distribution of strains $\varepsilon_{\|}$ in the HgCdTe epitaxial layer at 300 K deposited on GaAs (100) substrate.

Generated misfit dislocations have a very strong effect on the relaxation of lattice stresses and reduction of deformations of individual layers of the heterostructure. Figure 3 also shows the parameter p, which is the average distance between misfit dislocations lines which are located at interfaces of different epitaxial layers. A very dense grid of dislocations (p= 2.66nm) appears at the border between the buffer and the substrate. Fortunately, in the other interfaces, the density of dislocations is magnitude smaller. Figure 4 shows the spatial distribution of the energy bands and of the cut off wavelength $\lambda_{co} = 1.24/E_g$ in the substrate and epitaxial layers. Calculations include the influence of lattice deformations on position of the band edges [3-5].

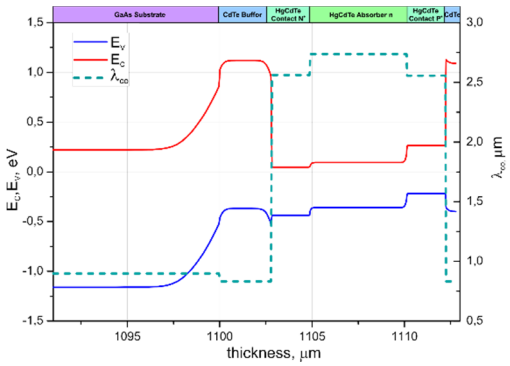

Fig. 4. Calculated band structure as a function of thickness in the epitaxial layer (solid lines). Dashed line shows spatial distribution of cut off wavelength λ_{co}.

III. Conclusion

Including misfit dislocations in the calculations of strain allows to estimate the real mechanisms of structure relaxation. By computing the minimum energy we can numerically determine the values of average distance between misfit dislocations lines in the interfaces of HgCdTe heterostructures.

Acknowledgment

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References

[1] K. Jóźwikowski, A. Jóźwikowska, M. Kopytko, A. Rogalski, and L.R. Jaroszewicz, "Simplified model of dislocations as a SRH recombination channel in the HgCdTe heterostructures," *Infrared Phys. Technol.,* 55 (1), 98, 2012.

[2] K. Jóźwikowski, M. Kopytko, A. Rogalski, A. Jóźwikowska, "Enhanced numerical analysis of current-voltage characteristics of long wavelength infrared n-on-p HgCdTe photodiodes," *J. Appl. Phys.,* vol. 108, nr 7, art. 074519, 2010.

[3] 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.

[4] S.C. Jain, T.J. Gosling, J.R. Willis, D.H.J. Totterdell and R. Bullough, "A new study of critical layer thickness, stability and strain relaxation in pseudomorphic ge_xsi_{1-x} strained epilayers," Phil. Mag. A 65, 1151, 1992.

[5] T. J. Gosling, R. Bullough, S. C. Jain, and J. R. Willis, "Misfit dislocation distribution in capped (buried) strained semiconductor layer", *J. Appl. Phys.,* 73, 8267-78, 1993.