CAN THE FORMATION OF COMPENSATING DONORS BE SUPPRESSED IN MODULATED P-DOPPED GALLIUM OXIDE QUANTUM WELLS?

T. Tchelidze[1,a], Z. Machavariani[1,2,b], E. Chikoidze[3]

[1] *Department of Exact and Natural Sciences, Tbilisi State University, 0179, Tbilisi, Georgia,* *[a]tchelidze@tsu.ge*

[2]*Doctoral School, Kutaisi International University, Youth Avenue, 5th Lane, 4600 Kutaisi, Georgia,* *[b]zaal.machavariani@tsu.ge*

[3] *University Paris Saclay, Grp Etud Matiere Condensee GEMaC, UVSQ CNRS, 45 Ave des Etats Unis, F-78035 Versailles, France*

Abstract. The actual problem of obtaining hole conductivity in ultra-wide bandgap semiconductor Ga_2O_3 is considered. It is proposed to use Aa_2O_3/Ga_2O_3 quantum structures for increasing hole concentration, and their mobility. The dependence of theses parameters on system geometry and composition is studied.

1. Introduction

One of the main goals of semiconductor material science is controlling the electrical and optical properties of materials, which is fulfilled by means of controlling charge carrier concentration. Most of the materials valuable for electronic application supper from monopolar doping problems; oxide semiconductors are easily n-doped, however, p-doping is a big challenge still. The difficulties of p-doping are connected to the creation of compensating donors, low mobility of holes, low lying valence band, high ionization energies of acceptors. Modulated doping, in which the impurities are separated from the layer where current flows, gives one possibility to decrease scattering with ionized impurities and increase carrier mobility. In this case, the barrier layers are doped, while carriers reside in quantum well layers and do not experience scattering with ions. However, it is counted that modulation doping cannot reduce the compensation processes. The essence of compensation is that the free energy of the pair [negatively charge acceptor-hole] is more than the free energy of the pair [negatively charge acceptor – positively charged donor]; that is why for crystal it is energetically more favorable to create a positively charged donor defect (hole killer) rather than to maintain a hole in a valence band. Therefore, the efficiency of compensation depends on the band-gap, the ionization energy of compensating donors, their creation enthalpy, and controlling of all these parameters is crucial to achieve the above mention goal.

Gallium oxide is ultra-wide band gap (~ 4.85 eV) material with great perspectives of application in optical and power electronics [1]. It also suffers from monopolar n-conductivity. High ohmic p-conductivity has been obtained [1,2], however, it low-ohmic samples suitable for practical application is still challenging.

2. Theoretical framework

It is expected that in nanostructures many desired properties that are impossible to realize in bulk materials can be obtained. This is connected to the appearance of now controlling parameters, such as size, shape, geometry. In the condition of space confinement all the characteristics, which are important to achieve high hole conductivity, change and become size dependent.

In this work, we study the possibilities of suppressing the formation of compensating intrinsic defects in modulated p-doped $AlGaO_3/Ga_2O_3$ quantum well heterostructures in order to obtain p-type gallium oxide layers.

The basic idea is that because of very high conduction band offset aluminum and gallium oxides [3], it is possible to construct two-step quantum wells with double barriers with different aluminum concentrations – $Al_{(1-x)}Ga_{(x)}O_3/Al_{(1-y)}Ga_{(y)}O_3/Ga_2O_3$ with y less than x. If the modulated doped barrier $Al_{(1-y)}Ga_{(y)}O_3$ that immediately borders Ga_2O_3 quantum well, is of a few nanometer sizes, the ionization energy of compensating donors will increase because of space confinement. The ionization energy of acceptors is expected to be much less affected by space confinement. This is mainly conditioned by a very low barrier for holes in the heterostructure, and also a big effective mass of holes, comparing with electron effective mass.

3. Results

We calculated the band structure and ionization energies of donors, acceptors for different thicknesses for quantum well and barrier of the $Al_{(1-x)}Ga_{(x)}O_3/Al_{(1-y)}Ga_{(y)}O_3/Ga_2O_3$ heterostructure in the frame of single-band effective mass approximation and perturbation theory. The obtained results then were used for the Kroger method of quasi-chemical reactions to define the equilibrium concentrations of careers, acceptor and donor

defects vs system geometrical parameters. Calculations revealed that the electronic structure of the system strongly depends on system geometry on the one hand, and impurity location on the other hand. For the quantum wells with total thickness bellow 5 nm increase of hole conductivity is predicted by thermodynamic analyses.

Acknowledgment:
The work is supported by Shota Rustaveli National Science Foundation of Georgia, Grant Number STEM-22-188.

References:

[1] Chikoidze E., et al. Materials Today Physics, 2017, 3, 118-126
[2] Chikoidze E., T. Tchelidze T., et al. Materials Today Physics, 2017, 15, 100263
[3] Shun Zhou et al. Journal of Vacuum Science & Technology, 2021, A 39, 030403.