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Short Communication

Some Aspects of Phosphorus Diffusion in Germanium in $In_{0,01}Ga_{0,99}As$ / $In_{0,56}Ga_{0,44}P$ / Ge Heterostructures

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The results of experimental and theoretical researches of phosphorus distribution in the first cascade of a multi cascade solar cell based on nanoscale structures AIIIBV / Ge are presented. Secondary ion mass spectroscopy has been applied to obtain profiles of phosphorus and gallium in $In_{0.01}Ga_{0.99}As$ / $In_{0.56}Ga_{0.44}P$ / Ge heterostructure. In the germanium surface there is a thin layer of about 26 nm, in which the gallium concentration exceeds the concentration of phosphorus. Therefore a nanoscale *p-n* junction forms that does not have a significant impact on the solar cells performance at room temperature. Phosphorus diffusion is much slower in this area than in area with electronic conductivity. The main *p-n* junction is formed at a distance of 130-150 nm from the surface of the germanium. Diffusivity of gallium ($D_{Ga} = 1,4\cdot10^{-15}$ cm²/s) is markedly higher than described in a literature. Diffusivity of *P* increase from $D_P = 3\cdot10$-15 cm²/s on the boundary of the heterostructure $In_{0,49}Ga_{0,51}P$ to $D_P = 5,2\cdot10^{-14}$ cm²/s in *n*-type Ge.

Keywords: Multi cascade solar cell, Diffusion of P in Ge, Diffusion of Ga in Ge, Heterostructure.

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1. INTRODUCTION

During the last decade Ge has received renewed attention as a potential material for nanoscale electronic. In particular the best multi cascade A^3B^5 solar cells are produced on the Ge substrate and transformation of the infrared part of solar energy to electric power is performed by Ge subelement [1-2]. *p-n* junction in the wide-gap semiconductor materials of multi cascade solar cells is produced during epitaxial growth, while phosphorus diffusion is used for the creation of the *p-n* junction in germanium subelement. The optimization of the *p-n* junction depth requires accurate dopant diffusion modeling in germanium. However, the current knowledge on dopant behavior in Ge is still rather poor as compared to that of Si. Although recent experimental data appear in complement to the earlier (40 years old) ones, the underlying physical mechanisms are not fully understood [3-9]. A vacancy-assisted mechanisms generally accepted, but details such as exact charge state of the defects, the roles of the simple exchange mechanism, or PV pair diffusion mechanism, are not clear. Experiments on the intrinsic (P concentration less than the intrinsic carrier concentration at the diffusion temperature) and extrinsic diffusion of the *n*-type dopants in Ge demonstrate an enhanced diffusion of these dopants with increasing doping level [5-8]. The ratio between the intrinsic D_{in} and extrinsic D_n diffusivities at a given temperature equals the squared [5] or cubic [7] ratio between the free electron concentration n and the intrinsic carrier concentration n_{in}. The diffusion model that describes these tendencies is based on the proposal of constant vacancy concentration and dominant role of V-P charged pairs in the diffusion [10]. Some experiments on co-diffusion have shown that P diffusion suppression [8, 9] demonstrates a strong dependence of diffusion process on the presence of other impurities in Ge. To produce comparatively shallow (less than 200 nm) *p-n* junction in Ge subelement, P diffusion should be make in heavily doped Ge. The aim of this work is to investigate the diffusion profiles of phosphorus in germanium in the $In_{0,01}Ga_{0,99}As$ / $In_{0,56}Ga_{0,44}P$ / Ge heterostructures.

2. EXPERIMENTAL DETAILS

The germanium *p*-type wafers, (100) orientation, heavily gallium doped ($N_{Ga} = 10^{18}$ cm^{-3}), were used.

The samples for the research were obtained by CVD method in the VEECO E450 LDM reactor. Three steps at $T = 635$ °C were used for Ge subelement creation: treatment at the phosphine flow (2.5 min), $In_{0,56}Ga_{0,44}P$ buffer layer growth (1 min), $In_{0,01}Ga_{0,99}As$ layer growth (1,6 min). Secondary ion mass spectrometry (SIMS) was carried out by PHI-6600 spectrometer for elements profiling. As it was shown previously [11] there were no significant changes in the element profiles when flux of phosphine increased from 600 to 1200 cm³/min. The main source of phosphorus in Ge substrate is $In_{0,56}Ga_{0,44}P$ buffer layer having thickness of about 24 nm, so the diffusion time is 2,6 min [11]. Electrochemical profiling was carried out by profilometer ECV Pro.

3. RESULTS AND DISCUSSION

Typical profiles of elements in the examined structures are shown on Fig. 1. The most surprising results are high P and Ga concentrations on the Ge surface and significant diffusion of Ga in Ge from buffer layer.

There are two regions on the P profile characterized by different phosphorus diffusivity D_P. In the germanium surface there is a thin layer of about 26 nm, in which gallium concentration exceeds the concentration of phosphorus. Therefore a nanoscale *p-n* junction forms

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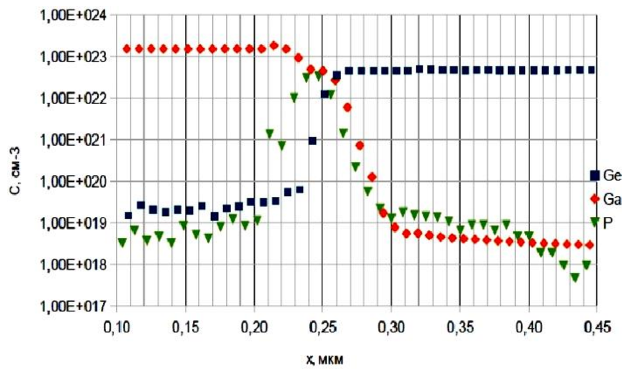

Fig. 1 – Profiles P, Ga and Ge in the investigated structures

that does not have a significant impact on the solar cell performance at room temperature. The existence of the additional *p-n* junction confirmed by electrochemical profiling (Fig. 2). Phosphorus diffusion is much slower in this area than in area with electronic conductivity. The main p-n junction is formed at a distance of 130-150 nm from the surface of the germanium.

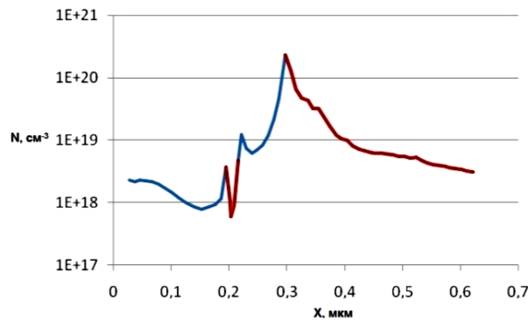

Fig. 2 – Results of electrochemical profiling of $In_{0.01}Ga_{0.99}As$ / $In_{0.56}Ga_{0.44}P$ / Ge heterostructure

Different diffusion mechanisms were analyzed to predict the dependence of the *p-n* junction depth. The *p*-type surface with low electron concentration leads to prediction of low diffusion coefficient D_p according to vacancy-assisted models [5, 7] (see Fig. 3). Using these diffusivities leads to very low P concentration. Together with high Ga concentration it leads to the inability to obtain *n*-type region in this structure. Experimental phosphorus diffusivity is greater than predicted one. The comparison of the literature data and calculated Ga and P diffusivities based on the 2-nd Fikes law are shown in Table 1. Experimental and calculated profiles for two regions are shown on the fig. 4, 5. As we can see, Ga diffusivity is higher than the literature data [4].

In contrary to previous experimental results, phosphorous diffusivity increase with drops of the P concentration. There are some reasons for observed distinctions. A vacancy-assisted mechanisms proposed existence of the thermal equilibrium concentration of vacancies in Ge. Really a high Ga and P concentration in the surface area may cause changing in the vacancy distribution. Moreover it may lead to changing VP charge diffusion mechanism to simple exchange or interstitial one. To calculate diffusion profiles in this case we need to include generation and recombination terms to continuity equation as it was done for diffusion profiles calculation in Si with taking into account kick-out mechanism [12].

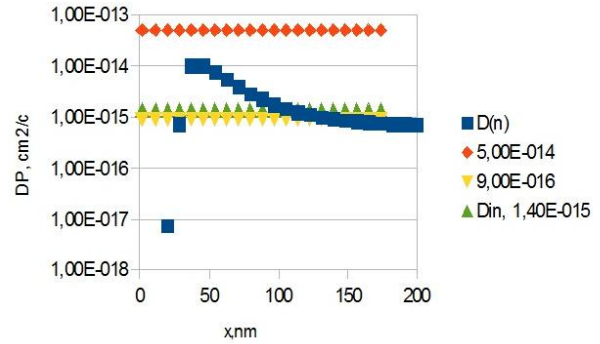

Fig. 3 – Diffusivity in P SIMS profiles of P (P(1)), Ga (Ga(1)) and calculated profiles: P (P(2), $D_P = 3 \cdot 10^{-15}$ cm²/s) and Ga (Ga(2), $D_{Ga} = 1{,}4 \cdot 10^{-15}$ cm²/s) in germanium

Table 1 – The diffusion coefficients ($D \cdot 10^{15}$, cm²/s) in the surface area at T = 635 °C

P [3]	P [8]	P [7]	Ga [4]	Ga [4]	Ga	P (1)	P (2)
43	1,40	0,88	0,23	0,06	1,4	3,0	52

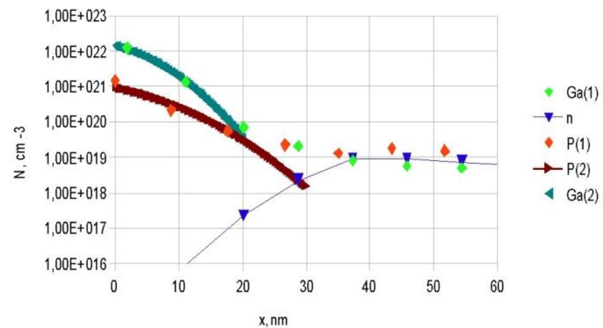

Fig. 4 – SIMS profiles of P (P(1)), Ga (Ga(1)) and calculated profiles: P (P(2), $D_P = 3 \cdot 10^{-15}$ cm²/s) and Ga (Ga(2), $D_{Ga} = 1{,}4 \cdot 10^{-15}$ cm²/s) in germanium.

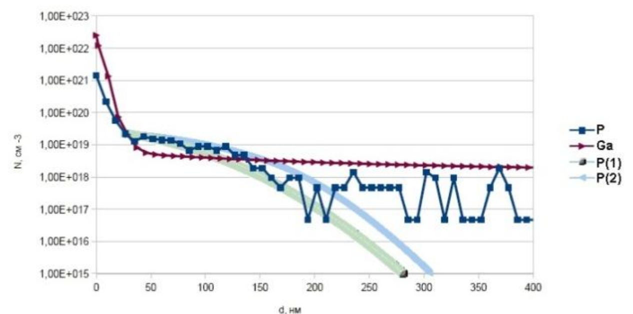

Fig. 5 – SIMS profiles of P, Ga and calculated profiles: P ($D_P = 5{,}2 \cdot 10^{-14}$ cm²/s, P(1)-based on the second Fick's law), P (P(2) – taking into account field effect)

4. CONCLUSIONS

Co-diffusion of Ga and P has been observed in $In_{0,56}Ga_{0,44}P$ / Ge heterostructure at 635 °C. The presence of high P and Ga concentration in the surface area leads to a significant acceleration of the Ga diffusion and influence on the P diffusion. It was demonstrated that when phosphorus concentration decreased from $2 \cdot 10^{22}$ cm^{-3} to $1{,}5 \cdot 10^{19}$ cm^{-3}, then D_P increased from $3 \cdot 10^{-15}$ cm²/s to $5{,}2 \cdot 10^{-14}$ cm²/s.

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