Identification of conditions for the formation of deep states of mismatch dislocations and DX centers in heteroepitaxial lightly doped $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs-layers

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High-voltage gradual p^0-i-n^0-junctions of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}As_{1-y}Sb_y$ with a maximum content of x from 0.15 to 0.6 and y to 0.02, obtained by liquid-phase epitaxy due to autodoping with background impurities, have been studied using methods of capacitance-voltage characteristics and deep-level transient spectroscopy. It was found that the effective recombination trap in the heteroepitaxial layers of $Al_xGa_{1-x}As$/GaAs and $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs with x more than 0.23, regardless of the antimony content, is the DX center of background donor impurities Si, Se, or Te, while these heterostructures lacked deep levels associated with dislocations. In the $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs heterostructures with $x \sim 0.15-0.19$ and $y \sim 0.02$ and $GaAs_{1-y}Sb_y$/GaAs with $y \sim 0.02$, the deep HD3 level associated with mismatch dislocations is an effective recombination trap.

Keywords: AlGaAsSb, p^0-i-n^0-junction, capacitance spectroscopy, DLTS, DX center, mismatch dislocations, liquid-phase epitaxy.

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1. Introduction

Wide-band weakly doped heteroepitaxial layers of AlGaAs/GaAs and AlGaAsSb/GaAs used in the manufacture of pulsed high-voltage $p-i-n$-diodes capable of operating in the megahertz pulse repetition frequency range and at high temperatures, $> 300\,^\circ$C [1–5], are currently of interest because of their potential applications in high-voltage high-speed and optoelectronic devices. The epitaxial growth of such heterostructures is accompanied by deformation of the growing layer, which occurs due to the difference in lattice parameters between it and the substrate [1–3,6,7]. If the epitaxial layer is thin enough, the mismatch of the lattice can be compensated by elastic deformation of the layer [5–7]. However, when the layer thickness exceeds a certain critical value, mismatch dislocations are generated at the interface to remove some of the deformation. The presence of mismatch dislocations at the interface between the layer and the substrate can lead to the appearance of deep energy states in the band gap, which act as traps for free charge carriers. Previously, it was found [3,4,6,8] that a two-dimensional grid of 60° mismatch dislocations was formed in weakly doped heteroepitaxial layers of InGaAs/GaAs and GaAsSb/GaAs due to the difference in lattice constants between GaAs and the ternary compound (with a Sb or In content of about $0.3-1.5\,\%$ and thicknesses of the heteroepitaxial layer of $\sim 50\,\mu$m). The heteroepitaxial InGaAs/GaAs and GaAsSb/GaAs layers with mismatch dislocations were characterized by the manifestation in the DLTS spectra of the so-called dislocation spatially localized (1D dimension) deep levels (DL) of the donor (ED1) and acceptor (HD3) types with thermal activation energies of 683 and 848 meV.

An unexpected result was obtained by capacitive spectroscopy when studying smooth p_0-i-n_0-junctions of $Al_xGa_{1-x}As_{1-y}Sb_y$ from x to 0.34 and y to 0.15, with thickness of $\sim 50\,\mu$m [2] — despite the fact that the antimony content in the heteroepitaxial layer was sufficient for the formation of dislocations, there were no peaks in the DLTS spectra, dislocation-related inconsistencies [4,6–8]. Instead, the DLTS peak of the DX center was observed in the spectra, characteristic of compounds $Al_xGa_{1-x}As$ at $x \geq 0.23$ [1,2,9–11]. It should be noted that the study of smooth p_0-i-n_0-junctions of $Al_xGa_{1-x}As_{1-y}Sb_y$ is a difficult task, since the presence of atoms of two types of groups III and V creates a non-trivial growth environment and creates a large space for interpreting experimental results.

The purpose of this paper is to identify the technological conditions under which defects with DL and mismatch dislocations occur in heteroepitaxial layers $Al_xGa_{1-x}As_{1-y}Sb_y$ smoothp_0-i-n_0-junctions with varying concentrations of aluminum (x) and antimony (y) compounds produced by liquid phase epitaxy (LPE). The diodes were studied using volt-faraday $(C-V)$ characteristics and deep-level transient spectroscopy (DLTS), which made it possible to detect both electron and hole traps in $Al_xGa_{1-x}As_{1-y}Sb_y$ in smooth p^0-i-n^0-junctions.

2. Experimental samples

High-voltage $p^+-p^0-i-n^0-n^+$-diodes based on heteroepitaxial layers $Al_xGa_{1-x}As$/GaAs and

$Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs were produced using a modified liquid-phase epitaxy method [1–5] in a graphite cartridge of a flowing type in a hydrogen atmosphere. Epitaxial growing of high-voltage weakly doped smooth p^0-i-n^0-junctions of solid solution of $Al_xGa_{1-x}As$ or $Al_xGa_{1-x}As_{1-y}Sb_y$ was conducted on p^+-GaAs (100) substrates doped with zinc to a concentration of $5 \cdot 10^{18}\,cm^3$, under forced cooling of limited solution-melts of Al–Ga–As or Al–Ga–As–Sb in the temperature range from 900–850 to 750–700 °C, after which heavily-doped n^+-GaAs emitter layers with a concentration of free electrons of $\sim 2 \cdot 10^{18}\,cm^{-3}$ were grown on them.

The work studied $p-i-n$-structures based on weakly doped layers of $Al_xGa_{1-x}As$, $Al_xGa_{1-x}As_{1-y}Sb_y$ and $GaAs_{1-y}Sb_y$ with a maximum content of x from 0.15 to 0.6 and y to 0.02, up to 50 μm thick, obtained by the liquid-phase epitaxy method due to auto-doping with background dopants. The method of manufacturing smooth p^0-i-n^0-junctions using the method used in the study from a single solution-melt due to autodoping with background impurities was described earlier in Refs. [1–5].

3. Results and discussion

3.1. Measurements of C–V-characteristics of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}As_{1-y}Sb_y$ diode $p^+-p^0-i-n^0-n^+$-heterostructures

Preliminary analysis of the chips manufactured by us (in this paper and earlier) with smooth p^0-i-n^0-$Al_xGa_{1-x}As$/GaAs and Al_xGa_{1-x}-heterojunctions of $As_{1-y}Sb_y$/GaAs suggests the presence in the epitaxial layers of the structure of donor impurities (Si, Se, Te) responsible for the formation of configurationally bistable DX centers [9–13].

Studies of $C-V$-characteristics at 300 and 87 K with different measurement conditions were conducted to identify DX centers in p^0-i-n^0-heterostructures. We have previously used the technique of such measurements to identify bistable defects in Refs. [2,5]. In the case of measurements at 87 K, the sample was pre-cooled either with the reverse bias voltage of $V_r < 0$ turned on, or at $V_r = 0$. $C-V$-measurements were carried out either in the dark or with optical illumination. A significant difference in $C-V$-characteristics was observed after pre-cooling the sample with $V_r < 0$ or $V_r = 0$. At $V_r < 0$ $C-V$-characteristic was determined by a change in the diffusion potential; the thickness W of the space charge layer (SCL) significantly increased at $V_r = 0$ and the effective concentration of free carriers decreased by almost an order of magnitude [2,5]. $C-V$-characteristic remained unchanged for a long time at a low temperature after switching off the lighting, which is explained by the so-called residual photoconductivity effect. The observed changes in the $C-V$-characteristics as shown in Ref. [5,10] are inherent in the DX center with negative correlation energy U and indicate the presence of donor impurities (Si, Se, Te) in epitaxial

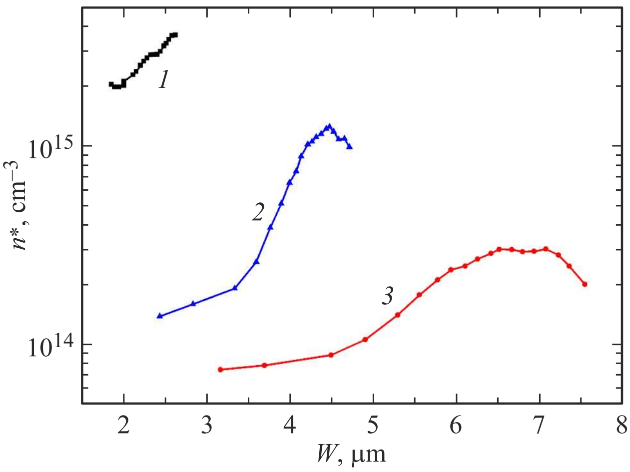

Figure 1. Distribution profiles of the effective concentration of free charge carriers n^* over the thickness W of the layer of a space charge of $p^+-p^0-i-n^0$-diode based on heteroepitaxial layers of $Al_xGa_{1-x}As$/GaAs c $x \sim 0.6$, measured at various temperatures T, K: *1* — 151; *2, 3* — 88; in darkness (*1, 3*) and with optical illumination (*2*).

layers $Al_xGa_{1-x}As_{1-y}Sb_y$ that have one delocalized DX^+-state of shallow donor and two deep localized DX^0- and DX-states. $C-V$-characteristics similar to those described above were observed for the epitaxial layers of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}As_{1-y}Sb_y$ with a maximum content of x from 0.23 to 0.6 and y to 0.02. Figure 1 shows the results of $C-V$-studies of a diode $p^+-p^0-i-n^0-n^+$ $Al_xGa_{1-x}As$/GaAs-heterostructure cooled with $V_r < 0$ either in the dark, or with optical illumination. The distribution profiles of the effective concentration of free carriers of charge n^* over the thickness of the space charge layer W were calculated from the measured $C-V$-characteristics (see Figure 1). The curve *1* was obtained for the temperature of measurements of $C-V$-characteristics $T = 151$ K, and the curves *2* and *3* were measured at $T = 88$ K and, respectively, with optical illumination and in the dark. Similar dependences on the measurement temperature and the presence of illumination in the profiles $n^*(W)$ were observed for the layers of $Al_xGa_{1-x}As_{1-y}Sb_y$. The effect of residual photoconductivity in the $C-V$-characteristic was not observed in the case when the molar composition of x did not exceed 0.20 (Figure 2). For these heterostructures, the thickness of the SCL increased with a decrease in the temperature of the sample measurement as noted in our paper [5], the increase in the thickness of the SCL with a temperature change from 300 to 86 K significantly exceeded the values calculated for the temperature behavior of the diffusion potential. The dependence of the effective concentration of free charge carriers (n^*) on the presence of optical illumination of the sample was also revealed for this $Al_xGa_{1-x}As_{1-y}Sb_y$-heterostructure with $y \sim 0.02$ (Figure 2, curve *2*). The illumination of the structure led to a decrease in the thickness of the SCL at both 90, 200, and 300 K. The most probable reason for these changes in the thickness of

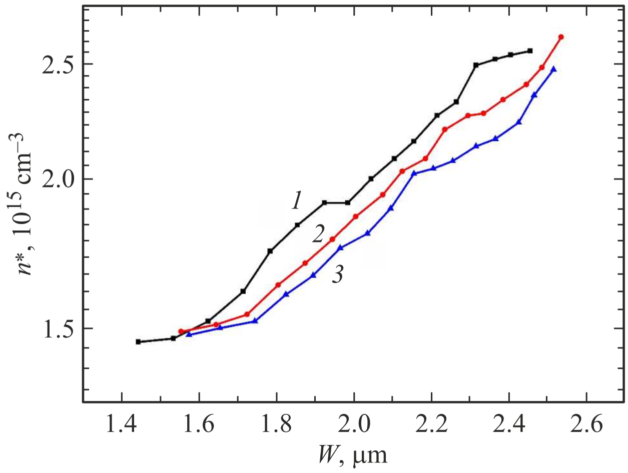

Figure 2. Distribution profiles of the effective concentration of free charge carriers n^* over the thickness W of the space charge layer of $p^+-p_0-i-n_0$-diode based on heteroepitaxial layers of $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs with $x \sim 0.2$ and $y \sim 0.02$ measured at different temperatures T, K: *1* — 200; *2, 3* — 90; in the dark (*1, 3*) and with optical illumination (*2*).

SCL with temperature and illumination is the deep interface states of the donor and acceptor types at the heterogeneous boundaries of the $p^+-p^0-i-n^0-n^+$-structure. The effect of the density of interface states N_{ss} on the $C-V$-characteristic of the $p-n$-junction was studied in detail in Ref. [4]:

$$\frac{1}{C^2} = -\frac{2(\varepsilon_n N_d + \varepsilon_p N_a)}{q\varepsilon_n\varepsilon_p N_d N_a}(U - U_0) - \frac{N_{SS}^2}{\varepsilon_n\varepsilon_p N_d N_a}, \qquad (1)$$

where U_0 is the diffusion potential, U is the reverse displacement, ε_n and ε_p is the dielectric constants n- and p-layers, N_d and N_a is the concentration of donors and acceptors in n- and p-layers, respectively.

The first member of the ratio (1) is related to the capacitance of the $p-n$-junction, which varies with the applied bias voltage and distribution of concentrations N_d and N_a in n- and p-layers, and the second member with a density of interface states N_{ss}, the occupation of which can vary with the measurement temperature and the position of the Fermi level in the structure. Optical illumination of $p^+-p^0-i-n^0-n^+$-heterostructure can lead to a change in the position of the Fermi level and, accordingly, to a change in the population of localized interface states by carriers when deep levels of donor and acceptor defects are present in the epitaxial layers at concentrations comparable to those of shallow levels. Therefore, the presence of interface states may be associated with the formation of mismatch dislocations at the heterogeneous boundaries of the structures under study.

In the case of p^0-i-n^0-structures based on GaAs, studies have shown no changes of $C-V$-characteristics depending on the conditions of pre-cooling of the sample at $V_r < 0$ or at $V_r = 0$ and with optical illumination.

3.2. DLTS-measurements of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}As_{1-y}Sb_y$ of diode $p^+-p^0-i-n^0-n^+$-heterostructures

For diode $Al_xGa_{1-x}As_{1-y}Sb_y$-heterostructures with $x = 0.00$, ~ 0.20, ~ 0.30, ~ 0.60 and $y = 0.00$, ~ 0.01, ~ 0.02 DLTS spectra were measured at different bias voltages V_r and fill-in pulses V_f (Figures 3–6). It turned out that the DLTS spectra of the studied $p^+-p^0-i-n^0-n^+$-diodes significantly differ depending on the molar composition (x and y) of the layers forming these heterostructures. Two types of heterostructures can be distinguished based on the obtained DLTS spectra. The first type includes structures with layers of triple $Al_xGa_{1-x}As$ (Figure 3) and quadruple $Al_xGa_{1-x}As_{1-y}Sb_y$ (Figure 4) compounds with x from 0.23 to 0.60, for which peaks with a positive sign

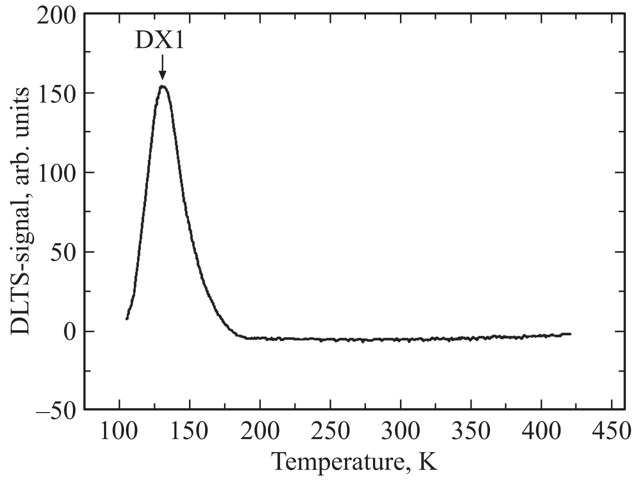

Figure 3. DLTS spectrum of $p^+ - p^0-i-n^0-n^+$-diodes of $Al_xGa_{1-x}As$/GaAs with $x \sim 0.6$ obtained at a window temp of 200 s^{-1}, bias voltage $V_r = -2.98$ V and fill-in pulse voltage of $V_f = +0.87$ V.

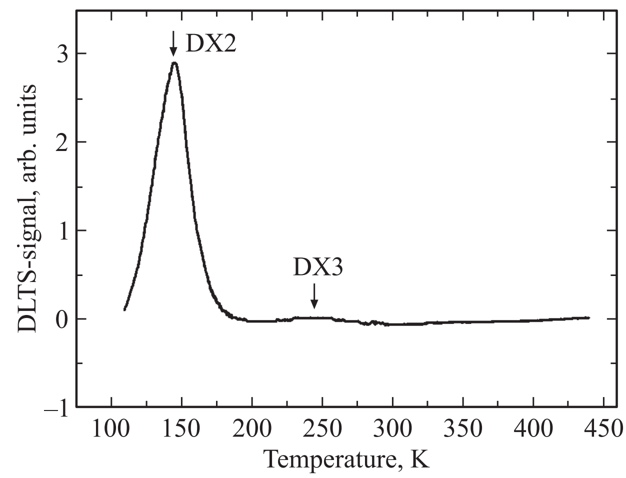

Figure 4. DLTS spectrum of $p^+-p^0-i-n^0-n^+$-diodes of $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs with $s \sim 0.3$ and $y \sim 0.02$, obtained at a window temp of 200 s^{-1}, bias voltage of $V_r = -1.12$ V and fill-in pulse voltage of $V_f = +0.54$ V.

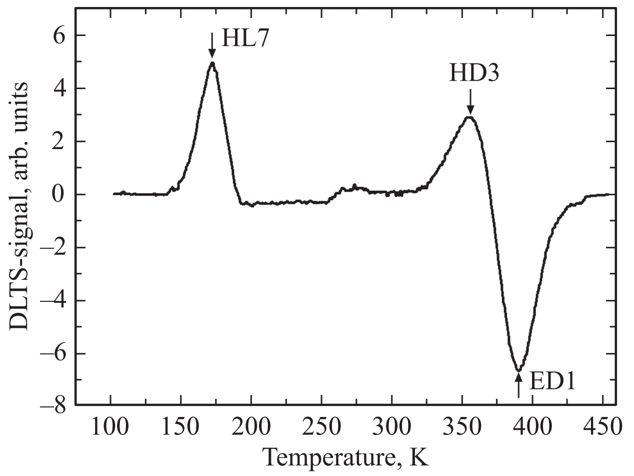

Figure 5. DLTS-spectrum of $p^+-p^0-i-n^0-n^+$-diodes of $GaAs_{1-y}Sb_y/GaAs$ with $y \sim 0.02$ obtained at a window temp of $200\,s^{-1}$, bias voltage of $V_r = -3.0\,V$ and the voltage of the fill-in pulse of $V_f = +0.50\,V$.

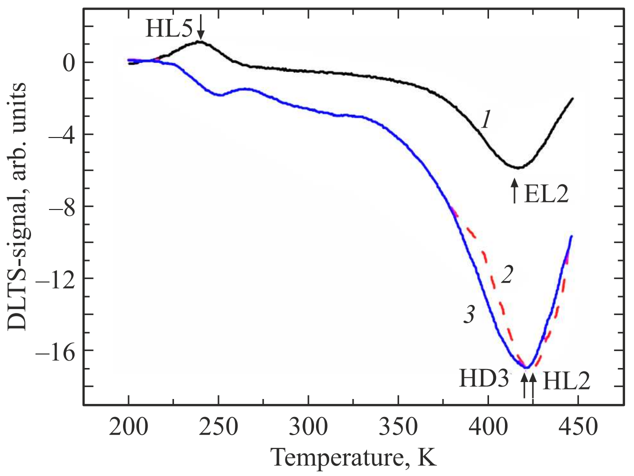

Figure 6. DLTS -spectrum of $p^+-p^0-i-n^0-n^+$-diodes of $Al_xGa_{1-x}As_{1-y}Sb_y/GaAs$ c x up to 0.19 and $y \sim 0.02$, obtained at a window temp of $200\,s^{-1}$, bias voltage of $V_r = -3.0\,V$ and fill-in pulse voltage of $V_f = +0.93\,V$ (*1*); at $V_r = +0.05\,V$ and $V_f = +0.93\,V$, in the dark (*2*) and with optical illumination (*3*).

associated with the acceptor-like state of the DX-center are detected in the DLTS spectra. These DX-states are traps of the main carriers (electrons) [5]. The thermal activation energy $E_t = 342\,meV$(DX1) and the electron capture cross section $\sigma_n = 8.91 \cdot 10^{-11}$ were determined from the Arrhenius dependence for the studied layer of $Al_xGa_{1-x}As$ with $x \approx 0.60\,cm^2$. In epitaxial layers of quadruple compounds of $Al_xGa_{1-x}As_{1-y}Sb_y$ containing antimony atoms with $y = 0.01$ and aluminum with $x \sim 0.30$, the DX-level had the following parameters, respectively: $E_t = 234\,meV$ (DX2) and $\sigma_n = 5.29 \cdot 10^{-15}\,cm^2$. The parameters of the DX^--level of these two structures indicate that the DX center detected in the DLTS spectra is apparently formed by background donor impurities Te and Se [5,14].

A higher temperature peak with parameters $E_t = 416\,meV$ and $\sigma_n = 5.08 \cdot 10^{-15}\,cm^2$ (DX3), which may be related to the DX level of the Si donor impurity, was also observed in the DLTS spectra for $Al_xGa_{1-x}As_{1-y}Sb_y$-structures with $y = 0.01$ and $x \sim 0.30$. Similar DLTS peaks were found for all $Al_xGa_{1-x}As_{1-y}Sb_y$structures with x from 0.23 to 0.60, with the difference that the capture cross-section σ_n increased for the structure with $x \sim 0.60$.

The second type of heterostructures includes structures with smooth p^0-i-n^0-junctions, such as $GaAs_{1-y}Sb_y/GaAs$ [7] and $Al_xGa_{1-x}As_{1-y}Sb_y$ with $x \sim 0.15-0.19$ and $y \sim 0.02$, for which peaks associated with mismatch dislocations are detected in the DLTS spectra (Figures 5 and 6). The traps of the majority and minor carriers were detected by conducting measurements at different bias voltages V_r and fill-in pulses V_f. For identifying the properties inherent in localized states of dislocations, additional studies of the effect of optical illumination on their filling with carriers were conducted. This technique was first used by us in Ref. [5] to identify the localization of dislocation levels. Deep traps for electrons and holes are clearly detected in the structures of $GaAs_{1-y}Sb_y/GaAs$ with $y \sim 0.02$ (Figure 5), as well mismatches associated with dislocations, designated as ED1 and HD3, the parameters of which were respectively: $E_t = 651\,meV$ and $\sigma_n = 2.15 \cdot 10^{-15}\,cm^2$ and $E_t = 721\,meV$ and $\sigma_p = 3.34 \cdot 10^{-14}\,cm^2$. Previously, these traps have been thoroughly studied and described in a number of papers [6–8], including in our articles [4]. The conducted studies of DLTS spectra in $Al_xGa_{1-x}As_{1-y}Sb_y/GaAs$ heterostructures with smooth p^0-i-n^0-junction also revealed a deep level, which could be identified with dislocation HD3 (Figure 6). It was possible to distinguish two peaks and identify them for a wide DLTS peak formed during measurements of DLTS spectra with $V_r = +0.04\,V$ and $V_f = +0.93\,V$ in the dark and with optical illumination caused by the emission of holes from deep states in the p^0-layer. The illumination led to the manifestation of the second DLTS peak from low temperatures. The dependence of the peak amplitudes of DLTS signals on optical illumination is a characteristic feature of such spatially localized states as quantum dots [15] and mismatch dislocations [4]. This distinguishes them from point defects with deep levels distributed over the entire thickness of the epitaxial layer. The parameters of these two deep states were determined using the Arrhenius dependencies. For the deep states of holes associated with dislocations, they were respectively: $E_t = 735\,meV$ and $\sigma_p = 3.78 \cdot 10^{-16}\,cm^2$, and for the second state, which does not exhibit localization properties and is a point defect, they were: $E_t = 881\,meV$ and $\sigma_p = 1.8 \cdot 10^{-14}\,cm^2$. A similar level in the layers of $Al_xGa_{1-x}As$ with $x \sim 0.20$ was previously observed in Ref. [16]. We defined it as the condition of the HL2 [4] defect with a hole trap. It was not possible to identify the dislocation level for the electron traps located in the n^0-layer and causing the presence of a DLTS peak with a negative sign. The parameters of the electron trap were close to the level of the EL2 defect with $E_t = 837\,\text{meV}$ and $\sigma_n = 6.06 \cdot 10^{-14}\,\text{cm}^2$, which is not surprising for compounds grown at temperatures of $> 850\,^\circ\text{C}$ using the LPE method [17].

4. Conclusion

High-voltage $p^+{-}p^0{-}i{-}n^0{-}n^+$-diodes based on AlGaAs/GaAs and AlGaAsSb/GaAs heteroepitaxial layers, as well as GaAsSb/GaAs, obtained by liquid-phase epitaxy due to autodoping with background impurities, were studied in this work. Using methods of capacitance-voltage characteristics and deep-level transient spectroscopy it was found that the DX center of background donor impurities Si, Se or Te is the effective recombination trap in smooth $p^0{-}i{-}n^0$-heterojunctions of $Al_xGa_{1-x}As$ and $Al_xGa_{1-x}As_{1-y}Sb_y$ with $x > 0.23$, regardless of the antimony content, while the capture cross-section of the trap σn increased with the increase of the composition of x. No deep levels associated with dislocations were found in the studied $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs heterostructures with $x \geq 0.23$ and with a mismatch in the lattice parameter sufficient for the formation of mismatch dislocations. A deep HD3 level associated with mismatch dislocations is an effective recombination trap in $Al_xGa_{1-x}As_{1-y}Sb_y$/GaAs heterostructures with $x \sim 0.15{-}0.19$ and $y \sim 0.02$ and $GaAs_{1-y}Sb_y$/GaAs with $y \sim 0.02$. We have previously found a similar level in heteroepitaxial structures InGaAs/GaAs and GaAsSb/GaAs with mismatch dislocations.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] M.M. Sobolev, F.Yu. Soldatenkov. FTP, **57** (8), 644 (2023). (in Russian).
[2] F.Y. Soldatenkov, M.M. Sobolev, A.S. Vlasov, A.V. Rozhkov, Surface. Rentgenovskie, sinkhrotronnye i neytronnye issledovaniya, (in Russian). № 7, 19 (2024). DOI: https://doi.org/10.31857/S1028096024070037
[3] F.Yu. Soldatenkov, V.G. Danil'chenko, V.I. Korol'kov. FTP, **41** (2), 217 (2007).
[4] M.M. Sobolev, F.Y. Soldatenkov, L. Shul'pina. J. Appl. Phys., **123**, 161588 (2018). DOI: 10.1063/1.5011297
[5] M.M. Sobolev, F.Y. Soldatenkov, V.G. Danil'chenko. J. Appl. Phys., **128** (9), 095705 (2020). https://doi.org/10.1063/5.0018317
[6] T. Wosinski. J. Appl. Phys., **65** (4), 1566 (1989).
[7] T. Wosinski, O. Yastrubchak, A. Makosa, T. Figielski. J. Phys.: Condens. Mater., **12** (49), 10153 (2000). DOI: 10.1088/0953-8984/12/49/314
[8] O. Yastrubchak, T. Wosinski, A. Makosa, T. Figielski, S. Porowski, I. Grzegory, R. Czernecki, P. Perlin. Eur. Phys. J.: Appl. Phys., **27**, 201 (2004). https://doi.org/10.1051/epjap:2004139
[9] D.J. Chadi, K.J. Chang. Phys. Rev. B, **39**, 10063 (1989). DOI: https://doi.org/10.1103/PhysRevB.39.10063
[10] W.Y.-S. Su, V.C.-P. Lu, C.-B. Wu, J.-Sh. Wang, J.-L. Shen, K.-Ch. Chiu. Scientific Rep., **10**, 12503 (2020). DOI: https://doi.org/10.1038/s41598-020-69153-1
[11] M. Anbinderis, S. Ašmontas, A. Čerškus, J. Gradauskas, A. Lučun, A. Šilėnas, A. Sužiedėlis. Sensors, **21** (13), 4487 (2021). DOI: https://doi.org/10.3390/s21134487
[12] D.V. Lang, R.A. Logan, M. Jaros. Phys. Rev. B, **19**, 1015 (1979). https://doi.org/10.1103/PhysRevB.19.1015
[13] L. Dobaczewski, P. Kaczor. Phys. Rev. B, **44**, 8621 (1991). https://doi.org/10.1103/PhysRevB.44.8621
[14] P. Nubile, M. Zazoui, J.C. Bourgoin, R. Grey, A.L. Powell, P.A. Claxton, P.I. Rockett. J. Appl. Phys., **72** (8),3 530 (1992).
[15] M.M. Sobolev, A.R. Kovsh, V.V. Ustinov, A.Y. Egorov, A.E. Zhukov, Y.G. Musikhin. J. Electron. Mater., **28**, 491 (1999).
[16] D.V. Lang. J. Appl. Phys., **45**, 3023 (1974).
[17] M.M. Sobolev, P.N. Brunkov, S.G. Konnikov, M.N. Stepanova, V.G. Nikitin, V.P. Ulin, A.Sh. Dolbaya, T.D. Kamushadze, R.M. Majsuradze. FTP, **25** (6), 1058 (1989). (in Russian).

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