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EFFECT OF IMPURITY AND RADIATION DEFECTS ON ANISOTROPY OF Yb-DOPED GaS SINGLE CRYSTAL

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The effect of γ-quanta on the anisotropy of GaS layered single crystal, pure and alloyed with 0.1at% Yb, has been studied at a temperature range of 125-300K. Since the difference between the ionic radius of the Yb-atom and the ionic radius of the component atoms is relatively small when the studied GaS monocrystal is added with itterbium ions, the additive atom is likely to be located both inside the layers (replacing the Ga atom or between nodes) and in interlayer space. The location of impurity atoms and radiation defects in the interlayer region of the layered GaS (Yb) crystal weakens the anisotropic properties of the crystals, and the location inside the layer strengthens them. The mechanism of current flow in high electric fields follows the Frenkel model, regardless of the nature of the impurity atom.
Keywords: *Anisotropy; Defects; Impurity atom; Electrical conductivity; Activation; Thermal annealing*
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1. INTRODUCTION

Single crystals of gallium sulfide (GaS) have garnered significant attention due to their unique structural and electronic properties, which render them promising candidates for various applications in optoelectronics, photonics, and semiconducting devices [1,2]. One of the key characteristics that distinguishes GaS single crystals is their anisotropic behavior, wherein their physical and electronic properties exhibit directional dependence along different crystallographic axes [3,4].

The anisotropy of GaS single crystals arises from the anisotropic arrangement of atoms within their crystal lattice, leading to variations in properties such as electrical conductivity, optical absorption, and mechanical strength along different crystallographic directions. Understanding and characterizing this anisotropy is crucial for tailoring the material's properties to specific applications and optimizing device performance.The study of anisotropy in semiconductor materials plays a crucial role in understanding their electronic, optical, and structural properties, which are fundamental for various technological applications[5,6]. The investigation of radiation-induced defects and their impact on the anisotropic properties of semiconductor materials holds significant importance in various fields of science and technology. Yb-doped GaS single crystals, with their unique electronic and optical properties, are of particular interest for optoelectronic applications. Understanding the effect of radiation defects on the anisotropy of Yb-doped GaS is crucial for optimizing their performance in radiation-sensitive devices such as radiation detectors and sensors [1,7-10].

Radiation defects, induced by exposure to ionizing radiation, can lead to the creation of vacancies, interstitials, and dislocations within the crystal lattice of semiconductor materials [11-14]. These defects can alter the material's electronic structure, transport properties, and optical characteristics, thereby influencing its anisotropic behavior along different crystallographic directions. In the case of Yb-doped GaS, the interaction between radiation and the crystal lattice can result in complex defect configurations, impacting its conductivity, mobility, and optical absorption properties [7,9].

Despite the potential applications of Yb-doped GaS in optoelectronic devices, limited research has been conducted to investigate the specific effects of radiation defects on its anisotropic behavior. Therefore, a comprehensive understanding of the interaction between radiation-induced defects and the anisotropy of Yb-doped GaS is essential for harnessing its full potential in practical applications.

In this study, we aim to explore the effect of radiation defects on the anisotropy of Yb-doped GaS single crystals. By employing advanced characterization techniques such as X-ray diffraction, photoluminescence spectroscopy, and electrical conductivity measurements, we seek to elucidate the underlying mechanisms governing the material's response to ionizing radiation. This research contributes to the fundamental understanding of semiconductor physics and facilitates the development of radiation-resistant optoelectronic devices with enhanced performance and reliability.

2. EXPERIMENTAL TECHNIQUES

The GaS and Yb doped GaS monocrystal investigated in this study was synthesized using the Bridgman–Stockbarger method at high temperatures. To ensure purity, the crucible contained materials with high degrees of purity

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for Ga (99.99%), S (99.999%), and Yb (0.1%). The material in the crucible was completely melted in the hot zone at 1360 K of a two-zone Bridgman furnace and then gradually transferred to the cold zone (823 K) at a speed of 1.2 mm/h. At the outset of synthesis, the furnace temperature was slowly increased to prevent potential explosions due to high temperatures. Homogenization of the melts was achieved by stirring them at the synthesis temperature through gentle shaking of the furnace, followed by cooling within the furnace. Subsequently, the resulting polycrystalline samples were sealed in conical-bottom quartz ampoules under a vacuum of better than 10^{-2} Pa.

The crystal structure and lattice parameters were determined through X-ray analysis, revealing dimensions of a = 3.54 Å, c = 16.6 Å [15]. GaS(Yb) single crystal has p-type conductivity and is $\rho \sim 10^9$ Ohm·cm. Indium was used to make ohmic contact. The electrical properties of GaS and GaS(Yb) samples were studied in the temperature range of 125-300 K, and during the measurement, the electric voltage of the sample was measured using a B7-27A voltmeter. The current generated in the crystal was recorded using a B7-30 voltmeter-electrometer amplifier.

3. DISCUSSION OF RESULTS

Figure 1 shows the dependence of electrical conductivity anisotropy on temperature (T=125-300K) of initial (curve-1) and doped with rare earth element ytterbium (Yb) GaS monocrystal (curve-2) and after irradiation (curve-3,4). It can be seen from the 1st curve in the graph that the $\sigma_{II}/\sigma_{\perp}$ ratio does not change with the increase in temperature in the interval 125-270 K in the GaS monocrystal, it decreases sharply with the subsequent increase in temperature. The existence of an interlayer potential barrier in A_3B_6 type crystals is a fact indicating that the conductivity in the σ_{II}-direction is lower than in the $\sigma_{\perp}$ - direction (Fig. 1, curve-1). The reduction of the $\sigma_{II}/\sigma_{\perp}$- ratio in the interval of 270-300 K occurs as a result of high conductivity in the $\sigma_{\perp}$ - direction. The stability of the $\sigma_{II}/\sigma_{\perp}$-ratio in the range of 125-270 K in the low-temperature region occurs as a result of thermal ionization of shallow energetic levels.

From the temperature dependence of the anisotropy of GaS monocrystal (Yb) (Figure 1, curve-2), it can be seen that the temperature range (190-210 K) where the maximum value of anisotropy is observed shifts to the lower temperature side. In the temperature range of 125-160 K, the value of anisotropy decreases depending on the temperature.The value of anisotropy increases in the next temperature range (160-210 K) and takes the maximum value at 200K.

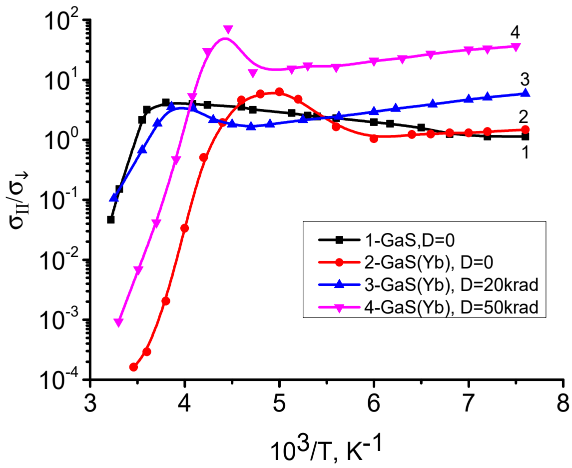

Figure 1. Temperature dependence of electrical conductivity anisotropy in GaS and GaS(Yb) monocrystals before and after irradiation

In the temperature range of 210-300 K, anisotropy sharply decreases with increasing temperature. Adding an additional Yb atom to the GaS crystal shifts the temperature corresponding to the maximum value of the $\sigma_{II}/\sigma_{\perp}$- ratio (curve-1) from 260 K to 230 K, moving it to a lower temperature region (curve-2). During the subsequent decrease in temperature, the $\sigma_{II}/\sigma_{\perp}$-ratio changes weakly. As a result of comparing perpendicular and parallel conductivity, it can be observed that during the addition, the Yb atom occupying the cation vacancy leads to a decrease in the value of the σ_{II} component directed in the parallel direction of the conductivity. Consequently, the maximum value of $\sigma_{II}/\sigma_{\perp}$ is observed at a temperature of 260 K corresponding to the V_{Yb} energy level.

The decrease in anisotropy observed in the 125-230 K temperature range in the GaS<Yb> 0.1 at % single crystal (curve-3) irradiated with a dose of D_γ = 20 krad is compared to the non-irradiated doped crystal (curve-1) and in the temperature range of 230-300 K, the anisotropy increases once again.

As can be seen from the graph, after irradiating the sample, the temperature region (190-210 K) where the maximum value of anisotropy is observed shifts to the higher temperature side. With further increase in temperature, the value of anisotropy decreases again in the temperature range of 210-300 K. When GaS(Yb) single crystal is irradiated with a dose of D_γ = 50 krad (curve-4, Fig. 1), the value of anisotropy in the temperature range of 125-200 K increases compared to (curves 1, 2 and 3). As can be seen from (Curve 4), in the temperature range of 125-220 K, the anisotropy decreases with increasing temperature, and with the subsequent increase in temperature, the anisotropy sharply increases in the temperature range of 220-230K, and it reaches its maximum value at 230 K. With further increase in temperature, the anisotropy decreases again.

A 2D (two-dimensional) [16,17] defect model was applied to clarify the results obtained from the temperature dependence of the anisotropy of the GaS single crystal doped with Yb and exposed to gamma radiation. According to the two-dimensional defect model, at the junction of the layers, the defects accumulated in the direction perpendicular to them create a potential barrier.These conditions lead to the formation of a large number of defects between the layers on the base surface of the GaS single crystal. The resulting defects form a potential barrier for charge carriers in the direction perpendicular to the layers.

The shape of the resulting potential barrier is determined by the degree of loading of defects. In relatively weak fields, the electrical conductivity in the perpendicular direction to the layers is found by the following equation:

$$\sigma\perp=\sigma_{II}\frac{U}{kT^2}\exp[-\frac{U}{kT}+A\frac{U^3}{(kT^3)}], \quad (1)$$

$$A = h/24d^2um^*, \quad (2)$$

σ_{II} - the electrical conductivity of the sample in the absence of a potential barrier, U - the height of the barrier, k - Bolsman's constant, d - the width of the barrier. Let's compare the results obtained for GaS(Yb) single crystal with (curve-1).

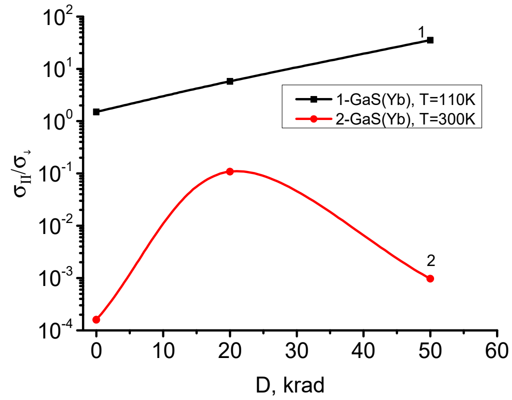

Figure 2. Dependence of the anisotropy of electrical conductivity in GaS(Yb) single crystal at different temperatures on the irradiation dose

Compared to experimental results (1), the passage of charge carriers through the potential barrier at lower temperatures (T < 200K) is tunnel-like and therefore weakly dependent on temperature.

In the temperature range of 220-300 K, the compatibility of the tunneling and activation mechanism removes the potential barrier for charge carriers, and depending on the value of A, different types of properties are revealed in the $\sigma_{II}/\sigma\perp = f(T)$ curve.

Based on the obtained experimental results, the dependence of $\sigma_{II}/\sigma\perp \sim f(D)$ was established at different temperatures. From the comparison of the graphs, we see that as a result of the thermal ionization of the shallow levels formed during irradiation at low temperatures, the dependence of $\sigma_{II}/\sigma\perp \sim f(D)$ increases proportionally, while T = 300K has an exponential character, and as a result of the donor-acceptor interaction of deep levels, an exponential dependence is observed.

According to the obtained experimental results, it can be concluded that the high value of the anisotropy of the electrical conductivity of GaS(Yb) single crystal and their temperature activation dependence are related to the potential barrier and the accumulation of defects between the layers.

Figure 3, Figures 4 and Figure 5 show the effect of thermal annealing on the conductivity anisotropy in the GaS(Yb) crystal $[(\sigma_o-\sigma_{ot})/\sigma_o-\sigma_{krad}) \sim f(t)]$.

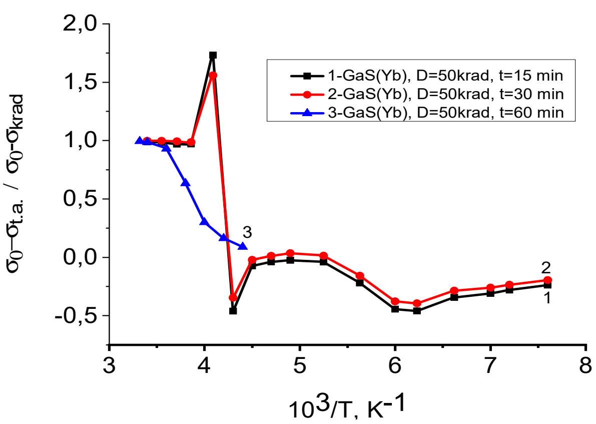

Figure 3. Temperature dependence of the $(\sigma_o/\sigma_{t.a})/(\sigma_o/\sigma_{rad})$ ratio for D = 50 rad of thermally annealed GaS(Yb) single crystal at different times (15 min, 30 min, 60 min).
σ_o – GaS(Yb) – D = 0, σ_{krad} – GaS(Yb) – D = 50 krad
$\sigma_{t.a}$ – GaS(Yb), D = 50 krad, thermal annealing at different times

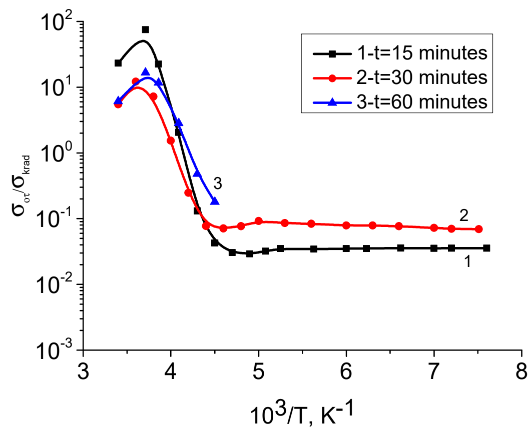

Figure 4. Temperature dependence of $(\sigma_o)/(\sigma_{krad})$ ratio of GaS(Yb) single crystal thermally annealed at different times (15 min, 30 min, 60 min) for D =50 krad:
σ_o – GaS(Yb) – D = 0; σ_{krad} – GaS(Yb) – D = 50 krad

It can be seen from Figure 3 that the ratio (σ_o-σ_{ot})/ σ_o-σ_{krad}) depends on the brewing time and consists of 4 stages. In the 1st stage, defects are settled; In the 2nd stage, the conductivity increases due to the recombination of defects, in the 3rd stage, the conductivity decreases due to the dissociation of complex defects [V_{Ga} Yb_i], and in the 4th stage, the conductivity changes weakly due to the stabilization of defects.

From the obtained results, it can be seen that the restoration of the value of electrical conductivity is complex, as the dependence varies depending on the nature and character of the defects created during exposure to ionizing rays.

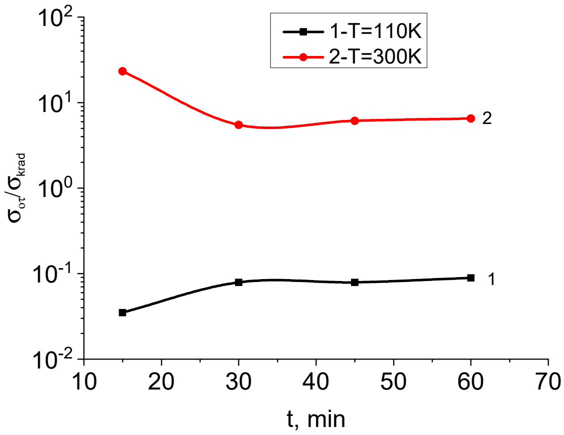

Figure 5. Dependence of the ratio (σ_o)/(σ_{krad}) of the thermally annealed GaS(Yb) single crystal at T = 110 K and 300 K for D = 50krad on the thermal annealing time. σ_o – GaS(Yb) – D = 0; σ_{krad} – GaS(Yb) – D = 50krad

CONCLUSIONS

It was found that partial filling of V_{Ga} occurs in GaS(Yb) crystal before irradiation. During irradiation, the arrangement of defects, formation of VS and complexes is observed. At high radiation doses, dissociation of complex defects occurs. During thermal annealing, the annealing process takes place in different stages depending on the rest energy of the defects. This can be explained by the fact that at the initial stage of annealing (t = 15 minutes), the amount of donor-type radiation defects is greater than the concentration of acceptor-type defects. At this stage, regrouping of defects occurs in the annealing process. During the subsequent period of brewing (15 min < t < 60min), the concentration of charge carriers increases, but the initial parameters of the sample are not restored, which is related to the formation of complex complexes in the process of reassembly of defects [V_S and V_{Ga}].

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ВПЛИВ ДОМІШОК ТА РАДІАЦІЙНИХ ДЕФЕКТІВ НА АНІЗОТРОПІЮ МОНОКРИСТАЛА GaS, ЛЕГОВАНОГО Yb

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Досліджено вплив γ-квантів на анізотропію шаруватого монокристала GaS, чистого та легованого 0,1 ат.% Yb, в діапазоні температур 125-300 К. Оскільки різниця між іонним радіусом атома Yb та іонним радіусом атомів компонента відносно невелика, коли досліджуваний монокристал GaS додається з іонами ітербію, адитивний атом, ймовірно, буде розташований всередині шарів (замінюючи Ga атом або між вузлами) і в міжшаровому просторі. Розташування домішкових атомів і радіаційних дефектів у міжшаровій області шаруватого кристала GaS (Yb) послаблює анізотропні властивості кристалів, а розташування всередині шару посилює їх. Механізм протікання струму в сильних електричних полях відповідає моделі Френкеля, незалежно від природи атома домішки.

Ключові слова: *анізотропія; дефекти; домішковий атом; електропровідність; активація; термічний відпал*