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Study of optical properties of CdTe/GaAs(100) epitaxial films grown in different temperature conditions

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The influence of the growth temperature of cadmium telluride epitaxial films grown by molecular beam epitaxy on semi-insulating GaAs(100) substrates on the optical and structural properties of CdTe was investigated. The spectra of ellipsometric parameters Ψ and Δ were determined by the spectroscopic ellipsometry. The study revealed that the Van Hove singularities E_1 and E_0 corresponding to 3.3 and 1.46 eV are the distinctive features of the CdTe compound. Surface roughness, resulting from non-optimal substrate temperatures, was identified as the primary factor increasing the oscillation amplitude Ψ(λ) in the transparent spectral region ($E < E_g$). A correlation between ellipsometric parameters Ψ and Δ and RMS roughness R_q of the film surface was established. The non-optimal temperature was found to result in development of surface morphology and reduction of range Δ(λ). Thus, the average value Δ(λ) is an indirect criterion for evaluating the surface morphology of CdTe epitaxial films. The range of optimal growth temperatures for CdTe epitaxial structures to achieve the minimum surface roughness was determined. The obtained data will be useful for growing CdHgTe on GaAs(100) substrate using CdTe buffer layers.

Keywords: CdTe, spectral ellipsometry, molecular beam epitaxy.

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Introduction

The advancement of optoelectronics requires the materials capable of absorbing long-wave radiation. For this reason compounds of the A_2B_6 chemical group, including ZnTe, CdTe, HgTe, CdHgTe, are widely used as base materials in various photodetectors [1, 2]. These compouds were selected among many other semiconductor structures based on the data obtained from strategic objects in the IR wavelength range of 1–12 μm. However, mechanical stresses in the crystal lattice of these materials result –

cause scattering of electromagnetic radiation. As a result, the obtained images become blurred and difficult to analyze.

In turn, the structural quality of the resulting A_2B_6-compounds, like that of other materials, is directly dependent on their synthesis method. One of the main modern methods for producing single-crystal semiconductor compounds is molecular beam epitaxy (MBE) [3–6]. The main advantage of this method is its precise control over parameters that affect growth mechanisms. Such parameters are the temperature of the substrate and molecular sources. These parameters critically affect the growth rate of compounds and the crystalline quality of epitaxial films. Non-optimal selection of these parameters leads to either the polycrystalline structure formation of A_2B_6-compounds or in numerous defects within the material bulk [7]. Low growth temperatures of A_2B_6-compounds decrease the binding energy between Cd, Te, Hg and Zn atoms, which potentially causing amorphous phase formation on the growing film surface [4, 8–10]. Conversely, exceeding the optimal epitaxial growth temperatures can lead to the accumulation of non-stoichiometric tellurium inclusions throughout the film volume [11].

The substrate material and orientation critically affects important role in the epitaxy of A_2B_6-compounds. A significant lattice mismatch between the substrate and the deposited material promotes the formation of structural defects in the grown material. In the case of A_2B_6-compounds, the most thermodynamically favorable substrate is $Cd_{0.96}Zn_{0.04}Te$. The mole fraction of zinc variation enables tuning the lattice parameter of $Cd_{1-x}Zn_xTe$, thereby reducing the mismatch with $Cd_xHg_{1-x}Te$ [12]. However, high-quality $Cd_xHg_{1-x}Te$-based substrates are prohibitively expensive and limited in size, so GaAs is used as an alternative [13]. Despite the high mismatch between $Cd_xHg_{1-x}Te$ and GaAs (about 20 %). Successful epitaxial growth is achieved through the implementation of CdTe, ZnTe buffer layers [1, 3, 7, 13, 14]. These buffer layers, preserve the substrate orientation and prevent defect propagation into the upper layers [3, 14, 15]. Importantly, the infrared absorption characteristics depend not only on the CMT active region quality, but also on the structural perfection of both the substrate and buffer layers. Therefore, performance of optoelectronic devices depends not only on the active region of $Cd_xHg_{1-x}Te$ structures, but also on the crystalline quality of the entire heterostructure system [12, 16].

The crystalline quality of grown samples is evaluated through comprehensive analysis of these structural and optical characteristics, which directly correlate with the epitaxial growth conditions. They are directly related to the conditions of epitaxial growth of the layers under study [16]. Therefore, to develop the technology for production of A_2B_6-compounds using molecular beam epitaxy, many different methods are required for post-growth analysis of resulting samples. Key parameters including surface roughness and optical spectra characteristics are crucial for optimizing growth conditions. In this study, the optical ellipsometry (OE) and atomic force microscopy (AFM) were employed to characterize optical and structural parameters. Ellipsometric measurements provided the spectra of $\Psi(\lambda)$ and $\Delta(\lambda)$ parameters [17]. The ellipsometric parameters Ψ and Δ represent components of the elliptical polarization of the beam reflected from the surface. These parameters provide information on the roughness and composition of sample compounds [18]. Optical ellipsometry is a rapid method for analyzing optical and structural characteristics of the grown films. Based on the data obtained by combination of OE and AFM, optimal growth temperatures for A_2B_6 based films can be determined.

The goal of this study is to determine the dependence of ellipsometric parameters Ψ(λ) and Δ(λ) in epitaxial CdTe films on different temperatures of growth conditions by the optical ellipsometry ns using optical ellipsometry. Additionally, we seek to determine the range of optimal growth temperatures to achieve minimum surface roughness of samples. The results of this work will be useful for determining the optimal temperature conditions for epitaxial growth of A_2B_6-compounds, and enable in situ monitoring of molecular beam epitaxy for $Cd_xHg_{1-x}Te$ layers on various substrates.

Experiment procedure

CdTe films (samples Nos. 5, 8, 15, and 18) were grown by molecular beam epitaxy in Riber Epineat Cluster ultra-high vacuum multi-chamber setup We used semi-insulating epi-ready GaAs(100) substrates and a binary CdTe source. The temperature was controlled using a thermocouple integrated in the sample heater. Molecular flows were measured with a Bayard-Alpert sensor. Pre-growth treatment of the GaAs substrate included two stages. First, the sample holder with the substrate was degassed to remove volatile compounds and water vapour in the pre-treatment chamber at the temperature of 350 °C for 20 minutes. Secondly, in the growth reactor for A_3B_5 group materials, natural oxides were desorbed in the arsenic flow at the temperature of 680 °C for 5 minutes, followed by growth of the GaAs buffer layer of 0.5 μm in thickness. Then, to perform the epitaxial synthesis of CdTe films, the holder with the substrate was placed in the growth chamber for A_3B_5 group materials. CdTe structures were grown at substrate temperatures of 250, 325, 400 and 450 °C.

After epitaxial growth and ellipsometric measurements of CdTe films, the CdTe/GaAs(100) samples were unloaded from the MBE setup and measured by the atomic force microscopy method using NT-MTD Ntegra Maximus microscope in contact mode in the 10×10 μm field. The average roughness (R_q) values of the samples are given in Table 1.

Table 1

Energy values and wavelengths corresponding to critical points E_1 and E_0 depending on the substrate temperature

Sample number	Substrate temperature, °C	R_q, nm	Thickness, nm	λ, nm	E_1, eV	λ, nm	E_g, eV
8	250	17.00	4058	365	3.39	846	1.46
9	325	4.90	4256	376	3.30	842	1.47
18	400	0.85	4071	372	3.33	846	1.46
15	450	1.17	1452	373	3.34	893	1.39

SEC-1000 spectral ellipsometric complex (Russia, Novosibirsk, Institute of Semiconductor Physics of the Russian Academy of Science) was used as analytical equipment for obtaining ellipsometric spectra Ψ(λ) Δ(λ) in the wavelength range of 350÷1000 nm (from 1.2 to 3.5 eV) [17]. The angle of incidence of linearly-polarized light on the sample under study was 70°. The highly stable OSRAM halogen lamp was used as a radiation source. Instrumentation errors in measurement of the refractive index

and thickness are 0.005 and 5 Å, respectively. Spectr software was used to analyze the ellipsometric spectra $\Psi(\lambda)$ $\Delta(\lambda)$.

Discussion of the results

Different crystal structures exhibit distinct electronic properties, characterized by critical points (Van Hove singularities) in their band structure. These singularities manifest as maxima in the dielectric function spectra [$\varepsilon_1(\lambda)$ and $\varepsilon_2(\lambda)$] or as features in the electronic band structure [19–21]. Lattice strains induced by defects (e.g., impurities, dislocations, vacancies) significantly alter the spectral positions and amplitudes of these critical points.

The structural quality of layers growing by the molecular beam epitaxy is directly dependent on the growth conditions, including temperatures of the substrate and molecular sources. A_2B_6-compound such as CdTe exhibit a low binding energy of about 572.6 eV, for which reason growth temperatures above 500 °C may be too high for the single crystal to grow [10]. Although CdTe films deposit on GaAs substrates below 200 °C, the growth mode transitions to 3D islanding [16], yielding polycrystalline films. This occurs due to insufficient kinetic energy for complete adatom dissociation and surface diffusion to stable lattice sites [22].

Substrate surface preparation is critical for growing high-quality CdTe epitaxial layers. Thermal decomposition of amorphous oxide layers with GaAs at temperatures above 700 °C is the main method of pre-growth treatment. High temperature causes the Ga-O and Ga-As bonds to break, facilitating oxygen, arsenic while exposing clean gallium-terminated surfaces. If thermal impact is insufficient, the near-surface oxygen or other near-surface defects can transite the orientation of growing CdTe from (100) to (111) [10, 23–26].

The in-situ optical research method such as ellipsometry can be found useful for describing the structure properties. This method measures two parameters, such as Ψ and Δ, corresponding to the ratio of amplitudes and phase difference of two components of the reflected elliptically-polarized wave. Their values are directly dependent on the optical characteristics of the material, such as the refractive index and absorption coefficient. The spectrum of imaginary permittivity is often used to analyze crystal features. However, parameter Δ taken into account in this calculation can affect the qualitative identification of Van Hove singularities due to sensitivity to the film roughness [18], so it is advisable to analyze the spectra Ψ [19]. Here the dependence $\Psi(\lambda)$ was used to determine the structural features of epitaxial films of cadmium telluride. The spectrum $\Delta(\lambda)$ describing the development of the sample surface morphology was compared to the findings of atomic force microscopy.

The study examined four epitaxial CdTe films (samples No. 8, 9, 15, and 18) grown directly on semi-insulating GaAs(100) substrates. The growth temperatures varied between 250 °C and 450 °C, while the film thickness differed among samples (see Table 1). All other growth parameters and substrate pretreatment conditions were kept identical.

The wavelength range from 350 nm to approximately 850 nm ($E > E_g$) is particularly important for optical characterization, as this spectral region the film absorbs incident radiation, and Van Hove singularities in the spectrum $\Psi(\lambda)$ will be observed. Figure 1 shows the ellipsometric spectra of parameter Ψ for CdTe samples Nos. 8, 9, 15 and 18, and results of determining the energy position of

the critical points are given in Table 1. Van Hove singularity E_1 equaling to approximately 3.3 eV can be observed in each spectrum and is in good agreement with the literature data [27]. Comparison of spectra Ψ(λ) revealed that the growth temperature in this case significantly influences the singularity's linewidth. Specifically, CdTe layers grown at 450 °C exhibit a narrower E_1 feature compared to samples prepared at lower temperatures. The reason is the additional absorption of incident radiation caused by defects found in samples Nos. 8, 9 and 18 near critical point E_1. Structural imperfections generated during CdTe growth at suboptimal temperatures (250–325 °C) likely contribute to this additional absorption. AFM measurements confirm that growth at 400 °C (sample No. 15) yields the smoothest surface, with the lowest root-mean-square roughness R_q (Table 1).

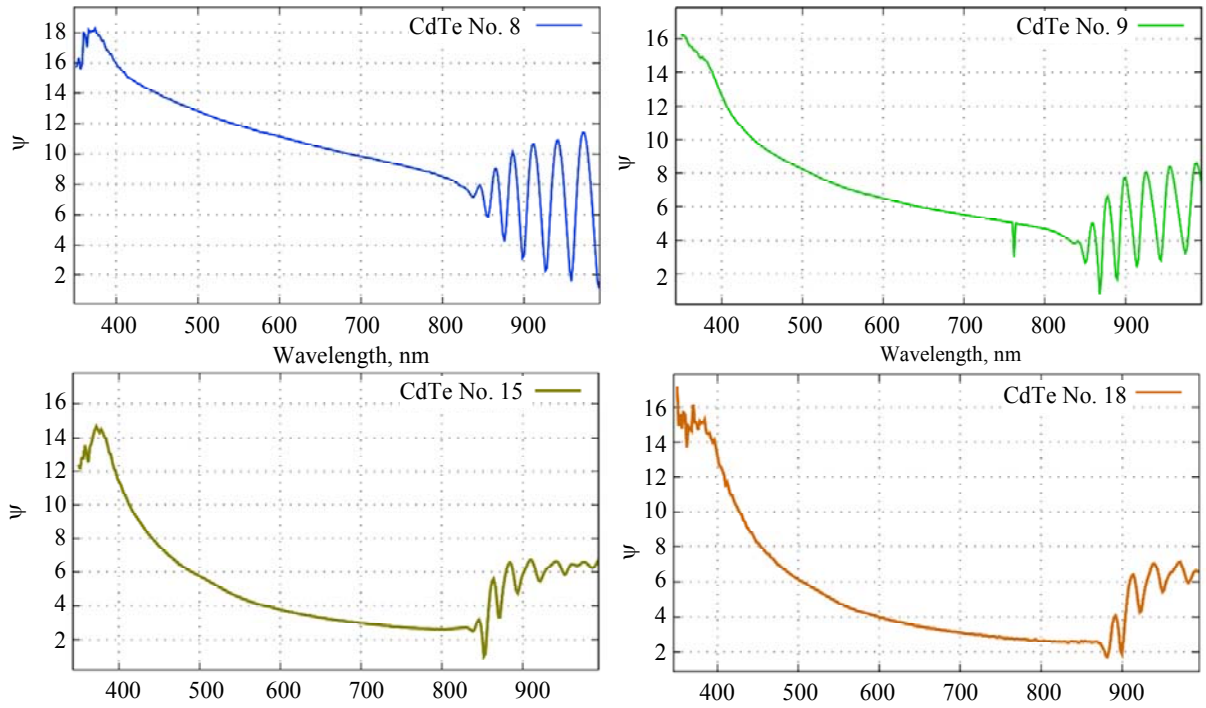

Fig. 1. Ellipsometric spectra of parameter ψ of CdTe/GaAs. Blue line – CdTe No. 8 (upper left corner); green line – CdTe No.9 (upper right corner); dark green line – CdTe No. 15 (lower left corner); orange line – CdTe No.18 (lower right corner)

The band gap is also directly dependent on characteristics of the crystal structure. In ellipsometric spectrum Ψ(λ), the critical point corresponding to E_g of CdTe is the first minimum before the start of interference oscillations in the CdTe film. According to the values of Table 1, E_g corresponds to the literature data in the case of samples Nos. 8, 9 and 18 [27]. Large thickness of samples of about 4 μm reduces to zero the probability of formation of interference oscillations in region $E > E_g$ due to the excessive depth of light penetration into the sample. For this reason no extremes are observed in this energy range ($E > E_g$) in the spectra Ψ(λ), and the band gap width is determined most

accurately. In the case of sample No. 15, which is about 1.5 μm in thickness, the mismatch of E_g and literature data is due to incomplete absorption of incident radiation in this spectrum region and, consequently, the influence of interference observed in the film.

The oscillations observed in spectrum Ψ(λ) shown in Figure 1 within the wavelength range from approximately 850 to 1000 nm ($E < E_g$) correspond to interference in the grown CdTe films [28]. Comparison of the dependencies under study has revealed that sample No. 8 has the highest oscillation amplitude, while decrease in the amplitude of these oscillations in other samples indicates a high absorption rate in CdTe films [28]. Figure 2 shows the ellipsometric spectra Δ(λ) for CdTe/GaAs(100) samples Nos. 8, 9, 15, 18. The above parameter is the phase difference of components of the elliptically-polarized radiation reflected from the film surface, and therefore it is used to analyze the roughness of grown structures.

According to the data obtained by the atomic force microscopy method (see Table 1), sample No. 8 has the most developed morphology (R_q = 17 nm), which is consistent with the OE findings Δ(λ), since the average value $\bar{\Delta}$ (70°) differs from the optimal one (140–150°) in the spectral region of 350–850 nm [29]. The low value of parameter Δ corresponds to the developed morphology of the film surface; the average value of parameter Δ for samples Nos. 15 and 18 was within the acceptable limits: 145°±5°. Thus, the data obtained by the spectral ellipsometry method indicate the low value of the RMS surface roughness of samples Nos. 15 and 18, which was confirmed by the atomic force microscopy method (see Table 1).

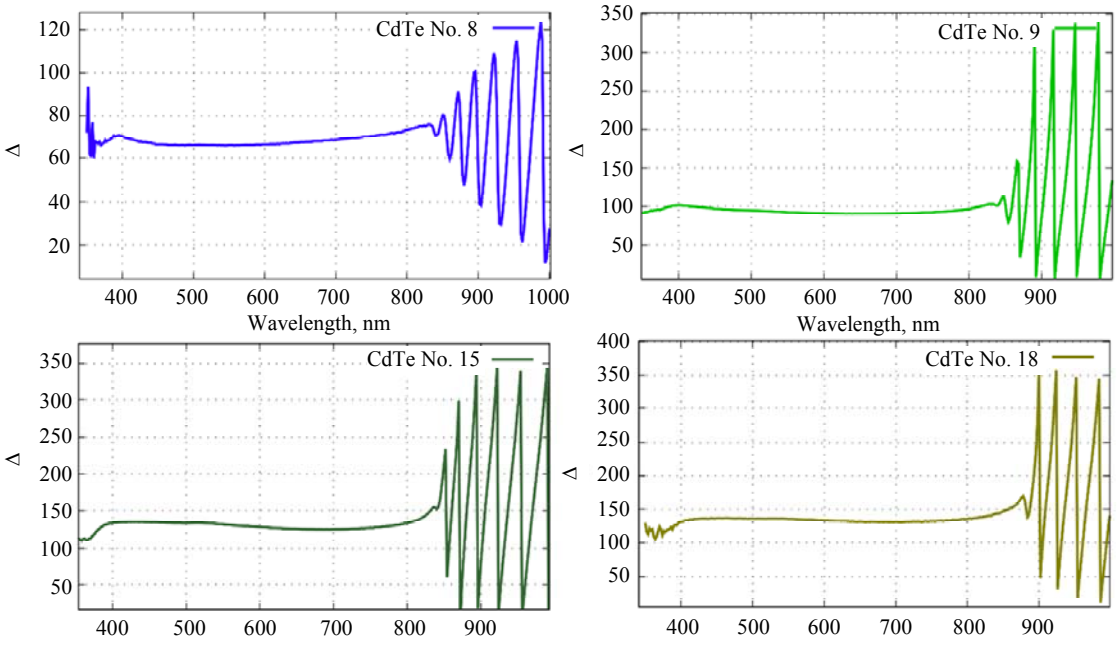

Fig. 2. Ellipsometric spectra of parameter Δ of CdTe/GaAs samples. Blue line – sample 8; light green line – sample 9; dark green line – sample 15; brown line – sample 18

Conclusion

This research analyzed the ellipsometric spectra of parameters Ψ, Δ as a function of the growth temperature of CdTe films. A correlation between ellipsometric parameters Ψ and Δ and RMS roughness R_q of the film surface was established. Comparison of the dependencies Ψ(λ) revealed that CdTe/GaAs(100) samples Nos. 15 and 18 synthesized at temperatures of 450 °C and 400 °C, respectively, scatter the optical radiation less than the others. This indicates a lower defect density in these films. Analysis of spectrum Δ(λ) allowed to establish that since the parameter Δ values for samples Nos. 15 and 18 were within the range of 145°±5°, the surface roughness of their CdTe films should be the lowest as compared to the other samples. The CdTe/GaAs(100) film No. 8 developed surface morphology confirmed by the atomic force microscopy measurements (R_q = 17 nm) and could be observed in spectrum Δ(λ) ($\bar{\Delta}$ = 70°). Thus, the optimal temperature range for epitaxial growth of CdTe films is 400–450 °C, as this minimizes formation of surface morphology on the film surface. The critical point E_1 (3.3 eV), corresponding to the CdTe compound, manifests as a maximum in the Ψ(λ) spectrum for light energies $E > E_g$. The half-width of this extremum provides a qualitative measure of defect formation in the growing CdTe structure. The findings of this work will be useful as the express method for determining the crystal structure features of A_2B_6-compounds and monitoring the epitaxial growth of CdTe, ZnTe, and CdHgTe.

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REFERENCES

1. Pan W. W., Gu R. J., Zhang Z. K., Lei W., Umana-Membreno G. A., Smith D. J., Antoszewski J. and Faraone L., J. Electron. Mater. **51**, 4869–4883 (2022). https://doi.org/10.1007/s11664-022-09725-1

2. Scarpulla M. A., McCandless B., Phillips A. B., Yan Y., Heben M. J., Wolden C., Xiong G., Metzger W. K., Mao D., Krasikov D., Sankin I., Grover S., Munshi A., Sampath W., Sites J. R., Bothwell A., Albin D., Reese M. O., Romeo A., Nardone M., Klie R., Walls M., Fiducia T., Abbas A. and Hayes S. M., Solar Energy Materials and Solar Cells. **255**, 112289 (2023). https://doi.org/10.1016/j.solmat.2023.112289

3. Dvoretsky S. A., Mikhailov N. N., Remesnik V. G., Sidorov Y. G., Shvets V. A., Ikusov D. G., Varavin V. S., Yakushev M. V., Gumenjuk-Sichevska J. V., Golenkov A. G., Lysiuk I. O., Tsybrii Z. F., Shevchik-Shekera A. V., Sizov F. F., Latyshev A. V. and Aseev A. L., Opto-Electronics Review **27**, 282–290 (2019). https://doi.org/10.1016/j.opelre.2019.07.002

4. Varavin V. S., Dvoretskii S. A., Mikhailov N. N., Remesnik V. G., Sabinina I. V., Sidorov Yu. G., Shvets V. A., Yakushev M. V. and Latyshev A. V., Optoelectron. Instrument. Proc. **56**, 456–469 (2020). https://doi.org/10.3103/S8756699020050143

5. Vogt A., Shutt S., Frei K. and Fiederle M., Journal of Crystal Growth. **477**, 114–117 (2017). https://doi.org/10.1016/j.jcrysgro.2017.02.048

6. Sidorov Yu. G., Dvoretsky S. A., Varavin V. S., Mikhailov N. N., Yakushev M. V. and Sabinina I. V., Semiconductors **35** (9), 1045–1053 (2001).

7. Wichrowska K., Wosinski T., Domagala J. Z., Kret S., Chusnutdinow S. and Karczewski G., Semicond. Sci. Technol. **36** (4), 045022 (2021). https://doi.org/10.1088/1361-6641/abbd0d

8. Ahmed T., Tan X., Li B. Y., Cook E., Williams J., Tiano S. M., Coffey B., Tenney S. M., Hayes D. and Caram J. R., ACS Nano. **19** (3), 3944–3952 (2025). https://doi.org/10.1021/acsnano.4c17596

9. Kozlov D. V., Rumyantsev V. V., Kadykov A. M., Fadeev M. A., Kulikov N. S., Utochkin V. V., Mikhailov N. N., Dvoretskii S. A., Gavrilenko V. I., Hubers H. W., Teppe F. and Morozov S. V., JETP Letters **109** (10), 657–662 (2019).

10. Feldman R. D., Austin R. F., Kisker D. W., Jeffers K. S. and Bridenbaugh P. M., Appl. Phys. Lett. **48**, 248–250 (1986). https://doi.org/10.1063/1.96571

11. Sidorov Y. G., Dvoretskii S. A., Varavin V. S., Mikhailov N. N., Yakushev M. V. and Sabinina I. V., Semiconductors **35**, 1045–1053 (2001). https://doi.org/10.1134/1.1403569

12. Varavin V. S., Dvoretskii S. A., Mikhailov N. N., Remesnik V. G., Sabinina I. V., Sidorov Yu. G., Shvets V. A., Yakushev M. V. and Latyshev A. V., Optoelectronics, Instrumentation and Data Processing. **56**, 456–469 (2021). https://doi.org/10.3103/S8756699020050143

13. Tyagi S., Goyal A., Rana S. S., Meena U. R., Mishra P., Pandey R. K., Dalal S., Pandey A., Garg A. K., Kumar S. and Singh R., J Mater Sci: Mater Electron. **35**, 982 (2024). https://doi.org/10.1007/s10854-024-12724-z

14. Svitashev K. K., Dvoretsky S. A., Sidorov Yu. G., Shvets V. A., Mardezhov A. S., Nis I. E., Varavin V. S., Liberman V. and Remesnik V. G., Crystal Research and Technology **29** (7), 931–937 (1994). https://doi.org/10.1002/crat.2170290703

15. Bratina G., Sorba L., Antonini A., Ceccone G., Nicolini R., Biasiol G., Franciosi A., Angelo J. E. and Gerberich W. W., Phys. Rev. B **48**, 8899 (1993). https://link.aps.org/doi/10.1103/PhysRevB.48.8899

16. Hwang Y., Ngugen V. Q., Choi J. S., Park S., Cho S., Kim T. H., Ha Y. and Ahn C. W., J. Korean Phys. Soc. **79**, 1057–1062 (2021). https://doi.org/10.1007/s40042-021-00337-2

17. Shvets V. A., Spesivtsev E. V., Rykhlitskii S. V. and Mikhailov N. N., Nanotechnol Russia **4**, 201–204 (2009). https://doi.org/10.1134/S1995078009030082

18. Shvets V. A., Marin D. V., Kuznetsova L. S., Azarov I. A., Yakushev M. V. and Rykhlitskii S. V., Journal of Optical Technology **91** (7), 496–501 (2024). https://doi.org/10.1364/jot.91.000091

19. Shvets V. A., Azarov I. A., Marin D. V., Yakushev M. V. and Rykhlitskii S. V., Semiconductors **53**, 132–137 (2019).

20. Moss T., Barrel G. and E`llis B. Poluprovodnikovaya optoe`lektronika. Moscow, Mir, 1976.

21. Shalimova K. V. Fizika poluprovodnikov. Mowcow, Energoatomizdat, 1985.

22. Yin J., Huang Q. and Zhou J., J. Appl. Phys. **79**, 3714–3717 (1996). https://doi.org/10.1063/1.361204

23. Mcgibbon A. J., Pennycook S. J. and Angelo J. E., Science **269** (5223), 519–521 (1995). https://doi.org/10.1126/science.269.5223.519

24. Kolodziejski L. A., Gunshor R. L., Otsuka N. and Choi C., J. vac. Sci. Technol. A **4**, 2150–2152 (1986). https://doi.org/10.1116/1.574045

25. Faurie J. P., Hsu C., Sivananthan S. and Chu X., Surface Science **168** (1-3), 473–482 (1986). https://doi.org/10.1116/1.574045

26. Zhang S., Zhang J., Qiu X., Wu Y. and Chen P., Journal of Crystal Growth. **546**, 125756 (2020). https://doi.org/10.1016/j.jcrysgro.2020.125756

27. Adachi S., Kimura T. and Suzuki N., J. Appl. Phys. **74**, 3435 (1993). https://doi.org/10.1063/1.354543

28. Shvets V. A., Marin D. V., Yakushev M. V. and Rykhlitskii S. V., Semiconductors **57** (6), 464–469 (2023).

29. Shvets V. A., Marin D. V., Yakushev M. V. and Rykhlitskii S. V., Semiconductors **58**, 67–72 (2024). https://doi.org/10.1134/S1063782624010147

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