UDC 621.315.592

Control of elastic stress during the growth of heterostructures (Al)GaN/SiC

© E.E. Zavarin[1,2], S.N. Rodin[1,2], B.Yu. Kluev[2], W.V. Lundin[1], A.E. Nikolaev[1], D.S. Arteev[1,2], A.V. Sakharov[1,2], A.F. Tsatsulnikov[1,2]

[1] Ioffe Institute,
194021 St. Petersburg, Russia
[2] Submicron Heterostructures for Microelectronics Research and Engineering Center of the Russian Academy of Sciences,
1904021 St. Petersburg, Russia
E-mail: zavarin@yandex.ru

Received May 5, 2025
Revised June 27, 2025
Accepted July 3, 2025

An analysis based on *in situ* optical reflectometry of elastic stresses during the growth of AlGaN/SiC HEMT heterostructures by MOVPE is presented. It is shown that changing the growth conditions of the nucleation AlN and buffer GaN layers makes it possible to control the compressive strain. The effect of GaN doping by Fe and C atoms on elastic stresses is compared. Growth conditions of structures with bow of less than 20 microns for substrates up to 3 inches in diameter have been obtained.

Keywords: AlGaN, SiC, HEMT, strain, curvature, deflection.

DOI: 10.61011/SC.2025.06.62051.8026

Field effect transistors based on III-N compounds have already found practical applications for power and high-frequency applications. Currently, high-power microwave transistors are manufactured mainly on the basis of AlGaN/GaN heterostructures on SiC substrates with maximum thermal conductivity from commercially available options (sapphire, silicon, silicon carbide). Epitaxy on a SiC substrate faces 2 problems: the first is the mismatch of the crystal parameters of the AlGaN and GaN lattices with the substrate, the second is the impossibility of dense homogeneous nucleation of GaN at high ($\sim 1000\,^\circ$C) temperature. These problems are successfully solved by choosing the appropriate growth conditions and choosing the composition of the initial layer. Buffer and nucleation layers of AlN or AlGaN between SiC and GaN were proposed back in the late 1990s [1]. However, there is also a more complex problem — elastic stresses that occur in structures due to mismatch of lattice parameters, as well as differences in the thermal expansion coefficients (TEC) of the grown layers and the substrate. The TEC is 5.59 and $4.3 \cdot 10^{-6}\,\mathrm{K}^{-1}$ for GaN and SiC, respectively, when cooled from the typical epitaxy temperature at $1000\,^\circ$C to room temperature, this creates a mismatch $\sim 10^{-3}$, leading to the appearance of tensile stresses in the layers of the structure and possible cracking. This problem can be solved by intentionally creating a compressive stress in the GaN layer when growing on Al(Ga)N, which compensates for the tensile stress that occurs later during cooling, which reduces the overall built-in stresses in the epitaxial structure. Our experience shows that stress compensation and crack suppression are possible in a very wide range of growing conditions, compositions, and thicknesses of buffer and nucleation layers of AlGaN, however, in most cases, excessive stress compensation is observed, and after cooling, structures are compressed in the substrate plane and have a relatively high curvature and bow. The transition to higher and higher operating frequencies requires a reduction in Feature size, imposes restrictions on the permissible bending of the final structure during lithography, which, combined with the ever-growing diameter of the substrates [2], leads to the need to control the bending of the structure more precisely, i.e. stresses in the layers, during the growth of the structure.

The bending of the structure during growth can be estimated by measuring the curvature. The curvature of the growing structure is determined by the Stoney formula [3]:

$$k = 6 \cdot S \cdot (1 - n_s)/E_s \cdot h_f/h_s^2,$$

where S is the amount of elastic deformation, E_s is the Young's modulus of the substrate material, n_s is the Poisson's ratio of the substrate material, h_f is the thickness of the grown layer, h_s is the thickness of the substrate. The wafer bow is related to the curvature by the following expression:

$$b = k \cdot d^2/8,$$

where k is the curvature, d is the diameter of the substrate. The amount of elastic deformation of the growing layers is determined by the difference between the lattice constants of the underlying and growing layers, which, in the absence of relaxation, leads to a linear change in the curvature of the structure with layer thickness. This is the compression stress for gallium nitride using a pair of Al(Ga)N/GaN-layers where the structure bends so that the center rises above the edges of the substrate, the curvature increases. During cooling, due to the difference between TEC of SiC and nitrides, the layers experience tensile stress, which leads to compensation of compressive stresses and bending of the structure in the other direction, the curvature decreases.

The authors found in Ref. [4] that the initial compression stress, relaxation, and transition to tensile stress in the SiC/AlN/AlGaN sequence are determined by the properties of the AlN layer grown at various V/III ratios. The author of Ref. [5] examines several mechanisms affecting the occurrence and relaxation of stresses in the process of AlGaN growth on SiC: mismatch of lattice parameters; the generation of threading dislocations at the boundary between AlGaN islands and the AlN nucleation layer; the process of coalescence of AlGaN islands; the generation of threading dislocations on the surface irregularities of a continuous layer; dislocation slope in response to compressive stress as the layer grows. The authors of Ref. [6] found that AlGaN Si doping leads to an increase in the angle of inclination of threading dislocations and stress relaxation in the growing layer. These studies show that the initial stages of growth of buffer and nucleation layers on SiC affect the stresses in the layers, which in turn affects the wafer bow after the epitaxy process. The purpose of this work is to study the effect of the initial stages of growth of the GaN buffer layer and its doping on the final curvature (bow) of the structure.

All experiments were carried out using the Dragon D175 installation, which has a low-pressure horizontal flow reactor, with inductive heating and multi-zone injection, with substrate holder configuration 7×2, 3×3, 1×4, 1×6 inches of substrates. Insulating substrates $4H$-SiC with a diameter of 2 and 3 inches and a thickness of $358\,\mu$m were used. The reactor is equipped with a Burattino reflectometry system with 4 measuring heads, which allow measuring, in addition to the reflection coefficient, changes in the geometry (curvature) of the substrate during growth at two wavelengths of 638 and 405 nm simultaneously. The SiC substrates had an initial curvature of $\pm10\,\text{km}^{-1}$. Changes in curvature as a result of epitaxy were normalized by this value. The basic structure design had the following sequence of layers (from substrate): AlN nucleation layer with a thickness of ~15 nm, GaN:Fe thickness $\sim1.1\,\mu$m (growth at a pressure of 400 mbar), undoped GaN with thickness of $\sim0.6\,\mu$m (growth at a pressure of 400–800 mbar), active region of HEMT transistor. The curvature after epitaxy for such a structure was $-40\,\text{km}^{-1}$. Experiments were made with changing the growth conditions of the structure with the basic structure described above. First, structures were grown in which the pressure changed at the beginning of the growth of the GaN buffer (100, 750 mbar). Secondly, for structures in which the buffer layer was grown at a pressure of 750 mbar, the effect of the thickness of the nucleation layer (15 and 10 nm) on their curvature was studied. The effect of Fe and C doping of GaN buffer on stress development during growth for structures with identical sequence layers was also investigated. The dependence of the stress relaxation of the GaN buffer layer on the composition of the first AlGaN layer is described in detail by the authors in Ref. [7]. In a series of experiments, the total thickness, the growth rate of the buffer layers, and the active region of the structure remained unchanged, so the development of curvature can be compared with the experimental time.

It is known that an increase in pressure affects the severity of islet growth of the initial stages of GaN on sapphire substrates and affects its dislocation structure. Three experiments were carried out in this study, differing in the growth pressure of the GaN buffer layer at the initial stages: 100, 400, 750 mbar. A strong influence of pressure on the nucleation of islands on the AlN nucleation layer was found (Figure 1, a). At a pressure of 100 mbar, a layered (2D) growth of the GaN layer is observed from the very beginning of its growth, while at 400 mbar, a decrease in reflection is observed at this stage, which indicates a pronounced formation of the surface relief. This corresponds to islet (3D growth) growth at the initial stage, with further smoothing of the surface and transition to layered growth. This effect becomes even more pronounced at a pressure of 750 mbar. Figure 1, b shows the dependence of the curvature of the grown layers. The slope of the dependence decreases with an increase in pressure, which indicates a greater relaxation of stresses. Thus, a more pronounced islet growth at the initial stages of growth of the GaN buffer layers is accompanied by a greater relaxation of stresses in it. As a result, the final curvature of the structure for a pressure of 750 mbar was $< 20\,\text{km}^{-1}$.

The properties of the AlN nucleation layer can also have a significant effect on the initial growth stages of the GaN buffer layer. Two experiments were conducted with different thickness of the AlN nucleation layer and identical growth conditions of the GaN buffer layer. The growth of the GaN buffer layer was carried out at a pressure of 750 mbar. The thickness of the AlN nucleation layer was 15 and 10 nm. Islet growth was observed in both cases at the initial stages of GaN growth (Figure 2, a). However, as the thickness of the AlN layer decreased, islet growth became much more pronounced, and surface smoothing with layered growth took much longer. The curvature dependences for these structures (Figure 2, b) show that a more pronounced three-dimensional growth is accompanied by greater stress relaxation in the growing GaN layer, which is reflected in the final curvature of the entire structure after epitaxy. With a layer thickness of AlN 10 nm, the final curvature was practically zero, which indicates the absence of bow associated with epitaxy. Thus, there is no deformation of the structure, but, of course, different layers of the structure may have local tensile and compressive stresses that compensate each other.

As was shown in Ref. [5], the doping of layers with Si atoms can affect the stress pattern in the layers during GaN growth on SiC substrates. Experiments were conducted with doping by Fe and C atoms of GaN buffer layers, with a dopant concentration of $\sim 1{-}3\cdot10^{18}\,\text{cm}^{-3}$, standard

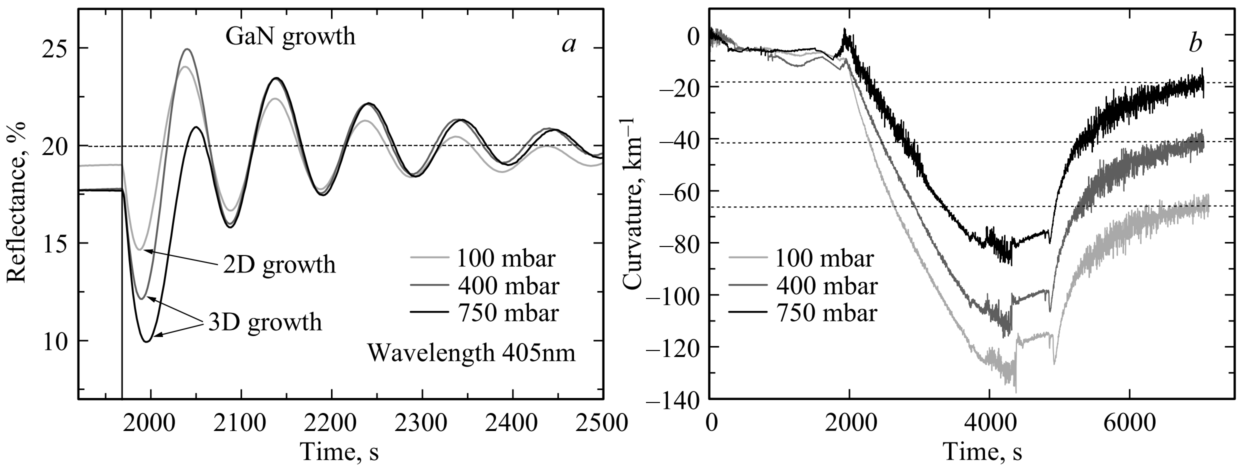

Figure 1. Influence of pressure at the initial stages of growth of the buffer layer GaN: *a* — dependence of the reflection coefficient; *b* — dependence of the curvature of the substrate.

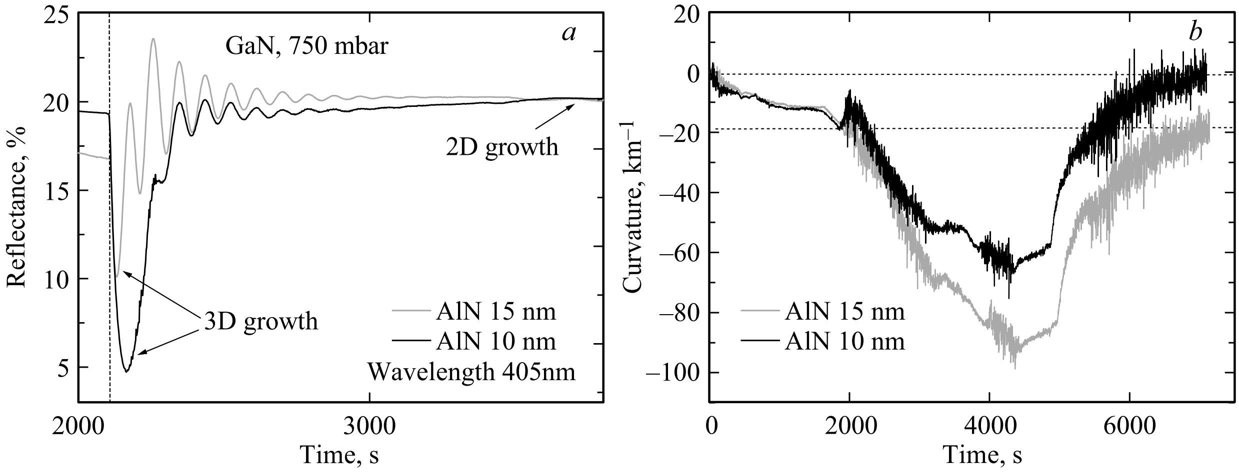

Figure 2. Influence of the thickness of the nucleation layer AlN: *a* — dependence of the reflection coefficient; *b* — dependence of the curvature of the substrate.

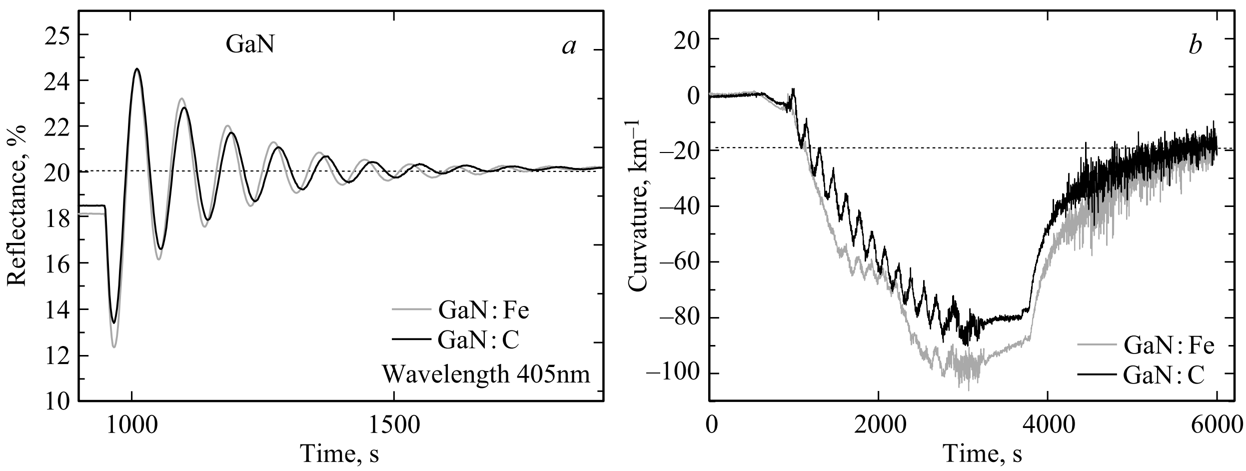

Figure 3. The effect of replacing the doping impurity Fe with C on the growth of the structure: *a* — dependence of the reflection coefficient; *b* — dependence of the curvature of the substrate.

for HEMT structures on SiC. This level of doping by both Fe and C has no significant effect on the character (island or layered) of the initial growth stage of the GaN buffer layer (Figure 3, *a*). As a result, the difference in the type of doping affects the final curvature of the structure after cooling by less than $10\,\text{km}^{-1}$ (Figure 3, *b*). However, it is known that high levels of doping by both Fe and C can affect the morphology of growing layers and, thus, affect stress relaxation, which requires additional research.

Thus, this paper presents the results of a systematic in situ analysis of optical reflectometry of elastic stresses arising from the growth of AlGaN heterostructures for field-effect transistors on SiC substrates by gas-phase epitaxy from metallorganic compounds. The possibility of precise control of the magnitude of the embedded compression stresses during epitaxy of the layers of III-N, compensating for the tensile stresses that occur during cooling, has been demonstrated, which has significantly reduced the final curvature of the structure. It is shown that the initial growth conditions of the GaN buffer layer and the thickness of the AlN nucleation layer significantly affect stress relaxation in it. Stress relaxation can be associated with the severity of islet growth at the initial stages of growth of the buffer layer of GaN. It is shown that doping of the buffer layer with deep impurities of different types (Fe and C), at standard concentrations for field-effect transistors on SiC, does not lead to a significant change in the degree of relaxation depending on the type of impurity and affects the final curvature of structures by less than $10\,\text{km}^{-1}$. The modes of reproducible production of structures with a bow of $< 20\,\mu$m for substrates up to 3 inches in diameter are determined.

Conflict of interest

The authors declare no conflict of interest.

References

[1] I. Nikitina, M. Sheglov, Y. Melnik, K. Irvine, V. Dmitriev. Diamond. Rerlat. Mater., 6, 1524 (1997). DOI: 10.1016/S0925-9635(97)00122-2

[2] https://compoundsemiconductor.net/article/121133/Infineon_starts_200mm_SiC_product-roll_out

[3] Maria Rosa Ardigo, Maher Ahmed, Aurélien Besnard. ISSN: 1662-8985, v. 996, pp 361-366. DOI: 10.4028/www.scientific.net/AMR.996.361

[4] J. Acord, S. Raghavan, D. Snyder, J. Redwing. J. Cryst. Growth, **272**, 65 (2004). DOI: 10.1016/j.jcrysgro.2004.08.033

[5] J.D. Acord. *In situ stress measurements during MOCVD growth of aluminum gallium nitride on silicon carbide*, Ph.D. thesis (Pennsylvania State University, 2007). 2007.3284895

[6] J. Acord, I. Manning, X. Weng, D. Snyder, J. Redwing. Appl. Phys. Lett., **93**, 111910 (2008). DOI: 10.1063/1.2986448

[7] M.E. Rudinsky, E.V. Yakovlev, W.V. Lundin, A.V. Sakharov, E.E. Zavarin, A.F. Tsatsulnikov, L.E. Velikovskiy. Phys. Status Solidi A, **213** (10), 2759 (2016). DOI: 10.1002/pssa.201600210

Translated by A.Akhtyamov