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Studies of structural and mechanical properties of AlGaN thin films on nano-SiC/Si hybrid substrates

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An experimental study of the structural characteristics of the surface and the parameters of hardness and elastic modulus of thin AlGaN films grown on nano-SiC/Si hybrid substrates was carried out. AlGaN layers on nano-SiC on Si with orientations (001), (011) and (111) have been investigated using atomic force microscopy and nanoindentation method. It is shown that the orientation of the Si substrate has a significant effect on the surface structure of AlGaN films and the elastic modulus parameter of AlGaN near the surface. The surface roughness and structural characteristics of AlGaN layers grown on nano-SiC on Si hybrid substrates have been determined. The elastic modulus parameters of AlGaN films near the surface and in the film volume have been measured. The hardness parameters of AlGaN thin films on nanoSiC on Si were experimentally determined.

Keywords: thin films, AFM, nanoindentation, heterostructures, nano-SiC/Si, AlGaN.

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AlGaN aluminium-gallium nitride thin films have unique physical and mechanical properties, making them an ideal material for creating high-performance electronic and optoelectronic devices such as LEDs, lasers, transistors and others. They have high thermal stability, high electrical conductivity and a wide range of optical properties. Optimization of growth conditions and crystal direction can further improve the properties of these structures for a variety of practical applications. The integration of AlGaN layers with silicon technologies is of great importance for microelectronics, as it allows for increased capabilities and improved device performance. In particular, this enables the creation of high-efficiency LEDs and lasers that are ideal for use in lighting, displays, and optical communications. Also, the integration of AlGaN layers with silicon technology enables the creation of high-frequency transistors and other electronic devices with high performance and reliability. In addition, the integration of AlGaN layers with silicon technologies can reduce manufacturing costs and improve the cost-effectiveness of electronic device manufacturing. Overall, the integration of AlGaN layers with silicon technologies is an important step in the development of microelectronics and the creation of new high-performance and efficient devices.

One of the main problems in the growth of AlGaN layers on silicon Si crystals is the mismatch of lattice constants and thermal expansion coefficients between AlGaN and Si. This leads to defects in the structure such as dislocations, crystal orientation disorders and others. In addition, the growth of AlGaN layers on Si wafers presents problems in controlling the composition and concentration of impurities in the structure. This can lead to changes in the optical and electrical properties of the material and reduce the performance of the device. Another challenge is the high growth temperature of high-quality AlGaN layers on Si crystals, which can lead to structure degradation and device performance degradation. To solve these problems, it is necessary to optimize the growth conditions of AlGaN layers on Si crystals, including the choice of optimal parameters of temperature, pressure and growth rate. Various methods can also be used to compensate for the mismatch of lattice constants, in particular, various kinds of buffer layers [1,2] are created on the silicon surface.

In the present work, we propose to use Si substrates with a nanometer-thick nano-SiC [3] layer of silicon carbide pre-synthesized by the method of coordinated atom substitution [3] for the growth of AlGaN thin films [4]. This nano-SiC/Si hybrid substrate configuration is used for the growth of AlGaN thin films for the first time. The main feature of the nano-SiC configuration used is that the wafer surface is not noticeably upgraded as a result of the synthesis. As a result, the growth of AlGaN layers is performed on a SiC layer with a surface roughness of 0.5 nm, which is comparable to commercial SiC crystals. Such structures can be synthesized on Si of any crystalline direction. In the present work, only structures grown on Si with (001), (011) and (111) orientations are investigated. These silicon wafer orientations are the most commonly used in industry. Thus, investigating the surface morphology and mechanical properties of AlGaN on nano-SiC thin films on Si with orientations (001), (011) and (111) is an important task for materials science.

Si substrates with nanoscale SiC layer were used for the growth of AlGaN layers. SiC layers were synthesized by atom substitution method on Si*p*- substrates of conduction

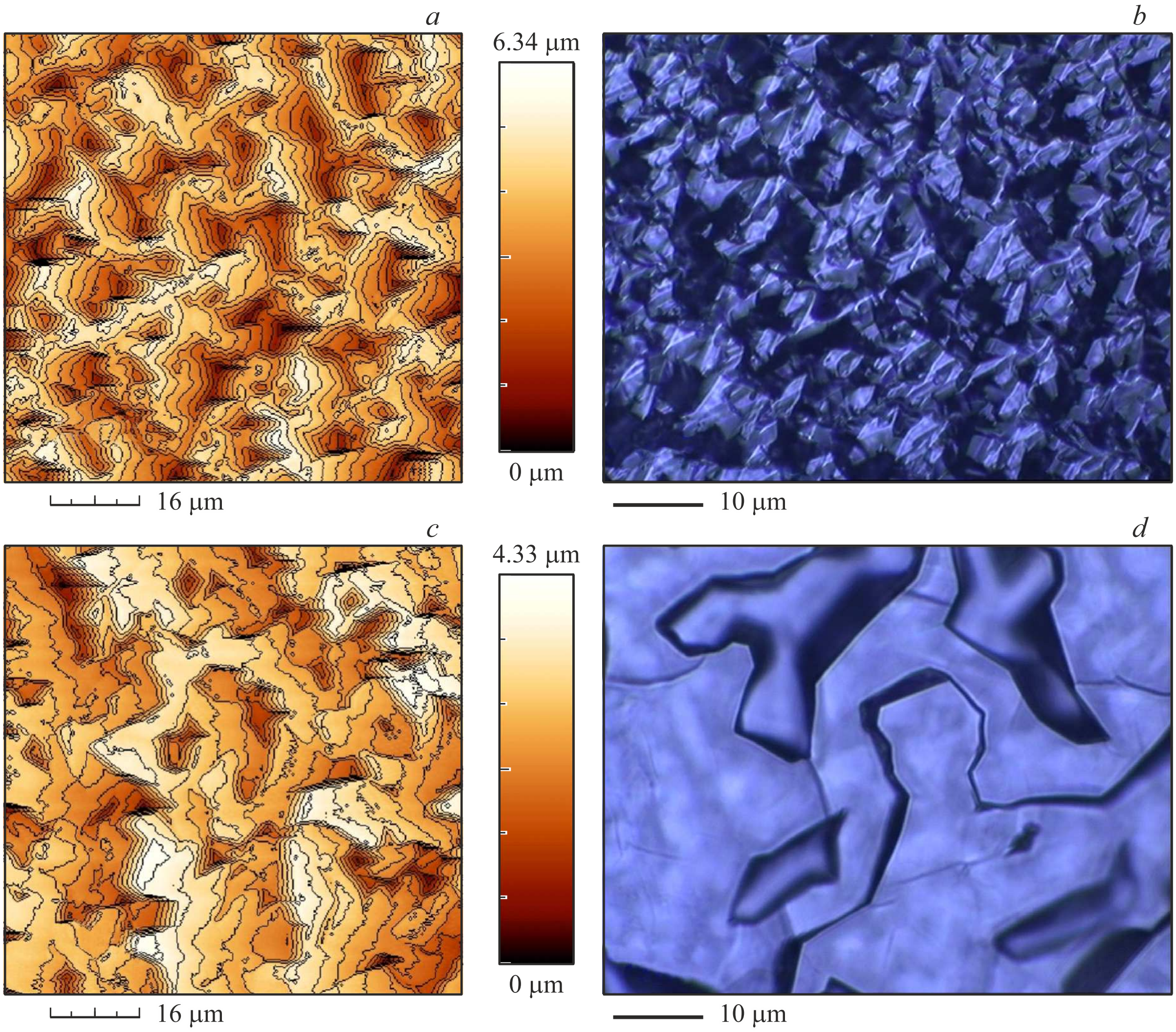

Figure 1. AFM images of AlGaN/SiC/Si(001) (*a*), AlGaN/SiC/Si(011) (*c*) and optical images of AlGaN/SiC/Si(001) (*b*), AlGaN/SiC/Si(011) (*d*) heterostructures. (The colored version of the figure is available on-line).

type doped with boron and with crystallographic directions (001), (011) and (111). The Si substrates with orientation (011) and (111) were without deviation from the base direction, while the Si substrate with orientation (001) was deflected by 4° to the (111) direction. The synthesis of SiC layers was carried out for 10 min at 1100°C and pressures inside the reactor of 0.5, 0.7 and 2.3 Torr for substrates with crystal-lattice orientations (001), (011) and (111), respectively. The thickness of synthesized SiC layers, according to spectral ellipsometry data, is 4 nm, the surface roughness, according to optical profilometry data, is 0.5 ± 0.2 nm. The growth of AlGaN layers was carried out by chloride-hydride epitaxy (HVPE) [5,6] at 1020°C in ammonia and argon atmospheres with a total flux of 1 and 4 l/min, respectively. A hydrogen chloride flow rate of 0.2 and 0.1 l/min was used to transfer aluminium and gallium atoms. The thickness of the AlGaN layers formed on the nano-SiC/Si hybrid substrates was $6-9\,\mu$m. The surface morphology of AlGaN films was investigated by atomic-force microscopy (AFM) using a Nanosurf Easy Scan microscope, and the hardness and modulus of elasticity parameters of AlGaN layers were measured by nano-indentation on a NanoTest 600 device made by Micromaterials.

According to AFM data, the surface structure of AlGaN on nano-SiC films on Si with orientations (001), (011) and (111) is significantly different. In the case of AlGaN layer on nano-SiC/Si(001) hybrid substrate (Figure 1, *a* and *b*), the surface structure consists of crystal clusters in the form of ridges. The slope planes are tilted at $45 \pm 5^\circ$ and $20 \pm 3^\circ$ relative to the general plane of the sample surface, with the projection areas of these slopes occupying 40 and 60% of the total area of the AFM image. The height of the ridge-shaped clusters is $2-4\,\mu$m. The rms roughness of the AlGaN surface in this case is $0.8\,\mu$m.

The surface structure of the AlGaN film formed on the nano-SiC/Si(011) hybrid substrate presents smooth terraces up to $20\,\mu\text{m}^2$ (Figure 1, *c* and *d*) with sharp slopes at the edges. Terraces occupy > 70% of the total area of the AFM image. The slope of the terraces and slopes surface relative to the general plane of the sample surface is 5 ± 1 and 25 ± 5°. The height of slopes of such structure, according to AFM data, is equal to 2.0–0.3 μm. The surface structure of the AlGaN layer on nano-SiC/Si(011) has a rms roughness of 0.5 μm.

Analysis of AFM data of AlGaN film on nano-SiC/Si(111) showed that the surface structure of this sample is the smoothest. The rms surface roughness of the AlGaN layer in this case is 60 nm. The surface structure of AlGaN formed on nano-SiC/Si(111) consists of clusters in the form of hills with a height of 200–400 nm (Figure 2). According to AFM data, the hills have a rounded shape with base diameters ranging from 10 to 30 μm. The slope of the side slopes of the hill-shaped surface structure of the AlGaN layer relative to the general plane of the sample is 0.5–1.8°. Growth pits were found in AlGaN films on nano-SiC/Si(111). These growth defects, known as „pits (pit)“, occur during the growth of AlGaN films on defective sites of hybrid nano-SiC/Si substrates.

The mechanical properties of AlGaN films grown on nano-SiC/Si were measured by nano-indentation near the surface and inside the AlGaN layer. The initial stage of nano-indentation (Figure 3), when predominantly elastic deformation occurs, was analyzed using the modernized Hertz [7] relation. Comparison of the experimental data with the upgraded Hertz relation showed that the parameters of the reduced modulus of elasticity near the surface for AlGaN on nano-SiC on Si films with orientations (001), (011) and (111) are significantly different. Near the surface, the reduced modulus of elasticity is 150 ± 50, 190 ± 50 and 310 ± 40 GPa for AlGaN/SiC heterostructures on Si with orientation (001), (011) and (111), respectively.

The hardness and reduced modulus of elasticity parameters within the AlGaN films were determined using the Oliver–Farrah [8] method. Analysis of nano-indentation data showed that the average value of modulus of elasticity inside AlGaN films for all investigated samples is equal to 300 GPa. The highest standard deviation from the mean value of the reduced modulus of elasticity of 100 GPa was observed in the nano-indentation of AlGaN/SiC/Si(001) heterostructure. In the case of AlGaN films on nano-SiC on Si with orientations (011) and (111), the standard deviation from the mean value of the reduced modulus of elasticity is 40 GPa. According to nano-indentation data, the hardnesses of AlGaN films on nano-SiC on Si with orientation (001), (011) and (111) are 15 ± 4, 12 ± 1 and 18 ± 3 GPa, respectively. In [9] the phenomenon of self-organization during the growth of AlGaN films on nano-SiC/Si hybrid substrates was discovered, which leads to the formation of interlayers (domains) with AlGaN composition close to stoichiometric. These interlayers are located between layers $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$ with low Al ~ 20%. Thus, the top layer of AlGaN film on nano-SiC/Si is a composite material $\mathrm{Al}_{0.2}\mathrm{Ga}_{0.8}\mathrm{N}$. Since the thickness of the $\mathrm{Al}_{0.2}\mathrm{Ga}_{0.8}\mathrm{N}$ layer is greater than 1 μm [9], the nano-indentation measures the mechanical characteristics of this particular layer. The modulus of elasticity of AlN and GaN, according to nano-indentation [10,11], is 320 and 295 GPa. Using Wegard's law and the values of the moduli of elasticity of AlN and GaN from [10,11], the concentration of Al and Ga in the investigated AlGaN films can be estimated. The nano-indentation results confirm that the concentration of Al and Ga is 20 and 80%, respectively, which is consistent with the results of [9].

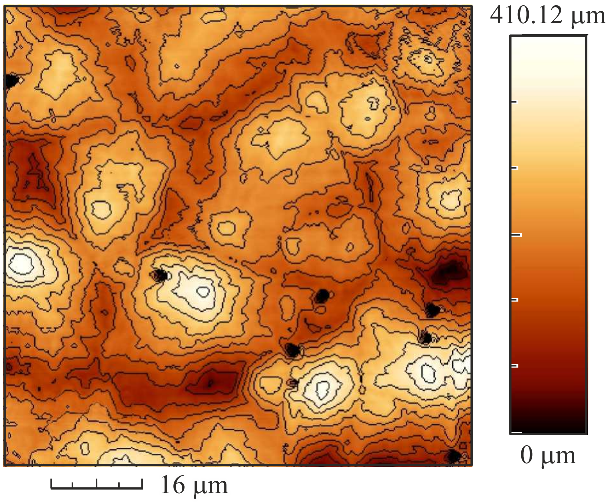

Figure 2. AFM images of AlGaN/SiC/Si(111) heterostructures.

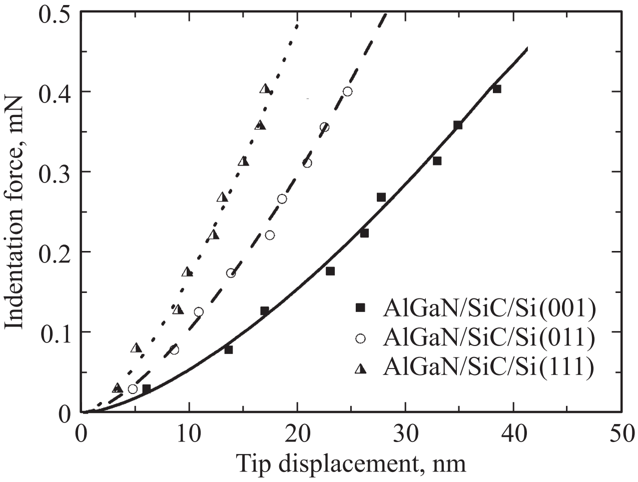

Figure 3. Dependences of indentation force on indenter displacement at the initial stage of nano-indentation of AlGaN/SiC/Si heterostructures. Dots — experimental data, lines — modernized Hertz ratios.

Thus, in the present work, the structural and mechanical characteristics of AlGaN thin films formed by CGE on nano-SiC/Si substrates with Si(001), (011) and (111) orientation were investigated for the first time. The characteristic structural parameters of the surface of AlGaN layers on nano-SiC/Si have been determined by AFM method. It is shown that the surface structure of AlGaN layers grown on Si substrates with (001), (011) and (111) orientations is dramatically different. The RMS surface roughness of AlGaN on nano-SiC on Si layers with orientations (001), (011) and (111) was determined to be 800, 500 and 60 nm, respectively. It should be noted that the creation of microelectronic and optoelectronic devices with high accuracy and reliability requires crystal surfaces with very low roughness, usually < 1 nm. The parameters of hardness and modulus of elasticity of AlGaN layers grown on nano-SiC/Si hybrid substrates were measured by nano-indentation method for the first time.

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Conflict of interest

The authors declare that they have no conflict of interest.

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