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SEMIPOLAR GaN ON Si(001): THE ROLE OF SiC BUFFER LAYER SYNTHESIZED BY METHOD OF SUBSTRATE ATOM SUBSTITUTION

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Abstract. The new HVPE method has been developed for synthesis of semipolar gallium nitride on the substrate of Si(100) deviated on 2°-7° from the direction <100>. The method is based upon the formation of two buffer layers. First, the thin buffer layer (20-30nm) of SiC is formed, which is grown using the technology of substitution of part of silicon atoms in substrate of Si by carbon atoms, then the layer of AlN is deposited on this surface. It has been shown that the misorientation of Si substrate from the direction <100> and formation of the thin SiC layer permit to form the epitaxial layers of semipolar gallium nitride. The polar axis "c" of wurtzite crystal appeared to be deflected by 55° from the plane (100) of Si substrate. The obtained films of semipolar GaN had a half-width of the rocking curve FWHM of the order of ω_θ ~24'. The thickness of GaN films was in the limits of 10-14 microns. The structure GaN/AlN/SiC/Si(100) formed during this process exhibited a bending of a cylindrical form. The formation of this bending is explained by anisotropy of the deformation of semipolar GaN on silicon.

1. Introduction

Epitaxial structures based upon semipolar GaN play important role in development of light diodes [1] and laser diodes [2]. Semipolar GaN structure can reduce or eliminate the polarization-induced quantum confined Stark effect [3] responsible for wavelength blueshift and limited radiative efficiency [4]. Among various materials such as (Al_2O_3, SiC, Si) namely the silicon is the most attractive substrate for such a light emitted structures. This high merit is attributed to the opportunity of using of large size substrates (up to 300 mm) in diameter, comparatively low cost, high electric and thermal conductivity, however the large difference in the constants of crystalline lattices and Coefficients of the Thermal Expansion (CTE) between GaN and Si leads to the appearance of the cracks during the epitaxial growth of thick GaN layers on the silicon substrates [5]. To suppress the chemical reactions between the silicon substrate and the gaseous phase containing the components necessary for formation of GaN layer the thin buffer layer of AlN is used [6]. During recent years the significant number of papers have been published on the growth of thin (~ 1 micron) GaN layers in semipolar directions by the method of Metal Organic Vapor Phase Epitaxy (MOVPE) on the substrates of Si(113) [7], Si(100) [8,9] and Si(112) [10]. The papers [8] and [11] describe the formation of the light diode and laser structures on the "template" of (1-101) GaN/Si(100) by MOVPE

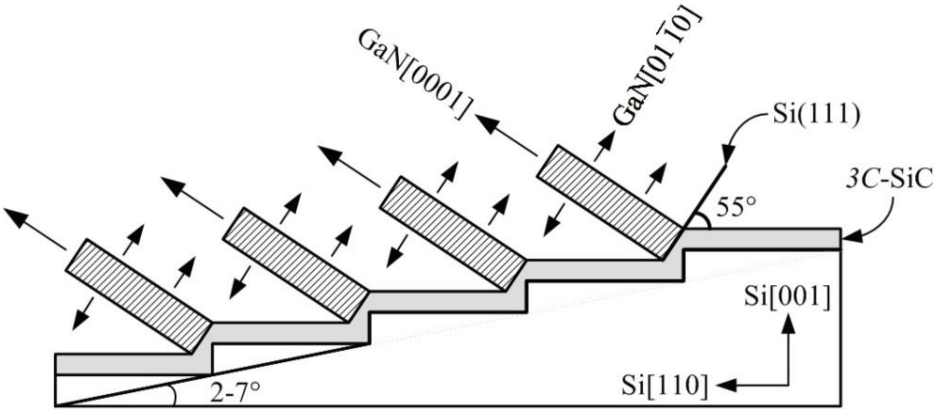

Fig. 1. Scheme of the process of synthesis of semipolar GaN on the 3C-SiC(111) quasi surface.

The XRD results indicate the presence of homogeneously ordered GaN layers with the layer deviation from the polar position of the *c* axis of the wurtzite crystal by an angle of 42° for the substrate Si(001) with a disorientation of 7°. Analysis of the electron diffraction pattern (Fig. 2) recorded at the interface of the heterostructure GaN/AlN/3C-SiC/Si(001) showed that the polar axis *c* of gallium nitride was parallel to the direction [111] of the silicon substrate; i.e., the layer deviation from the polar position of the *c* axis of wurtzite crystal was about 55° without taking into account the substrate disorientation (Fig. 2a).

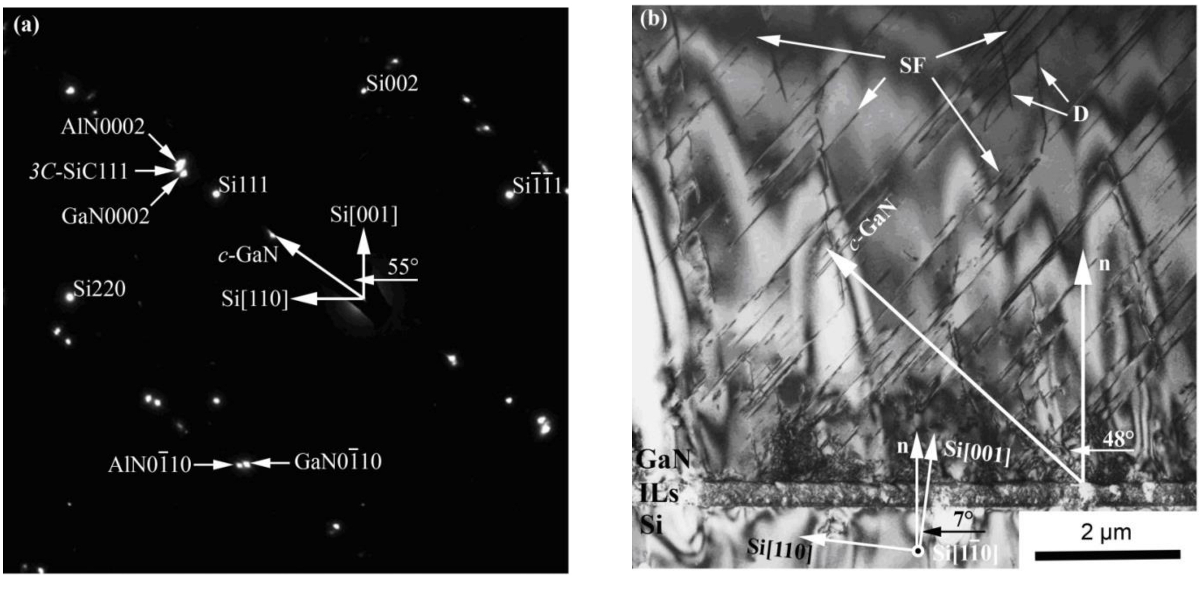

Fig. 2. (a) Electron diffraction pattern and (b) TEM image of the heterostructure of GaN/AlN/3C-SiC/Si(001). Arrows in the gallium nitride layer indicate stacking faults (SF), dislocations (D), and intermediate layers (IL) of AlN and 3C-SiC.

TEM image of the structure showed that the angle between the normal to the substrate and the perpendicular direction to lines of the stacking faults in the direction [0001] GaN was 48° and 51° for structures synthesized on substrates with cutoff angles 7° and 4°, respectively (Fig. 2b), which is in agreement with the microelectron diffraction pattern analysis results. The sum of the XRD and TEM results enables one to assume that the combined technology of solid-

structure GaN(1-101)/AlN/SiC/Si(011) seems to related with the difference of the coefficients of thermal expansion along the directions “a”-<11-20> and “c”-<11-23> of the wurtzite semipolar crystal of gallium nitride. In fact, the values of CTE in the lattice of gallium nitride in the direction of axes “c” and “a” are different at the room temperature (α_c GaN ~ $3.52\cdot10^{-6}$ 1/K, α_a GaN ~ $3.93\cdot10^{-6}$ 1/K [21]). They differ also from the CTE of silicon equals $\alpha_{Si} \sim 2.6\cdot10^{-6}$ 1/K [5].

As known, at the cooling of the structures of polar gallium nitride, synthesized on the silicon substrate the layer of gallium nitride is in the state of isotropic compression because the CTE of GaN for lattice “a” is higher than CTE of Si. With the increase of the thickness of the GaN layer the curvature radius of the structure bending is reducing. Let us assume that the contribution of thin interlayers of SiC and AlN in the bending of the structure GaN/AlN/SiC/Si(100) is insignificant. From here follows, that at the cooling of the layer of semipolar gallium nitride on the silicon substrate from the temperature of epitaxy down to room temperature the bending of the structure GaN/Si will be determined only by difference in CTE between GaN and Si. The CTE for lattices GaN and Si differ not only along the direction “a” of GaN lattice, but also along the direction “c” of the lattice GaN and Si (Fig.4).

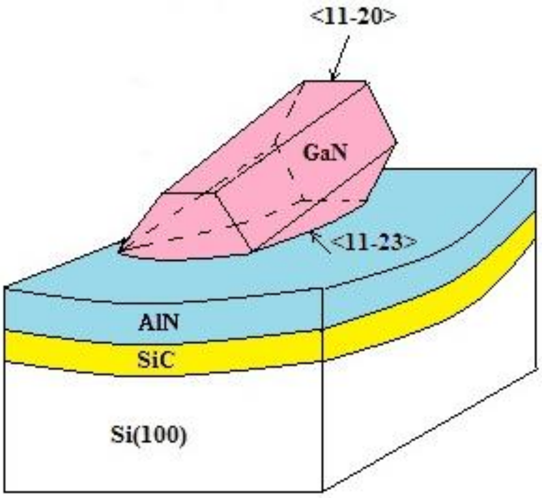

Fig. 4. Schematic drawing of the synthesis of the GaN(1-101)/AlN/SiC/Si(100) structure.

Since the CTE of lattices “a” and “c” are different, the cooling of the film of semipolar gallium nitride on the silicon substrate will lead to the anisotropic bending of the structure GaN/AlN/SiC/Si(100). That to confirm this hypothesis we estimated by formula [22] the anisotropic bending of the semipolar GaN on Si(100) substrate , assuming that CTE of GaN in the semipolar plane will be equal to CTE of GaN in the plane (100).

$$\frac{1}{R} = 6m\varepsilon\left(\frac{h}{h_2}\right)\left(\frac{1+h}{1+mh(4+6h+4h^2)+m^2h^4}\right),$$

where: $m = \frac{E_1}{E_2}$, $h = \frac{h_1}{h_2}$, $\varepsilon = (\alpha_1 - \alpha_2)\Delta T$,

- E_1 – Young modulus of GaN =210 GPa, E_2 = 165,6 GPa – Young modulus of Si
- h_1- thickness of GaN , h_2 – thickness of Si.
- α_1- CTE of the lattice GaN “a” and “c” respectfully, α_2 – CTE of lattice Si.
- ΔT – Difference between growth and room temperature.

The estimates obtained on the GaN layer bending radii in the directions of <11-23> and <11-20> on the substrate Si(100) are presented in the Table I.

Table 1. Dependences of the radii of curvature of the heterostructure in the direction of disorientation of substrate (R_a) and in the perpendicular direction (R_b) on the GaN layer thickness.

GaN layers Thickness, μm	Disorientation, deg	Experiment	
		R_a, m	R_b, m
~ 2	2	-1,6	-1,8
10	4	-0,4	-1,6
14	7	-0,25	-1,4

It is seen that appearance of anisotropic deformation in the layer of semipolar GaN synthesized on the substrate of Si(100) is in accordance with the hypothesis according to which this deformation is due to two reasons: difference in the thermal expansion coefficients for lattices SiC and lattices GaN, and anisotropy of the coefficients of thermal expansion along the plane of semipolar GaN.

5. Conclusions

Thus, the new approach to the growing of the semipolar layers of gallium nitride by HVPE method on the planar substrate of Si(100) deviated from the plane (100) towards the plane Si(011) has been proposed and implemented. The semipolar direction of the GaN synthesis has been given by the formation of the three-dimensional prisms of SiC covered by the planes (111). The formation of given structures became possible due to development of the method of solid- phase epitaxy of SiC on Si and favorable matching of these films with the properties of AlN and GaN films. As a result of our studies we have grown the layers of GaN on the silicon carbide “template “ with orientation of the surface parallel to planes (10-12) or (1-101) and with value of half-width of x-ray diffraction of FWHM ω_θ~24'. The proposed approach, given in this paper, permits to grow thick layers (>10 micron) of gallium nitride and could be perspective at the formation of “templates” for the structures of gallium nitride based optoelectronics.

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