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Curvature and bow of III-N HEMT structures during epitaxy on silicon substrates

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Abstract. High Electron Mobility Transistor (HEMT) heterostructures based on III-N semiconductors (nitrides of Al and Ga) have become increasingly widespread in recent years. They are used in the manufacture of microwave transistors, high-power transistors for power electronics, etc. However, mass application of such transistors requires a reduction in the cost of heterostructures due to the use of cheap substrates and an increase in the area of one substrate. Thus, substrates of single-crystal Si(111) are of great interest. They are available in diameters up to 300 mm, and the possibility of growing III-N structures has already been demonstrated for them. Nevertheless, the epitaxy of III-N HEMT structures on Si substrates is complicated due to a number of technological difficulties in the epitaxy of such structures. In this paper, the dynamics of curvature and residual bow of III-N HEMT structures were experimentally studied during epitaxy and after cooling for Si(111) substrates with a diameter of 100 mm and various thicknesses of substrates and grown semiconductor films. It has been shown that the technology developing and optimization should be carried out on thin substrates, while device structures should be grown on thick substrates. Furthermore, the mechanical stresses can be controlled accurately enough so after epitaxy the bow of the structure is minimal.

Keywords: MOVPE, HEMT, elastic strain, silicon

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Кривизна и прогиб III-N HEMT структур при эпитаксии на кремниевых подложках

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Аннотация. В настоящей работе проведено экспериментальное исследование динамики кривизны и остаточного прогиба III-N HEMT структур во время и после эпитаксии для подложек Si(111) диаметром 100 мм различной толщины; была определена динамика кривизны от толщины структуры во время роста, что позволяет определить параметры эпитаксии для получения необходимого прогиба структур после остывания.

Ключевые слова: ГФЭ МОС, полевые транзисторы, упругие напряжения, кремний

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Introduction

High Electron Mobility Transistor (HEMT) heterostructures based on III-N semiconductors (nitrides of Al and Ga) have become increasingly widespread in recent years [1]. They are used for manufacturing microwave transistors, high-power transistors for power electronics, etc. However, the mass application of such transistors requires a reduction in the cost of heterostructures through the use of cheap substrates and an increase in the area of each of them. From this point of view, substrates of single-crystal Si(111) are of great interest. They are available in diameters up to 300 mm [2] and have already been shown to grow III-N structures. However, epitaxy of III-N HEMT structures on Si substrates is very difficult due to the significant difference in lattice parameters and in thermal expansion coefficients (TEC) of the substrate and III-N layers [3]. There are also a number of technological difficulties in the epitaxy of such structures associated with the solubility of Ga in Si, warping of large-diameter substrates due to temperature inhomogeneity, leading to their plastic deformation, etc.

Materials and Methods

Equipment. The experiments were carried out on a MOVPE Dragon D-125 growth system [4] with an inductively heated susceptor and custom-built gas injector allowing high growth rate and uniformity. The setup has a horizontal flow reactor and a laser reflectometry system with the ability to measure the structures curvature in-situ.

Structure growth method on silicon. One of the main epitaxy problems is the difference between the TEC of the substrate and III-N layers, which leads to a strong contortion of the structure after epitaxy and cooling. To eliminate this effect, the technique of creating mechanical stresses in the growing III-N layers during growth is used [5–9] to compensate for the stresses that arise during the cooling of the structure. Since the structures are highly stressed, after the epitaxy process, they can have a different bow, which affects the subsequent stages of transistor fabrication. The order of growing HEMT structures is shown in Fig. 1.

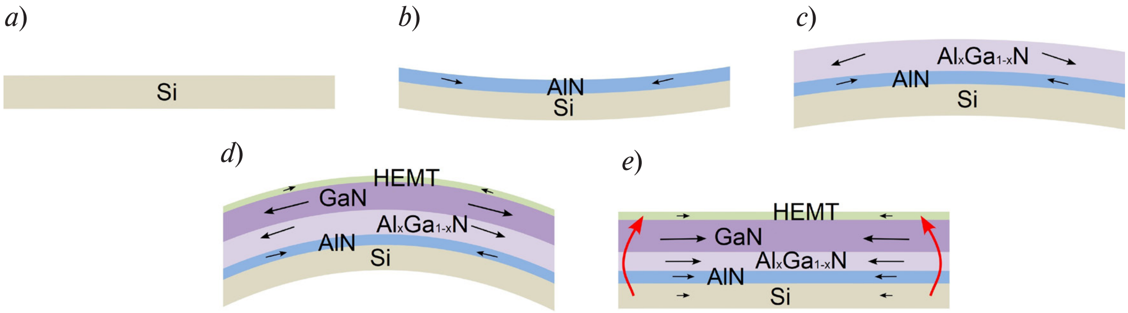

Fig. 1. Order of growing HEMT structures: flat silicon substrate (*a*); first AlN layer protecting Si from Ga and creating initial stresses (*b*); AlGaN buffer of several variable composition layers to maintain the coherence of GaN growth on AlN and stress accumulation (*c*); GaN layer for the accumulation of mechanical stresses, the creation of a non-conductive buffer layer and the active region of the HEMT (*d*); structure distortion during cooling after epitaxy (*e*).
The black arrows show the direction of layer contortion at each stage; the red ones show the distortion of the whole structure during cooling

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Structure growth starts with substrate annealing (T = 1130 °C; p = 100 mbar) to get rid of silicon oxide covering the substrate (Fig. 1, *a*). After that an AlN layer is deposited (T = 1100 °C [10]; p = 110 mbar; growth rate ≈ 0.5 μm/h) to prevent etching of Si by Ga melt (Fig. 1,*b*). Then a set of AlGaN layers (T = 1050 °C; p = 100 mbar; 6 layers of different composition; composition being controlled by concentration of Al and Ga ratio; Al concentration in solid solution: 80%, 60%, 45%, 35%, 15%, 10%) for stress compensation are grown (Fig. 1,*c*). HEMT structure is finalized (T = 1050–1100 °C; p = 100−400 mbar) with doped with Fe and C and undoped GaN layers, AlN spacer (f = 1 nm), $Al_{0.23}Ga_{0.77}N$ barrier layer (f = 23 nm) and in-situ deposited SiN (f = 5 nm) (Fig. 1,*d*). At the end of epitaxy grown structure is cooled down (t ≈ 30 min) to the room temperature (Fig. 1, *e*).

Geometry of the structures. The curvature coefficient, defined as the reciprocal of the curvature, at constant mechanical stresses in the structure layers according to the Stoney equation (1) is directly proportional to the thickness of the grown film and inversely proportional to the square of the substrate thickness:

$$k = \frac{1}{R} \sim \frac{f}{H^2}, \tag{1}$$

where k is the curvature coefficient, R is the curvature, f is the film thickness, H is the substrate thickness.

Based on geometric considerations (Fig. 2) and the smallness of bow h in relation to the curvature R and substrate diameter d, we can obtain expression (2) for calculating h.

$$h = \frac{d^2}{8R} = \frac{kd^2}{8}. \tag{2}$$

The structure bow is proportional to the square of the substrate diameter, so as substrates increase in size, it is necessary to significantly reduce the residual curvature. The condition for post-growth processing is a bow of no more than 50 μm, which corresponds to a curvature of 40 km^{-1} for a 100 mm substrate.

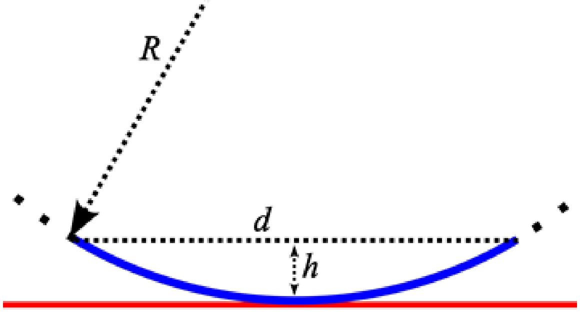

Fig. 2. Relation between curvature R and substrate diameter d and bow h

Results and Discussion

The curvature of the grown structure, as well as the growth rate of each layer, was determined from data in-situ measured during growth for each layer. The structure layers thicknesses were calculated based on the known growth times and corresponding for each layer rates, and the bow was calculated based on the curvatures and structure geometric dimensions.

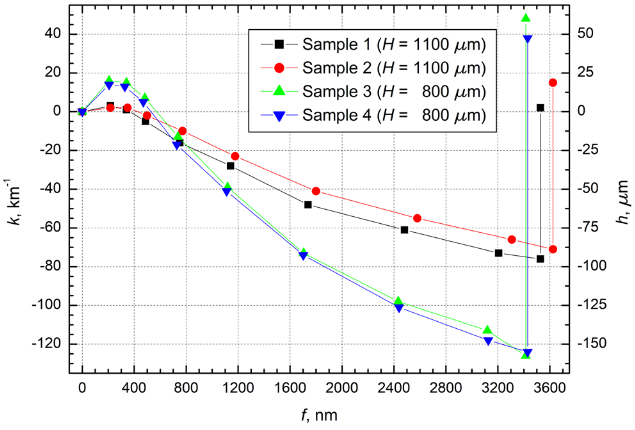

Fig. 3. Graph of the curvature k and bow h vs thickness of the growing structure f at different thicknesses of substrate H
(given in brackets for each sample)

Dependence on substrate thickness. Fig. 3 shows the curvature and bow dependence on thickness of the growing structure at different thicknesses of substrate. It is clearly seen that the thinner substrate is contorting more than thick one.

Dependence on structure thickness. Fig. 4 shows the curvature and bow dependence on thickness of the growing structure for different thicknesses of final films. Substrate thicknesses were equal. It is seen that controlling compositions and thicknesses of the buffer layers allow to control the

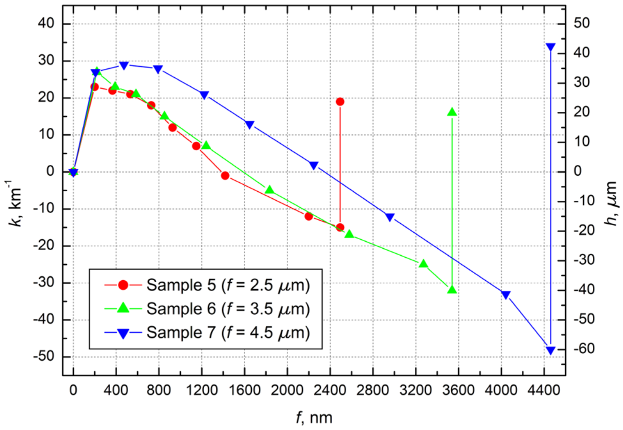

Fig. 4. Graph of the curvature k and bow h vs thickness of the growing structure f at different total thicknesses of structure (given in brackets for each sample)

mechanical stresses in the layers during the growth.

Table 1 shows the final bows of the heterostructures. The best result was demonstrated by sample 1, while sample 3 did not fit into the tolerance at all (II.C).

Table 1

Final bow of heterostructures after cooling

Sample	1	2	3	4	5	6	7
h, µm	2.5	18.8	60.0	47.5	23.8	20.0	42.5

Conclusion

To conclude, it has been shown that under certain mechanical stresses in the layers, the curvature and bow of the structure are inversely proportional to the square of the substrate thickness. Therefore, the technology developing and optimization should be carried out on thin substrates so that the sensitivity is higher and the response to stress changes is more noticeable, while device structures should be grown on thick substrates so that the final bow is minimal.

Furthermore, the mechanical stresses can be controlled accurately enough by compositions and thicknesses of the buffer layers so that after epitaxy the bow of the structure is minimal.

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