Comparative study on stress in AlGaN/GaN HEMT structures grown on 6H-SiC, Si and on composite substrates of the 6H-SiC/poly-SiC and Si/poly-SiC

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Abstract. The stresses in GaN-based HEMT structures grown on both single crystal 6H SiC(0001) and Si(111) have been compared to these in the HEMT structures grown on new composite substrates engendered as a thin monocrystalline film attached to polycrystalline 3C-SiC substrate. By using HRXRD technique and wafer curvature method we show that stress of monocrystalline layer in composite substrates of the type mono-Si/poly-SiC is lower than 100 MPa and residual stress of epitaxial GaN buffer grown on the composite substrate does not exceed 0.31 GPa, but in the cases of single crystal SiC or Si substrates the GaN buffer stress is compressive in the range of -0.5 ÷ -0.75 GPa. The total stress of the HEMT structure calculated from strains is consistent with the averaged stress of the multilayers stack measured by wafer curvature method. The averaged stress of HEMT structure grown on single crystals is higher than those in structures grown on composites substrates.

1. Introduction

Currently, GaN-based high electron mobility transistors (HEMTs) are considered as the most promising devices for high power and high temperature operation [1]. A key issue in exploiting the properties of III-nitride materials for these applications is the fabrication of high thermal conductivity substrates with good lattice and thermal match. Due to the lack of native III-nitride substrates, the devices are commonly fabricated on mismatched sapphire and silicon wafers, which results in highly stressed AlGaN/GaN heterostructures. The most suitable SiC substrate, owing to superior thermal conductivity and similar wurtzite structure with almost good matched lattice parameters, remains extremely expensive. To solve this problem, two novel composite substrates tailored for GaN-based HEMTs have been recently developed by Smart Cut™ technology [2, 3]. First one is a SiCopSiC structure, where a thin film of monocrystalline SiC is bonded onto an oxidized polycrystalline SiC wafer. Due to multiple usages of high quality single crystal SiC as seed layer and to high thermal conductivity of the inexpensive polycrystalline SiC, this substrate would significantly improve the cost

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of GaN-based HEMT structure grown on it. The second substrate, SopSiC, is a monocrystalline Si bonded onto oxidized polycrystalline SiC. Here, silicon as seed layer will provide large diameter substrates and the polycrystalline SiC will significantly improve the thermal conductivity as opposed to bulk silicon.

In this paper we present the results of stress measurements in the AlGaN/GaN HEMT structures grown on mono-SiC 6H, on mono-Si and on composite substrate SopSiC and SiCopSiC. Two complementary techniques for stress measurement have been applied: Wafer Curvature Method (WCM) and High Resolution X-ray Diffractometry [4, 5].

**Experimental**

The SiCopSiC wafer consisted of the polycrystalline SiC 3C, followed by ~230 nm SiO2 and 280 nm of monocrystalline 6H-SiC. For SopSiC, 480 nm thick (111)-oriented Si was applied as the top seed layer. AlGaN/GaN heterostructures on SiC, Si and on composite SopSiC substrates were grown by Molecular Beam Epitaxy (MBE), while those on SiCopSiC substrates were grown by Metalorganic Vapour Phase Deposition (MOCVD). The epitaxial growth began typically with deposition of a low temperature nucleation AlN film, than 25/25 nm thick (Al)GaN/AlN buffers, followed by a thick additional GaN buffer, a monolayer channel, and an AlGaN barrier on the top. The details on samples under investigation are given in the table 1.

| Sample        | Substrate                  | Buffer 1 | Buffer 2 | Barrier       |
|---------------|----------------------------|----------|----------|---------------|
| SopSiC        | 3C-poly-SiC/SiO2/(111)Si   | -        | -        | -             |
| SiCopSiC      | 3C-poly-SiC/SiO2/(0001)SiC 6H | -        | -        | -             |
| HEMT M1 MBE   | (0001)SiC 6H               | AlGaN/AiN | GaN(1400 nm) | AlGaN(22 nm) |
| HEMT M2 MBE   | (111)Si                    | AlGaN/AiN | GaN(800 nm)  | AlGaN(26 nm)  |
| HEMT M3 MBE   | 3C-poly-SiC/SiO2/(111)Si   | AlGaN/AiN | GaN(1400 nm) | AlGaN(23 nm)  |
| HEMT M4 MOVPE | 3C-poly-SiC/SiO2/(0001)SiC 6H | AlGaN/AiN | GaN(1700 nm) | AlGaN(22 nm)  |

Measurements of film stress were conducted by: HRXRD measurement of film strain using PHILIPS X’Pert MRD diffractometer and wafer-bending technique using ADE Ultragauge Map Shape Metrology System and Tencor FLX-2320 Stress Measurements System. HRXRD was used to inspect crystal structure and to measure lattice parameters in epitaxial film. The lattice parameters are determined from positions of the diffraction peaks precisely measured in the triple-axis mode. The geometry of the samples included symmetrical and asymmetrical cases in reflection, as well as grazing-incidence mode. The lattice parameters $c$ are directly extracted from 00.2 lattice spacing, but the parameter $a$ is extracted from asymmetrical reflection of the -1-1.24 peak. Taking into account that hexagonal GaN film growth in c-axis direction is confirmed by HRXRD, a bi-axial stress state in film plane can be applied in terms of elastic theory to calculate the film stress. Biaxial modulus $E/(1-\nu)$ is a factor of proportionality in the function of stress $\sigma$ vs. strain $\varepsilon$ in the film plain, where: $E$ – Young modulus, $\nu$ – Poisson coefficient, $\varepsilon_c$ and $\varepsilon_a$ – strain in c- and a-axis direction, respectively. Calculation of $\varepsilon_c$ and $\varepsilon_a$ strains requires true values of relaxed lattice parameters assigned as $c_{\text{relx}}$ and $a_{\text{relx}}$. Relaxed lattice parameters of epitaxial film have been calculated from the experimental values of $c$ and $a$ using the formula applicable for biaxial stress state:

$$\frac{c - c_{\text{relx}}}{c_{\text{relx}}} = \frac{2\nu}{\nu - 1} \frac{a - a_{\text{relx}}}{a_{\text{relx}}}$$

The ratio of $c_{\text{relx}}/a_{\text{relx}} = 1.626$ is known for hexagonal GaN structures. The value of the Poisson parameter being $\nu = 0.23$ was assumed for epitaxial Al-Ga-N films. For stress calculation, biaxial modulus $E/(1-\nu)$ in the (0001) plain was assumed to be 396 GPa, 430 GPa, 566 GPa for GaN, AlN [6]
and 6H-SiC [7], respectively. Total stress of the film stack is obtained as a sum of ratios of each i-th film force per line $\sigma_i$, ($t_i$ - thickness of i-th film) by the total thickness of the stack.

Based on measured wafer bows, corresponding radii of curvature are calculated, and next the average stress is calculated using Stoney’s equation, where biaxial modulus of 466 GPa and 229 GPa are taken here for the poly-SiC 3C and (111)Si substrates [7], respectively.

**Results and discussion**

The stress in the Si/SiO$_2$ bilayer measured on the SopSiC series using wafer-bending technique is in the range of +/-100 MPa. The stress was verified by strain measurement in (111)Si plane on the SopSiC sample, where lattice parameter of 0.5431039 nm was applied for perfect single Si crystal at relaxed state. The calculated stress of -16 MPa is compressive, and it is within the error range. In the case of SiCopSiC substrates the stress of the SiC/SiO$_2$ bilayer is evaluated from wafer bending as tensile close to 250 MPa with an error 30%. The positive value for the stress seems to be confirmed by strain measurement of $4.5 \times 10^{-4}$ in a plane of 6H SiC film, if we take reference for relaxed SiC lattice $a = 3.03086\AA$ according to available data [7].

The results of HRXRD measurements are shown in the figure 1. Here, reciprocal space maps of samples around the -1-1 4 Bragg reflections are essential to explain strain relations between the epitaxial layers. A signal corresponding to the AlGaN barrier is located above the main GaN peak from the thick buffer indicating pseudomorphic growth of the top AlGaN film. The position of the AlN signal shows strained properties of the film relative to neighbours. The reflections on the buffer layers GaN and AlGaN are partially overlapped, what increases the error of calculated parameter $a$.

The stress calculations from strains obtained for GaN, AlN, and AlGaN layers grown on the 6H-SiC and Si substrate are displayed in the table 1. These results show similar values of stress in the bottom layers grown on SiC as those in the structure grown on (111)Si substrate: compressive in AlGaN ($-1.22$ GPa), tensile in AlN ($3.97$ GPa), and only slightly higher compressive stress in GaN film ($-0.73$ GPa). The high positive stress in the intermediate AlN film is a result of tension by epi-films GaN and Al$_{0.1}$GaN with higher lattice parameter $a$, and in contradiction, the adjacent films are compressed. In the cases of the HEMT M3 and M4 grown on SopSiC and SiCopSiC, all films are tensely stressed in range described in the table 3. The positive stress is usually expected for these films with respect to the mismatching of thermal expansion coefficients of substrate and epitaxial materials.

| Film     | $c(\AA)$ | $a(\AA)$ | $\varepsilon_{rel}(%)$ | $\varepsilon_a$ | $\sigma$ (GPa) |
|----------|----------|----------|------------------------|-----------------|----------------|
| AlGaN   | 5.1104   | 3.1836   | 5.1262                 | 3.1672          | 0.0053         |
| GaN     | 5.1891   | 3.1845   | 5.1849                 | 3.1892          | -0.0014        |
| AlN     | 4.9565   | 3.144    | 4.9849                 | 3.1143          | 0.00955        |
| AlGaN   | 5.1718   | 3.1802   | 5.1690                 | 3.1832          | -0.001         |

The lower stress in the films could be explained by the presence of the SiO$_2$ film in composite substrates, which acts as a ‘stress buffer’ due to plastic relaxation at high temperature. The average stress calculated from radii of wafer is in good agreement with the total stress in the HEMT M3. Discrepancies in these stresses for other structures come from the lack of initial radius of the substrate. The average stress in the M1 or M2 structure is most probably lower than presented in the table, as could be suggested from the high wafer bows. Microscopy observations revealed some microcracks at a interlayer of the HEMT structure grown on single crystals, while similar HEMT structure grown on SiCopSiC or SopSiC substrate are free or almost free from these defects. This notes are well corresponding with the lower stress in HEMT structures grown on the composites substrates.
Table 3. Comparison of stress $\sigma$ in the HEMT structure grown on different substrates. Total stress of the film stack is calculated from the strains (HRXRD), the average stress is measured by the WCM.

| Film                      | $\sigma$ in HEMT M2 on (11)Si (GPa) | $\sigma$ in HEMT M3 on SopSiC (GPa) | $\sigma$ in HEMT M1 on (0001)SiC 6H (GPa) | $\sigma$ in HEMT M4 on SiCopSiC (GPa) |
|---------------------------|-----------------------------------|-----------------------------------|------------------------------------------|--------------------------------------|
| AlGaN barrier             | 2.1                               | 2.1                               | 1.74                                     | 3.7                                  |
| GaN buffer 2              | -0.54                             | 0.11                              | -0.73                                    | 0.31                                 |
| AlN buffer 1              | +4.1                              | 1.34                              | 3.97                                     | 0.35                                 |
| (Al)GaN buffer 1          | -0.4                              | 0.57                              | -1.22                                    | -                                    |
| Total stress              | -0.025                            | 0.250                             | -0.31                                    | 0.25                                 |
| Average stress            | 0.280                             | 0.274                             | -0.6                                     | -                                    |

Summary

The stress in the GaN buffer film of the HEMT structure grown on composites substrates SopSiC and SiCopSiC is in the range of $110 \div 310$ MPa, while in the case of (111)Si and (0001)SiC 6H substrates the buffer stress is compressive in the range of $-540 \div -730$ MPa. The total stress in the HEMT structure calculated enabling HRXDR is concurrent with result obtained by wafer curvature method.

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Fig. 5. The reciprocal lattice mapping of the -1-1. 4 Bragg reflections on the HEMT structures M1 grown on (0001)SiC 6H (a) and M2 on (111)Si (b), respectively.