Mat. Res. Soc. Symp. Vol. 639 © 2001 Materials Research Society

Simulation of Stress Generation during GaN Lateral Epitaxial Overgrowth

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ABSTRACT

To facilitate an understanding of defect production in gallium nitride during lateral epitaxial overgrowth, computer models have been developed to simulate the complete mechanical stress and strain fields. The virtual process included the deposition of a GaN seed layer on a sapphire substrate followed by a silicon dioxide stencil mask through which, and over which, the GaN product layer evolved and then cooled down to room temperature. Lattice mismatch and thermal strain were continuously assessed. Shear stresses on different crystallographic planes were analyzed to predict dislocation generation.

INTRODUCTION

Gallium nitride (GaN) is being developed for applications such as blue-light lasers and advanced data storage devices. Lateral epitaxial overgrowth (LEO) continues to be a promising technique for producing GaN films, but during the film growth, high stresses generated by thermal expansion and lattice mismatch between the GaN and sapphire substrates lead to dislocations which adversely affect the film quality and characteristics of subsequent devices. Characterizing the stress distribution at each stage of GaN growth is important for understanding the mechanism of dislocation generation, and consequently, improvements in process procedures. It is very difficult to directly measure the stresses in real time because of the stringent laboratory conditions. Computational simulation of stress evolution is more feasible.

The stress distribution in the selectively overgrown GaN hexagonal structure was analyzed and compared with experimental observations by Liu et al. [1]. Finite element (FE) models simulating the stress generation and development during the entire GaN LEO process, (not just one or several special steps), are discussed in this paper. The models were analyzed by transient algorithms, and both lattice and thermal mismatch were considered simultaneously. Shear stresses on different crystallographic planes have been analyzed. Based on the shear stress assessment, the possibility of dislocation generation and development was evaluated.

GaN LEO PROCESS AND SIMULATION MODELS

The lateral epitaxial overgrowth process was divided into ten principal steps, as shown with the simulation cell in Figure 1. At Step 1 and 2 the seed layer was prepared. At Steps 3, 4 and 5 the SiO_2 was deposited on the seed layer and windows were etched to form a stencil mask. Then the GaN was regrown through the windows, vertically and laterally (Steps 6, 7).

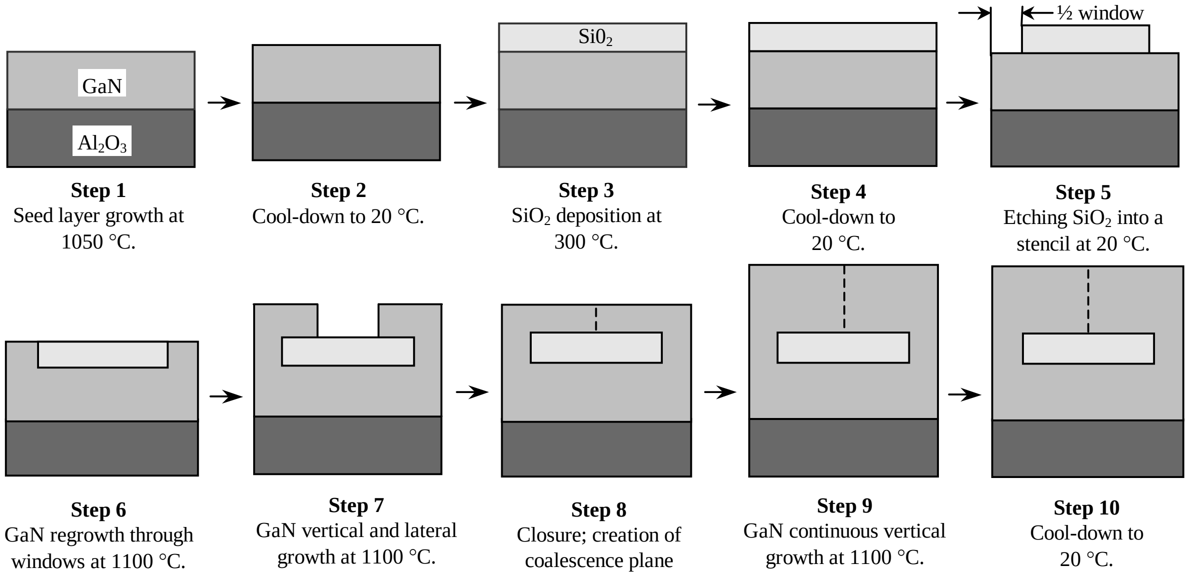


Figure 1. *Simulation cell illustrating the principal steps of the LEO process. Model simulates 800 cells / cm.*

The lateral overgrowth stopped when the gaps were closed (Step 8), but the GaN continued vertical growth. After the GaN reached its maximum thickness (Step 9), it was cooled down to room temperature (Step 10). Three-dimensional transient models were created for simulating the ten steps and the stress analysis was carried out continuously, although the growth process was divided into steps. The output results from last step were used as initial conditions for current step, and results of current step would be input as initial conditions for next step. The windows were 2 μm wide, and the stencil mask periodicity was 12 μm. There were approximately 800 windows and simulation cells per cm on the SiO_2, which made the growing GaN discontinuous with gaps formed in the GaN at Steps 6 and 7 (Figure 1). To simulate the complicated geometry by 3-D FE models, submodeling techniques had to be used. Stresses and displacements of the parent model were applied as boundary conditions for the submodel.

Different constraint conditions between the SiO_2 and the GaN grown above SiO_2 were tested. It was determined that the most representative model corresponded to the GaN and SiO_2 having the same out-of-plane displacements at corresponding points on the interface, but there was no in-plane constraint between each material.

Numerical simulation tests demonstrated that the effect of viscosity of SiO_2 at 1100 ºC on stresses in GaN and sapphire was negligible. Thus, for computational efficiency, all three materials were treated as purely elastic, with the material properties cited in Table I.

COMPARISON WITH EXPERIMENTAL RESULTS (STEPS 1 – 2)

As stated above, it is very difficult to measure the stresses during GaN growth. Only a few experimental results have been published. In-plane stresses during seed layer deposition on sapphire followed by cool-down (Steps 1 to 2), were analyzed by the present technique and compared with other published experimental results [2,3]. Table II shows that the computed stresses are in good agreement with the measured values.

Table I. Material properties utilized in the FE models.

	Elastic Modulus (GPa)	**Poisson's Ratio (m/m)**	**Coefficient of Thermal Expansion (ppm /° C)**
Sapphire	425	0.30	7.50
GaN	196	0.30	5.45
SiO_2	73	0.30	0.55

Table II. Comparison of in-plane normal stress in GaN obtained by analysis and experiments.

		Analysis (MPa)	**Experiment (MPa)**	**Experimental Data Ref.**
Test Case 1*	Lattice mismatch only (1050 °C)	275	140 ~ 290	[2]
	Thermal mismatch only (1050 °C down to 20 °C)	- 580	- 560 ~ - 760	[2]
	Lattice + thermal mismatch (20 °C)	- 305	0 ~ 660	[2]
Test Case 2**	Thermal mismatch only (1050 °C down to 20 °C)	- 530	- 570	[3]

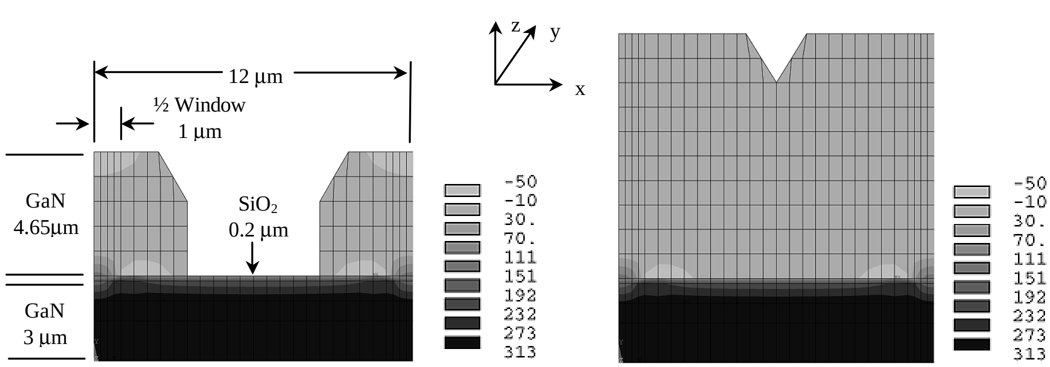
* Effective lattice mismatch strain = 0.1%, two layers (GaN and sapphire) only, GaN thickness = 3 µm, sapphire thickness = 330 µm.

** Two layers (GaN and sapphire) only, GaN thickness = 3 µm, sapphire thickness = 300 µm.

STRESS DEVELOPMENT IN GaN (STEPS 5 – 10)

Stresses in the LEO GaN were very low at growth temperature. Figure 2 (a) shows contours of the in-plane normal stress σ_x, which is the main component of the stress tensor during GaN growth. The tensile stresses in the GaN seed layer caused by lattice mismatch remained at a relatively high level of 300 MPa, but decreased quickly in the GaN above the windows and SiO_2**.** About 2 µm above the SiO_2, the σ_x magnitudes and the corresponding strain energy were nearly zero. The low strain energy cannot support dislocation formation or motion. Figure 2 (b) shows σ_x contours following gap closure. If the coalescence is perfect, without voids or other defects, the σ_x in the GaN above SiO_2 was still negligible, precluding new dislocation generation.

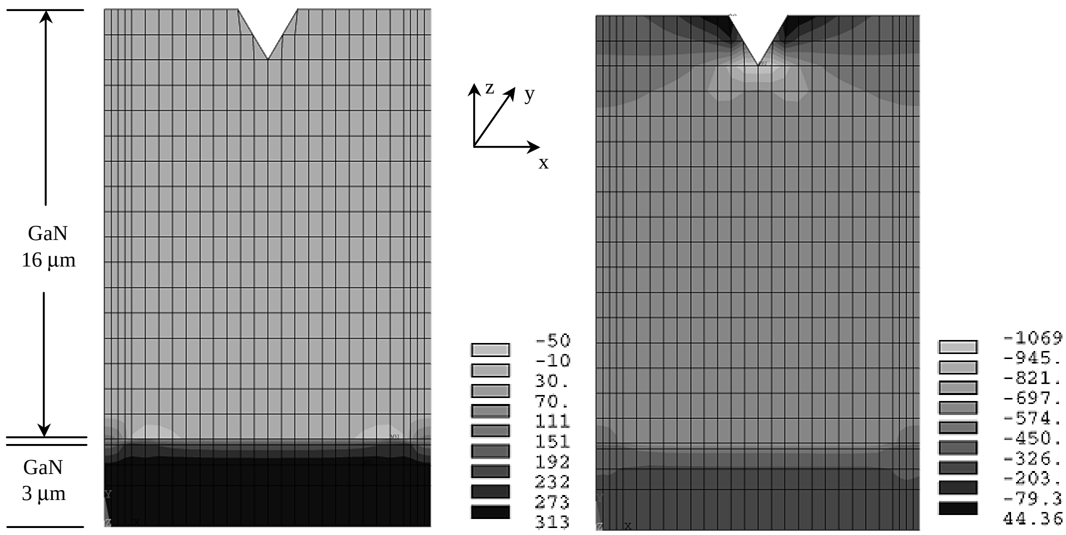
Figure 3 (a) shows the σ_x contours when GaN reached its maximum thickness of 16 µm at 1100 °C. In the GaN above the SiO_2, σ_x remained very low, and it is unlikely that dislocations would emerge and develop in these regions of negligible stress.



(Sapphire Thickness = 432 µm) (Sapphire Thickness = 432 µm)

(a) (b)

***Figure 2**. Contours of normal stress σ_x for (a) Step 7, gap existing and (b) Step 8, gap closed. FE scale in MPa.*



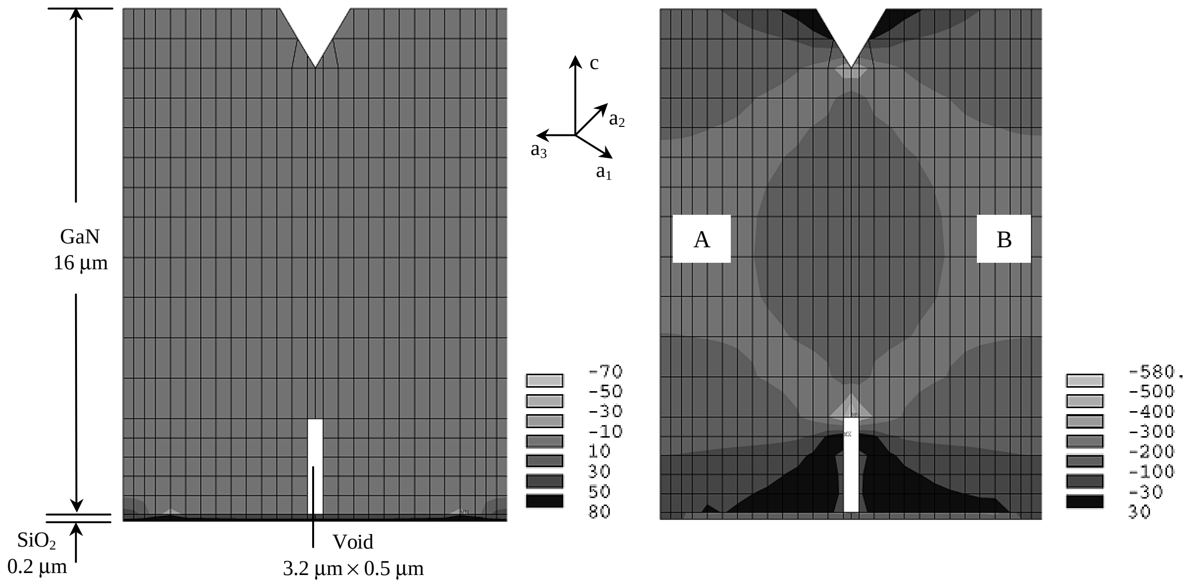
(a) (b)

Figure 3. *Contours of normal stress σ_x for (a) T = 1100 °C, at end of Step 9 and (b) T = 20 °C, at end of Step10. FE scale in MPa.*

During the temperature decrease from 1100 °C to 20 °C, thermal expansion mismatch leads to very large compressive stresses in the GaN. At most nodes, σ_x was about -600 MPa. In the stress concentration area around the tip of the V-trench, it became -1000 MPa (Figure 3 (b)). Associated with the large in-plane compressive normal stresses, high shear stresses may occur on some crystallographic planes.

SHEAR STRESSES AND DISLOCATIONS

A more complicated test case was used to characterize the effects of stress on the dislocation microstructure. In this case the GaN incompletely coalesced and 3.2 µm × 0.5 µm voids remained on the interface surfaces. Dislocation slip and generation depend on the shear stresses. On particular crystallographic planes and in different directions the shear stresses will vary. Finite element analysis outputs all six independent components of a stress tensor in the normal Cartesian coordinate system. Based on the tensor, the shear stress on different crystallographic planes and in different directions can be calculated. As an example, Figure 4 shows the contours of shear stress in $[\bar{1}2\bar{1}0]$ direction on the $(10\bar{1}0)$ plane. At 1100 °C, the shear stress in GaN above the SiO_2 was negligible (Figure 4 (a)), and the strain energy was not sufficient to generate new dislocations or move existing dislocations. After the GaN was cooled down to room temperature, high shear stress was caused by the thermal mismatch (Figure 4(b)). Stress concentration occured at the top of the void and the tip of the V-trench. The maximum value of the shear stress at the top of void was about 580 MPa. In the two symmetric zones A and B, the shear stresses were in the range of 200 to 300 MPa. Yielding and dislocation glide may start in the stress concentration areas and then propagate in zones A and B. In other words, the stress concentrations are yield kernels and A, B are yielding zones.



(a) (b)

Figure 4*. Contours of shear stresses on* $(10\bar{1}0)$ *plane, in* $[\bar{1}2\bar{1}0]$ *direction for (a) T = 1100 °C, at end of Step 9 and (b) T = 20 °C, at end of Step 10. FE scale in MPa.*

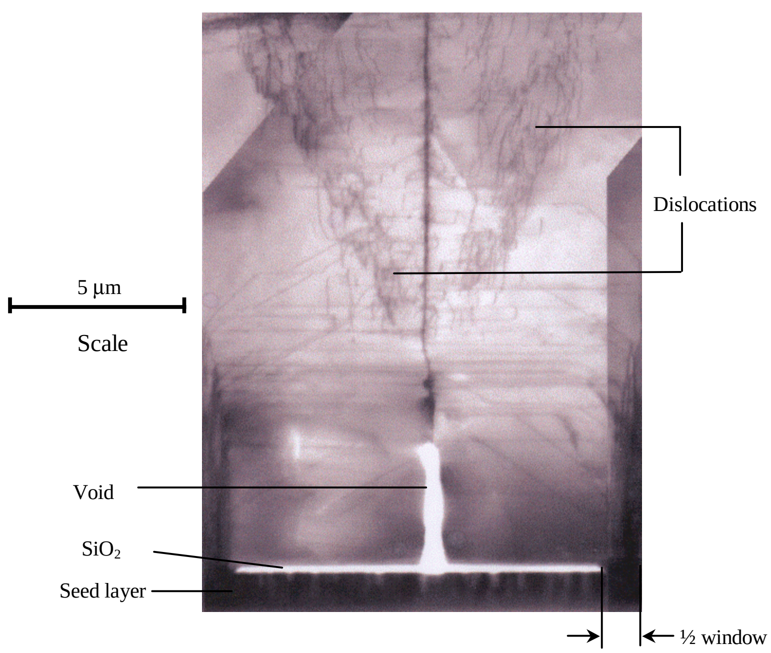


Figure 5. *TEM micrograph showing V-shaped dislocation network [4]. The central coalescence plane runs vertically through the micrograph.*

Glide can result in regions of high dislocation density. Figure 5 is a TEM image of the dislocation microstructure in a film with the same geometry as the simulation model. A set of dislocation loops that originate at the coalescence plane and propagate into the LEO material form a V-shaped network in the final microstructure with the same characteristics as the yield zone in the simulation model, Figure 4 (b). Analysis of the character (line vector and Burger's vector) of these particular dislocations indicate that they accommodate thermal expansion mismatch rather than lattice mismatch at the growth temperature [4] and that they can glide in $(10\bar{1}0)$.

CONCLUSIONS

Finite element models have been created and used to simulate the entire process of GaN lateral epitaxial overgrowth, from seed layer growth on sapphire, to film lateral overgrowth and cool-down to room temperature. The 3-D stresses caused by lattice mismatch and temperature change have been assessed.

For GaN LEO at 1100 °C, normal and shear stress in the GaN were negligible. During cool-down, high shear stress resulted in yielding and dislocations.

The present simulation technique can be used for analyzing stresses, demonstrating the dislocation mechanism, predicting dislocation generation and optimizing parameters in GaN LEO to produce low-defect films.

ACKNOWLEDGMENTS

This research is sponsored by the ONR MURI on Compliant Substrates (C. Wood) with additional support from the NSF MRSEC. The authors are grateful to Dr. Kathleen Dunn for the TEM image used in Figure 5.

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