RELAXATION PHENOMENA IN GaN/ AlN/ 6H-SiC HETEROSTRUCTURES

N.V. Edwards,*¤ A.D. Batchelor,† I.A. Buyanova,* L.D. Madsen,* M.D. Bremser,‡# R.F. Davis,‡
D.E. Aspnes,‡ and B. Monemar*

*Linköping universitet, Materiefysik, Linköping, Sverige, S-58183
¤ginger@ifm.liu.se
†Analytical Instrumentation Facility, Box 7531, N.C. State University, Raleigh, NC, USA 27695
†North Carolina State University, Raleigh, NC, USA 27695
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ABSTRACT

We have developed a method to modulate the strain state (normally > 4 kbar, tensile) of moderately thick (~2 μm) GaN based structures grown on 6H-SiC to a range 0 to -2 kbar of compressive stresses by introducing a strain-mediating layer (SML) above the standard high-temperature AlN buffer layer. The strain characteristics of subsequently deposited nitride layers can be modulated by changing the growth parameters of the SML layer. This is achieved by *in-situ* techiniques during crystal growth without degrading the optical and structural properties of the deposited layers.

INTRODUCTION

By conventional wisdom, simple structures grown on Al_2O_3 are in compression,[1-4] while those grown on 6H-SiC are in tension.[1,5,6,7] It is usually assumed for growth on 6H-SiC that compressive lattice-mismatch stresses[3,4] are relieved after a few nanometers of growth[8] and tensile thermal mismatch stresses[3,4] persist thereafter. Optical data in the literature also give the impression that compressive stress is the inevitable result of growth on Al_2O_3 substrates,[9,10] while the relative scarcity of data for GaN on 6H-SiC has reinforced the impression that only tensile material can be grown on this substrate.[5,11,12]

However, for GaN film/ AlN buffer/ 6H-SiC substrate heterostructures, we have observed a greater versatility in achievable residual stresses than predicted by conventional wisdom or observed thus far for films on Al_2O_3 substrates.[13] Here GaN films are mostly compressive for films less than about 0.7μm thick, are tensile up to about 2μm, then abruptly become less tensile with stress values near 1 kbar thereafter. Despite this increased flexibility, the thickness dependence means that a given combination of growth and material parameters nonetheless dictates a unique value of stress in the overlying film. However, the inclusion of a negligibly thin (~375-750Å) strain mediating layer (SML) of GaN or AlGaN between the AlN buffer layer and overlying GaN film can potentially circumvent these trends for moderately thick (~2μm) GaN layers (normally >4kbar, tensile), yielding a range of stresses between 0 and -2kbar, compressive. Thus the SML, when used in conjunction with current buffer layer technology, provides even greater flexibility than the AlN/ SiC combination alone. In fact, it enables otherwise unachievable combinations of growth temperatures, film thicknesses and residual stresses.

Such capability is potentially of interest for nitride valence band engineering and device processing applications. But these applications require that residual stress be controlled in device active regions without sacrificing material quality or violating device design parameters. To demonstrate the suitability of the SML approach for potential device applications, we report the interfacial properties, surface morphology, crystalline quality, and optical properties of GaN films grown with SMLs relative to those grown without them. We find that the SML has the capacity to alter the growth rate and stress state of the GaN film but does not appreciably degrade its optical, structural or surface properties.

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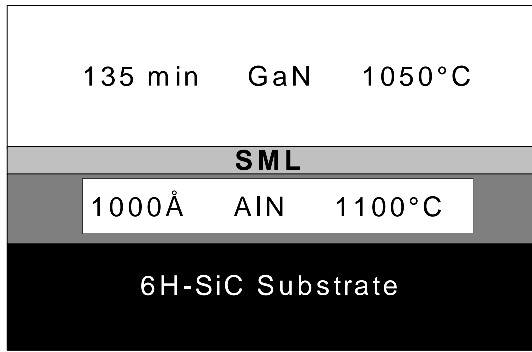

Fig. 1. Structure, compositions, layer thicknesses, and growth parameters common to all SML samples.

EXPERIMENTAL DETAILS

In-plane residual stresses (σ_{xx}) were determined from the energies E_A, E_B, and E_C of the A, B, and C excitons observed in optical data obtained with a single-beam low-temperature reflectometer as described previously.[12] The samples were imaged in cross-section with a JEOL 6400FE field emission scanning electron microscope (SEM). Photoluminescence (PL) was excited by the UV line (334.5 nm) of an Ar^+ ion laser and dispersed using a 0.5 m Jobin-Yvon monochromator with a GaAs photomultiplier tube. Sample surfaces were characterized by a Digital Instruments (DI) Dimension 3000 Scanned Probe Microscope (SPM) operated in tapping mode®. X-ray diffraction (XRD) was carried out with a Philips MRD system using the high resolution optics (triple axis mode).

Four SML samples were examined in the context of twenty-five other GaN films[13] grown by metal organic chemical vapor deposition (MOCVD)[14] with the same V-III ratio and no doping. The structures were all grown on 6H-SiC substrates. All included a 1000 Å AlN buffer layer grown at 1100°C and were subjected to the same rate of post-growth cooling. The structure of the four SML-containing samples is shown in Fig. 1; SML growth parameters are given in Table I. Except for the presence of the SML these samples are nominally identical to Sample 5, which does not have a SML.

RESULTS & CONCLUSIONS

The effect of the SML is apparent in Fig. 2. Here film thickness vs. E_A and σ_{xx} is plotted for samples with and without SMLs, represented by the numbered X's and filled circles, respectively. General stress trends for simple GaN/ AlN/ 6H-SiC heterostructures, as described previously,[13] are apparent in the main sequence of filled circles.

Table I. Properties of SMLs and associated GaN films. Note that the SML *d* is projected from known growth rates* while the GaN film *d* was measured by cross-section SEM.

	SML Properties			**Properties of Associated GaN Film**				
	Material	time at T(°C)	~*d* (Å)	*d* (μm)	σ_{xx} (kbar)	PL Linewidth (meV)	XRD FWHM (arcsec)	AFM Rms Roughness (Å)
1	GaN	2 min 1000	375	0.9	0.26	3.56	53	3.95
2	GaN	6 min 1120	450	2.1	-1.02	3.27	56	4.49
3	GaN	4 min 1000	750	2.2	-0.44	4.26	59	6.85
4	$Al_{0.13}Ga_{0.87}N$	2 min 1000	375	1.2	-1.98	4.35	59	2.72
5	------	------	---	1.9	4.63	8.13	52	2.61

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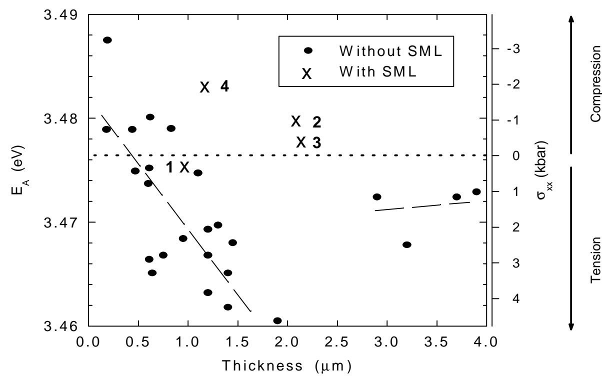
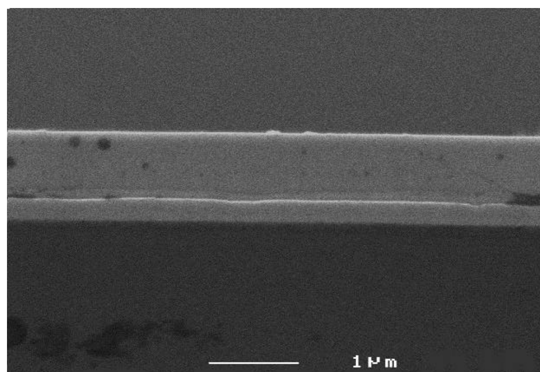


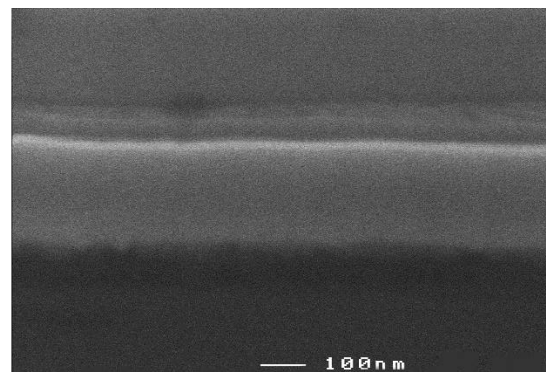
Fig. 2. E_A and σ_{XX} vs. thickness d for GaN films on 6H-SiC. Points [•] represent samples without strain mediating layers (SML); X's represent samples with SMLs.

Sample 1 has a GaN SML that was grown for 2 minutes at 1000°C, corresponding to a projected layer thickness of ~375Å.[14] The SML/ film interface was not resolvable with the SEM (Figs. 3a and b). But instead we found a heavily striated region above the 1000Å AlN buffer layer—suggesting the possibility of strain anisotropy in the (0001) direction—that is divided by a crack extending fully across the sample. Not surprisingly, this sample is nearly relaxed.[15] Here σ_{xx} = 0.26 kbar instead of the 4.63 kbar tensile observed for Sample 5. A cracked sample is not ostensibly useful for device purposes, but it is reported because of relevance for the recognized device processing problem of lifting nitride epilayers from their substrates.

Similar layered regions of differing contrast are observed in Sample 2 for a GaN SML ~450Å thick, grown for 6 minutes at 1120°C. These regions are seen in low and high magnification in Figs. 4a and b, respectively. However, instead of cracking, the film has a division into two light and dark bands on the low magnification scale, in addition to the striations seen at high magnification. This film is slightly compressive, with σ_{xx} = -1.02 kbar. Surprisingly, SML parameters like these may prove to be useful if they can indeed create strain anisotropies in the (0001) direction without cracking the overlying GaN film. The introduction of strain anisotropies perpendicular to the direction of growth is currently thought to be the best option for optimizing nitride valence band configurations for minimal laser threshold currents.[16]

A simple change in SML growth parameters eliminates this c-plane anisotropy. If the SML of Sample 1 is grown for 4 min at 1000°C instead of 2 min, the resulting film (Sample 3; Fig. 4c) is without resolvable cracks or c-plane anisotropy at either high or low magnification and becomes slightly compressive. If the SML growth parameters of Sample 1 are reproduced with $Al_{0.13}Ga_{0.87}N$ instead of GaN, the resulting film (Sample 4; Fig. 4d) is also free from cracks and c-plane anisotropy. But the σ_{xx}=-1.98 kbar achieved here is comparable to compressive stresses obtained on Al_2O_3 substrates.[15] These can be contrasted to the interfacial properties of Sample 5, shown in Fig. 4e. Without the SML to "getter" the residual stress, the film is not only the most tensile in the set, but it also suffers from cracks distributed throughout the film, which precludes any useful removal of the epilayer from the substrate.





Figs. 3a and b. Lower magnification SEM micrograph of Sample 1, left. Right shows high magnification view of the buffer layer/ SML/ overlying GaN film interfaces for the same sample.

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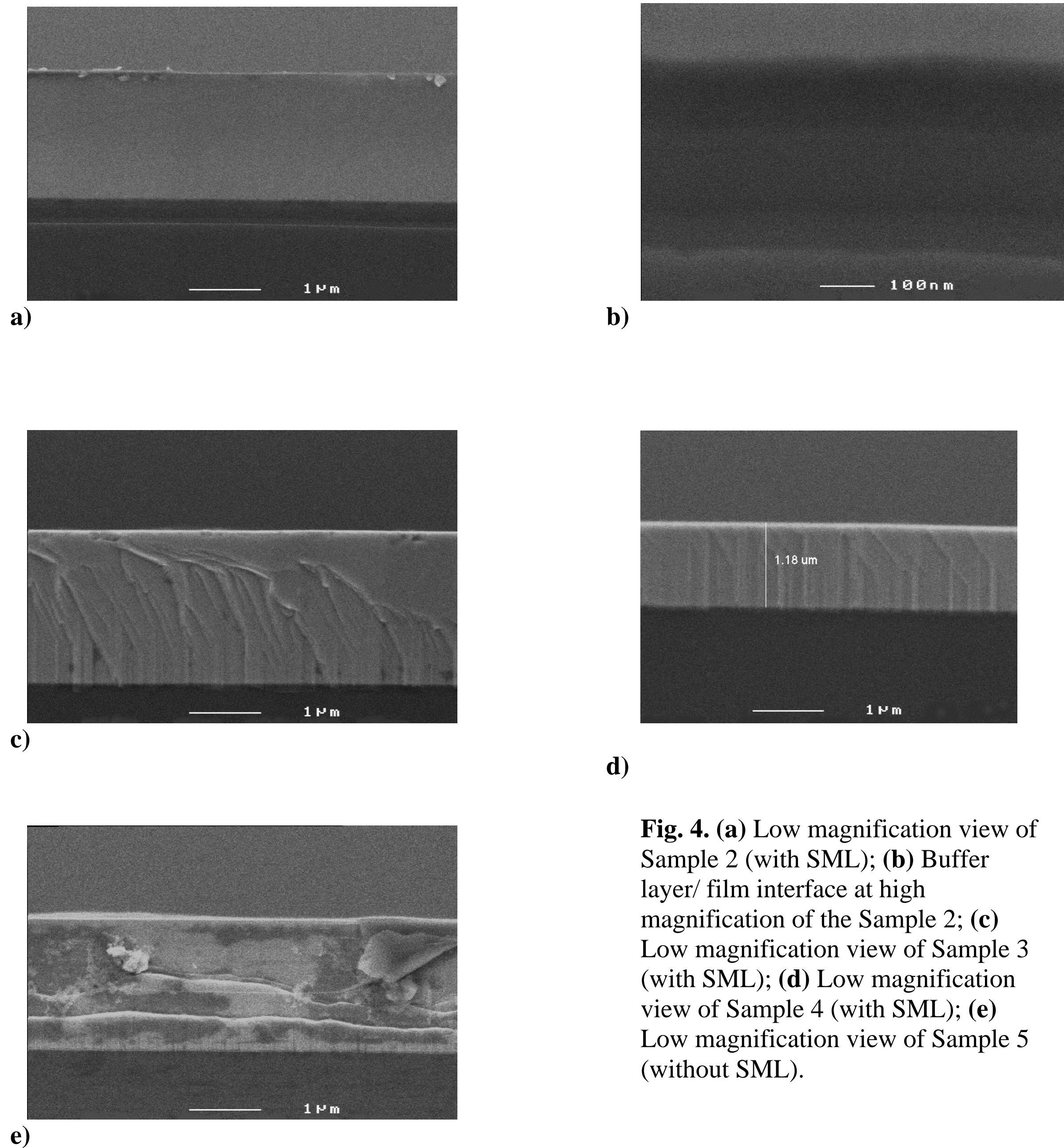

Fig. 4. (a) Low magnification view of Sample 2 (with SML); **(b)** Buffer layer/ film interface at high magnification of the Sample 2; **(c)** Low magnification view of Sample 3 (with SML); **(d)** Low magnification view of Sample 4 (with SML); **(e)** Low magnification view of Sample 5 (without SML).

We also find that growth of the overlying GaN film for 135 minutes at 1050°C does not always result in the expected[14] 2μm thickness for this layer if an SML is used. Sample 1 has a total thickness of only 0.97μm, while Sample 4 is only 1.2μm thick. Both samples have SMLs with projected thicknesses <400Å. Samples 2 and 3 are by contrast the expected thickness, and their SMLs are >400Å. To explain this behavior we must consider the anticipated morphology of the SML. Initial investigations of GaN growth on the high-temperature AlN buffer layer determined that growth was layer-by-layer only after an initial coalescence of two-dimensional, flat-topped islands that occurs *after ~400Å of growth*.[14] It is plausible that the samples with reduced growth rates had SMLs that were not fully planarized and that growth was in fact occurring on non-(0001) planes. Growth on such planes occurs at significantly reduced rates, due in theory to reduced Ga incorporation relative to that for the (0001) direction.[17] The degree of reduction of growth rate would then depend on the degree of coalescence of the thin SML.

By contrast how the SML modifies the sample stress is not straightforward since the relaxation

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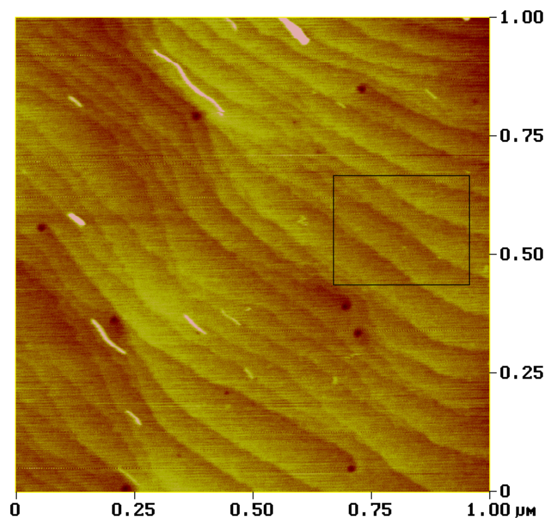

Fig. 5. SPM micrograph of the surface of Sample 4 (with SML). Image rms roughness was 2.7Å; rms roughness in boxed region is 0.15Å.

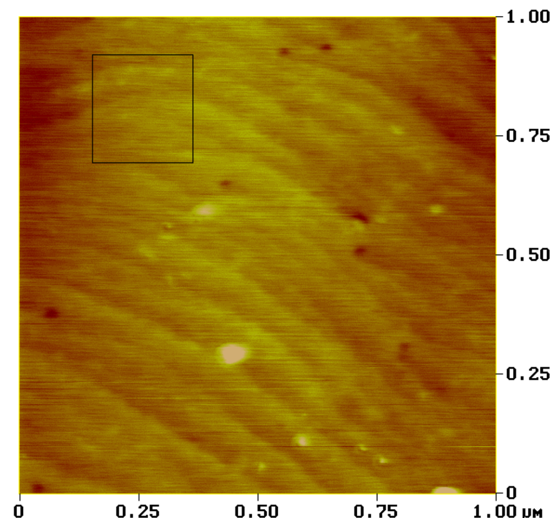

Fig. 6. SPM micrograph of the surface of Sample 5 (without SML). Image rms roughness was 2.61Å; rms roughness in boxed region is 1.48Å.

phenomena in GaN/ AlN/ 6H-SiC heterostructures are not well-understood.[13] Neglecting microstructural explanations, the "stress-trend" behavior of Fig. 2 for samples without SMLs is consistent with a gradual relaxation of pseudomorphic growth and predominance of tensile stresses upon cooling with increasing film thickness described in Ref. 13. We have hypothesized that the specific thicknesses at which these processes occur vary with substrate orientation and growth temperature, but it remains unclear whether the SML merely modifies the thickness at which these relaxation processes occur or circumvents them altogether. Nonetheless—and despite such marked differences in the interfacial character of the films—our film characterizations indicate that there is very little variation in the optical quality, surface morphology and structure of GaN films grown on SMLs. SPM measurements yielded root mean square (rms) roughnesses on the order of 3 to 7 Å, comparable to any of the smoothest films in Fig. 2.[18] Fig. 5 shows the morphology of a representative SML-containing sample (Sample 4), and it is remarkably similar to the morphology of Sample 5, shown in Fig. 6. Representative broadband PL spectrum of typical

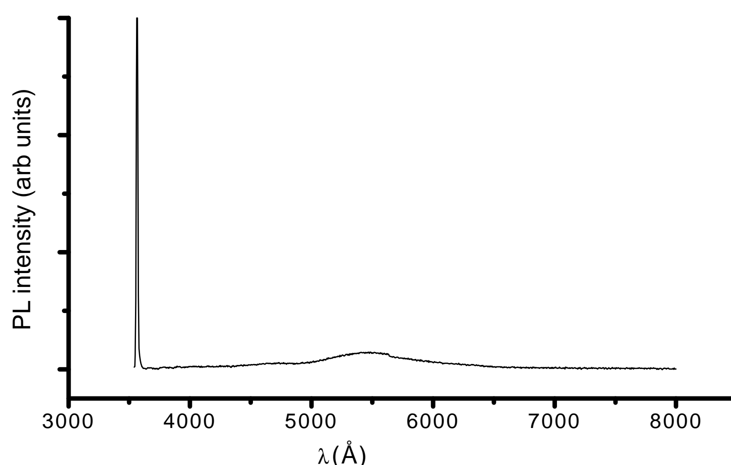

Fig. 7. Representative broadband PL spectrum of SML containing samples. (Sample 4)

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quality is shown in Fig. 7; we see that the spectra are dominated by (predominantly bound) excitonic emission with relatively weak yellow-band emission, typical of good-quality, strained MOCVD-grown films. The linewidth of the excitonic emission ranged from 3 to 5 meV, also indicative of good material quality. Linewidth variations occurred as expected with residual stress. XRD θ-2θ full width at half-maximum (FWHM) intensity values were in the 53-59 arcsec range, and, like the PL linewidths, are not significantly different from the FWHM obtained for Sample 5 (accounting for variations in residual stress). Thus the SML has the capacity to alter the growth rate and stress state of a GaN film, but *does not appreciably degrade its optical, structural or surface properties*.

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