THERMAL RESIDUAL STRESS MODELING IN AlN AND GaN MULTI LAYER SAMPLES

Kai Wang and Robert R. Reeber

Department of Materials Science and Engineering
North Carolina State University, Raleigh, NC 27695-7907

ABSTRACT

Thermal residual stresses can detrimentally affect the electronic and optical properties of epitaxial films thereby shortening device lifetime. Based on our earlier work on thermal expansion of nitrides, we provide a finite element modeling analysis of the residual stress distribution of multilayered GaN and AlN on 6H-SiC. The effects of thickness and growth temperatures are considered in the analysis.

INTRODUCTION

Group III-nitride based semiconductors have direct band gaps that can provide blue or ultraviolet light-emitting devices and high temperature optoelectronics. Recent work [1-3] has highlighted some of the difficulties and successes with their thin film device fabrication. Processing such devices often relies on the high temperature growth of epitaxial layers on different substrates with different coefficients of thermal expansion. Residual stresses introduced by cooling or heating may detrimentally affect device long term performance and lifetime.

The stress-strain distribution in these electronic composite structures can be calculated from the temperature dependence of their thermoelastic properties. The results provide a guide for optimizing interfacial processing.

For an axially symmetric problem without a body force, the equilibrium equations of the system are:

$$\frac{1}{r}\frac{\partial(r s_{rr})}{\partial r} - \frac{s_{qq}}{r} - \frac{\partial s_{rz}}{\partial z} = 0 \qquad (1)$$

$$\frac{\partial s_{rz}}{\partial r} + \frac{\partial s_{zz}}{\partial z} + \frac{s_{rz}}{r} = 0 \qquad (2)$$

Where the σ_{ij} are the components of the stress tensor for a coordinate system (r, θ, z). After assuming displacements U and V along the r and z directions respectively, the strain tensor is

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$$
\begin{aligned}
e_{rr} &= \frac{\partial U}{\partial r} \\
e_{qq} &= \frac{U}{r} \\
e_{zz} &= \frac{\partial V}{\partial z} \\
e_{rz} &= \frac{\partial U}{\partial z} + \frac{\partial V}{\partial r}
\end{aligned} \qquad (3)
$$

Hooke's law is then

$$
\begin{bmatrix} s_{rr} \\ s_{qq} \\ s_{zz} \\ s_{rz} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 \\ C_{12} & C_{11} & C_{13} & 0 \\ C_{13} & C_{13} & C_{33} & 0 \\ 0 & 0 & 0 & C_{44} \end{bmatrix} \begin{bmatrix} e_{rr} - \overline{a_{\perp}}\Delta T \\ e_{qq} - \overline{a_{\perp}}\Delta T \\ e_{zz} - \overline{a_{II}}\Delta T \\ e_{rz} \end{bmatrix} \qquad (4)
$$

Where $\overline{a_{\perp}}$ and $\overline{a_{II}}$ are the mean coefficients of thermal expansion along the a- and the c-axes and the C_{ij} are the elastic constants. For a hexagonal crystal, there are five independent elastic constants.

A 2-D code, PDEase2, developed by SPDE, Inc. and distributed by Macsyma, is applied to calculate the stress-strain distributions of multilayer GaN/AlN or GaN/SiC structures. This code permits calculation of the stress/strain distribution for a cylindrically symmetrical system as shown in Fig. 1,

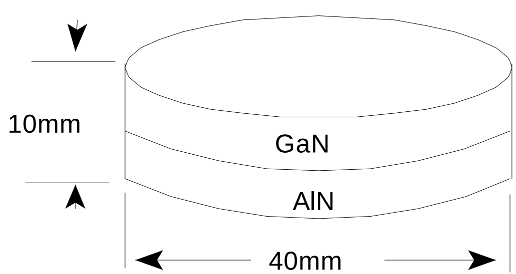

Figure 1. Geometry of the disk-shaped sample.

where the two layers are separated by a sharp interface. The GaN layer is either on top of AlN or SiC. For simplicity, a linear elastic continuum model for anisotropic samples was utilized. The c-axis is assumed to be perpendicular to the interface.

Thermoelastic property measurements for AlN and GaN have been reviewed [4] and high temperature thermal expansion was calculated semiempirically. These results, plus work on -SiC thermal expansion [5], permit us to calculate the stress-strain distributions for disk-shaped samples. The mean thermal expansion between 298^{o}K and high temperatures are provided in Fig. 2. The lattice mismatches for the a-axis between GaN and SiC and for AlN and SiC are also plotted. Their elastic constants were chosen from Polian *et al*. [6], McNeil *et al* [7]. and

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Kamitani *et al* [8] and tensile strengths from Kosolapova's handbook [9].

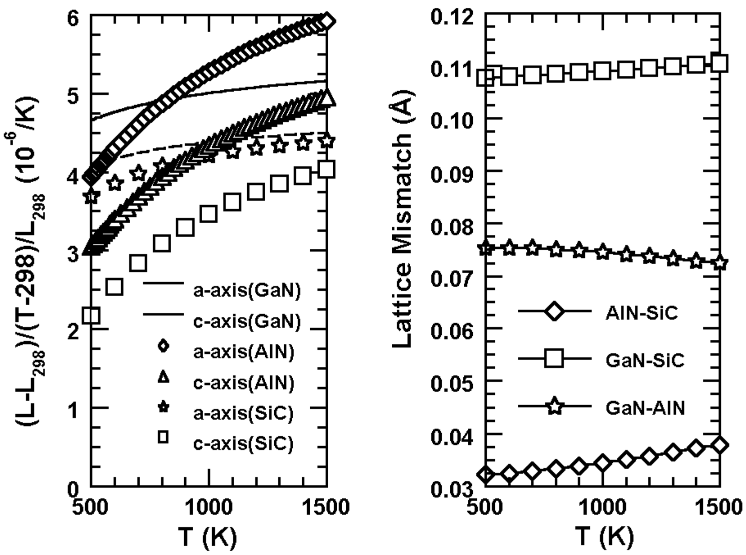

Figure 2. Mean thermal expansion and lattice mismatch.

The samples are assumed cooled to 298°K from a growth temperature of 1300°K. Selected materials properties are listed in Table 1. Residual stress distributions are calculated from the thermoelastic properties. The effects of thickness and growth temperatures are considered in the analysis.

Table 1. Selected thermoelastic properties of GaN, AlN and SiC

		GaN	AlN	SiC
Thermal Expansion $(10^{-6}K^{-1})$	a-axis	5.11	5.72	4.34
(298~1300°K)	c-axis	4.47	4.75	3.74
	C_{11}	390.0	410.5	501
	C_{12}	145.0	148.5	111
Elastic Constants	C_{13}	106.0	98.9	52
(GPa)	C_{33}	398.0	388.5	553
	C_{44}	105.0	124.6	163
Young's Modulus (GPa)		302.7	329.7	444
Poisson's Ratio		0.26	0.239	0.164

RESULTS

Fig. 3(a) through 3(c) provide r-z plane stress distributions for a disk-shaped GaN on AlN sample. In fig. 3(a), the distribution of axial stress σ_{zz}, is peripherally concentrated along the sample and is tensile in GaN and compressive in AlN. Fig. 3(b) provides the shear stress σ_{rz} distribution. The shear stresses concentrate along the interface and also close to the edge. Fig. 3(c), the radial stress σ_{rr} distribution, is primarily a GaN/AlN interfacial stress. The σ_{rr} is compressive in GaN and tensile for AlN. The maximum calculated tensile stresses are 139.7MPa for GaN and 146.3MPa for AlN.

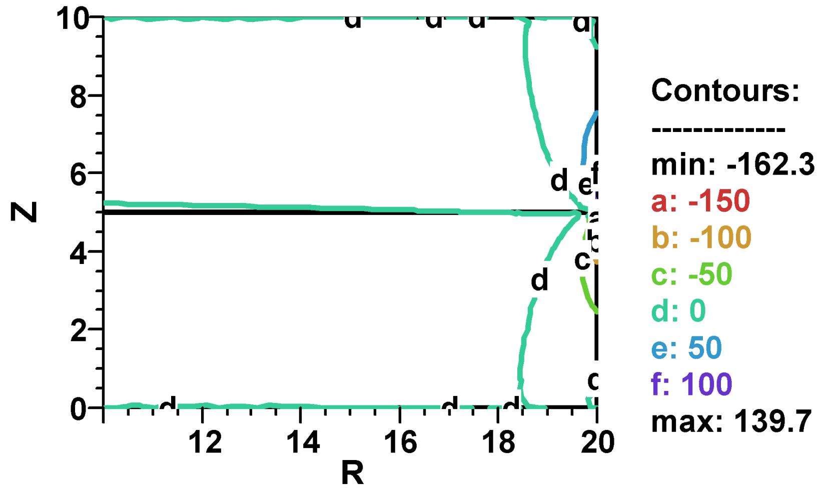

Figure 3(a). Distribution of σ_{zz}.

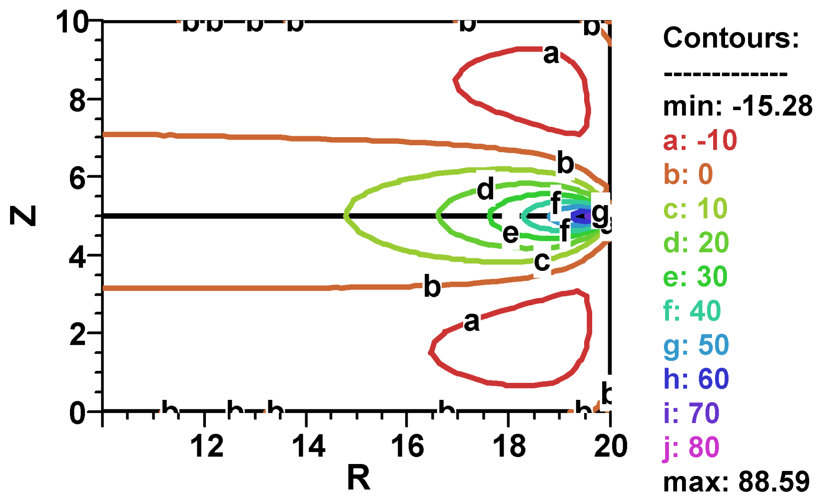

Figure 3(b). Distribution of σ_{rz}.

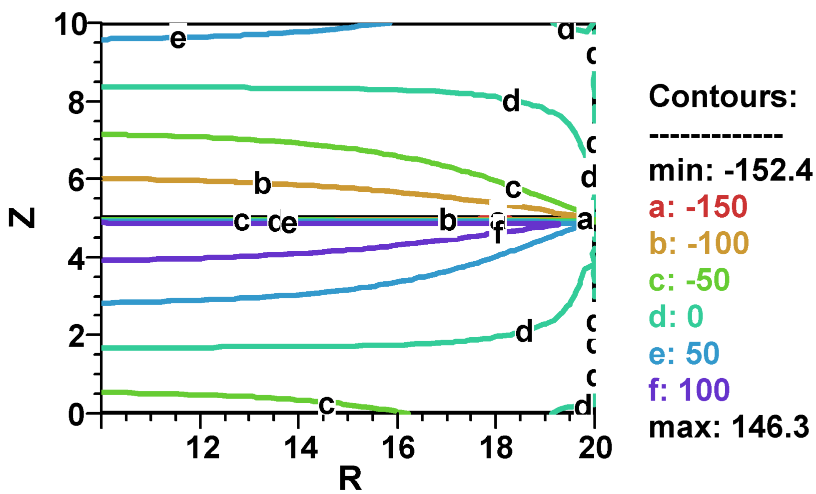

Figure 3(c). Distribution of σ_{rr}

The stress distributions for a disk-shaped GaN on 6H-SiC sample were also calculated. The

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distributions are similar to that of GaN on AlN sample except that the signs of the stresses are reversed. This is because the thermal expansion for SiC is smaller than GaN. The axial σ_{zz}, is peripherally concentrated along the sample and is compressive in GaN and tensile in SiC. The maximum σ_{zz} is 149MPa in GaN and 298MPa in SiC. The radial stress σ_{rr} distribution is also primarily a GaN/SiC interfacial stress. The σ_{rr} is tensile in GaN and compressive in AlN. The maximum σ_{rr} is 200 for GaN and 211MPa for SiC.

The thickness dependence of the maximum residual stresses was also calculated. The residual stresses do not change much except for the tensile radial stress in GaN. This varies from about 200MPa to 350MPa in GaN and indicates, within a thin layer of GaN grown on SiC, that the maximum tensile stress decreases with the GaN thickness. The maximum axial tensile stress fluctuates between 290MPa to 400MPa in SiC.

Figure 4 illustrates the temperature dependence of the maximum residual stress in a GaN on SiC substrate. The residual stresses increase with increasing growth temperature.

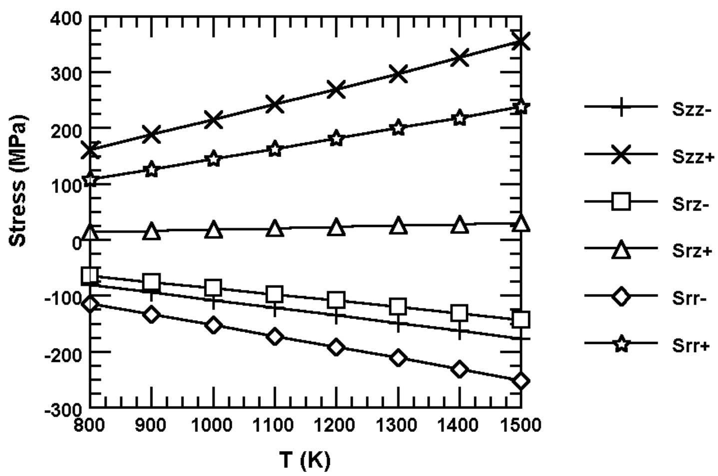

Figure 4. Growth temperature dependence of residual stresses in GaN over SiC sample.

Finally, we have calculated the maximum residual stress distribution for an AlN over SiC substrate grown at 1300^{o}K. The distributions of the residual stresses are similar to that of the GaN on SiC except the maximum stresses are larger than in the GaN on SiC sample. This is easily understood as the differences of thermal expansion between AlN and SiC are larger than equivalent differences between GaN and SiC. The maximum tensile stress is 370MPa in AlN and 519MPa in SiC. The maximum compressive stress is 279PMa in AlN and 382MPa in SiC.

DISCUSSION AND CONCLUSIONS

Our calculations indicate that the residual stresses primarily concentrate along the interface and at the edge of the multilayered samples. The tensile strength indicated for a SiC single crystal is within the range of 180 to 200MPa [9]. GaN and AlN tensile strengths are expected to be smaller than SiC. Comparing the maximum residual stresses and the strength data of the materials studied, we see that the residual tensile stresses in SiC and AlN are larger than their strength. Similar results are expected for GaN. This should cause cracking and other defects during processing as has been observed [2]. The effect of these residual stresses on the band gap can be illustrated by a simple calculation. Assume that the maximum stress is in the order of 400MPa in GaN. Since the band gap pressure coefficient is about 4.2×10^{-5} eV/MPa in GaN[10], the small shift of the band gap due to this stress is about 0.017eV. Increasing the thickness of GaN on SiC will slightly reduce the radial residual stress at the interface. Raising the growth temperature for GaN on SiC introduces higher residual stresses at room temperature. The residual stress reduction for AlN on SiC with decrease in growth temperature has been observed [11] experimentally as a decrease in crystal roughness from 1473^oK to 1323^oK.

In summary, we have performed a finite element modeling analysis of the residual stress distribution of multilayered GaN and AlN unbuffered on 6H-SiC. The effects of layer thickness and growth temperatures are analyzed. Residual stresses if unrelaxed during cooling probably introduce cracks and other defects. The effect of the stresses on the band gap is estimated and is minimal. More calculations should be performed on growing GaN and AlN on other substrates with different growth conditions and with varying thickness buffer layer. Such calculations can provide insights for optimizing the processing conditions of these important nitrides.

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