Interlayers structural design and thermal stress analysis of GaN epilayers grown on Si substrate

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In order to analyze and design interlayers structure of GaN epilayers grown on Si substrate, finite element model based on coupled field was established. Theoretical simulation results showed that HT-AlN buffer with double LT-AlN interlayers can evident relax the tensile stress induced by the thermal mismatch between Si and GaN. Changed the thickness of the LT-AlN, the optimum value was between 20-27nm. Compared with no LT-AlN layer, thermal stress decreased was 24.1%. Optical microscopy images were corresponding to calculation results. This research shows that thermal residual stress of GaN epilayer can be effectively reduced by finite element structural and it provide a new design method for epitaxial growth using MOCVD.

(Received March 20, 2013; accepted November 7, 2013)

Keywords: Si substrates, GaN film, AlN interlayer, Finite element, Thermal stress

1. Introduction

As the next generation light sources, LED have significant advantages in energy saving, luminous efficiency, electronic control, life time, et al. GaN-based LED developed rapidly since Nichia company introduced the first commercial GaN-based LED [1-3]. GaN has strong chemical bond and high melting point, therefore synthesis of single crystal GaN needs to be controlled at high temperature and high pressure or non-equilibrium conditions. Single crystal GaN material has many defects such as crystal orientation uncertain, small scale, easy bending and crackly [4-5]. Therefore GaN-based materials and devices are all grown on heterogeneous substrate.

Sapphire (Al_2O_3) and silicon carbide (SiC) are two widely used heterogeneous substrates for GaN-based LED. Compared with Al_2O_3 and SiC, Si substrate is gaining more and more interest as a better selection for its good thermal conductivity, low cost, easy to obtain large size, and becoming research hotspot in recent years [6-8]. However, large lattice mismatch and thermal expansion coefficient difference between Si and GaN easily lead to GaN epilayers subject to large tensile stress and affect the performance of epitaxial wafer. In response to resolve this problem, researchers proposed different buffer layers and interlayer structures, which including low temperature AlN (LT-AlN) interlayers, [9-12]. AlGaN superlattice buffer layers, [13] $Al_xGa_{1-x}N$ interlayers, [14-15] Si_xN_y interlayers, [16-17] high temperature AlN (HT-AlN) buffer layer, [18] et al.

In order to deeply understand the interlayers' structure effect on thermal residue stress of GaN epilayers, a three dimensional thermal-stress coupled finite element model of GaN epilayers grown on Si substrate was established. The relationship between LT-AlN interlayers' structure and GaN epilayers thermal stress were analyzed. Experimental results were consonant with numerical simulation and verified the effectiveness of this model.

2. Finite model and experiment

Deposition process, heat treatment technology and mechanical characters of materials affect to residual stress of GaN epilayers. Residual stress can be divided into internal stress and external stress. The former is related to lattice mismatch, dislocations, doping concentration, et al, and can be reduced by improved deposition technology. External stress is mainly thermal tensile stress. Growth temperature of GaN epilayers is about 1000-1200^{o}C, and difference in thermal expansion coefficient results in high density cracks during the cooling of GaN epilayers on Si substrate to room temperature. In this process, GaN epilayers thermal stress is, [17-18]

$$\sigma_{th} = E_f\left(\alpha_f - \alpha_s\right)\Delta T \tag{1}$$

where E_f is young's module of GaN, α_f and α_s is thermal expansion coefficient of GaN and Si respectively, ΔT is temperature variable quantity. The stress induced thermal strain ε_{th} and elastic strain ε_{el} can be represented as,

$$\varepsilon_{thx} = \varepsilon_{thy} = \varepsilon_{thz} = \Delta\alpha \cdot \Delta T \tag{2}$$

$$\begin{cases} \varepsilon_{elx} = \dfrac{1}{E_f}[\sigma_{elx} - v(\sigma_{ely} + \sigma_{elz})] \\ \varepsilon_{ely} = \dfrac{1}{E_f}[\sigma_{ely} - v(\sigma_{elx} + \sigma_{elz})] \\ \varepsilon_{elz} = \dfrac{1}{E_f}[\sigma_{elz} - v(\sigma_{elx} + \sigma_{ely})] \end{cases} \tag{3}$$

where ε_{thx} and ε_{elx} , ε_{thy} and ε_{ely} , ε_{thz} and ε_{elz} are thermal strain and elastic strain of x, y, z direction respectively. Heat dissipation ignores thermal radiation and only considers heat convection and heat conduction. Thermal boundary condition can be expressed as,

$$-\lambda \frac{\partial T}{\partial n}\bigg|_{\tau} = h \cdot \Delta T \tag{4}$$

where λ is thermal conductivity coefficient, h is surface heat transfer coefficient, τ is heat transfer boundary. Based on finite element method and simultaneous equations, thermal stress of GaN epilayers can be obtained. For simplified calculation, we make some hypotheses for finite element model: without consider the effect of cracks on thermal stress release, materials parameters have temperature independent. Table 1 shows the materials parameters, where ρ , c and P are density, heat capacity and Poisson ratio respectively.

Table 1. Parameters of materials.

	Si	AlN	GaN
$\lambda\,(W/m\cdot K)$	150	285	130
$\rho\,(Kg/m^3)$	2330	3235	6150
$\alpha\,(1/K)$	3.59×10^{-6}	4.2×10^{-6}	5.59×10^{-6}
$c\,(J/Kg\cdot K)$	700	60	80
$E\,(GPa)$	160	310	299.5
P	0.27	0.2	0.49

Schematic diagram of GaN epilayers grown on Si is shown in Fig. 1. The substrate surface was pre-deposited Al avoid the formation of Si_xN_y. Then a 100 nm thick. High temperature (HT) AlN buffer layer was deposited at 1100℃. Subsequently, GaN and LT-AlN interlayers were grown alternant at 1050℃ and 820℃ respective, followed by 1.5 μm thick GaN epilayers. In experiments, GaN epilayers on Si substrate were grown in metal organic chemical vapor deposition (MOCVD) reactor. Trimethylgallium (TMGa), trimethylaluminum (TMAl) and ammonia (NH_3) were used as Ga, Al, and N precursors, respectively. H_2 used as the carrier gas.

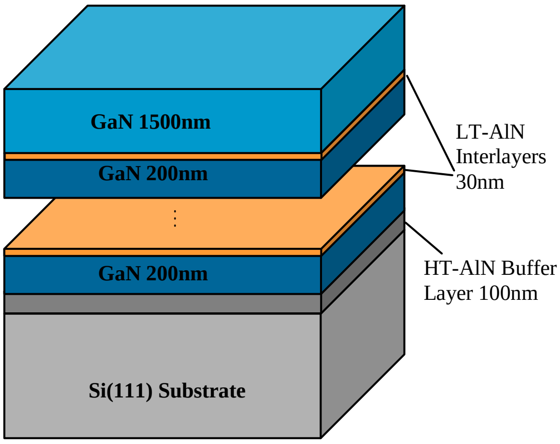

Fig. 1. Schematic drawing of GaN epilayers grown on Si substrates using HT-AlN and multilayer interlayers.

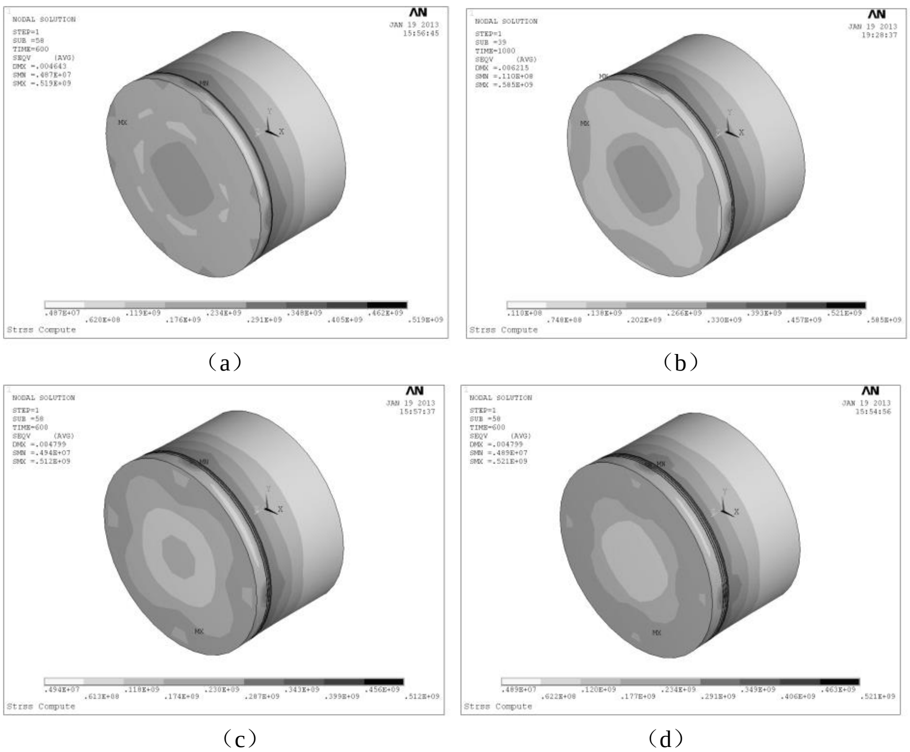

Fig. 2. Thermal stress simulation results of GaN epilayer with different number of LT-AlN (a:0, b:1, c:2, d:3).

3. Results analysis

When the thickness of LT-AlN was 30nm, Fig. 2 shows the thermal stress simulation results of GaN epilayers with different number of interlayers. As seen in Fig. 2(a), without any interlayer the maximum thermal stress of GaN upper surface was near center area and it was approximate 0.162GPa. The thermal stress of lower surface was also near center area and calculation result was 0.193GPa. When there was one LT-AlN interlayer, the maximum thermal stress was 0.179GPa of upper surface and 0.196GPa of lower surface (Fig. 2(b)). It was slightly larger than Fig. 2(a). However, light gray region was markedly enlarged and showed that the whole stress of GaN was smaller. From Fig. 2(c) and Fig. 2(d), we could find that the maximum stress of GaN was near edge area and calculation result was 0.134GPa and 0.147GPa. Compare with Fig. 2(b), stress distributed more uniform and reduced significant. It was obviously that more LT-AlN interlayers could reduce residual thermal tensile stress of GaN epilayer for it introduced a compression stress. However, the introductions of LT-AlN interlayers not only brought tensile stress, but also generated new dislocation. Especially too many interlayers would make AlN layers discontinuous and weaken effect of compression stress. Calculation results also showed that double layers of LT-AlN was superior to three layers and compared with Fig. 2(a) the maximum thermal stress decreased 17.28%.

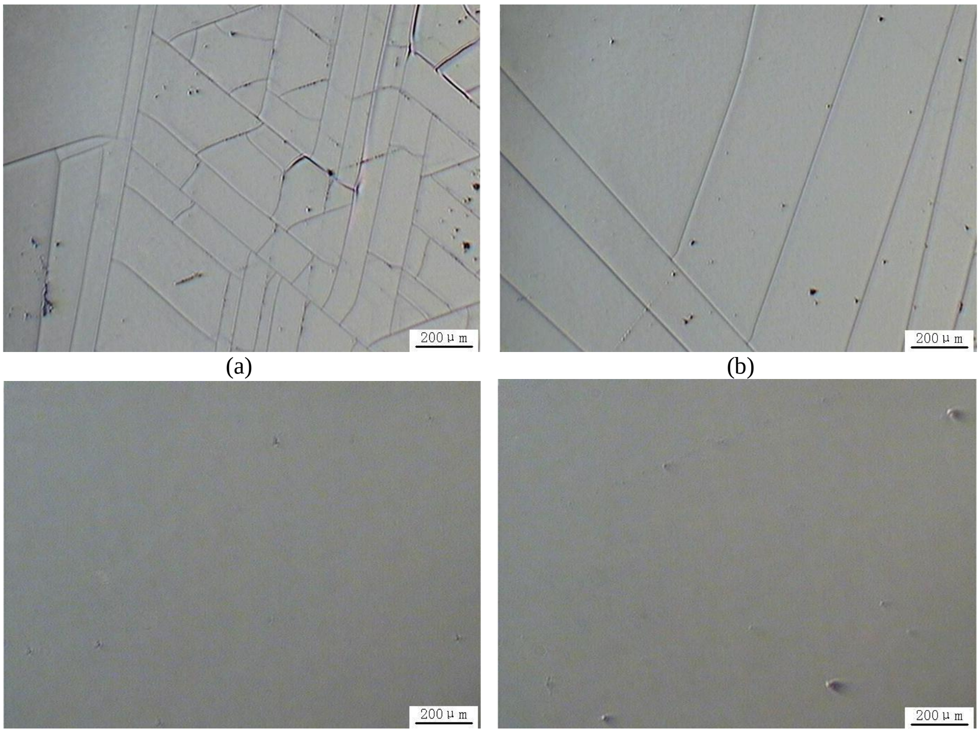

Fig. 3. OM images of crack density of GaN epilayer surface of four samples (a-d:0-3 LT-AlN interlayers).

Four samples with same structures according to Fig. 2 were synthesized. The crack density of the GaN epilayer was investigated by optical microscopy (OM) and shown in Fig. 3. Compared these images, we found that cracks of the samples were evidently dependent on the number of LT-AlN interlayers. The surface of sample (a) with all over cracks and defects meant that GaN epilayer was crushed by tensile stress. Although there were still many cracks, the surface of sample (b) is much better than sample (a). It was proved that LT-AlN interlayer could balance the tensile stress. The surfaces of sample (c) and (d) were specular to naked eye. However, OM images showed some defects on sample (d), while few in sample (c). In short, experimental results coincided with simulation calculations. It means that even neglect the effect of crystalline quality, such as cracking, dislocation density, interface flatness, and point-defects expected in LT growth, finite simulation can still be guide epitaxial growth structure design of MOCVD.

Furthermore, the study on the LT-AlN thickness based on double interlayers analysis and optimization design were performed. The maximum thermal stresses of GaN upper surfaces with different interlayer thickness were shown in Fig. 4. The image implied that the thickness of LT-AlN interlayers influence the thermal stress of GaN. The best thickness of LT-AlN was 25nm. Compared with no LT-AlN, the maximum thermal stress of GaN decreased 24.1%. When thickness of LT-AlN interlayers exceeded 25nm, the maximum thermal stress increased sharply. So we could predict that the interlayer thickness between 20-27nm was optimum. This result is consonant with the early paper of Xiang et al. [11].

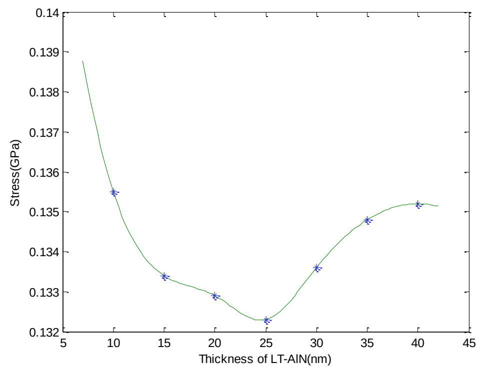

Fig. 4. Maximum thermal stress of GaN with different thickness of LT-AlN.

4. Conclusion

In summary, we have presented a study on the effects of structure of LT-AlN interlayers on GaN epilayers grown on Si substrate. Finite element simulation results showed that LT-AlN interlayers could provide the GaN epilayer a compression stress, which helped to reduce the tensile stress. Calculations indicated that double LT-AlN interlayers was optimum and coincided with OM images of experiments. Furthermore, through simulation we predicted that optimal thickness range of interlayer was 20-27nm for double LT-AlN layers. The thermal stress of GaN epilayer could be controlled under 0.132GPa and achieved a nearly crack free surface of GaN with 1.5 μm thickness. By thermal-stress coupled finite element model, external thermal stress changes of GaN epilayers in the cooling process can be calculated. Therefore, simulation using finite element principle can provide a reference for LED chip structure design and reduce the cost of growth by MOCVD.

Acknowledgments

This work is supported by National Nature Sciences Foundation of China (Grant no. 61177050); LED Lighting Scientific & Technology Innovation Team of Zhejiang Province (Grant no. 2010R20020), Foundation of Zhejiang Education Committee (Grant no. Y201018862).

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