LATTICE PARAMETERS OF GALLIUM NITRIDE AT HIGH TEMPERATURES AND RESULTING EPITAXIAL MISFITS WITH ALUMINA AND SILICON CARBIDE SUBSTRATES

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ABSTRACT

Lattice constants of single phase gallium nitride were measured from room temperature to 1273 K using high temperature x-ray powder diffraction. The data were used to calculate the epitaxial misfits using the epitaxial relationships, GaN(0001)||Al_2O_3(0001) and GaN[$10\bar{1}0$]||Al_2O_3[$11\bar{2}0$] and GaN(0001)||6H-SiC(0001) and GaN[$10\bar{1}0$]||6H-SiC[$10\bar{1}0$], reported in the literature. Using the above relationships epitaxial misfits of – 13.62 % and –3.57% were calculated between GaN and Al_2O_3 and between GaN and 6H-SiC, respectively, at 1273 K. From these epitaxial misfits, layer strains of –0.22% and 0.16%, respectively, were calculated for cooling from 1273 K to room temperature.

INTRODUCTION

Gallium nitride (GaN), with a direct band gap of 3.4 eV [1], is a promising material in the development of short-wavelength light emitting devices [2,3]. Other optical device applications for GaN include semiconductor lasers and optical detectors. The crystal structure of GaN was first reported by Juza and Hahn [4]. GaN crystallizes in the hexagonal crystal system and the x-ray powder diffraction pattern was indexed using space group $P6_3mc$ (186) [4]. Balkas *et al.* [5] gave an indexed powder pattern and refined lattice parameters of a = 3.18907(8) and c = 5.1855(2) Å.

It has recently become possible to grow epitaxial films of GaN on various substrates by the

metal-organic chemical vapor deposition (MOCVD) technique [6,7], at a usual growth temperature of 1273 K [8]. However, any difference in thermal expansion between a film and substrate induces thermal strain when subsequently cooled to room temperature [9]. In order to calculate these thermal strains, one needs to know the lattice parameters of GaN and the substrates at the deposition temperature.

The work presented here compares the lattice parameters at 1273 K of GaN with Al_2O_3 and 6H-SiC, which are the most common substrates used for epitaxial growth of GaN. A more detailed report of the thermal expansion of GaN, calculated from the data presented here, will be compared to previous studies [10-14] and reported elsewhere. Only one of these previous studies collected data above 900 K [11]. The work presented here was undertaken, in part, to verify the higher temperature study [11].

EXPERIMENTAL

High purity GaN powder was prepared by Prof. R. F. Davis at North Carolina State University from the reaction of molten Ga with flowing NH_3 in a hot walled furnace [5].

High temperature x-ray diffraction (HTXRD) measurements were conducted using a Scintag PAD X vertical θ/θ goniometer equipped with a modified Buehler HDK-2 diffraction furnace, CuKα radiation (45 kV and 40mA), and a Si(Li) Peltier-cooled solid state detector. The data were collected as step scans, with a step size of 0.02 °2θ and a count time of 1 sec/step between 30 and 85 °2θ. All data were collected in 1 atm of flowing He gas. The sample temperature was monitored with a Pt/Pt-10%Rh thermocouple spot-welded to a Pt-30%Rh heater strip on which a thin layer of GaN powder was dispersed. The readings of the thermocouple were checked with an optical pyrometer (Pyrometer Instrument Company, Inc., Bergenfeild, NJ, model 95) and were within 5% of the set temperature. For a discussion of thermal gradients across the strip and over the sample using the same heater configuration the reader is referred to [15]. Data were collected at 295 K and on heating to set points of 473, 673, 873, 1073 and 1273 K at a rate of 50

°K/min. The sample was held at the desired temperature for 60 sec before data collection started.

Peak positions were determined by profile fitting individual peaks using a pseudo-Voigt profile, and the unit cell refinements were carried out using the JADE 5.0.13 [Materials Data Inc. Livermore, CA] cell refinement option. Twelve well resolved peaks in the 30 to 85 °2θ range were used to refine the lattice constants. For the x-ray diffraction data collected at 473 K the (104) reflection (room temperature relative intensity of 2, $2\theta = 82.112°$) was not well resolved so only eleven peaks were used in the refinement. Refinement on the sample displacement was included for all data sets.

RESULTS AND DISCUSSION

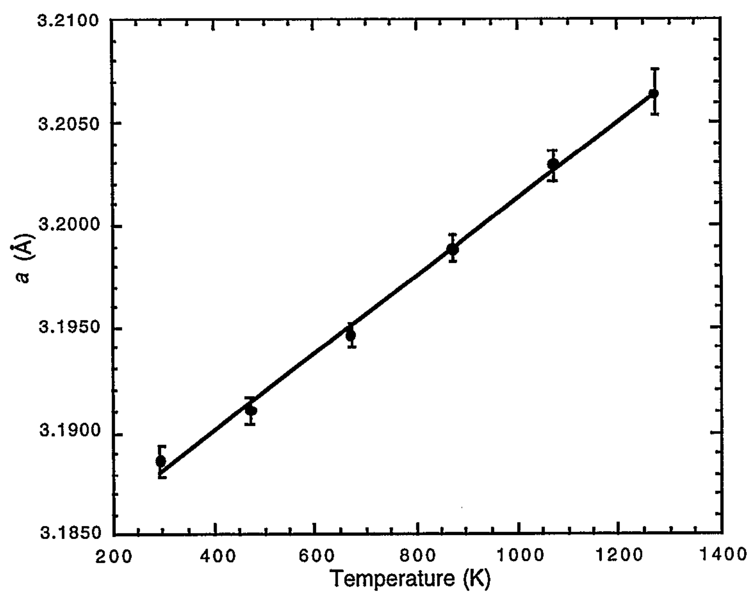
High temperature x-ray powder diffraction. The refined lattice constants and volumes from the high temperature x-ray diffraction data are given in Table I and are shown plotted against temperature in Figure 1. Fitting straight lines to $\Delta a/a_0$ and $\Delta c/c_0$ yield thermal expansion coefficients approximately 10% higher than those given by Ejder [11] and the lattice parameters are in good agreement with those reported by Reeber and Wang [14].

Table I. Refined lattice constants and volumes from the high temperature x-ray diffraction data.

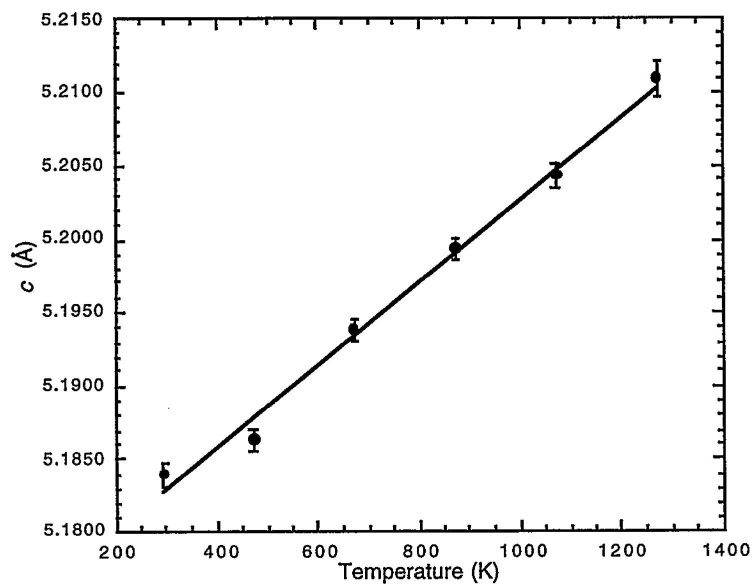
Temperature (K)	*a* (Å)	*c* (Å)	Volume (Å^3)
295	3.1886(7)	5.1840(8)	45.64(2)
473	3.1910(6)	5.1864(7)	45.73(1)
673	3.1947(6)	5.1938(7)	45.91(1)
873	3.1989(7)	5.1994(7)	46.08(2)
1073	3.2029(8)	5.2043(8)	46.23(2)
1273	3.2064(11)	5.2109(12)	46.39(2)

Epitaxial misfits. The lattice mismatch between an epitaxial GaN film and a single crystal sapphire substrate is calculated from the $(10\bar{1}0)$ and $(11\bar{2}0)$ planes of GaN and Al_2O_3,

Figure 1. Lattice constants a) *a* and b) *c* as a function of temperature.



(a)



(b)

respectively [16]. Using the GaN layer as the reference layer, the room temperature lattice mismatch, *f*, is calculated by:

$$f = \frac{d_{(Al_2O_3)} - d_{(GaN)}}{d_{(GaN)}} = -13.84\%$$

resulting in a compressive strain in the GaN layer near the interface. Using the thermal expansion of Al_2O_3 [17] to calculate the lattice constant $d_{(11\bar{2}0)}$ of Al_2O_3 at 1273 K and the refined *a* lattice parameter of GaN, given in Table I, to calculate the lattice constant $d_{(10\bar{1}0)}$ of GaN at 1273 K yields a lower calculated lattice mismatch of –13.62% at 1273 K corresponding to a change in layer strain of –0.22% for cooling from 1273 K to room temperature.

The 6H-SiC polytype is another substrate material for growing GaN films. From the data of Taylor and Jones [18] the lattice parameters of 6H-SiC have been derived for room and elevated temperatures. The lattice mismatch between the GaN film and a 6H-SiC substrate is calculated by comparing the $(10\bar{1}0)$ planes of GaN and 6H-SiC. Using the GaN layer as the reference layer the room temperature lattice mismatch, *f*, is calculated by

$$f = \frac{d_{(6H-SiC)} - d_{(GaN)}}{d_{(GaN)}} = -3.41\%.$$

By using the refined *a* lattice constant of GaN, given in Table I, and the data of Taylor and Jones [18] to calculate the $d_{(10\bar{1}0)}$ of 6H-SiC a lattice mismatch of –3.57% was calculated for 1273 K corresponding to a change in layer strain of 0.16 % when cooling from 1273 K to room temperature.

CONCLUSIONS

Lattice constants of single phase powder GaN are reported up to 1273 K, which is the typical growth temperature of GaN films. The epitaxial misfits at high temperature between GaN and two common substrates, Al_2O_3 and 6H-SiC, have been calculated. The epitaxial misfit between GaN and Al_2O_3 decreased at 1273 K and a layer strain of –0.22% was calculated for cooling from 1273 K to room temperature. The epitaxial misfit between GaN and 6H-SiC increased at 127K and a layer strain of 0.16% was calculated for cooling from 1273 K to room temperature.

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