



Contract number

MORGaN

Materials fOr Robust Gallium Nitride

Additional Report

Temperature Dependent Properties of GaN

Scientific project Coordinator :Sylvain Delage
Company: Alcatel-Thales III-V Lab

Date of issue: Feb 20th 2009

Revision: V1

**Report written by Michael Edwards
University of Bath (UoB)**

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Temperature Dependent Properties of GaN.

Michael Edwards, Department of Mechanical Engineering and Department of Electronics and Electrical Engineering, University of Bath, BA2 7AY.
20th February 2009

This document has been created with the aim of bringing together the large numbers of values for GaN material properties found in the literature. There is some variation in these numbers due to crystalline imperfections that exist in all GaN samples and the accuracy of the equipment used to take the measurements.

1. Elastic Coefficients.

The elastic coefficients of wurtzite GaN are given in a stiffness matrix, as shown below.

$$c_{ij} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11} - c_{12}}{2} \end{bmatrix}$$

(1)

As the stiffness matrix shows, there are only five elastic coefficients c_{11} , c_{12} , c_{13} , c_{33} and c_{44} that need to be defined. There are a variety of reported values for these coefficients found in the literature, as shown in Table 1.

c_{11} (GPa)	c_{12} (GPa)	c_{13} (GPa)	c_{33} (GPa)	c_{44} (GPa)	Ref
370	145	110	390	90	1
296±18	130±10	158±5	267±17	24±2	2
390±15	145±20	106±20	398±20	105±10	3
374	106	70	379	101	4
396	144	100	392	91	5, 6
367	135	103	405	95	7
365	135	114	381	189	8
377	160	114	209	81.4	9
373	141	80.4	387	93.6	10
373	141	80	387	94	11
374.2	141.4	98.1	388.6	98.3	12
368.7	138.5	103.0	362.1	96.6	Average

(All measurements taken at or near 300K.)

Table 1: Room temperature values for the elastic coefficients of GaN.

As GaN expands as it is heated, the elastic coefficients are temperature dependent and decrease in value as the material is heated. Reeber and Wang¹² have determined the temperature dependent elastic coefficients of GaN within 7% of their probable values.

T (K)	c ₁₁ (GPa)	c ₃₃ (GPa)	c ₁₂ (GPa)	c ₁₃ (GPa)	c ₄₄ (GPa)
0	376.4	387.1	142.4	99.1	98.5
50	376.4	387.1	142.4	99.1	98.5
100	376.1	386.8	142.3	99.0	98.5
150	375.7	386.5	142.1	98.9	98.5
200	375.4	385.8	141.9	98.7	98.4
250	374.8	385.2	141.7	98.4	98.4
300	374.2	384.4	141.4	98.1	98.3
400	372.6	382.3	140.6	97.4	98.1
500	370.7	380.0	139.8	96.7	97.9
600	368.5	377.8	138.8	96.0	97.7
700	366.3	375.5	137.7	95.3	97.5
800	364.1	373.3	136.7	94.5	97.3
900	362.0	371.1	135.6	93.8	97.1

Table2: Temperature dependent GaN elastic coefficients ¹².

Table 2 shows that the changes in elastic coefficients are small when considering the variation in literature values at room temperature.

2. Coefficients of Thermal Expansion (CTE).

GaN has two coefficients of thermal expansion (CTEs), one for the c-axis (<001> direction) and another for the a-axis (<110> and < $\bar{1}\bar{1}0$ > directions). Both CTEs are temperature dependent, with higher temperature dependency at higher temperatures. Another paper by Reeber and Wang¹³ includes data showing temperature dependence of the CTEs, as well as the equivalent lattice constants, presented in *Table 3*.

Temperature (K)	$\alpha_a (10^{-6}/K)$	$\alpha_c (10^{-6}/K)$	$a_0 (\text{\AA})$	$c_0 (\text{\AA})$
0	0.0000	0.0000	3.1868	5.1828
25	0.0242	0.0308	3.1868	5.1828
50	0.0468	0.0565	3.1868	5.1828
75	0.1799	0.1688	3.1868	5.1828
100	0.5765	0.5110	3.1868	5.1829
125	1.1465	1.0141	3.1869	5.1830
150	1.7433	1.5486	3.1870	5.1831
175	2.2861	2.0389	3.1871	5.1834
200	2.7501	2.4596	3.1873	5.1837
225	3.1370	2.8104	3.1876	5.1840
250	3.4577	3.0991	3.1878	5.1844
275	3.7241	3.3372	3.1881	5.1848
300	3.9469	3.5342	3.1884	5.1852
350	4.2945	3.8356	3.1891	5.1862
400	4.5495	4.0506	3.1898	5.1872
450	4.7420	4.2083	3.1905	5.1883
500	4.8906	4.3270	3.1913	5.1894
550	5.0077	4.4183	3.1921	5.1905
600	5.1013	4.4900	3.1929	5.1917
650	5.1773	4.5472	3.1937	5.1929
700	5.2398	4.5936	3.1946	5.1941
800	5.3351	4.6632	3.1962	5.1965
900	5.4033	4.7120	3.1980	5.1989
1000	5.4537	4.7476	3.1997	5.2014
1100	5.4918	4.7743	3.2015	5.2038
1200	5.5213	4.7948	3.2032	5.2063
1300	5.5446	4.8109	3.2050	5.2088
1400	5.5633	4.8238	3.2068	5.2113
1500	5.5786	4.8342	3.2086	5.2139
1600	5.5911	4.8427	3.2103	5.2164
1700	5.6016	4.8498	3.2121	5.2189
1800	5.6104	4.8558	3.2139	5.2214
1900	5.6179	4.8609	3.2158	5.2240

*Table 3: Recommended temperature dependent lattice constants and CTEs for GaN.*¹³

3. Piezoelectric Coefficients.

GaN is a piezoelectric material, which means that when a strain is applied on the material it will induce a voltage. GaN will also strain under the application of a potential difference (electric field). The piezoelectric behaviour of GaN can be described in the following stress matrix.

$$e_{ij} = \begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix}$$

(2)

As the piezoelectric stress matrix shows, there are three piezoelectric stress coefficients e_{31} , e_{33} and e_{15} that are used to define the piezoelectric properties of GaN. There are various numeric values for these coefficients found in the literature, see *Table 4*.

e_{31}	e_{33}	e_{15}	Ref
-	0.44	-	14
0.22	0.65	0.21	
-	0.73	-0.3	
0.33	1.00	-	
-		0.33	
0.36			
-			
0.49			
-	0.67	-	15
0.33		0.37	
-	1	-0.3	16
0.36			
-	0.44	-	17
0.22		0.22	
-	0.65	-	18
0.33		0.33	
-	0.70	0.29	Average
0.33			

Table 4: Piezoelectric stress coefficients of GaN.

There are no agreed values for the piezoelectric stress coefficients in the literature, so a literature average value has been included for completeness.

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