Chapter 10

Wurtzite Gallium Nitride (α-GaN)

10.1 STRUCTURAL PROPERTIES

10.1.1 Ionicity

Table 10.1.1 *Phillips's ionicity f_i for α-GaN [1.1].*

f_i
0.500

[1.1] J. C. Phillips, *Bonds and Bands in Semiconductors* (Academic, New York, 1973).

10.1.2 Elemental Isotopic Abundance and Molecular Weight

- **Isotopic abundance**

Table 10.1.2 *Isotopic abundance in percent for gallium and nitrogen [1.2].*

Isotope	% nat. abundance	Isotope	% nat. abundance
^{69}Ga	60.108±0.009	^{14}N	99.634
^{71}Ga	39.892±0.009	^{15}N	0.366

[1.2] D. R. Lide, *CRC Handbook of Chemistry and Physics*, 78th Edition (CRC Press, Boca Raton, 1997).

• **Molecular weight**

Table 10.1.3 *Molecular (average atomic) weight M for α-GaN.*

M (amu)
83.730

10.1.3 Crystal Structure and Space Group

Table 10.1.4 *Crystal structure and its space and pint groups for α-GaN.*

Crystal structure	Space group	Point group
Wurtzite (Hexagonal)	$P6_3mc$	C_{6v}^4

10.1.4 Lattice Constant and Its Related Parameters

• **Lattice constant**

Table 10.1.5 *Lattice constant (a, c) for α-GaN at 300 K.*

a (Å)	c (Å)	Ref.
3.1890±0.0003	5.1864±0.0001	[1.3]
3.1885±0.0003	5.1850±0.0001	[1.4]
3.1892±0.0009	5.1850±0.0005	[1.5]
3.1896±0.0002	5.1855±0.0002	[1.6]

[1.3] Bulk [M. Leszczynski, H. Teisseyre, T. Suski, I. Grzegory, M. Bockowski, J. Jun, K. Pakula, J. M. Baranowski, C. T. Foxon, and T. S. Cheng, *Appl. Phys. Lett.* **69**, 73 (1996)].

[1.4] Bulk [See, M. Leszczynski, T. Suski, J. Domagala, and P. Prystawko, in *Properties, Processing and Applications of Gallium Nitride and Related Semiconductors*, EMIS Datareviews Series No. 23, edited by J. H. Edgar, S. Strite, I. Akasaki, H. Amano, and C. Wetzel (INSPEC, London, 1999), p. 6].

[1.5] Relaxed layer on sapphire [T. Detchprohm, K. Hiramatsu, K.; Itoh, and I. Akasaki, *Jpn. J. Appl. Phys.* **31**, L1454 (1992)].

[1.6] Relaxed layer on GaN substrate [T. Deguchi, D. Ichiryu, K. Toshikawa, K. Sekiguchi, T. Sota, R. Matsuo, T. Azuhata, M. Yamaguchi, T. Yagi, S. Chichibu, and S. Nakamura, *J. Appl. Phys.* **86**, 1860 (1999)].

• **Lattice constant and molecular density**

Table 10.1.6 *Lattice constant (a, c) and molecular density (d_M) for α-GaN at 300 K.*

Parameter	Value
Lattice constant a (Å)	3.1896
c (Å)	5.1855
Molecular density d_M (10^{22} cm^{-3})	4.3776

• **Crystal density**

Table 10.1.7 *Crystal density g for α-GaN at 300 K.**

g (g/cm^3)
6.0865

*Calculated using a=3.1896 Å and c=5.1855 Å.

10.1.5 Structural Phase Transition

Table 10.1.8 *Structural phase transition in α-GaN at high pressures.*

Structure	Transition pressure (GPa)
Wurtzite ($P6_3mc$)	Normal pressure
Rocksalt (NaCl)	47 [1.7]
	37 [1.8]
	52.2 [1.9]
	53.6 [1.10]

[1.7] P. Perlin, C. Jauberthie-Carillon, J. P. Itie, A. S. Miguel, I. Grzegory, and A. Polian, *Phys. Rev. B* **45**, 83 (1992).
[1.8] H. Xia, Q. Xia, and A. L. Ruoff, *Phys. Rev. B* **47**, 12925 (1993).
[1.9] M. Ueno, M. Yoshida, A. Onodera, O. Shimomura, and K. Takemura, *Phys. Rev. B* **49**, 14 (1994).
[1.10] S. Uehara, T. Masamoto, A. Onodera, M. Ueno, O. Shimomura, and K. Takemura, *J. Phys. Chem. Solids* **58**, 2093 (1997).

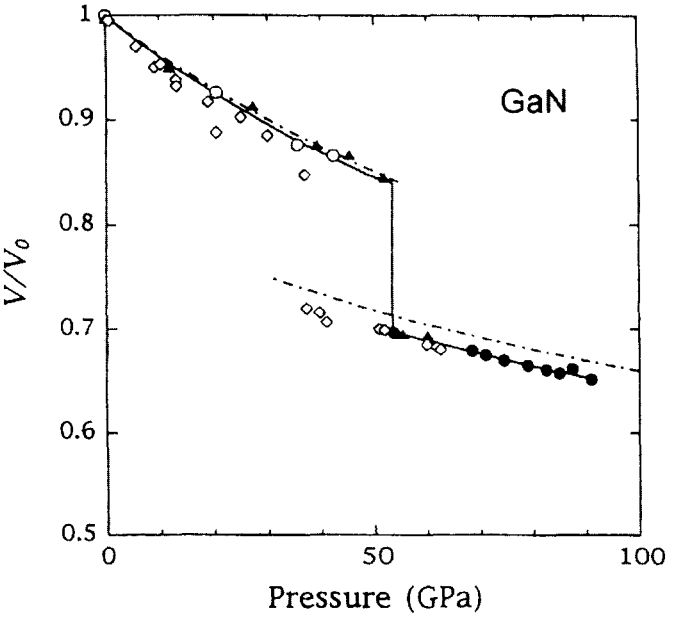

Fig. 10.1.1 Measured equation of state for GaN. [From S. Uehara, T. Masamoto, A. Onodera, M. Ueno, O. Shimomura, and K. Takemura, *J. Phys. Chem. Solids* **58**, 2093 (1997).]

10.1.6 Cleavage Plane

Table 10.1.9 *Crystallographic plane most readily cleaved for α-GaN.**

Cleavage plane
$(11\bar{2}0)$, $(10\bar{1}0)$

*Expected.

10.2 THERMAL PROPERTIES

10.2.1 Melting Point and Its Related Parameters

Table 10.2.1 *Melting point T_m and its related parameters for α-GaN [2.1].*

Parameter	Value
Melting point T_m (K)	2791
Pressure coefficient dT_m/dp (°C/kbar)	−2.5
Heat of fusion ΔH_m (kcal/mol)	44.68
Entropy of fusion ΔS_m (cal/mol K)	16.01

[2.1] Calculated [J. A. Van Vechten, *Phys. Rev. B* **7**, 1479 (1973)].

10.2.2 Specific Heat

Table 10.2.2 *Specific heat C_p (at constant pressure) for α-GaN [2.2].*

Temperature (K)	C_p (mJ/g K)	Temperature (K)	C_p (mJ/g K)
5.4	0.196	152.5	261.6
11.1	1.80	161.2	273.4
21.2	11.4	169.6	284.2
30.2	25.2	181.8	300.0
40.3	46.0	197.1	317.4
51.8	75.7	209.5	331.5
59.3	95.3	220.5	343.2
69.1	116.7	231.1	353.5
79.4	139.7	241.4	362.8
91.6	165.3	251.5	373.5
100.6	181.8	260.9	381.3
110.8	199.3	270.5	390.3
119.2	212.6	283.1	402.1
130.4	229.5	292.9	417.9
140.5	244.6	305.4	423.7

[2.2] The data are taken from tabulation by S. Krukowski, M. Leszczynski, and S. Porowski [in *Properties, Processing and Applications of Gallium Nitride and Related Semiconductors*, EMIS Datareviews Series No. 23, edited by J. H. Edgar, S. Strite, I. Akasaki, H. Amano, and C. Wetzel (INSPEC, London, 1999), p. 21].

• Functional expression

Table 10.2.3 *Specific heat C_p (at constant pressure) as a function of temperature T for α-GaN.*

C_p (J/g K)
$0.521+1.03\times10^{-4}T-5.78\times10^{3}T^{-2}$ ($800\leq T\leq1050$ K) [2.3]

[2.3] K. Yamaguchi, K. Itagaki, and A. Yazawa, *J. Jpn. Inst. Metals* **53**, 764 (1989).

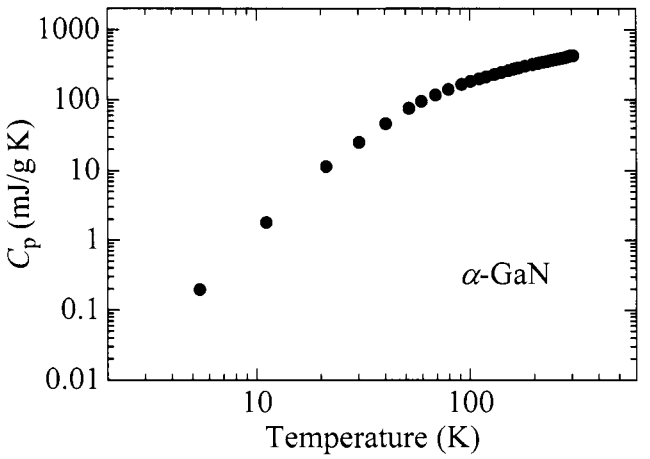

Fig. 10.2.1 Specific heat C_p (at constant pressure) versus temperature for α-GaN. The data are taken from tabulation by S. Krukowski, M. Leszczynski, and S. Porowski [in *Properties, Processing and Applications of Gallium Nitride and Related Semiconductors*, EMIS Datareviews Series No. 23, edited by J. H. Edgar, S. Strite, I. Akasaki, H. Amano, and C. Wetzel (INSPEC, London, 1999), p. 21].

10.2.3 Debye Temperature

Table 10.2.4 *Debye temperature θ_D for α-GaN [2.4].*

Temperature (K)	θ_D (K)	Temperature (K)	θ_D (K)
20	558	400	846
35	503	500	855
50	514	600	861
100	597	800	868
150	700	1000	873
200	765	1500	873
250	798	2000	874
300	821		

[2.4] J. C. Nipko, C.-K. Loong, C. M. Balkas, and R. F. Davis, *Appl. Phys.* **73**, 34 (1998).

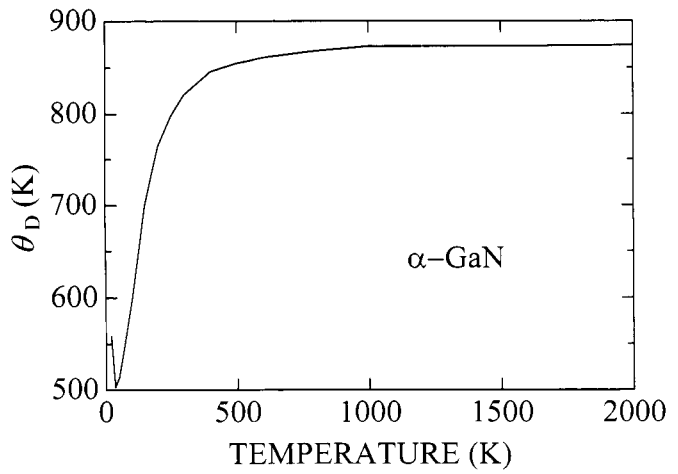

Fig. 10.2.2 Debye temperature θ_D for α-GaN. The data are obtained from J. C. Nipko, C.-K. Loong, C. M. Balkas, and R. F. Davis [*Appl. Phys.* **73**, 34 (1998)].

10.2.4 Thermal Expansion Coefficient

Table 10.2.5 *Thermal expansion coefficient α_{th} for α-GaN [2.5].*

Temperature (K)	α_{th} (10^{-6} K^{-1})		Temperature (K)	α_{th} (10^{-6} K^{-1})	
	α_a	α_c		α_a	α_c
100	1.249	1.145	700	5.122	4.487
150	2.473	2.228	800	5.185	4.541
200	3.340	2.979	900	5.235	4.581
250	3.898	3.456	1000	5.276	4.613
298	4.249	3.755	1100	5.312	4.643
300	4.261	3.765	1200	5.342	4.666
400	4.678	4.117	1300	5.369	4.689
500	4.898	4.302	1400	5.396	4.709
600	5.033	4.413	1500	5.420	4.727

[2.5] K. Wang and R. R. Reeber, *Mat. Res. Soc. Symp. Proc.* **482**, 863 (1998).

Table 10.2.6 *Thermal expansion coefficient α_{th} for α-GaN. The numerical data are obtained from a linear fit of the temperature-dependent lattice parameters a and c in the given temperature ranges.*

Temperature (K)	α_{th} (10^{-6} K^{-1})		Comment
	α_a	α_c	
≤100	−0.2±0.6	0.7±0.4	Bulk and homoepitaxial crystals [2.6]
100–250	2.7±0.6	1.9±0.5	
250–600	5.0±0.7	4.5±0.4	

[2.6] V. Kirchner, H. Heinke, D. Hommel, J. Z. Domagala, and M. Leszczynski, *Appl. Phys. Lett.* **77**, 1434 (2000).

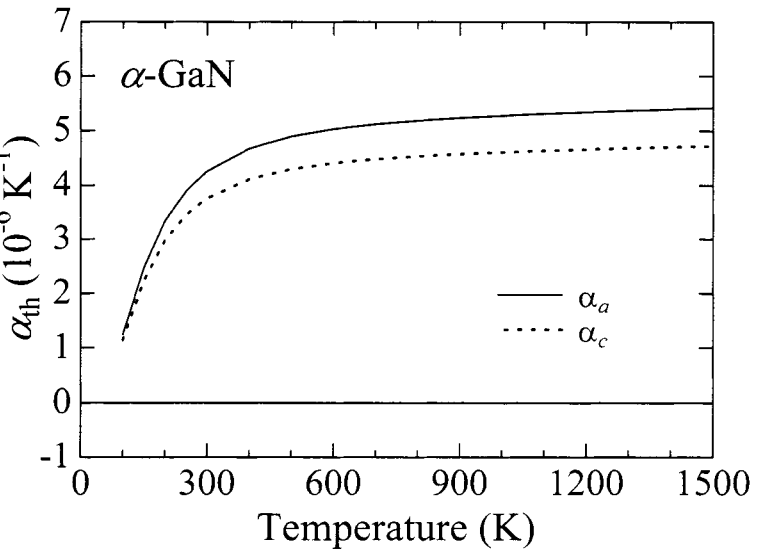

Fig. 10.2.3 Thermal expansion coefficient α_{th} versus temperature for α-GaN. The data are taken from K. Wang and R. R. Reeber [*Mat. Res. Soc. Symp. Proc.* **482**, 863 (1998)].

10.2.5 Thermal Conductivity and Diffusivity

• Room-temperature value

Table 10.2.7 *Thermal conductivity K for α-GaN at 300 K. LEOF=lateral epitaxial overgrown film; HVPE=hydride vapor phase epitaxy.*

K (W/cm K)	Comment
1.21	Bulk crystal [2.7]
>1.55	LEO film [2.8]*
1.35	HVPE film [2.8]
1.95	HVPE film, n~6.9×10^{16} cm^{-3} [2.9]
2.00<K<2.10	LEO film [2.10]*

[2.7] E. K. Sichel and D. I. Pankove, *J. Phys. Chem. Solids* **38**, 330 (1977).
[2.8] C.-Y. Luo, H. Marchand, D. R. Clarke, and S. P. DenBaars, *Appl. Phys. Lett.* **75**, 4151 (1999).
[2.9] D. I. Florescu, V. M. Asnin, L. G. Mourokh,F. H. Pollak, and R. J. Molnar, *Mat. Res. Soc. Symp. Proc.* **595**, w3.89.1 (2000).
[2.10] D. I. Florescu, V. M. Asnin, F. H. Pollak, A. M. Jones, J. C. Ramer, M. J. Schurman, and I. Ferguson, *Appl. Phys. Lett.* **77**, 1464 (2000).
*It should be noted that the dramatic reduction in dislocation densities in GaN films can be achieved by using a lateral epitaxial overgrowth (LEO) technique.

• Temperature dependence

Table 10.2.8 *Thermal conductivity K for α-GaN [2.11].**

Temperature (K)	K (W/cm K)	Temperature (K)	K (W/cm K)
25	0.42	134	1.20
27	0.43	153	1.24
31	0.49	165	1.27
34	0.54	167	1.40
40	0.61	182	1.42
44	0.64	195	1.40
52	0.71	214	1.42
63	0.74	224	1.38
77	0.80	253	1.32
97	0.85	300	1.21
114	1.10	365	1.20

[2.11] E. K. Sichel and D. I. Pankove, *J. Phys. Chem. Solids* **38**, 330 (1977).
*Thick film grown by hydride vapor phase epitaxy (heat flow is along the c-axis).

Table 10.2.9 *Thermal conductivity K for α-GaN [2.12].**

Temperature (K)	K (W/cm K)	Temperature (K)	K (W/cm K)
40	8.19	200	2.53
60	9.26	220	2.46
80	10.07	240	2.10
100	8.81	260	1.84
120	8.14	280	1.61
140	6.00	300	1.61

Table 10.2.9 *Continued.*

Temperature (K)	K (W/cm K)	Temperature (K)	K (W/cm K)
160	5.96	320	1.48
180	4.71		

[2.12] C. Luo, D. R. Clarke, and J. R Dryden, *J. Electron. Mater.* **30**, 138 (2001).
*Lateral epitaxially overgrown film.

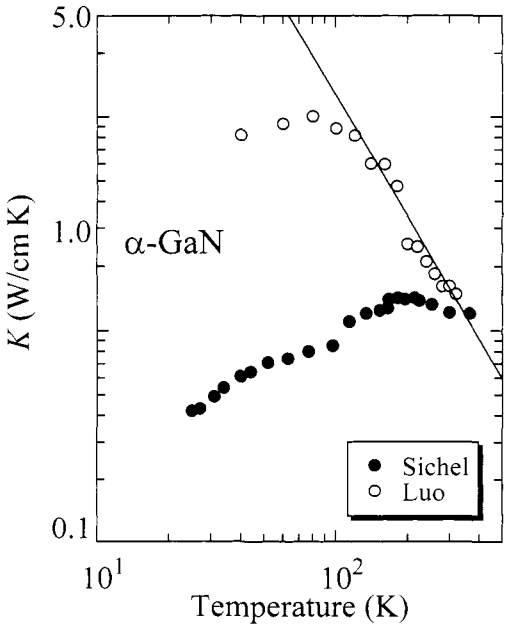

Fig. 10.2.4 Thermal conductivity K for α-GaN. The experimental data are taken from E. K. Sichel and D. I. Pankove [*J. Phys. Chem. Solids* **38**, 330 (1977); solid circles (a thick film grown by hydride vapor phase epitaxy)] and from C. Luo, D. R. Clarke, and J. R Dryden [*J. Electron. Mater.* **30**, 138 (2001); open circles (a lateral epitaxially overgrown film by hydride vapor phase epitaxy)]. The solid line represents the calculated result of $K=AT^{n}$ with A=80000 W/cmK$^{-0.9}$ and n= −1.90.

• Doping dependence

The thermal conductivity K as a function of carrier concentration n for α-GaN measured by D. I. Florescu, V. M. Asnin, F. H. Pollak, R. J. Molnar, and C. E. C. Wood [*J. Appl. Phys.* **88**, 3295 (2000)] suggested that K decreases with increasing n.

10.3 ELASTIC PROPERTIES

10.3.1 Elastic Constant

• Room-temperature value

Table 10.3.1 *Elastic stiffness constant C_{ij} for α-GaN at 300 K. XRD=X-ray diffraction; BS=Brillouin scattering; RU=resonance ultrasound; SAW=surface acoustic wave.*

C_{ij} (10^{11} dyn/cm^2)						Comment
C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	
29.6±1.8	13.0±1.1	15.8±0.6	26.7±1.8	2.41±0.2	8.3	Polycrystal, XRD [3.1]
39.0	14.5	10.6	39.8	10.5	12.3	Needle-like bulk crystal, BS [3.2]
37.7	16.0	11.4	20.9	81.4	10.9	Epitaxial film, RU [3.3]

Table 10.3.1 *Continued.*

C_{ij} (10^{11} dyn/cm^2)						Comment
C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	
36.5±0.2	13.5±0.4	11.4±1.6	38.1±0.1	10.9±0.3	11.5±0.1	Epitaxial film, BS [3.4]
37.3±0.2	14.1±0.4	8.0±1.6	38.7±0.1	9.4±0.3	11.8±0.1	Bulk single crystal, BS [3.5]
37.0	14.5	10.6	39.8	10.5	12.3	Epitaxial film, SAW [3.6]
37.3	14.1	8.04	38.7	9.36	11.8	Lateral epitaxially overgrown layer, BS [3.7]

[3.1] V. A. Savstenko and A. U. Shieleg, *Phys. Status Solidi A* **48**, K135 (1978).
[3.2] A. Polian, M. Grimsditch, and I. Grzegory, *J. Appl. Phys.* **79**, 3343 (1996).
[3.3] R. B. Schwarz, K. Khachaturyan, and E. R. Weber, *Appl. Phys. Lett.* **70**, 1122 (1997).
[3.4] M. Yamaguchi, T. Yagi, T. Azuhata, T. Sota, K. Suzuki, S. Chichibu, and S. Nakamura, *J. Phys.: Condens. Matter* **9**, 241 (1997).
[3.5] M. Yamaguchi, T. Yagi, T. Sota, T. Deguchi, K. Shimada, and S. Nakamura, *J. Appl. Phys.* **85**, 8502 (1999).
[3.6] C. Deger, E. Born, H. Angerer, O. Ambacher, M. Stutzmann, J. Hornstein, E. Riha, and G. Fischeruer, *Appl. Phys. Lett.* **72**, 2400 (1998).
[3.7] T. Deguchi, D. Ichiryu, K. Toshikawa, K. Sekiguchi, T. Sota, R. Matsuo, T. Azuhata, M. Yamaguchi, T. Yagi, S. Chichibu, and S. Nakamura, *J. Appl. Phys.* **86**, 1860 (1999).

Table 10.3.2 *Room-temperature elastic stiffness (C_{ij}) and compliance constants (S_{ij}) for α-GaN (recommended values).*

C_{ij} (10^{11} dyn/cm^2)					
C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}*[1]
37.3	14.1	8.0	38.7	9.4	11.6
S_{ij} (10^{-13} cm^2/dyn)*[2]					
S_{11}	S_{12}	S_{13}	S_{33}	S_{44}	S_{66}*[1]
3.20	−1.12	−0.43	2.76	10.6	8.64

*[1] $C_{66}=\frac{1}{2}(C_{11}-C_{12})$; $S_{66}=2(S_{11}-S_{12})$.
*[2] Calculated from C_{ij} values.

10.3.2 Third-Order Elastic Constant

No detailed data are available for α-GaN.

10.3.3 Young's Modulus, Poisson's Ratio, and Similar

• Young's modulus

Table 10.3.3 *Young's modulus Y for α-GaN at 300 K.**

Direction	Y (10^{12} dyn/cm^2)
$c \perp l$	3.13
$c \parallel l$	3.62

*Calculated using $S_{11}=3.20\times10^{-13}$ and $S_{33}=2.76\times10^{-13}$ cm^2/dyn.
l: directional vector.

• **Poisson's ratio**

Table 10.3.4 *Poisson's ratio P for α-GaN at 300 K.**

Direction	*P*
$c \perp l$	0.23
$c \parallel l$	0.19

*Obtained from a definition $B_u = Y/[3(1-2P)]$, where B_u and Y are bulk and Young's moduli, respectively.
l: directional vector.

• **Bulk modulus, shear modulus, etc.**

Table 10.3.5 *Bulk modulus, B_u, pressure derivative of B_u, dB_u/dp, and linear compressibility, C_o, for α-GaN at 300 K.*

Parameter	Value
B_u (10^{12} dyn/cm^2)	1.92 [3.8]
dB_u/dp	3.2, 4.3 [3.9]
	4.5 [3.10]
C_o (10^{-13} cm^2/dyn)	
$c \perp l$	1.65 [3.8]
$c \parallel l$	1.90 [3.8]

[3.8] Calculated using $C_{11}=3.73\times10^{12}$ dyn/cm^2, $C_{12}=1.41\times10^{12}$ dyn/cm^2, $C_{13}=8.00\times10^{11}$ dyn/cm^2, $C_{33}=3.87\times10^{12}$ dyn/cm^2, $S_{11}=3.20\times10^{-13}$ cm^2/dyn, $S_{12}=-1.12\times10^{-13}$ cm^2/dyn, $S_{13}=-4.30\times10^{-14}$ cm^2/dyn, and $S_{33}=2.76\times10^{-13}$ cm^2/dyn.
[3.9] Exper. [see, K. C. Stampfl and C. G. Van de Walle, *Phys. Rev. B* **59**, 5521 (1999)].
[3.10] T. Tsuchiya, K. Kawamura, O. Ohtaka, H. Fukui, and T. Kikegawa, *Solid State Commun.* **121**, 555 (2002).
l: directional vector.

10.3.4 Microhardness

Table 10.3.6 *Microhardness H for α-GaN.*

H (GPa)
10.2 [3.11]

[3.11] Vickers's microhardness, (0001) basal plane [I. Yonenaga, T. Hoshi, and A. Usui, *Jpn. J. Appl. Phys.* **39**, L200 (2000)].

10.3.5 Sound Velocity

Table 10.3.7 *Sound velocity propagating in α-GaN at 300 K.* LA=longitudinal acoustic; TA1, TA2=transverse acoustic.*

Propagation direction ***a***	Direction of polarization π	Mode	Sound velocity (10^5 cm/s)
$a \parallel c$	$\pi \parallel c$	LA	7.97
$a \parallel c$	$\pi \perp c$	TA1, TA2	3.93
$a \perp c$	$\pi \perp c$	LA	7.83
$a \perp c$	$\pi \perp c$	TA1	4.37
$a \perp c$	$\pi \parallel c$	TA2	3.93

*Calculated using $C_{11}=3.73\times10^{12}$ dyn/cm^2, $C_{12}=1.41\times10^{12}$ dyn/cm^2, $C_{33}=3.87\times10^{12}$ dyn/cm^2, $C_{44}=9.4\times10^{11}$ dyn/cm^2, and $g=6.0865$ g/cm^3.

10.4 PHONONS AND LATTICE VIBRONIC PROPERTIES

10.4.1 Phonon Dispersion Relation

• Dispersion curves and phonon density of states

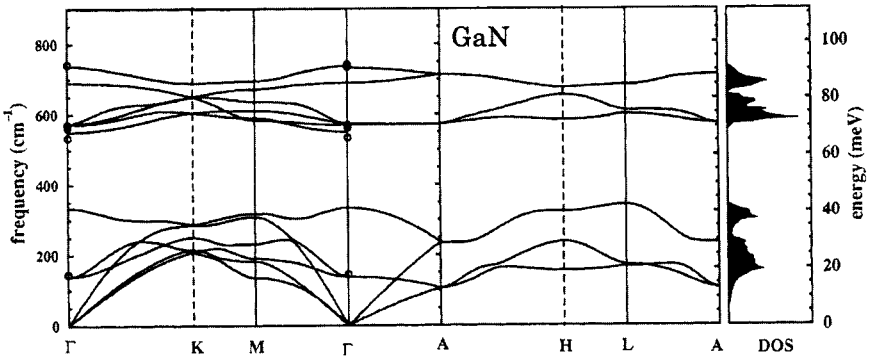

Fig. 10.4.1 Phonon dispersion curves and density of states (DOS) in α-GaN. The symbols represent the Raman data. [From C. Bungaro, K. Rapcewicz, and J. Bernholc, *Phys. Rev. B* **61**, 6720 (2000).]

10.4.2 Phonon Frequency

• Room-temperature value

Table 10.4.1 *Long-wavelength ($q \to 0$) phonon frequencies for α-GaN.*

Phonon frequency (cm^{-1})						Comment
E_2 low	A_1 (TO)	E_1 (TO)	E_2 high	A_1 (LO)	E_1 (LO)	
144	531	560	568			Exper. [4.1]
	534	563	572	736	745	Exper. [4.2]
144	533	561	569	735	743	Exper. [4.3]
	533	561	570	735	742	Exper. [4.4]
	537	556	571	737		Exper. [4.5]
144.0	531.8	558.8	567.6	734.0	741.0	Exper. [4.6]
144.1	531.7	558.2	567.0	736.5	742	Exper. [4.7]
144	533	560	569	736	743	Mean value (Exper.)
144.7	545.2	571.7	581.0	751.2	752.2	Theor. [4.8]

[4.1] P. Perlin, C. Jauberthie-Carillon, J. P. Itie, A. S. Miguel, I. Grzegory, and A. Polian, *Phys. Rev. B* **45**, 83 (1992).
[4.2] T. Kozawa, T. Kachi, H. Kano, Y. Taga, M. Hashimoto, N. Koide, and K. Manabe, *J. Appl. Phys.* **75**, 1098 (1994).
[4.3] T. Azuhata, T. Sota, K. Suzuki, and S. Nakamura, *J. Phys.: Condens. Matter* **7**, L129 (1995).
[4.4] H. Siegle, L. Eckey, A. Hoffman, C. Thomsen, B. K. Meyer, D. Schikora, M. Hankeln, and K. Lischka, *Solid State Commun.* **96**, 943 (1995).
[4.5] T. Tabata, R. Enderlein, J. R. Leite, S. W. da Silva, J. C. Galzerani, D. Schikora, M. Kloidt, and K. Lischka, *J. Appl. Phys.* **79**, 4137 (1996).
[4.6] V. Yu. Davydov, Yu. E. Kitaev, I. N. Goncharuk, A. N. Smirnov, J. Graul, O. Semchinova, D. Uffmann, M. B. Smirnov, A. P. Mirgorodsky, and R. A. Evarestov, *Phys. Rev. B* **58**, 12899 (1998).
[4.7] A. R. Goñi, H. Siegle, K. Syassen, C. Thomsen, and J.-M. Wagner, *Phys. Rev. B* **64**, 35205 (2001).
[4.8] T. Ruf, J. Serrano, M. Cardona, P. Pavone, M. Pabst, M. Krisch, M. D'Astuto, T. Suski, I. Grzegory, and M. Leszczynski, *Phys. Rev. Lett.* **86**, 906 (2001).

• **Temperature dependence**

Table 10.4.2 *Temperature variation of the long-wavelength ($q \to 0$) phonon frequency in α-GaN grown on sapphire substrate [4.9].*

$$\omega_q(T) = \omega_q(0) - \frac{A}{e^{B\hbar\omega_q(0)/kT} - 1}$$

ω_q	$\omega_q(0)$ (cm^{-1})	A (cm^{-1})	B	Comment
E_2 high	568.4±0.05	19.9±1.1	1.13±0.03	Free standing
	568.2±0.2	17.9±2.4	0.99±0.08	Attached to substrate
A_1 (LO)	741.2±0.4	8.78±3.0	0.37±0.10	Free standing
	743.6±0.4	7.08±3.6	0.38±0.15	Attached to substrate

[4.9] M. S. Liu, L. A. Bursill, S. Prawer, K. W. Nugent, Y. Z. Tong, and G. Y. Zhang, *Appl. Phys. Lett.* **74**, 3125 (1999).

Table 10.4.3 *Temperature variation of the long-wavelength ($q \to 0$) phonon frequency in α-GaN grown on sapphire substrate [4.10].*

$$\omega_q(T) = \omega_q(0) - aT - bT^2$$

ω_q	$\omega_q(0)$ (cm^{-1})	a (10^{-3} cm^{-1}/K)	b (10^{-6} cm^{-1}/K^2)
A_1 (TO)	537.79	10.11	3.99
E_1 (TO)	564.09	8.92	6.38
E_2 high	572.60	7.14	9.42
A_1 (LO)	741.78	20.00	9.60
E_1 (LO)	750.03	22.00	8.50

[4.10] W. S. Li, Z. X. Shen, Z. C. Feng, and S. J. Chua, *J. Appl. Phys.* **87**, 3332 (2000).

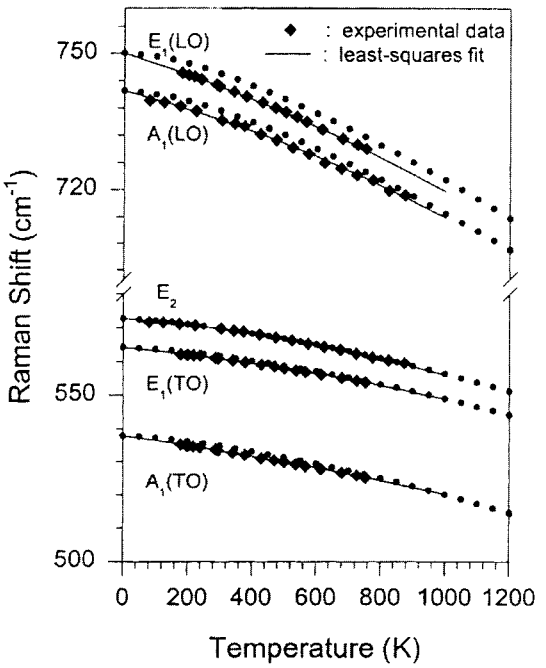

Fig. 10.4.2 Temperature dependence of the long-wavelength ($q \to 0$) phonon frequency in α-GaN grown on sapphire substrate. The solid lines represent the best fit using an empirical expression. The solid circles also represent the theoretical fit to the data. [From. W. S. Li, Z. X. Shen, Z. C. Feng, and S. J. Chua, *J. Appl. Phys.* **87**, 3332 (2000).]

• **Pressure dependence**

Table 10.4.4 *Pressure variation of the long-wavelength (q→0) phonon frequency in bulk α-GaN [4.11].*

$$\omega_q(p) = \omega_q(0)+ap+bp^2$$

ω_q	$\omega_q(0)$ (cm^{-1})	a (cm^{-1}/GPa)	b (cm^{-1}/GPa^2)
E_2 low	144	−0.25	−0.0017
A_1 (TO)	531	4.06	−0.0127
E_1 (TO)	560	3.68	−0.0078
E_2 high	568	4.17	−0.0017

[4.11] P. Perlin, C. Jauberthie-Carillon, J. P. Itie, A. S. Miguel, I. Grzegory, and A. Polian, *Phys. Rev. B* **45**, 83 (1992).

• **Temperature and/or pressure coefficient**

Table 10.4.5 *Linear pressure coefficient $d\omega_q/dp$ of the long-wavelength (q→0) phonon frequency in α-GaN grown on sapphire substrate.*

Phonon	$d\omega_q/dp$ (cm^{-1}/GPa)	Ref.
E_2 low	−0.3±0.1	[4.12]
A_1 (TO)	3.9±0.1	[4.12]
	3.1	[4.13]
E_1 (TO)	3.94±0.03	[4.12]
E_2 high	4.24±0.03	[4.12]
	3.75	[4.13]
A_1 (LO)	4.4±0.1	[4.12]

[4.12] A. R. Goñi, H. Siegle, K. Syassen, C. Thomsen, and J.-M. Wagner, *Phys. Rev. B* **64**, 35205 (2001).
[4.13] C. Wetzel, H. Amano, I. Akasaki, J. W. Ager III, I. Grzegory, M. Topf, and B. K. Meyer, *Phys. Rev. B* **61**, 8202 (2000).

10.4.3 Mode Grüneisen Parameter

Table 10.4.6 *Mode Grüneisen parameter for the long-wavelength (q→0) phonons in α-GaN.*

Phonon	Mode Grüneisen parameter			
	a	b	c	d
E_2 low	−0.426	−0.4		−0.4±0.1
A_1 (TO)	1.184	1.51		1.47±0.04
E_1 (TO)	1.609	1.41		1.41±0.01
E_2 high	1.798	1.50	1.47	1.50±0.01
A_1 (LO)		1.20	1.53	1.20±0.05
E_1 (LO)				

[a] P. Perlin, C. Jauberthie-Carillon, J. P. Itie, A. S. Miguel, I. Grzegory, and A. Polian, *Phys. Rev. B* **45**, 83 (1992).
[b] H. Siegle, A. R. Goñi, C. Thomsen, C. Ulrich, K. Syassen, B. Schöttker, D. J. As, and D. Schikora, *Mat. Res. Soc. Symp. Proc.* **468**, 225 (1997).
[c] See, A. Link, K. Bitzer, W. Limmer, R. Sauer, C. Kirchner, V. Schwegler, M. Kamp, D. G. Ebling, and K. W. Benz, *J. Appl. Phys.* **86**, 6256 (1999).
[d] A. R. Goñi, H. Siegle, K. Syassen, C. Thomsen, and J.-M. Wagner, *Phys. Rev. B* **64**, 35205 (2001).

10.4.4 Phonon Deformation Potential

Table 10.4.7 *Long-wavelength phonon deformation potential (PDP) for α-GaN.*

Definition: $\Delta\Omega = 2ae_{xx} + be_{zz}$

Phonon	PDP (cm^{-1})		Comment
	a	*b*	
E_2 low	77	7	Calc. [4.12]
	115±25	−80±35	Exper. [4.13]
A_1 (TO)	−639	−690	Calc. [4.12]
	−630±40	−1290±80	Exper. [4.13]
E_1 (TO)	−718	−592	Calc. [4.12]
	−820±25	−680±50	Exper. [4.13]
E_2 high	−740	−727	Calc. [4.12]
	−850±25	−920±60	Exper. [4.13]
	−818±14	−797±60	Exper. [4.14]
A_1 (LO)	−663	−877	Calc. [4.12]
	−685±38	−997±70	Exper. [4.14]
E_1 (LO)	−776	−704	Calc. [4.12]

[4.12] J.-M. Wagner and F. Bechstedt, *Appl. Phys. Lett.* **77**, 346 (2000).
[4.13] *T*=300 K [V. Yu. Davydov, N. S. Averkiev, I. N. Goncharuk, D. K. Nelson, I. P. Nikitina, A. S. Polkovnikov, A. N. Smirnov, M. A. Jacobson, and O. K. Semchinova, *J. Appl. Phys.* **82**, 5097 (1997)].
[4.14] *T*=77 K [F. Demangeot, J. Frandon, M. A. Renucci, O. Briot, B. Gil, and R. L. Aulombard, *Solid State Commun.* **100**, 207 (1996)].

10.5 COLLECTIVE EFFECTS AND RELATED PROPERTIES

10.5.1 Piezoelectric Constant

Table 10.5.1 *Theoretically obtained piezoelectric constant e_{ij} for α-GaN.*

e_{ij} (C/m^2)			Comment
e_{15}	e_{31}	e_{33}	
	−0.32	0.63	First-principles total energy calculation [5.1]
	−0.34	0.67	Berry-phase approach [5.2]
	−0.44	0.86	Local density approximation [5.3]
	−0.34	0.67	Generalized gradient approximation [5.3]

[5.1] K. Shimada, T. Sota, and K. Suzuki, *J. Appl. Phys.* **84**, 4951 (1998).
[5.2] F. Bernardini, V. Fiorentini, and D. Vanderbilt, *Phys. Rev. B* **63**, 193201 (2001).
[5.3] A. Zoroddu, F. Bernardini, P. Ruggerone, and V. Fiorentini, *Phys. Rev. B* **64**, 45208 (2001).

Table 10.5.2 *Piezoelectric constant e_{ij} for α-GaN estimated from cubic phase data (in C/m^2) [5.4].*

e_{15}	e_{31}	e_{33}
−0.22[a]	−0.22[a]	0.44[a]
−0.33[b]	−0.33[b]	0.65[b]

[5.4] A. D. Bykhovski, B. L. Gelmont, and M. S. Shur, *J. Appl. Phys.* **81**, 6332 (1997).
[a] From e_{14}=0.375 C/m^2.
[b] From e_{14}=0.56 C/m^2.

Table 10.5.3 *Experimentally determined piezoelectric stress (e_{ij}) and strain constants (d_{ij}) for α-GaN.*

e_{ij} (C/m^2)			d_{ij} (10^{-12} m/V)			Ref.
e_{15}	e_{31}	e_{33}	d_{15}	d_{31}	d_{33}	
					2.0±0.1	[5.5]
					2.13	[5.6]
			3.1±0.2			[5.7]
	−0.55	1.12		−1.9	3.7	[5.8]
					3.1	[5.9]

[5.5] S. Muensit and I. L. Guy, *Appl Phys. Lett.* **72**, 1896 (1998).
[5.6] C. M. Lueng, H. L. W. Chan, C. Surya, W. K. Fong, C. L. Choy, P. Chow, and M. Rosamond, *J. Non-Cryst. Solids* **254**, 123 (1999).
[5.7] S. Muensit, E. M. Goldys, and I. L. Guy, *Appl. Phys. Lett.* **75**, 3965 (1999).
[5.8] I. L. Guy, S. Muensit, and E. M. Goldys, *Appl. Phys. Lett.* **75**, 4133 (1999).
[5.9] C. M. Lueng, H. L. W. Chan, C. Surya, and C. L. Choy, *J. Appl. Phys.* **88**, 5360 (2000).

10.5.2 Fröhlich Coupling Constant

Table 10.5.4 *Fröhlich coupling constant α_F of α-GaN.*

α_F
0.48 [5.10]
0.37 [5.11]
0.43 [5.12]

[5.10] See, V. W. L. Chin, T. L. Tansley, and T. Osotchan, *J. Appl. Phys.* **75**, 7365 (1994).
[5.11] Electron–LO-like-phonon coupling (α_L) [M. E. Mora-Ramos, F. J. Rodríguez, and L. Quiroga, *J. Phys.: Condens. Matter* **11**, 8223 (1999)].
[5.12] Electron–TO-like-phonon coupling (α_T) [M. E. Mora-Ramos, F. J. Rodríguez, and L. Quiroga, *J. Phys.: Condens. Matter* **11**, 8223 (1999)].

10.6 ENERGY-BAND STRUCTURE: ENERGY-BAND GAPS

10.6.1 Basic Properties

• Electronic energy-band structure

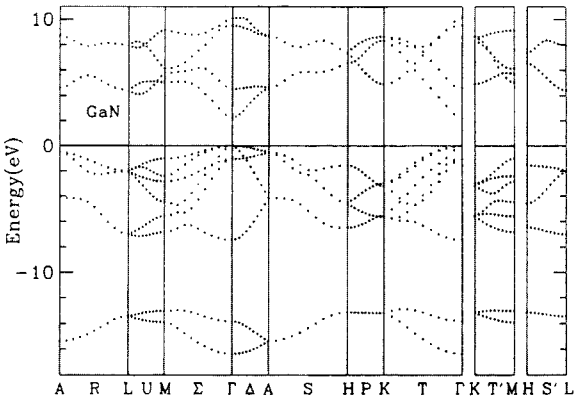

Fig. 10.6.1 Electronic energy-band structure of α-GaN calculated in the GW approximation. [From A. Rubio, J. L. Corkill, M. L. Cohen, E. L. Shirley, and S. G. Louie, *Phys. Rev. B* **48**, 11810 (1993).]

• Electronic density of states

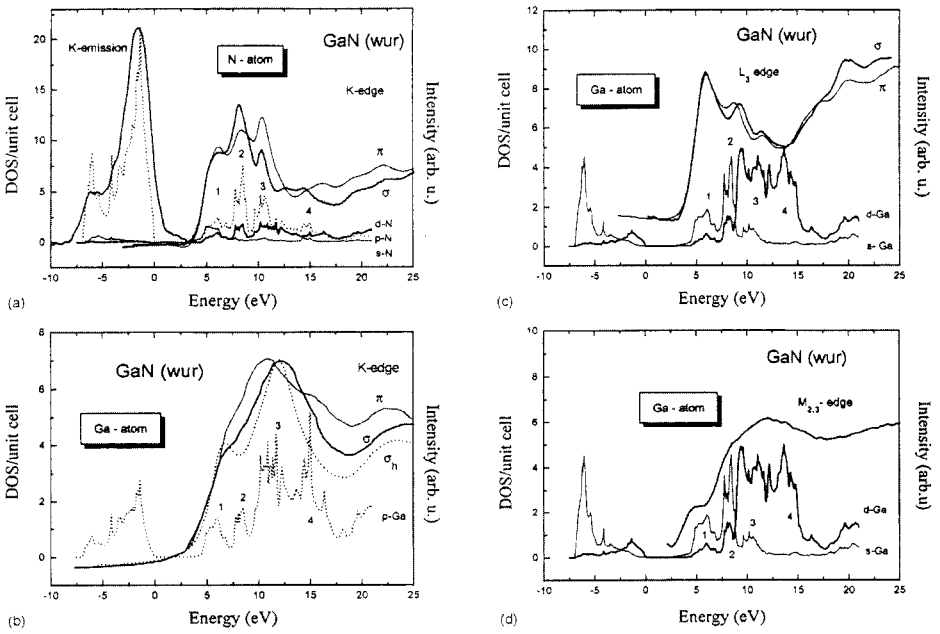

Fig. 10.6.2 Projected density of states (PDOS) for α-GaN (s, thin line; p, dotted line; d, thick line). (a) Projected on the N atom and compared with N K emission and absorption spectra measured for π and σ polarization geometry. (b) Projected on the Ga atom: p PDOS compared with Ga K absorption spectra measured for π and σ polarization geometry, additionally the high-resolution σ spectrum is shown (dotted line). (c) Projected on the Ga atom: s and d PDOS compared with Ga L_3 absorption spectra measured for π and σ polarization geometry. (d) Projected on the Ga atom: s and d PDOS compared with Ga $M_{2,3}$ absorption spectrum. [From K. Lawniczak-Jablonska, T. Suski, I. Gorczyca, N. E. Christensen, K. E. Attenkofer, R. C. C. Perera, E. M. Gullikson, J. H. Underwood, D. L. Ederer, and Z. L. Weber, *Phys. Rev. B* **61**, 16623 (2000).]

• **Energy eigenvalue**

Table 10.6.1 *Energy eigenvalues at the critical points for the valence and first few conduction bands of α-GaN calculated in the GW approximation [6.1].*

Critical point	Level	Value (eV)	Critical point	Level	Value (eV)
Γ	Γ_1^v	−18.2	L	$L_{1,3}^v$	−15.4
	Γ_3^v	−15.7		$L_{1,3}^v$	−7.6
	Γ_3^v	−8.0		$L_{2,4}^v$	−2.2
	Γ_5^v	−1.2		$L_{1,3}^v$	−2.2
	Γ_5^v	−1.2		$L_{1,3}^c$	6.0
	Γ_1^v	0.0		$L_{1,3}^c$	9.9
	Γ_6^v	0.0			
	Γ_6^v	0.0			
	Γ_1^c	3.5			
	Γ_3^c	5.9			
	Γ_1^c	12.1			
	Γ_6^c	11.9			
K	K_3^v	−15.2	H	$H_{1,3}^v$	−15.1
	K_3^v	−15.2		H_3^v	−7.1
	K_1^v	−6.1		$H_{1,2}^v$	−4.9
	K_3^v	−6.1		H_3^v	−1.6
	K_3^v	−6.1		H_3^c	8.3
	K_3^v	−3.5		$H_{1,2}^c$	9.4
	K_3^v	−3.5			
	K_2^v	−3.2			
	K_2^c	6.6			
	K_3^c	10.6			
	K_3^c	10.6			
	K_1^c	10.8			
M	M_1^v	−15.8	A	$A_{1,3}^v$	−17.2
	M_3^v	−15.0		$A_{1,3}^v$	−4.6
	M_1^v	−7.4		$A_{5,6}^v$	−0.6
	M_3^v	−6.1		$A_{5,6}^v$	−0.6
	M_1^v	−4.9		$A_{1,3}^c$	6.1
	M_2^v	−3.1		$A_{5,6}^c$	10.8
	M_3^v	−2.6			
	M_4^v	−1.1			
	M_1^c	6.5			
	M_3^c	7.4			
	M_3^c	8.1			
	M_1^c	11.5			

[6.1] A. Rubio, J. L. Corkill, M. L. Cohen, E. L. Shirley, and S. G. Louie, *Phys. Rev. B* **48**, 11810 (1993).

10.6.2 E_0-Gap Region

• Temperature dependence

Table 10.6.2 *Excitonic energy gap $E_{0\alpha}$ (α=A, B, or C) for α-GaN determined at various temperatures. Values in parentheses give the band-gap energy.*

Substrate	$E_{0\alpha}$ (eV)			Comment
	A	*B*	*C*	
Bulk GaN	3.477 (3.504)	3.482	3.489	*T*=4.2 K [6.2]
	3.4780±0.0004	3.4831±0.0005	3.5018±0.0010	*T*=7 K [6.3]
GaN	3.4767±0.0003	3.4815±0.0003	3.4986±0.0008	*T*=1.8 K [6.4]
	3.4769±0.0003	3.4821±0.0003	3.4993±0.0008	*T*=4.2 K [6.5]
Al_2O_3	3.485	3.493	3.518	*T*=15 K [6.6]
	3.420	3.428		*T*=300 K [6.6]
	(3.503)			*T*=10 K [6.7]
	3.4857 (3.504±0.001)			*T*=10 K [6.8]
	3.4831 (3.5031±0.0005)	3.4896 (3.5116±0.0005)	3.518	*T*=2 K [6.9]
	3.4770	3.4865	3.5062	*T*=2 K [6.10]
	(3.523)			*T*=1.5 K, thin film [6.11]
	(3.506)			*T*=1.5 K, strain-free film [6.11]
	3.491	3.499	3.528	*T*=10 K [6.12]
	3.478 (3.504)			*T*=10 K, strain-free value [6.13]
	3.4867	3.4923		*T*=6 K [6.14]
	(3.522±0.002)			*T*=2 K [6.15]
	(3.507)			*T*=77 K [6.16]
	(3.452±0.001)			*T*=295 K [6.16]
	(3.479±0.003)			*T*=9 K, weakly strained [6.17]
	3.4791±0.0002 (3.5025)	3.4844±0.0002 (3.5080)	3.5027±0.0002	*T*=10 K, strain-free value [6.18]
	3.4764±0.0005	3.4822±0.0005	3.4983±0.0005	*T*=10 K, strain-free value [6.19]
6H-SiC	(3.497)			*T*=1.5 K, thin film [6.11]
	3.470	3.474	3.491	*T*=10 K [6.12]
	3.470	3.489		*T*=6 K [6.20]
	3.470	3.470	3.486	*T*=10 K [6.21]
	3.477	3.487	3.498	*T*=20 K [6.22]
ZnO	3.375	3.386		*T*=4.2 K [6.23]
Si	3.454	3.454	3.475	*T*=10 K [6.21]

Table 10.6.2 *Continued.*

Substrate	$E_{0\alpha}$ (eV)			Comment
	A	*B*	*C*	
GaAs (GaP)	3.42±0.02			*T*=300 K [6.24]

[6.2] T. Ogino and M. Aoki, *Jpn. J. Appl. Phys.* **19**, 2395 (1980).
[6.3] M. Steube, K. Reimann, D. Fröhlich, and S. J. Clarke, *Appl. Phys. Lett.* **71**, 948 (1997).
[6.4] R. Stępniewski, K. P. Korona, A. Wysmołek, J. M. Baranowski, K. Pakuła, M. Potemski, G. Martinez, I. Grzegory, and S. Porowski, *Phys. Rev. B* **56**, 15151 (1997).
[6.5] R. Stępniewski, M. Potemski, A. Wysmołek, K. Pakuła, J. M. Baranowski, J. Łusakowski, I. Grzegory, S. Porowski, G. Martinez, and P. Wyder, *Phys. Rev. B* **60**, 4438 (1999).
[6.6] W. Shan, T. J. Schmidt, X. H. Yang, S. J. Hwang, J. J. Song, and B. Goldenberg, *Appl. Phys. Lett.* **66**, 985 (1995).
[6.7] M. Smith, G. D. Chen, J. Z. Li, J. Y. Lin, H. X. Jiang, A. Salvador, W. K. Kim, O. Aktas, A. Botchkarev, and H. Morkoç, *Appl. Phys. Lett.* **67**, 3387 (1995).
[6.8] M. Smith, G. D. Chen, J. Y. Lin, H. X. Jiang, M. S. Khan, C. J. Sun, Q. Chen, and J. W.. Yang, *J. Appl. Phys.* **79**, 7001 (1996).
[6.9] D. C. Reynolds, D. C. Look, W. Kim, Ö. Aktas, A. Botchkarev, A. Salvador, H. Morkoç, and D. N. Talwar, *J. Appl. Phys.* **80**, 594 (1996).
[6.10] M. Tchounkeu, O. Briot, B. Gil, J. P. Alexis, and R.-L. Aulombard, *J. Appl. Phys.* **80**, 5352 (1996).
[6.11] D. Volm, K. Oettinger, T. Streibl, D. Kovalev, M. Ben-Chorin, J. Diener, B. K. Meyer, J. Majewski, L.Eckey, A. Hoffmann, H. Amano, I. Akasaki, K. Hiramatsu, and T. Detchprohm, *Phys. Rev. B* **53**, 16543 (1996).
[6.12] W. Shan, B. D. Little, A. J. Fischer, J. J. Song, B. Goldenberg, W. G. Perry, M. D. Bremser, and R. F. Davis, *Phys. Rev. B* **54**, 16369 (1996).
[6.13] A. Shikanai, T. Azuhata, T. Sota, S. Chichibu, A. Kuramata, K. Horino, and S. Nakamura, *J. Appl. Phys.* **81**, 417 (1997).
[6.14] J. A. Freitas, Jr., K. Doverspike, and A. E. Wickenden, *Mat. Res. Soc. Symp. Proc.* **395**, 485 (1996).
[6.15] C. Merz, M. Kunzer, U. Kaufmann, I. Akasaki, and H. Amano, *Semicond. Sci. Technol.* **11**, 712 (1996).
[6.16] J. F. Muth, J. H. Lee, I. K. Shmagin, R. M. Kolbas, H. C. Casey, Jr., B. K. Keller, U. K. Mishra, and S. P. DenBaars, *Appl. Phys. Lett.* **71**, 2572 (1997).
[6.17] M. Leroux, B. Beaumont, N. Grandjean, C. Golivet, P. Gibart, J. Massies, J. Leymarie, A. Vasson, and A. M. Vasson, *Mater. Sci. Eng. B* **43**, 237 (1997).
[6.18] K. Torii, T. Deguchi, T. Sota, K. Suzuki, S. Chichibu, and S. Nakamura, *Phys. Rev. B* **60**, 4723 (1999).
[6.19] N. V. Edwards, M. D. Bremser, A. D. Batchelor, I. A. Buyanova, L. D. Madsen, S. D. Yoo, T. Wethkamp, K. Wilmers, C. Cobet, N. Esser, R. F. davis, D. E. Aspnes, and B. Monemar, *Thin Solid Films* **364**, 98 (2000).
[6.20] D. K. Nel'son, Yu. V. Nel'nik, A. V. Sel'kin, M. A. Yakobson, V. A. Dmitriev, K. J. Irvine, and C. H. Carter, Jr., *Phys. Solid State* **38**, 455 (1996).
[6.21] S. Chichibu, T. Azuhata, T. Sota, H. Amano, and I. Akasaki, *Appl. Phys. Lett.* **70**, 2085 (1997).
[6.22] D. Y. Lin, Y. . Huang, Y. F. Chen, and K. K. Tiong, *Solid State Commun.* **107**, 533 (1998).
[6.23] F. Hamdani, M. Yeadon, D. J. Smith, H. Tang, W. Kim, A. Salvador, A. E. Botchkarev, J. M. Gibson, A. Y. Polyakov, M. Skowronski, and H. Morkoç, *J. Appl. Phys.* **83**, 983 (1998).
[6.24] D. E. Lacklison, J. W. Orton, I. Harrison, T. S. Cheng, L. C. Jenkins, C. T. Foxon, and S. E. Hooper, *J. Appl. Phys.* **78**, 1838 (1995).

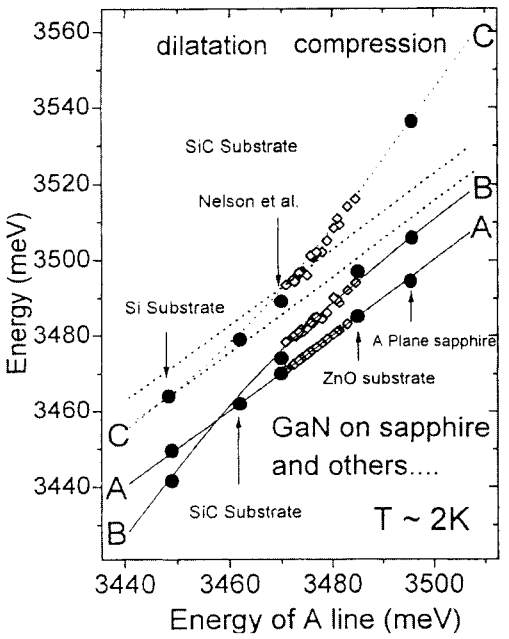

Fig. 10.6.3 Evolution of the excitonic transition energies at the E_0 edge of GaN epilayers grown on various substrates with strain along the [0001] direction. Line A shifts linearly with strain if spin-exchange interaction is ignored. Its position is thus an excellent probe of the strain. Black circles on the right-hand side correspond to growth on *A*-plane sapphire. [From A. Alemu, B. Gil, M. Julier, and S. Nakamura, *Phys. Rev. B* **57**, 3761 (1998).]

Table 10.6.3 *Empirical equation for the excitonic $E_{0\alpha}$-gap (α=A, B, or C) energy variation with temperature T for α-GaN.*

$$E_{0\alpha}(T) = E_{0\alpha}(0) - \frac{\alpha T^2}{T + \beta}$$

Parameter			Comment
$E_{0\alpha}(0)$ (eV)	α (10^{-4} eV/K)	β (K)	
3.486 (*A*)	8.32	835.6	Epilayer on Al_2O_3, *T*=15–300 K [6.25]
3.494 (*B*)	10.9	1194.7	
3.510 (*A*)	8.58	700	Epilayer on Al_2O_3, *T*=110–630 K [6.26]
3.512 (*A*)	5.66	737.9	Epilayer on Al_2O_3 (MOCVD), *T*=13–300 K [6.27]
3.458 (*A*)	11.56	1187.4	Epilayer on Al_2O_3 (MBE), *T*=13–300 K [6.27]
3.484 (*A*)	12.8	1190	Epilayer on Al_2O_3, *T*=15–475 K [6.28]
3.490 (*B*)	12.9	1280	
3.512 (*C*)	6.6	840	
— (*A*, *B*)	11.8	1414	Epilayer on Al_2O_3, *T*=10–475 K [6.29]
3.480 (*A*)	5.0	400	Epilayer on Al_2O_3, *T*=12–200 K [6.30]
3.488 (*B*)	5.2	450	
3.481 (*A*)	3.75	270	Epilayer on Al_2O_3, *T*=9–300 K [6.31]
3.489 (*B*)	3.75	310	
3.497 (*A*)	10	1000	Epilayer on Al_2O_3, *T*=2–240 K [6.32]
3.508 (*B*)	10	1000	

[6.25] W. Shan, T. J. Schmidt, X. H. Yang, S. J. Hwang, J. J. Song, and B. Goldenberg, *Appl. Phys. Lett.* **66**, 985 (1995).
[6.26] J. Petalas, S. Logothetidis, S. Boultadakis, M. Alouani, and J. M. Wills, *Phys. Rev. B* **52**, 8082

(1995).
[6.27] M. O. Manasreh, *Phys. Rev. B* **53**, 16425 (1996).
[6.28] C. F. Li, Y. S. Huang, L. Malikova, and F. H. Pollak, *Phys. Rev. B* **55**, 9251 (1997).
[6.29] A. J. Fischer, W. Shan, J. J. Song, Y. C. Chang, R. Horning, and B. Goldenberg, *Appl. Phys. Lett.* **71**, 1981 (1997).
[6.30] A. K. Viswanath, J. I. Lee, S. Yu, D. Kim, Y. Choi, and C. Hong, *J. Appl. Phys.* **84**, 3848 (1998).
[6.31] A. K. Viswanath, J. I. Lee, C. R. Lee, J. Y. Leem, and D. Kim, *Solid State Commun.* **108**, 483 (1998).
[6.32] H. Haag, P. Gilliot, R. Lévy, B. Hönerlage, O. Briot, S. Ruffenach-Clur, and R. L. Aulombard, *Phys. Rev. B* **59**, 2254 (1999).

Table 10.6.4 *Empirical equation for the excitonic $E_{0\alpha}$-gap (α=A, B, or C) energy variation with temperature T for α-GaN.*

$$E_{0\alpha}(T) = E_B - \frac{a_B}{\exp(\Theta/T) - 1}$$

Parameter			Comment
E_B (eV)	a_B (eV)	Θ(K)	
3.489 (*A*)	0.472	692	Epilayer on Al_2O_3, *T*=110–630 K [6.33]
3.510 (*A*)	0.0755	289.0	Epilayer on Al_2O_3 (MOCVD), *T*=13–300 K [6.34]
3.457 (*A*)	0.1193	307.9	Epilayer on Al_2O_3 (MBE), *T*=13–300 K [6.34]
3.4776 (*A*)	0.121	316	Epilayer on GaN, *T*=4.2–390 K [6.35]
3.4827 (*B*)	0.121	316	
3.484 (*A*)	0.220	405	Epilayer on Al_2O_3, *T*=15–475 K [6.36]
3.490 (*B*)	0.224	420	
3.512 (*C*)	0.114	340	
3.479 (*A*)	0.126	334	Epilayer on Al_2O_3, *T*=5–300 K [6.37]
3.485 (*B*)	0.126	334	
3.503 (*C*)	0.126	334	
3.480 (*A*)	0.162	366	Strain-free epilayer on Al_2O_3, *T*=7–300 K [6.38]
3.4866 (*A*)	0.110	309	Epilayer on Al_2O_3, *T*=10–270 K [6.39]

[6.33] J. Petalas, S. Logothetidis, S. Boultadakis, M. Alouani, and J. M. Wills, *Phys. Rev. B* **52**, 8082 (1995).
[6.34] M. O. Manasreh, *Phys. Rev. B* **53**, 16425 (1996).
[6.35] K. P. Korona, A. Wysmołek, K. Pakuła, R. Stępniewski, J. M. Baranowski, I. Grzegory, B. Łucznik, M. Wróblewski, and S. Porowski, *Appl. Phys. Lett.* **69**, 788 (1996).
[6.36] C. F. Li, Y. S. Huang, L. Malikova, and F. H. Pollak, *Phys. Rev. B* **55**, 9251 (1997).
[6.37] L. Siozade, S. Colard, M. Mihailovic, J. Leymarie, A. Vasson, N. Grandjean, M. Leroux, and J. Massies, *Jpn. J. Appl. Phys.* **39**, 20 (2000).
[6.38] S. F. Chichibu, K. Torii, T. Deguchi, T. Sota, A.Setoguchi, H. Nakanishi, T. Azuhata, and S. Nakamura, *Appl. Phys. Lett.* **76**, 1576 (2000).
[6.39] L. Bergman, M. Dutta, M. A. Stroscio, S. M. Komirenko, R. J. Nemanich, C. J. Eiting, D. J. H. Lambert, H. K. Kwon, and R. D. Dupuis, *Appl. Phys. Lett.* **76**, 1969 (2000).

Table 10.6.5 *Empirical equation for the excitonic $E_{0\alpha}$-gap (α=A, B, or C) energy variation with temperature T for α-GaN.*

$$E_{0\alpha}(T) = E_{0\alpha}(0) - \frac{\alpha\Theta_p}{2}\left[\sqrt[p]{1+\left(\frac{2T}{\Theta_p}\right)^p} - 1\right]$$

$E_{0\alpha}(0)$ (eV)	p	α (meV/K)	Θ_p (K)	Comment
3.470	2.62	0.599	504	T=2–1067 K [6.40]

[6.40] R. Pässler, *Phys. Status Solidi B* **216**, 975 (1999).

Table 10.6.6 *Empirical equation for the excitonic $E_{0\alpha}$-gap (α=A, B, or C) energy variation with temperature T for α-GaN.*

$$E_{0\alpha}(T) = E_{0\alpha}(0) - \alpha\sum_{i=1,2}\frac{W_i\Theta_i}{\exp(\Theta_i/T)-1}$$

$E_{0\alpha}(0)$ (eV)	α (10^{-4} eV/K)	Θ_1 (K)	Θ_2 (K)	W_1	W_2	Comment
3.470	6.14	270	755	0.34	0.66	T=2–1067 K [6.41]

[6.41] R. Pässler, *J. Appl. Phys.* **89**, 6235 (2001).

- **Pressure dependence**

Table 10.6.7 *Empirical equation for the excitonic $E_{0\alpha}$-gap (α=A, B, or C) energy variation with pressure p for α-GaN.*

$$E_{0\alpha}(p) = E_{0\alpha}(0) + ap + bp^2$$

	Parameter		
$E_{0\alpha}(0)$ (eV)	a (10^{-2} eV/GPa)	b (10^{-4} eV/GPa^2)	Comment
3.41–3.46 (A)	4.7	–18	Bulk GaN, T=300 K [6.42]
3.4725 (A)	4.0	–3.4	Epilayer on (100)GaAs, T=10 K [6.43]
3.4875 (A)	3.90	–1.8	Epilayer on Al_2O_3, T=10 K [6.44]
3.479 (A)	4.14	–3	Epilayer on Al_2O_3, T=10 K [6.45]
3.487 (B)	4.10	–2	
3.507 (C)	4.05	–2	
3.4762 (A)	4.27	–3.9	Epilayer on GaN, T=10 K [6.46]
3.4813 (B)	4.29	–3.9	
3.498 (C)	4.30	–4	
3.497 (A)	4.30	–4	Epilayer on GaN, band gap, T=10 K [6.46]

[6.42] P. Perlin, I. Gorczyca, N. E. Christensen, I. Grzegory, H. Teisseyre, and T. Suski, *Phy.s. Rev. B* **45**, 13307 (1992).
[6.43] S. J. Hwang, W. Shan, R. J. Hauenstein, J. J. Song, M.-E. Lin, S. Sitrite, B. N. Sverdlov, and H. Morcoç, *Appl. Phys. Lett.* **64**, 2928 (1994).
[6.44] W. Shan, T. J. Schmidt, R. J. Hauenstein, J. J. Song, and B. Goldenberg, *Appl. Phys. Lett.* **66**, 3492 (1995).

[6.45] Z. X. Liu, S. Pau, K. Syassen, J. Kuhl, W. Kim, H. Morkoç, M. A. Khan, and C. J. Sun, *Phys. Rev. B* **58**, 6696 (1998).
[6.46] Z. X. Liu, K. P. Korona, K. Syassen, J. Kuhl, K. Pakuła, J. M. Baranowski, I. Grzegory, and S. Porowski, *Solid State Commun.* **108**, 433 (1998).

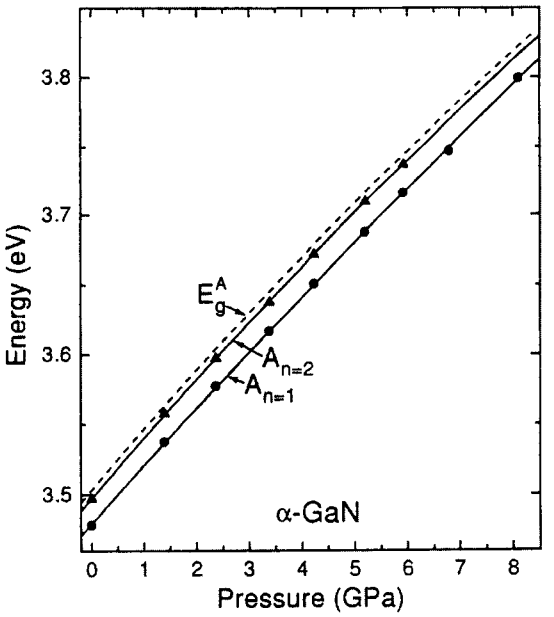

Fig. 10.6.4 *A*-exciton and band-gap energies in α-GaN as a function of hydrostatic pressure at 10 K. [From Z. X. Liu, S. Pau, K. Syassen, J. Kuhl, W. Kim, H. Morkoç, M. A. Khan, and C. J. Sun, *Phys. Rev. B* **58**, 6696 (1998).]

- **Temperature and/or pressure coefficient**

Table 10.6.8 *Linear temperature and pressure coefficients of the excitonic energy gap* $E_{0\alpha}$ *(α=A, B, or C) for α-GaN.*

Coefficient	Value	Comment
$dE_{0\alpha}/dT$ (10^{-4} eV/K)	−4.8	Bulk GaN, T=100–350 K [6.47]
	−4.5	Epilayer on Al_2O_3, T~300 K [6.48]
	−5.3	Bulk GaN, T~300 K [6.49]
	−3.70	Epilayer on Al_2O_3, T=200–300 K [6.49]
	−3.6±0.2	Epilayer on GaN, T~300 K [6.50]
	−4.4	(Mean value)
$dE_{0\alpha}/dp$ (10^{-2} eV/GPa)	4.6	Bulk GaN, T=77 K [6.51]
	4.2	Bulk GaN, T=295 K [6.51]
	4.7	Bulk GaN, T=300 K [6.52]
	4.4±0.1	Epilayer on Al_2O_3, T=9 K [6.53]
	4.7±0.1	Epilayer on Al_2O_3, T=300 K [6.53]
	3.0±0.2	Bulk GaN & epilayer on Al_2O_3, T=300 K [6.54]
	4.37±0.02	Epilayer on GaAs, T=7 K [6.55]
	4.3	(Mean value)

[6.47] J. I. Pankove, S. Bloom, and G. Harbeke, *RCA Review* **36**, 163 (1975).
[6.48] H. Teisseyre, P. Perlin, T. Suski, I. Grzegory, S. Porowksi, J. Jun, A. Pietraszko, and T. D. Moustakas, *J. Appl. Phys.* **76**, 2429 (1994).
[6.49] S. Chichibu, T. Azuhata, T. Sota, and S. Nakamura, *J. Appl. Phys.* **79**, 2784 (1996).

[6.50] K. P. Korona, A. Wysmołek, K. Pakuła, R. Stępniewski, J. M. Baranowski, I. Grzegory, B. Łucznik, M. Wróblewski, and S. Porowski, *Appl. Phys. Lett.* **69**, 788 (1996).
[6.51] D. L.Camphausen and G. A. N. Connell, *J. Appl. Phys.* **42**, 4438 (1971).
[6.52] P. Perlin, I. Gorczyca, S. Porowski, T. Suski, N. E. Christensen, and A. Polian, *Jpn. J. Appl. Phys.* **32** (Suppl. **32-1**), 334 (1992).
[6.53] S. Kim, I. P. Herman, J. A. Tuchman, K. Doverspike, L. B. Rowland, and D. K. Gaskill, *Appl. Phys. Lett.* **67**, 380 (1995).
[6.54] T. Suski, P. Perlin, H. Teisseyre, M. Leszczyński, I. Grzegory, J. Jun, M. Boćkowski, S. Porowski, and T. D. Moustakas, *Appl. Phys. Lett.* **67**, 2188 (1995).
[6.55] M. Steube, K.Reimann, O. Brandt, H. Yang, and K. H. Ploog, *Phys. Status Solidi B* **211**, 57 (1999).

• Doping dependence

Table 10.6.9 *Change in the excitonic energy gap $E_{0\alpha}$ (α=A, B, or C) with doping for α-GaN [6.56].*

$$\Delta E_{0\alpha} = -K(n^{1/3}+p^{1/3})$$

K (10^{-8} eV cm)
2.4±0.5

[6.56] X. Zhang, S.-J. Chua, W. Liu, and K.-B. Chong, *Appl. Phys. Lett.* **72**, 1890 (1998).

• Crystal-field and spin–orbit–splitoff energies

Table 10.6.10 *Theoretical crystal-field and spin-orbit–splitoff energies Δ_1, Δ_2, and Δ_3 for α-GaN (in meV). Note that in the quasi-cubic approximation, $\Delta_{cr}=\Delta_1$ and $\Delta_{so}=3\Delta_2=3\Delta_3$.*

Δ_1 (Δ_{cr})	Δ_2	Δ_3	Δ_{so}	Ref.
72.9	5.2	5.2		[6.57]
16	4	4	12	[6.58]
42			13	[6.59]
22			11	[6.60]
36	5.0	5.9		[6.61]
24	5.4	6.8		[6.62]
19			13	[6.63]
12.5	5.95	5.95		[6.64]
21	3.7	3.7	11	[6.65]
30			11	[6.66]
22.3	3.7	3.7		[6.67]

[6.57] M. Suzuki, T. Uenoyama, and A. Yanase, *Phys. Rev. B* **52**, 8132 (1995).
[6.58] S. L. Chuang and C. S. Chang, *Phys. Rev. B* **54**, 2491 (1996).
[6.59] S.-H. Wei and A. Zunger, *Appl. Phys. Lett.* **69**, 2719 (1996).
[6.60] J.-B. Jeon, Yu. M. Sirenko, K. W. Kim, M. A. Littlejohn, and M. A. Stroscio, *Solid State Commun.* **99**, 423 (1996).
[6.61] K. Kim, W. R. L. Lambrecht, B. Segall, and M. van Schilfgaarde, *Phys. Rev. B* **56**, 7363 (1997).
[6.62] J. A. Majewski, M. Städele, and P. Vogl, *Mat. Res. Soc. Symp. Proc.* **449**, 887 (1997).
[6.63] W. W. Chow, A. F. Wright, A. Girndt, F. Jahnke, and S. W. Koch, *Mat. Res. Soc. Symp. Proc.* **468**, 487 (1997).
[6.64] Y. Sirenko, J. B. Jeon, K. W. Kim, and M. A. Littlejohn, *Electrochem. Soc. Proc.* **97-34**, 177 (1997).
[6.65] Y. C. Yeo, T. C. Chong, and M. F. Li, *J. Appl. Phys.* **83**, 1429 (1998).
[6.66] S. K. Pugh, D. J. Dugdale, S. Brand, and R. A. Abram, *Semicond. Sci. Technol.* **14**, 23 (1999).
[6.67] D. J. Dugdale, S. Brand, and R. A. Abram, *Phys. Rev. B* **61**, 12933 (2000).

Table 10.6.11 *Experimental crystal-field and spin-orbit-splitoff energies Δ_1, Δ_2, and Δ_3, for α-GaN (in meV). Note that in the quasi-cubic approximation, $\Delta_{cr}=\Delta_1$ and $\Delta_{so}=3\Delta_2=3\Delta_3$.*

Δ_1 (Δ_{cr})	Δ_2	Δ_3	Δ_{so}	Technique
22±2			11^{+5}_{-2}	Optical spectroscopy [6.68]
10±0.1	6.2±0.1	5.5±0.1		Reflectivity [6.69]
35	5	7		Photoluminescence [6.70]
21			16	Photoreflectance [6.71]
24.7			17.3	Optical spectroscopy [6.72]
9.3±0.3			19.7±1.5	Reflectivity [6.73]
10±0.1	6.2±0.1	5.5±0.1		Optical spectroscopy [6.74]
19.2			10.4	Photoluminescence [6.75]
17±2			12±2	Optical spectroscopy [6.76]
22	5	5	15	Photoreflectance [6.77]
9.8±1.0			17±1	Reflectivity [6.78
13.1±0.4	6.6±0.4	5.3±0.4		Magnetooptics [6.79]
8.8±0.8			17.9±1.2	Optical spectroscopy [6.80]
11.0			14.5	Reflectivity [6.81]
3.7±1.4			17.3±3.4	Optical spectroscopy [6.82]
10	5.5	6.0		Optical spectroscopy [6.83]
12.3±0.1			18.3±0.5	Magnetooptics [6.84]
15.2	5.8	5.7	15.5	Mean value

[6.68] R. Dingle, D. D. Sell, S. E. Stokowski, and M. Ilegems, *Phys. Rev. B* **4**, 1211 (1971).
[6.69] B. Gil, O. Briot, and R.-L. Aulombard, *Phys. Rev. B* **52**, R17028 (1995).
[6.70] D. Volm, K. Oettinger, T. Streibl, D. Kovalev, M. Ben-Chorin, J. Diener, B. K. Meyer, J. Majewski, L. Eckey, A. Hoffmann, H. Amano, I. Akasaki, K. Hiramatsu, and T. Detchprohm, *Phys. Rev. B* **53**, 16543 (1996).
[6.71] S. Chichibu, A. Shikanai, T. Azuhata, T. Sota, A. Kuramata, K. Horino, and S. Nakamura, *Appl. Phys. Lett.* **68**, 3766 (1996).
[6.72] D. C. Reynolds, D. C. Look, W. Kim, Ö. Aktas, A. Botchkarev, A. Salvador, H. Morkoç, and D. N. Talwar, *J. Appl. Phys.* **80**, 594 (1996).
[6.73] K. P. Korona, A. Wysmołek, K. Pakuła, R. Stępniewski, J. M. Baranowski, I. Grzegory, B. Łucznik, M. Wróblewski, and S. Porowski, *Appl. Phys. Lett.* **69**, 788 (1996).
[6.74] M. Tchounkeu, O. Briot, B. Gil, J. P. Alexis, and R.-L. Aulombard, *J. Appl. Phys.* **80**, 5352 (1996).
[6.75] J. W.Orton, *Semicond. Sci. Technol.* **11**, 1026 (1996).
[6.76] L. Eckey, L. Podlowski, A. Göldner, A. Hoffmann, I. Broser, B. K. Meyer, D. Volm, T. Streibl, K. Hiramatsu, T. Detchprohm, H. Amano, and I. Akasaki, *Inst. Phys. Conf. Ser.* **142**, 943 (1996).
[6.77] A. Shikanai, T. Azuhata, T. Sota, S. Chichibu, A. Kuramata, K. Horino, and S. Nakamura, *Appl. Phys. Lett.* **81**, 417 (1997).
[6.78] N. V. Edwards, S. D. Yoo, M. D. Bremser, T. W. Weeks, Jr., O. H. Nam, H. Liu, R. A. Stall, M. N. Horton, N. R. Perkins, T. F. Kuech, and D. E. Aspnes, *Appl. Phys. Lett.* **70**, 2001 (1997).
[6.79] J. Campo, M. Julier, D. Conquillat, J. P. Lascaray, D. Scalbert, and O. Birot, *Phys. Rev. B* **56**, R7108 (1997).
[6.80] R. Stępniewski, K. P. Korona, A. Wysmołek, J. M. Baranowski, K. Pakuła, M. Potemski, G. Martinez, I. Grzegory, and S. Porowski, *Phys. Rev. B* **56**, 15151 (1997).
[6.81] M. A. Jacobson, D. K. Nelson, and A. V. Sel'kin, *Electrochem. Soc. Proc.* **97-34**, 103 (1997).
[6.82] B. J. Skromme, *Mater. Sci. Eng. B* **50**, 117 (1997).
[6.83] A. A. Yamaguchi, Y. Mochizuki, H. Sunakawa, and A. Usui, *J. Appl. Phys.* **83**, 4542 (1998).
[6.84] A. V. Rodina, M. Dietrich, A. Göldner, L. Eckey, Al. L. Efros, M. Rosen, A. Hoffmann, and B. K. Meyer, *Phys. Status Solidi B* **216**, 21 (1999).

10.6.3 Higher-Lying Direct Gap

• Room-temperature value

Table 10.6.12 *Higher-lying direct-gap energies for α-GaN measured at room temperature ($\boldsymbol{E}\perp c$).*

Band gap	Possible transition	Value (eV)	Ref.
E_1	L→L, M→M, U→U,	6.8	[6.85]
	Γ→Γ	7.0	[6.86]
		6.9	[6.87]
		6.86, 7.08	[6.88]
E_2	H→H, M→M, L→L	7.9	[6.86]
		8.0	[6.87]
E_3	K→K, T→T, P→P	9.5	[6.85]
		9.0	[6.86]
		9.3	[6.87]
E_4	A→A, L→L	10.7	[6.85]
		10.5–11.5	[6.87]
E_5	Γ→Γ, M→M, T→T,	12.2–13.4	[6.87]
	U→U, A→A, Σ→Σ,		
	L→L		
E_6	T→T, K→K, M→M,	13.9	[6.87]
	Γ→Γ		

[6.85] B. B. Kosicki, R. J. Powell, and J. C. Burgiel, *Phys. Rev. Lett.* **24**, 1421 (1970).
[6.86] S. Logothetidis, J. Petalas, M. Cardona, and T. D. Moustakas, *Phys. Rev. B* **50**, 18017 (1994).
[6.87] W. R. L. Lambrecht, B. Segall, J. Rife, W. R. Hunter, and D. K. Wickenden, *Phys. Rev. B* **51**, 13516 (1995).
[6.88] M. F. Al-Kuhaili, R. Glosser, A. E. Wickenden, D. D. Koleske, and R. L. Henry, *Appl. Phys. Lett.* **82**, 1203 (2003).

• Temperature dependence

Table 10.6.13 *Empirical equation for the higher-lying direct-gap energy variation with temperature T for α-GaN.*

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

Band gap	Parameter			Comment.
	$E_g(0)$ (eV)	α (10^{-4} eV/K)	β (K)	
E_1	7.10	8.9	621	T=80–570 K [6.89]
E_2	8.01	7.7	503	T=80–570 K [6.89]

[6.89] S. Logothetidis, J. Petalas, M. Cardona, and T. D. Moustakas, *Phys. Rev. B* **50**, 18017 (1994).

Table 10.6.14 *Empirical equation for the higher-lying direct-gap energy variation with temperature T for α-GaN.*

$$E_g(T) = E_B - 2a_B\left(\frac{1}{2} + \frac{1}{e^{\Theta/T} - 1}\right)$$

Band gap	Parameter			Comment
	E_B (eV)	a_B (meV)	Θ(K)	
E_1	7.23	140	461	T=80–570 K [6.90]
E_2	8.15	150	486	T=80–570 K [6.90]

[6.90] S. Logothetidis, J. Petalas, M. Cardona, and T. D. Moustakas, *Phys. Rev. B* **50**, 18017 (1994).

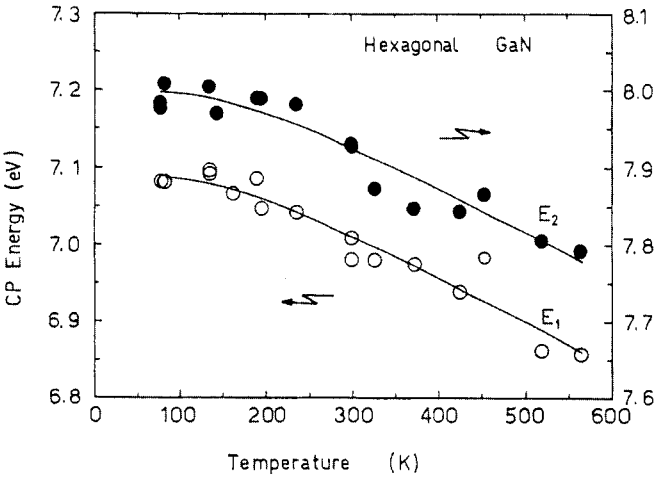

Fig. 10.6.5 Temperature dependence of the E_1- and E_2-gap energies for α-GaN as determined from spectroscopic ellipsometry ($E \perp c$). The solid lines represent the least-squares fits to the data using an empirical equation. [From S. Logothetidis, J. Petalas, M. Cardona, and T. D. Moustakas, *Phys. Rev. B* **50**, 18017 (1994).]

• Temperature and/or pressure coefficient

Table 10.6.15 *Linear temperature coefficient of the higher-lying band-gap energy for α-GaN.*

Band gap	Coefficient	Value	Comment
E_1	dE_g/dT (10^{-4} eV/K)	−5.5	T>300 K [6.91]
E_2	dE_g/dT (10^{-4} eV/K)	−5.4	T>300 K [6.91]

[6.91] S. Logothetidis, J. Petalas, M. Cardona, and T. D. Moustakas, *Mater. Sci. Eng. B* **29**, 65 (1995).

10.6.4 Lowest Indirect Gap

• Theoretical value

Table 10.6.16 *Theoretically obtained lowest indirect-gap energy for α-GaN.*

Band gap	Value (eV)	
	a	b
E_g^K ($\Gamma \rightarrow$K)	6.6	6.35
E_g^M ($\Gamma \rightarrow$M)	6.5	5.94
E_g^L ($\Gamma \rightarrow$L)	6.0	5.49
E_g^H ($\Gamma \rightarrow$H)	8.3	7.47
E_g^A ($\Gamma \rightarrow$A)	6.1	5.31

[a] A. Rubio, J. L. Corkill, M. L. Cohen, E. L. Shirley, and S. G. Louie, *Phys. Rev. B* **48**, 11810 (1993).
[b] N. E. Christensen and I. Gorczyca, *Phys. Rev. B* **50**, 4397 (1994).

• Pressure dependence

Table 10.6.17 *Theoretically obtained empirical equation for the lowest indirect-gap energy variation with pressure p for α-GaN [6.92].*

$$E_g^{ID}(p) - E_g^{ID}(0) = ap + bp^2$$

E_g^{ID}	Parameter	
	a (10^{-2} eV/GPa)	b (10^{-4} eV/GPa^2)
E_g^K ($\Gamma \rightarrow$K)	−0.18	−0.3
E_g^M ($\Gamma \rightarrow$M)	1.4	−1.7
E_g^L ($\Gamma \rightarrow$L)	1.7	−2.1
E_g^H ($\Gamma \rightarrow$H)	1.6	−1.6
E_g^A ($\Gamma \rightarrow$A)	3.6	−3.0

[6.92] N. E. Christensen and I. Gorczyca, *Phys. Rev. B* **50**, 4397 (1994).

10.6.5 Conduction-Valley Energy Separation

• Theoretical value

Table 10.6.18 *Theoretically obtained conduction-valley energy separation ΔE_g for α-GaN.*

ΔE_g	Value (eV)	
	a	b
K–Γ	3.1	2.91
M–Γ	3.0	2.50
L–Γ	2.5	2.05
H–Γ	4.8	4.03
A–Γ	2.6	1.87

[a] A. Rubio, J. L. Corkill, M. L. Cohen, E. L. Shirley, and S. G. Louie, *Phys. Rev. B* **48**, 11810 (1993).
[b] N. E. Christensen and I. Gorczyca, *Phys. Rev. B* **50**, 4397 (1994).

10.6.6 Direct–Indirect-Gap Transition Pressure

No detailed data are available for α-GaN.

10.7 ENERGY-BAND STRUCTURE: ELECTRON AND HOLE EFFECTIVE MASSES

10.7.1 Electron Effective Mass: Γ Valley

• Theoretical value

Table 10.7.1 *Theoretical effective masses $m_e^{\perp}$, $m_e^{//}$, and m_e^{Γ} at the Γ valley for α-GaN. $m_e^{\Gamma}=(m_e^{\perp 2}\, m_e^{//})^{1/3}$: density-of-states effective mass.*

$m_e^{\perp}/m_0$	$m_e^{\parallel}/m_0$	m_e^{Γ}/m_0	Ref.
0.22	0.20	0.21	[7.1]
0.18	0.20	0.19	[7.2]
0.198	0.197	0.198	[7.3]
0.19	0.17	0.18	[7.4]
0.23	0.19	0.22	[7.5]
0.20	0.18	0.19	[7.6]
		0.18	[7.7]
0.17	0.19	0.18	[7.8]
0.2	0.2	0.20	[7.9]
0.15	0.14	0.15	[7.10]
0.12	0.16	0.13	[7.11]
0.1846	0.2283	0.1981	[7.12]
0.18	0.16	0.17	[7.13]

[7.1] K. Miwa and A. Fukumoto, *Phys. Rev. B* **48**, 7897 (1993).
[7.2] M. Suzuki, T. Uenoyama, and A. Yanase, *Phys. Rev. B* **52**, 8132 (1995).
[7.3] T. Yang, S. Nakajima, and S. Sakai, *Jpn. J. Appl. Phys.* **34**, 5912 (1995).
[7.4] G. D. Chen, M. Smith, J. Y. Lin, H. X. Jiang, S.-H. Wei, M. A. Khan, and C. J. Sun, *Appl. Phys. Lett.* **68**, 2784 (1996).
[7.5] K. Kim, W. R. L. Lambrecht, B. Segall, and M. van Schilfgaarde, *Phys. Rev. B* **56**, 7363 (1997).
[7.6] J. A. Majewski, M. Städele, and P. Vogl, *Mat. Res. Soc. Symp. Proc.* **449**, 887 (1997).
[7.7] W. W. Chow, A. F. Wright, A. Girndt, F. Jahnke, and S. W. Koch, *Mat. Res. Soc. Symp. Proc.* **468**, 487 (1997).
[7.8] Y. C. Yeo, T. C. Chong, and M. F. Li, *J. Appl. Phys.* **83**, 1429 (1998).
[7.9] B. Jogai, *Solid State Commun.* **107**, 345 (1998).
[7.10] S. K. Pugh, D. J. Dugdale, S. Brand, and R. A. Abram, *J. Appl. Phys.* **86**, 3768 (1999).
[7.11] S. K. Pugh, D. J. Dugdale, S. Brand, and R. A. Abram, *Semicond. Sci. Technol.* **14**, 23 (1999).
[7.12] M. Goano, E. Bellotti, E. Ghillino, G. Ghione, and K. F. Brennan, *J. Appl. Phys.* **88**, 6467 (2000).
[7.13] C. Persson, B. E. Sernelius, A. F. da Silva, R. Ahuja, and B. Johansson, *J. Phys.: Condens. Matter* **13**, 8915 (2001).

• **Experimental value**

Table 10.7.2 *Experimental effective masses $m_e^{\perp}$, $m_e^{//}$, and m_e^{Γ} at the Γ valley for α-GaN. $m_e^{\Gamma}=(m_e^{\perp\,2}\ m_e^{//})^{1/3}$: density-of-states effective mass. 2DEG=two-dimensional electron gas; SdH=Shubnikov–de Hass.*

$m_e^{\perp}/m_0$	$m_e^{\parallel}/m_0$	m_e^{Γ}/m_0	Technique
		0.19	Optical absorption [7.14]
		0.25	Photoluminescence [7.15]
		0.25	Photoluminescence [7.16]
0.20±0.02	0.20±0.06	0.20±0.02	Infrared reflectivity [7.17]
		0.27±0.03	Faraday rotation [7.18]
		0.236±0.005	Infrared absorption [7.19]
		0.200±0.005	Cyclotron resonance [7.20]
		0.22±0.02	Infrared reflectivity & Hall effect [7.21]
0.23			2DEG cyclotron resonance [7.22]
0.223±0.011			2DEG cyclotron resonance [7.23]
0.230±0.005			2DEG cyclotron resonance [7.24]
0.18±0.02			SdH oscillation [7.25]
0.228			SdH oscillation [7.26]
0.2±0.03	0.2±0.03	0.2	Magnetooptics [7.27]
0.222			Magnetooptics [7.28]
0.21±0.01	0.22	0.21	Magnetooptics [7.29]
0.19			SdH oscillation [7.30]
0.23±0.01			SdH oscillation [7.31]
0.237±0.006	0.228±0.008	0.234	Infrared ellipsometry [7.32]
0.185±0.005			SdH oscillation [7.33]

[7.14] B. B. Kosicki, R. J. Powell, and J. C. Burgiel, *Phys. Rev. Lett.* **24**, 1421 (1970).
[7.15] R. Dingle and M. Ilegems, *Solid State Commun.* **9**, 175 (1971).
[7.16] R. D. Cunningham, R. W. Brander, N. D. Knee, and D. K. Wickenden, *J. Lumin.* **5**, 21 (1972).
[7.17] A. S. Barker, Jr. and M. Ilegems, *Phys. Rev. B* **7**, 743 (1973).
[7.18] B. Rheinländer and H. Neumann, *Phys. Status Solidi B* **64**, K123 (1974).
[7.19] B. K. Meyer, D. Volm, A. Graber, H. C. Alt, T. Detchprohm, A. Amano, and I. Akasaki, *Solid State Commun.* **95**, 597 (1995).
[7.20] M. Drechsler, D. M. Hofmann, B. K. Meyer , T. Detchprohm, H. Amano, and I. Akasaki, *Jpn. J. Appl. Phys.* **34**, L1178 (1995).
[7.21] P. Perlin, E. Litwin-Staszewska, B. Suchanek, W. Knap, J. Camassel, T. Suski, R. Piotrzkowski, I. Grzegory, S. Porowski, E. Kaminska, and J. C. Chervin, *Appl. Phys. Lett.* **68**, 1114 (1996).
[7.22] Y. J. Wang, R. Kaplan, H. K. Ng, K. Doverspike, D. K. Gaskill, T. Ikedo, I. Akasaki, and H. Amano, *J. Appl. Phys.* **79**, 8007 (1996).
[7.23] W. Knap, H. Alause, J. M. Bluet, J. Camassel, J. Young, M. Asif Khan, Q. Chen, S. Huant, and M. Shur, *Solid State Commun.* **99**, 195 (1996).
[7.24] W. Knap, S. Contreras, H. Alause, C. Skierbiszewski, J. Camassel, M. Dyakonov, J. L. Robert, J. Yang, Q. Chen, M. Asif Khan, M. L. Sadowski, S. Huant, F. H. Yang, M. Goiran, and J. Leotin, *Appl. Phys. Lett.* **70**, 2123 (1997).
[7.25] S. Elhamri, R. S. Newrock, D. B. Mast, M. Ahoujja, and W. C. Mitchel, *Phys. Rev. B* **57**, 1374 (1998).
[7.26] L. W. Wong, S. J. Cai, R. Li, K. Wang, H. W. Jiang, and M. Chen, *Appl. Phys. Lett.* **73**, 1391 (1998).
[7.27] L. Eckey, A. Hoffmann, P. Thurian, I. Broser, B. K. Meyer, and K. Hiramatsu, *Mat. Res. Soc. Symp. Proc.* **482**, 555 (1998).
[7.28] A. M. Witowski, K. Pakuła, J. M. Baranowski, M. L. Sadowski, and P. Wyder, *Appl. Phys. Lett.* **75**, 4154 (1999).

[7.29] A. V. Rodina, M. Dietrich, A. Göldner, L. Eckey, Al. L. Efros, M. Rosen, A. Hoffmann, and B. K. Meyer, *Phys. Status Solidi B* **216**, 21 (1999).
[7.30] T. Wang, J. Bai, S. Sakai, Y. Ohno, and H. Ohno, *Appl. Phys. Lett.* **76**, 2737 (2000).
[7.31] A. F. Braña, C. Diaz-Paniagua, F. Batallan, J. A. Garrido, E. Muñoz, and F. Omnes, *J. Appl. Phys.* **88**, 932 (2000).
[7.32] A. Kasic, M. Schubert, S. Einfeldt, D. Hommel, and T. E. Tiwald, *Phys. Rev. B* **62**, 7365 (2000).
[7.33] D. R. Hang, C.-T. Liang, C. F. Huang, Y. H. Chang, Y. F. Chen, H. X. Jiang, and J.Y. Lin, *Appl. Phys. Lett.* **79**, 66 (2001).

10.7.2 Electron Effective Mass: Satellite Valley

• Theoretical value

Table 10.7.3 *Theoretical effective masses at the Γ-second minimum (Γ_3^c) and satellite valleys in α-GaN [7.34].*

Valley	Direction	Mass (m_0)
Γ	Γ→M ($m^{\perp}$)	0.2856
	Γ→K ($m^{\perp}$)	0.2856
	Γ→A ($m^{\parallel}$)	3.6227
K	K→Γ	0.7673
	K→M	0.7719
	K→H	0.4357
M–L	(M–L)→(Γ–A)	3.0375
	(M–L)→(K–H)	0.3158
	(M–L)→M	0.3858
	(M–L)→L	0.3858

[7.34] M. Goano, E. Bellotti, E. Ghillino, G. Ghione, and K. F. Brennan, *J. Appl. Phys.* **88**, 6467 (2000).

10.7.3 Hole Effective Mass

• Luttinger's valence-band parameter

Table 10.7.4 *Theoretical Luttinger's valence-band parameter A_i for α-GaN. A_i (i=1–6) are in units of $\hbar^2/2m_0$ and A_7 is in units of eV/Å. Values in the parentheses correspond to those obtained in the quasi-cubic approximation.*

A_1	A_2	A_3	A_4	A_5	A_6	$\|A_7\|$	Ref.
–6.27	–0.96	5.70	–2.84	–3.18	–4.96	0.22	[7.35]
(–6.56)	(–0.91)	(5.65)	(–2.83)	(–3.13)	(–4.85)	(0.00)	
–6.37	–0.72	5.70	–2.82	–2.94	–4.29		[7.36]
–6.4	–0.50	5.9	–2.55	–2.56	–3.06	0.20	[7.37]
(–6.36)	(–0.51)	(5.85)	(–2.92)	(–2.60)	(–3.21)	(0.00)	
–6.40	–0.80	5.93	–1.96	–2.32	–3.02	0.35	[7.38]
–7.24	–0.51	6.73	–3.36	–3.35	–4.72		[7.39]
–7.71	–0.60	7.02	–3.08	–3.04	–4.00	0.19	[7.40]
–6.90	–0.73	6.11	–4.19	–3.94	–5.96		[7.41]
(–9.80)	(–0.41)	(9.39)	(–4.70)	(–4.28)	(–5.47)	(0.00)	
–7.706	–0.597	7.030	–3.076	–3.045	–4.000	0.194	[7.42]
–6.87	–0.68	6.27	–2.98	–3.05	–4.25	0.23	Mean value

[7.35] M. Suzuki, T. Uenoyama, and A. Yanase, *Phys. Rev. B* **52**, 8132 (1995).
[7.36] J.-B. Jeon, Yu. M. Sirenko, K. W. Kim, M. A. Littlejohn, and M. A. Stroscio, *Solid State Commun.* **99**, 423 (1996).
[7.37] K. Kim, W. R. L. Lambrecht, B. Segall, and M. van Schilfgaarde, *Phys. Rev. B* **56**, 7363 (1997).
[7.38] J. A. Majewski, M. Städele, and P. Vogl, *Mat. Res. Soc. Symp. Proc.* **449**, 887 (1997).
[7.39] Y. C. Yeo, T. C. Chong, and M. F. Li, *J. Appl. Phys.* **83**, 1429 (1998).
[7.40] S. K. Pugh, D. J. Dugdale, S. Brand, and R. A. Abram, *J. Appl. Phys.* **86**, 3768 (1999).
[7.41] S. K. Pugh, D. J. Dugdale, S. Brand, and R. A. Abram, *Semicond. Sci. Technol.* **14**, 23 (1999).
[7.42] D. J. Dugdale, S. Brand, and R. A. Abram, *Phys. Rev. B* **61**, 12933 (2000).

• Band and density-of-states masses

Table 10.7.5 *Theoretical band and density-of-states hole masses at the A, B, and C valence bands in α-GaN (in m_0). The superscripts $\perp$ and $\parallel$ stand for the perpendicular and parallel to the c-axis, and $m_\alpha^* = (m_\alpha^{\perp 2}\, m_\alpha^{\parallel})^{1/3}$ denotes the density-of-state mass. ESO and ISO mean excluding and including spin–orbit interaction, respectively.*

A			B			C			Comment
$m_A^\perp$	$m_A^\parallel$	m_A^*	$m_B^\perp$	$m_B^\parallel$	m_B^*	$m_C^\perp$	$m_C^\parallel$	m_C^*	
2.04	2.00	2.03	0.18	2.00	0.40	2.00	0.16	0.86	ESO [7.43]
0.34	2.00	0.61	0.35	1.19	0.53	1.27	0.17	0.65	ISO [7.43]
1.0908	1.0705		0.2853	1.0705		0.3771	0.1536		[7.44]

[7.43] K. Kim, W. R. L. Lambrecht, B. Segall, and M. van Schilfgaarde, *Phys. Rev. B* **56**, 7363 (1997).
[7.44] M. Goano, E. Bellotti, E. Ghillino, G. Ghione, and K. F. Brennan, *J. Appl. Phys.* **88**, 6467 (2000).

Table 10.7.6 *Experimental band and density-of-states hole masses at the A, B, and C valence bands in α-GaN (in m_0). The superscripts $\perp$ and $\parallel$ stand for the perpendicular and parallel to the c-axis, and $m_\alpha^* = (m_\alpha^{\perp 2}\, m_\alpha^{\parallel})^{1/3}$ denotes the density-of-state mass. OA=optical absorption; PL=photoluminescence; ABE=acceptor binding energy; TPA=two-photon absorption; MO=magnetooptics.*

A			B			C			Technique
$m_A^\perp$	$m_A^\parallel$	m_A^*	$m_B^\perp$	$m_B^\parallel$	m_B^*	$m_C^\perp$	$m_C^\parallel$	m_C^*	
		≥0.6							OA [7.45]
		1–2							PL [7.46]
		0.40							ABE [7.47]
		1.0							PL [7.48]
		0.75							PL [7.49]
		0.54							PL [7.50]
		2.2±0.2							PL [7.51]
		1.0±0.1			1.1±0.2			1.6±0.5	TPA [7.52]
0.9±0.3	1.3±0.2	1.0							MO [7.53]

[7.45] B. B. Kosicki, R. J. Powell, and J. C. Burgiel, *Phys. Rev. Lett.* **24**, 1421 (1970).
[7.46] R. Dingle and M. Ilegems, *Solid State Commun.* **9**, 175 (1971).
[7.47] J. W. Orton, *Semicond. Sci. Technol.* **10**, 101 (1995).
[7.48] R. D. Cunningham, R. W. Brander, N. D. Knee, and D. K. Wickenden, *J. Lumin.* **5**, 21 '1972).
[7.49] D. Volm, K. Oettinger, T. Streibl, D. Kovalev, M. Ben-Chorin, J. Diener, B. K. Meyer, J. Majewski, L. Eckey, A. Hoffmann, H. Amano, I. Akasaki, K. Hiramatsu, and T. Detchprohm, *Phys. Rev. B* **53**, 16543 (1996).
[7.50] C. Merz, M. Kunzer, U. Kaufmann, I. Akasaki, and H. Amano, *Semicond. Sci. Technol.* **11**, 712 (1996).
[7.51] J. S. Im, A. Moritz, F. Steuber, V. Härle, F. Scholz, and A. Hangleiter, *Appl. Phys. Lett.* **70**, 631