MATERIALS PROPERTIES OF NITRIDES. SUMMARY

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Introduction

The interest in III-N materials (stimulated by pioneering work of Pankove, Akasaki, Nakamura, and many others) dates back to 1970s. High-power microwave/millimeter wave and optoelectronic applications of nitrides have emerged, with nitride-based visible LEDs already accounting for billion dollar markets. These applications demand the improved materials quality and better device design, which in turn require the knowledge of nitride materials parameters.

Our recent book published in 2001 [1] has listed important nitride parameters. However, intensive research on properties and device applications is continuing albeit with a saturated rate of growth (see Fig. 1.). The new results require revisions of the important parameters for these materials (the energy gap of InN being a dramatic example [25].) The goal of this Chapter is to provide such an update.

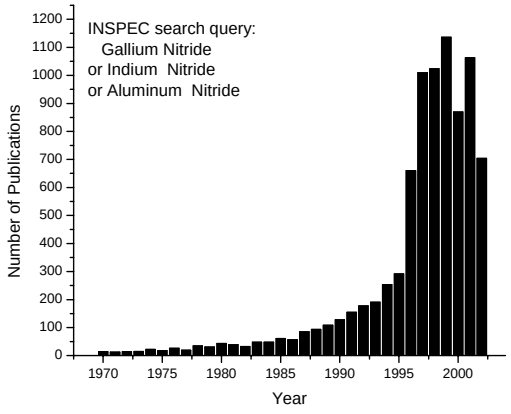

Fig. 1 Number of publication related to III-N materials versus year.

The discussion of semiconductor materials properties at a very basic level is given in [2] "Introduction to Electronic Devices", which also contains convenient tables summarizing the basic semiconductor equations and the definitions of basic semiconductor parameters. More detailed information is given in the two volumes "Survey of Semiconductor Physics" by Karl Boer [3].

In certain cases, tensor parameters (such piezoelectric constants or elastic modulus) might be represented in different (but related) forms. R. E. Newnhams book [4] can assist

you in converting these parameters from the form given in this Chapter to any other form.

We attempted to include into this Chapter most important parameters and be selective in providing the values that we found to be more accurate or reliable. More information can be found in many reviews, tutorials, and books on nitrides and nitride device published in recent years (as well as on the WEB) given below.

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Keywords: Nitrides; semiconductor parameters; materials properties.

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GALLIUM NITRIDE (GaN)

Crystal structure	Wurtzite	Zinc Blende
Group of symmetry	C_{6v}^4 $P6_3mc$	$T_d^2 - F\bar{4}3m$
Density (g/cm^3)	6.15[22,49]	
Dielectric constant		
Static	8.9-9.5[49,75,78,100]	9.7
high frequency	5.35[42,49,75,78,100]	5.3[42]
Electron affinity (eV)	4.1[88]; 3.4[61]	
Lattice constants (Å)	a = 3.189[109] c = 5.185[49,109]	4.52[49]- 4.50[78,109]
Optical phonon energy (meV)	91.8[27,49]	91.9[49]
Band structure		
Energy gap (eV)	3.51[109]	3.3[109]
Temperature dependence of the energy gap [109]	$3.582-9.09\times10^{-4}\times T^2/(T+830)$	$3.358-5.93\times10^{-4}\times T^2/(T+600)$
Conduction band		
Effective electron mass (in units of m_0) (for electron mass in two dimensional electron gas see ref. [125])	0.20- 0.22[80,109,111]	0.15[36]
Effective conduction band density of states (cm^{-3})	2.6×10^{18}	1.4×10^{18}
Ionization energies of shallow donors [44,79,118]		
Si (eV)	0.012-0.03	
O (eV)	0.004-0.01	
Valence band		
Energy of spin-orbital splitting E_{SO} (eV)	0.010- 0.018[99,109]	0.017[109]
Energy of crystal-field splitting E_{cr} (eV)	0.011- 0.022[99,109]	
Effective hole mass (in units of m_0)		

heavy	1.0[109]	1.3[36,67]
Effective valence band density of states (cm^{-3}) (For more details of the band structure see [109, 119] and references there in)	2.5×10^{19}	4.1×10^{19}
Ionization energies of shallow acceptors [5,44,100]		
Mg (eV)	0.14-0.21	
Zn (eV)	0.21	
Native defect V_{Ga} (eV)	0.14	
Electrical properties		
Breakdown field (Vcm^{-1})	$\sim5\times10^6$ [49]	$\sim5\times10^6$
Mobility ($cm^2\ V^{-1}\cdot s^{-1}$)		
Electrons (for temperature and concentration dependencies see also [22,40,59])	~1000[50,69,85]	≤1000[59]
Holes	≤ 200[40]	≤ 350[10,38]
Diffusion coefficient($cm^2\cdot s^{-1}$)		
Electrons	25	25
holes	5	9
Electron saturation velocity ($10^7 cm\ s^{-1}$)	2 [112](experiment) 2-2.5[8,15,60] (calc)	2.0[60]
Peak velocity ($10^7 cm\ s^{-1}$)	2 [112](experiment) 2.5-3 [8,15,60,112] (calc)	2.5[60]
Peak velocity field (kV/cm)	150-180[8,15,60]	100-150[60]
Recombination parameters		
Hole diffusion length (μm)	1-3.5 [21]	
Radiative recombination coefficient ($cm^3\ s^{-1}$)	10^{-8} [83]	
Optical properties		[36]
Infrared refractive index	2.3 [49]	
Refractive index spectra	[81,120]	[42]

Reflectance spectra	[16, 32, 99,121]	
Absorption spectra	[9, 32, 42,81, 82, 92]	
Photoluminescence spectra	[24, 54,77, 99,92]	[51,115]
Thermal properties		
Debye temperature (K)	820[86]	
Specific heat at 300K ($Jg^{-1}\,°C^{-1}$) 298<T<1773	0.49[86] $0.456+0.107\times10^{-3}T$[11]	
Thermal conductivity ($Wcm^{-1}°C^{-1}$)	>2.1 [38,63,95,123,124]	
Thermal diffusivity ($cm^2\,s^{-1}$)	0.65	
Thermal expansion, linear ($°C^{-1}$)	$\alpha_a = 5.59\times10^{-6}$ [49]	
	$\alpha_c = 3.17\times10^{-6}$ [49]	
Mechanical properties		
Elastic constants (GPa)(see also [30,113])		
C_{11}	390±15[90]	293[113]
C_{12}	145±20[90]	159[113]
C_{13}	106±20[90]	
C_{33}	398±20[90]	
C_{44}	105±10[90]	155[113]
Piezoelectric constants ($C\,m^{-2}$)[14,20,48,109,122]		
e_{15}	–0.30	
e_{31}	(–0.3)–(–0.55)	
e_{33}	0.6–1.12 1,27	
e_{14}		0.4[94]

ALUMINUM NITRIDE (AlN)

Crystal structure	Wurtzite
Space group	$C_{6v}^4 - P6_3mc$
Density (g cm^{-3})	3.257[96]
Dielectric constant	
static	8.5[49,78]
high frequency	4.68-4.84[100] 4.77[49,78]
Electron affinity (eV)	0.6[13]; 1.9[12,114]
Lattice constant (Å)	a=3.112[109] c=4.982[109]
Optical phonon energy (meV)	113[27,49]
Band structure	
Energy gap (eV)	6.23[109]
Temperature dependence of the energy gap[47,109]	$6.34-1.799\times10^{-3}\times T^2/(T+1462)$
Conduction band	
Effective electron mass (in units of m_0):	0.3[109]
Effective conduction band density of states (cm^{-3})	4.1×10^{18}
Ionization energies of donors[17,23,39, 43,53, 76, 98,105]	
Donor levels of N vacancies V_N (eV)	0.17; 0.5; 0.8-1.0
Donor level of N in Al sites N_{Al} (eV)	1.4-1.85
Donor level of Al in N sites Al_N (eV)	3.4-4.5
Donor level of C in Al sites C_{Al} (eV)	0.2
Valence band	
Effective hole masses (in units of m_0):	
Heavy:	
for k_z direction m_{hz}	3.53[102]
for k_x direction m_{hx}	10.42[102]
Effective valence band density of states (cm^{-3})	4.8×10^{20}
Ionization energies of acceptors [17,23,39, 43,53, 76, 98,102]	
Acceptor level of Al vacancies V_{Al} (eV)	0.5

Acceptor level of C in N sites C_N (eV)	0.4
Acceptor level of Zn in Al sites Zn_{Al} (eV)	0.2
Acceptor level of Mg in Al sites Mg_{Al} (eV)	0.1
(For more details of the band structure see [109], and references there in)	
Electrical properties	
Breakdown field (Vcm^{-1})	$(1.2 \div 1.8) \times 10^6$
Mobility ($cm^2\ V^{-1} \cdot s^{-1}$)	
Electrons	135[91]
holes	14[40]
Diffusion coefficient($cm^2 \cdot s^{-1}$)	
Electrons	3.3
holes	0.3
Electron saturation velocity ($10^7 cm\ s^{-1}$)	1.4[91]
Peak velocity ($10^7 cm\ s^{-1}$)	1.7[91]
Peak velocity field (kV/cm)	450[91]
Recombination parameters	
Radiative recombination coefficient ($cm^3 s^{-1}$)	0.4×10^{-10} [33]
Optical properties	
Infrared refractive index	2.15[49,100]
Refractive index spectra	[31,41, 42, 55,56,71, 118,]
Reflectance spectra	[7, 45,46,71]
Absorption spectra	[5, 31, 56, 71, 89]
Photoluminescence spectra	[66,101]
Thermal properties	
Debye temperature (K)	980[88]
Specific heat at 300K ($Jg^{-1}\ °C^{-1}$) At 300K<T<1800K[59] At 1800K<T<2700K[62]	0.73[62,74,87] $1.097+7.99\times10^{-5}\times T-0.358\times10^{5}\times T^{-2}$ $0.892+0.188\times10^{-3}\times T$
Thermal conductivity ($Wcm^{-1}°C^{-1}$)	2.85[97], 3.3[124]
Thermal diffusivity ($cm^2\ s^{-1}$)	1.47
Thermal expansion, linear,($°C^{-1}$)	$\alpha_a=4.2\times10^{-6}$ [49]
	$\alpha_a=5.3\times10^{-6}$ [49]

Mechanical properties		
Elastic constants (GPa)(see also[57, 113])		
C_{11}	410.5±10[73]	410[30]
C_{12}	148.5±10[73]	140[30]
C_{13}	98.9±3.5[73]	100[30]
C_{33}	388.5±10[73]	390[30]
C_{44}	124.6±4.5[73] 122±1[126]	120[30]
Piezoelectric constants (C m^{-2}) [14,19,48,68,84,102]		
e_{15}	(-0.33)-(-048)	
e_{31}	(-0.38)-(-0.82)	
e_{33}	1.26 – 2.1	

INDIUM NITRIDE (InN)

Crystal structure	Wurtzite
Space group	$C_{6v}^4 - P6_3mc$
Density (g cm^{-3})	6.81-6.89[106]
Dielectric constant	
static	15[106] 15.3[49, 78]
high frequency	6.7-8.4[49,78] ; 5.8-9.3[58]
Lattice constants (Å)	a = 3.54[49,109] c = 5.70[49,107]
Optical phonon energy (meV)	73[49, 58]
Band structure	
Energy gap (eV)	Early studies showed 1.9 – 2.05[47,104] Recent studies indicate 0.7-1.0 [25,26,29,52,72, 116,117]
Conduction band	
Effective electron mass (in units of m_0):	0.07-0.26[117]; 0.14 [58]
Effective conduction band density of states (cm^{-3})	$4.6\times10^{17} - 3.3\times10^{18}$
Ionization energy of donor[105]	
Donor level of N vacancies V_N (meV)	40-50
Valence band	
Effective hole mass (in units of m_0):	
heavy	1.63[65]
Electrical properties	
Mobility (cm^2 $V^{-1}\cdot s^{-1}$)	
Electrons	2700[103] 1000-1900[25,52,70,117]
Diffusion coefficient($cm^2\cdot s^{-1}$)	
Electrons	67 25-47
Optical properties	
Infrared refractive index	2.9[49]
Refractive index spectra	[118]

Reflectance spectra	[108,117]	
Absorption spectra	[25,47, 52,72,116,117]	
Photoluminescence spectra	[25,26, 29,72,116]	
Thermal properties		
Debye temperature (K)	660 [28]	
Specific heat ($Jg^{-1}\,°C^{-1}$) Temperature coefficient of Specific heat 298K<T<1273K[86]	0.30[28] 9.39×10^{-5}	
Thermal conductivity ($Wcm^{-1}°C^{-1}$)	0.45[64]	
Thermal diffusivity ($cm^2\,s^{-1}$)	0.2	
Thermal expansion, linear,($°C^{-1}$)	$\alpha_a = 3.8\times10^{-6}$ [93,110] $\alpha_c = 2.9\times10^{-6}$ [93,110]	
Mechanical properties		
Elastic constants (GPa)	[93, exper.]	(see refs. in [110], calc.)
C_{11}	190±7	271-298
C_{12}	104±3	92-124
C_{13}	121±7	70-109
C_{33}	182±6	25-278
C_{44}	10±1	46-89
Piezoelectric constants ($C\,m^{-2}$)[14,122]		
e_{31}	(–0.45)–(–0.56)	
e_{33}	0.81–1.09	

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