1 Introduction

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1.1 A Brief History

Considerable efforts to fabricate nitride devices began more than three decades ago. In 1971, Pankove *et al.* reported the first GaN-based lightemitting diode (LED) [1]. However, most of these early research programs were eventually abandoned due to fundamental materials problems. Since there was no suitable bulk-crystal technology for producing GaN substrates, epitaxy was done on highly lattice-mismatched substrates. The resulting heteroepitaxial films exhibited a high defect density and poor surface morphology. The high n-type background doping, coupled with the deep ionization levels of common acceptors, resulted in an inability to grow p-type materials.

It was not until the mid-1980s that these problems began to be overcome, due in large part to the work of Isamu Akasaki at Nagoya and Meijo Universities and Shuji Nakamura at Nichia Chemical Company in Japan. The use of AlN [2]or GaN [3] nucleation layers facilitated the growth of high-quality GaN films on sapphire substrates by metalorganic chemical vapor deposition (MOCVD). The first n-GaN/AlGaN transistor was demonstrated by Khan et al. in 1993 [4]. Another breakthrough was the first successful fabrication of ptype GaN by low-energy electron-beam irradiation (LEEBI) of Mg-doped GaN [5]. In 1992, Nakamura demonstrated that Mg-doped GaN could also be made conductive by thermal annealing in an N₂ ambient [6]. The development of high-quality InGaN films was the third main breakthrough towards the fabrication of InGaN/GaN high-brightness LEDs in 1994 [7]. Finally, Nakamura et al. succeeded, in 1995, in manufacturing the first nitride-based laser diode with continuous-wave room-temperature emission at 417 nm wavelength [8]. Soon thereafter, Nichia offered the first commercial GaN-based LEDs and laserdiodes. A detailed review of these developments can be found in [9].

Blue and green nitride LEDs are now widely used, for instance, in full-color displays and in traffic signals. Nitride laser diodes are key components in emerging high-definition DVD players. Other promising application areas

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are printing, sensors, communication, and medical equipment. However, despite intense research efforts worldwide, there still remains a strong need for a more detailed understanding of microscopic physical processes in nitride devices. Numerical simulation can help to investigate those processes and to establish quantitative links between material properties and measured device performance.

1.2

Unique Material Properties

The troubled history and the recent success of nitride semiconductor devices are both very much related to the unique material properties of GaN and its most relevant alloys InGaN and AlGaN. Depending on the alloy composition, the direct bandgap varies from about 0.7 eV to 6.2 eV, covering a wide wavelength range from red through yellow and green to blue and ultraviolet. While other compound semiconductors, such as GaAs and InP, are grown in the zinc blende crystal system, nitride devices are grown in the hexagonal (wurtzite) crystal system (Fig. 1.1). This leads to unique material properties, such as built-in electric fields due to spontaneous and piezoelectric polarization. Sapphire (Al₂O₃) or SiC are often used as substrates for GaN growth, which exhibit slightly different lattice constants *a* of 0.476 nm and 0.308 nm, respectively (GaN substrates became available only recently, a = 0.319 nm). The lattice-mismatched epitaxial growth causes a large number of dislocations in nitride devices, with dislocation densities that are more than five orders of magnitude higher than in other compound semiconductor devices. The surprisingly small impact of these defects on the performance of GaN-based light emitters is still not fully understood. Another unique property of nitrides is the high activation energy for acceptor (Mg) doping of about 170 meV. It requires high doping densities near 10²⁰ cm⁻³ to achieve free hole concentrations of about 10^{18} cm⁻³. The high doping density causes an extremely low hole mobility on the order of $10 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$. On the other hand, the high GaN electron mobility of up to 2000 cm²V⁻¹s⁻¹ and the large critical breakdown field of more than 3 MV cm⁻¹ are advantageous in high-speed and highpower electronics. The thermal conductivity in GaN is more than three times higher than in GaAs.

Despite the recent commercial success of GaN-based devices, internal physical mechanisms are often not completely understood. Advanced models and numerical simulations are needed to support further performance enhancement as well as the emergence of new GaN devices. Sophisticated theories and physics-based software have been developed for previous generations of semiconductor devices (see, e.g., [10,11]). However, the unique material prop-



Fig. 1.1 Wurtzite crystal with lattice constants *c* and *a*. The structure is formed by two intertwined hexagonal sublattices of, for instance, Ga and N atoms.

erties of nitrides present a new challenge. Comprehensive device simulations require the knowledge of a large number of material parameters, including their variation with material composition, defect or carrier density, internal temperature, built-in electric field, or with other physical conditions. The reliability of simulation results strongly depends on the accuracy of the material parameters used. Measured device characteristics can be utilized to adjust specific parameters in the simulation, in particular those parameters that are affected by the fabrication process [12, 13].

The past decade of intense research effort has tremendously improved our knowledge of nitride material properties. However, many material parameters are still not exactly known. An example is the thermal conductivity of ternary and quaternary nitride alloys. The first thermal conductivity measurements for AlGaN have only recently been published.

Thermal properties of nitrides are briefly reviewed in the next section. Other material parameters are covered in the following chapters.

1.3

Thermal Parameters

Self-heating often limits the performance of semiconductor devices. Heat is generated when carriers transfer part of their energy to the crystal lattice. In consequence, the thermal (vibrational) energy of the lattice rises, which is measured as an increase in its temperature, T_L . We here assume a local ther-

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mal equilibrium between lattice and carriers, i.e., the lattice temperature and the carrier temperature are considered identical ($T = T_L = T_n = T_p$). Virtually all material properties like energy band gap and carrier mobility, change with rising temperature.

Within the crystal lattice, thermal energy is dissipated by traveling lattice vibrations. The smallest energy portions of lattice waves are phonons, which can be treated like particles. Microscopic theories of lattice heat generation and dissipation are based on the phonon picture outlined in many solid-state textbooks, e.g., [14,16,17].

In practical device simulation, the main thermal parameters are thermal conductivity κ_L and specific heat C_L of the crystal lattice. Electrons and holes also contribute to specific heat and thermal conductivity. However, those contributions are usually negligible. The lattice thermal conductivity κ_L controls the heat flux density (W cm⁻²)

$$\vec{J}_{\text{heat}} = -\kappa_{\rm L} \nabla T \tag{1.1}$$

which is driven by the gradient of the temperature distribution $T(\vec{r})$. Conservation of energy requires that the temperature satisfies the heat flux equation

$$\rho_{\rm L}C_{\rm L}\frac{\partial T}{\partial t} = -\nabla \cdot \vec{J}_{\rm heat} + H_{\rm heat} \tag{1.2}$$

where $\rho_{\rm L}$ is the material's density and $H_{\rm heat}(\vec{r}, t)$ is the heat power density (W cm⁻³) generated by various sources. This equation relates the change in local temperature $(\partial T/\partial t)$ to the local heat flux (in or out) and to the local heat generation. All parameters in Eq. (1.2) generally depend on the material composition and on the temperature itself. Near room temperature (T = 300K) [14]

$$C_{\rm L}(T) = C_{\rm L}(300 \,\rm K) \frac{20 - (\Theta_{\rm D}/T)^2}{20 - (\Theta_{\rm D}/300 \,\rm K)^2}$$
(1.3)

with Θ_D giving the Debye temperature which itself may be temperature dependent. A recent review of Debye temperatures reported for GaN is given in [15]. Temperature effects on the thermal conductivity near room temperature can be described by a power law

$$\kappa_{\rm L}(T) = \kappa_{\rm L}(300 \,\mathrm{K}) \left(\frac{T}{300 \,\mathrm{K}}\right)^{\delta_{\rm K}} \tag{1.4}$$

Table 1.1 lists the above material parameters for binary nitride compounds and for some substrate materials.

The room-temperature thermal conductivity of bulk GaN was first measured in 1977 by Sichel and Pankove who reported a value of $130 \text{ Wm}^{-1}\text{K}^{-1}$

Tab. 1.1 Thermal material parameters at room temperature for binary nitrides and typical substrates (density ρ_L , specific heat C_L , Debye temperature Θ_D , thermal conductivity κ_L and its temperature coefficient δ_{κ}) [18–21].

Parameter Unit	${ ho_{ m L}\over { m gcm^{-3}}}$	$\stackrel{C_{\rm L}}{{\sf J}{\sf g}^{-1}{\sf K}^{-1}}$	Θ _D K	(W m ⁻¹ K ⁻¹)	δ_{κ}
GaN	6.15	0.49	600	160	–0.6 (250 K< T <370 K)
AIN	3.23	0.6	1150	210	-1.2 (150 K< T <300 K)
InN	6.81	0.32	660	45	
SiC	3.21	0.69	1200	380	-1.4 (200 K< T <600 K)
AI_2O_3	3.97	0.88	1032	38	−1.5 (300 K< T <600 K)



Fig. 1.2 GaN thermal conductivity as function of: (a) electron density of Si-doped samples (measured in [22]); (b) dislocation line density (calculated in [23]).

[24]. Although the crystal quality of their sample was not well known, this result is relatively close to the earlier theoretical prediction of 170 Wm⁻¹K⁻¹ by Slack [25]. The recent success of GaN devices has motivated a number of new investigations of the GaN thermal conductivity. Typical results at room temperature are between 130 and 200 Wm⁻¹K⁻¹. The largest values are obtained for high crystal quality, with a maximum of 225 Wm⁻¹K⁻¹ measured on free-standing GaN films [26]. The GaN thermal conductivity was found to drop significantly with increasing doping density (by about a factor of two per decade above 10^{17} cm⁻³ [22]) and for dislocation densities higher than 10^{11} cm⁻² [23]. Both dependencies are plotted in Fig. 1.2. The temperature dependence is shown in Fig. 1.3 [19]. Near room temperature, it can be described by (1.4) with $\delta_{\kappa} = -0.6$ (dashed line in Fig. 1.3). This empirical parameter also depends on the defect density, it is $\delta_{\kappa} = -1.2$ for low defect density [20] and $\delta_{\kappa} = -0.2$ for polycrystalline GaN samples [27]. Over a wider temperature



Fig. 1.3 GaN thermal conductivity vs. temperature. The dots show experimental results and the line plots Eq. (1.4) with $\delta_{\kappa} = -0.6$ [19].

range, the relation $\kappa_{\rm L}(T)$ is more complex due to different dominating scattering mechanisms [23]. For doping densities of 10^{16} – 10^{18} cm⁻³, the electronic contribution to the GaN thermal conductivity is about 1000 times smaller than that of the lattice [22]. The thermal conductivity anisotropy in GaN at 300K is 1% or less [20].

Thermal parameters of AlN and InN are summarized in Table 1.1. However, these binary materials are commonly not employed in nitride devices. Alloys of GaN with InN and/or AlN are of higher importance. The random distribution of alloy atoms in ternary or quaternary semiconductor compounds causes strong alloy scattering of phonons, which leads to a significant reduction of the thermal conductivity. For ternary alloys, like $Al_xGa_{1-x}N$, the thermal conductivity is typically estimated from binary values using [28]

$$\frac{1}{\kappa_{\rm L}(x)} = \frac{x}{\kappa_{\rm AIN}} + \frac{1-x}{\kappa_{\rm GaN}} + x(1-x)C_{\rm AlGaN}$$
(1.5)

with the empirical bowing parameter C_{AlGaN} . The same bowing parameters can be employed for the quaternary alloy $Al_x In_y Ga_{1-x-y} N$

$$\frac{1}{\kappa_{\rm L}(x,y)} = \frac{x}{\kappa_{\rm AlN}} + \frac{y}{\kappa_{\rm InN}} + \frac{1-x-y}{\kappa_{\rm GaN}} + xyC_{\rm AlInN} + x(1-x-y)C_{\rm AlGaN} + y(1-x-y)C_{\rm InGaN}$$
(1.6)

Thus far, this bowing effect has only been measured for AlGaN [27, 29] (Fig. 1.4). The significant difference between both results may be due to the different measurement methods or to different quality of the AlGaN films,



Fig. 1.4 Thermal conductivity of $Al_x Ga_{1-x}N$ (circles, solid lines) and $In_x Ga_{1-x}N$ (squares, dashed line). Open/solid symbols indicate theoretical/experimental results. Lines give the fit using Eq. (1.5).

that were both grown on sapphire (0001) substrates. It is interesting to note that the AlGaN thermal conductivity increases with temperature in one investigation [29] while it decreases in the other [27]. Using the bowing formula (1.5) and the binary data from Table 1.1, we obtain the room-temperature bowing parameters C_{AlGaN} of 0.1 Km W⁻¹ and 0.6 Km W⁻¹, respectively (see lines in Fig. 1.4).

More sophisticated models have been applied to calculate the alloy thermal conductivity from fundamental material parameters, including a virtualcrystal model [29] and a molecular dynamics model [30]. The latter was also used to estimate the InGaN thermal conductivity [31] (open squares in Fig. 1.4). However, the accuracy of such fundamental models very much depends on the material parameters used and fits to measurements are often required to obtain reliable results. The bowing parameters estimated from the theoretical results in Fig. 1.4 are $C_{InGaN} = 0.8 \text{ Km W}^{-1}$ and $C_{AlGaN} =$ 1.2 Km W^{-1} .

In practical device analysis, the internal temperature often needs to be known only for specific locations, for instance in the active region of a laser diode. If the heat power P_{heat} (W) is generated in the same location, then the heat flux from that location to the heat sink can be characterized by a thermal resistance R_{th} (K W⁻¹), giving the temperature difference

$$\Delta T = R_{\rm th} P_{\rm heat} \tag{1.7}$$

between the heat source and the heat sink. Similar to the electrical resistance, the thermal resistance depends not only on material properties (thermal con-

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ductivity) but also on the device geometry. The advantage of this approach is the thermal characterization of the device by one parameter R_{th} that usually can be measured. In cases with heat generation at different locations or multiple layers within the device, the single resistance R_{th} can be replaced by a thermal resistance network. In analogy to electrical circuits, simplified thermal models can be established this way. For homogeneous heat flux, the thermal resistance of a given layer of thickness *d* and cross-section *A* is linked to its thermal conductivity by

$$R_{\rm th} = dA^{-1}\kappa_{\rm L}^{-1} \tag{1.8}$$

Thermal resistances are also employed to characterize the heat flux through an interface. For instance, the thermal boundary resistance between GaN and the substrate depends on the transmission probability of phonons through that interface. Phonon scattering and reflection lead to a relatively large interface resistance value on the order of 10^{-3} Kcm²W⁻¹ which may have a considerable impact on the device performance [32].

Within thin semiconductor layers, interface scattering may reduce the phonon mean free path. As a consequence, the bulk thermal conductivity of this layer is reduced [33]. With an estimated GaN phonon mean free path of 88 nm at room temperature [27], nanometer-scale GaN layers are expected to exhibit a strongly reduced thermal conductivity.

References

- 1 J. I. Pankove, E. A. Miller and J. E. Berkeyheiser. *RCA Rev.*, 32:383, 1971.
- 2 H. Amano and N. Sawaki and I. Akasaki and T. Toyoda. *Appl.Phys.Lett.*, 48:353, 1986.
- **3** S. Nakamura *Japan. J. Appl.Phys., Part* 2, 30:L1705, 1991.
- 4 M. A. Khan, A. Bhattarai, J. N. Kuznia and D. T. Olson. *Appl. Phys. Lett.*, 63:1214, 1993.
- 5 H. Amano, M. Kito, K. Hiramatsu and I. Akasaki. *Japan. J. Appl. Phys., Part 1*, 28:L2112, 1989.
- 6 S. Nakamura, T. Mukai, M. Senoh and N. Iwasa. *Japan. J. Appl. Phys., Part 1*, 31:L139, 1992.
- **7** S. Nakamura, T. Mukai and M. Senoh. *Appl. Phys. Lett.*, 64:1687, 1994.
- 8 S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, H. Kiyoku and Y. Sugimoto. *Japan. J. Appl. Phys., Part* 1, 35:L74, 1996.

- **9** S. Nakamura, S. Pearton and G. Fasol. *The Blue Laser Diode*. Springer-Verlag, Berlin, 2000.
- **10** V. Palankovski and R. Quay. *Analysis and Simulation of Heterostructure Devices*. Springer, Wien, 2004.
- 11 J. Piprek, editor. Optoelectronic Devices: Advanced Simulation and Analysis. Springer, New York, 2005.
- 12 J. Piprek and S. Nakamura. *IEE Proc., Part J: Optoelectron.,* 149:145, 2002.
- 13 J. Piprek, T. Katona, S. P. DenBaars and S. Li. 3d simulation and analysis of UV Al-GaN/GaN LEDs. In *Light-Emitting Diodes: Research, Manufacturing and Applications VII*, volume 5366, Bellingham, 2004. SPIE-The International Society for Optical Engineering.
- 14 K. W. Boer. Survey of Semiconductor Physics, volume II. Van Nostrand Reinhold, New York, 1992.

References 11

- **15** C. Roder, S. Einfeldt, S. Figge and D. Hommel. *Phys. Rev. B*, 72:085218, 2005.
- 16 P. Y. Yu and M. Cardona. Fundamentals of Semiconductors. Springer-Verlag, Berlin, 1996.
- **17** Ch. Kittel. *Introduction to Solid State Physics*. Wiley, New York, 1996.
- 18 M. E. Levinshtein, S. L. Rumyantsev and M. S. Shur, editors. *Properties of Advanced Semiconductor Materials*. Wiley, New York, 2001.
- 19 M. Kamano, M. Haraguchi, T. Niwaki, M. Fukui, M. Kuwahara, T. Okamoto and T. Mukai. *Japan. J. Appl. Phys., Part* 1, 41:5034, 2002.
- **20** G. A. Slack, L. J. Schowalter, D. Morelli and Jaime A. Freitas. *J. Cryst. Growth*, 246:287, 2002.
- 21 Ch. Eichler. Thermal Management of Ganbased Laserdiodes. PhD thesis, University of Ulm, 2005.
- 22 D. I. Florescu, V. M. Asnin, F. H. Pollak, R. J. Molnar and C. E. C. Wood. *J. Appl. Phys.*, 88:3295, 2000.

- **23** J. Zou, D. Kotchetkov, A. A. Balandin, D. I. Florescu and F. H. Pollak. *J. Appl. Phys.*, 92:2534, 2002.
- 24 E. K. Sichel and J. I. Pankove. J. Phys. Chem. Sol., 38:330, 1977.
- 25 G. A. Slack. J. Phys. Chem. Sol., 34:321, 1973.
- **26** W. Liu, A. A. Balandin, C. Lee and H.-Y. Lee. *phys. stat. sol. (a)*, 202:R135, 2005.
- 27 B. C. Daly, H. J. Maris, A. V. Nurmikko, M. Kuball and J. Han. J. Appl. Phys., 92:3820, 2002.
- 28 J. Piprek. Semiconductor Optoelectronic Devices: Introduction to Physics and Simulation. Academic Press, San Diego, 2003.
- **29** W. Liu and A. A. Balandin. *J. Appl. Phys.*, 97:073710, 2005.
- **30** T. Kawamura, Y. Kangawa and K. Kakimoto. J. Cryst. Growth, 284:197, 2005.
- 31 T. Kawamura, Y. Kangawa and K. Kakimoto. *phys. stat. sol.* (c),3:1695, 2006.
- **32** V. O. Turin and A. A. Balandin. *Electron. Lett.*, 40:81, 2004.
- **33** J. Piprek, T. Troger, B. Schroter, J. Kolodzey and C. S. Ih. *IEEE Photon. Technol. Lett.*, 10:81, 1998.