Materials Physics and Mechanics. 2022;49(1): 97-107
Conference materials
http://dx.doi.org/10.18149/MPM.4912022_7

First-principles study of anisotropic thermal conductivity of GaN, AlN, and $Al_{0.5}Ga_{0.5}N$

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Abstract. The thermal stability of devices based on GaN, AlN, and $Al_{0.5}Ga_{0.5}N$ semiconductors is a critical property for efficient and reliable operation. The thermal conductivity of these materials has anisotropic nature. We proposed an approach for calculating the anisotropic thermal conductivity based on harmonic and anharmonic interatomic force constants of a lattice. The thermal-conductivity coefficient of GaN, AlN, and $Al_{0.5}Ga_{0.5}N$ in the [100], [001], and [111] directions were calculated using *ab initio* methods by solving the linearized Boltzmann transport equation. It equals $\lambda_{[100]}$ = 259.28, $\lambda_{[001]}$ = 335.96 and $\lambda_{[111]}$ = 309.56 W/(m·K) for GaN; $\lambda_{[100]}$ = 396.06 , $\lambda_{[001]}$ = 461.65 and $\lambda_{[111]}$ = 435.05 W/(m·K) for AlN; and $\lambda_{[100]}$ = 186.74, $\lambda_{[001]}$ = 165.24 and $\lambda_{[111]}$ = 177.62 W/(m·K) for $Al_{0.5}Ga_{0.5}N$ at 300 K. The dependence of the coefficient λ(T) on temperature in the range from 250 to 750 K is presented. A comparative analysis of the GaN thermal conductivity investigations has been carried out for experimental studies and theoretical calculations.
Keywords: aluminum nitride, first-principle calculation, gallium nitride, thermal conductivity

Acknowledgements*. This work was supported by grant 3.02.3 of Belarusian National Scientific Research Program "Convergence – 2025" and the grant of The Belarusian Republican Foundation for Fundamental Research for young scientists "Science M – 2021" (contract № F21M-122). Computing cluster of BSUIR was used for computer modeling.*

Citation: Hvazdouski DC, Baranava MS, Stempitsky VR. First-principles study of anisotropic thermal conductivity of GaN, AlN, and $Al_{0.5}Ga_{0.5}N$. *Materials Physics and Mechanics*. 2022;49(1): 97-107. DOI: 10.18149/MPM.4912022_7.

1. Introduction

The structures based on GaN, AlN, and AlGaN semiconductor nitrides are considered promising materials for electronic and optoelectronic technology. For many applications, GaAs is gradually changed by GaN because of its high polarization, chemical, and physical stability, and wide band gap. Gallium nitride appears as a perspective material for the development of the high-frequency, heat-resisting, and power semiconductor devices [1]. GaN transistors, unlike GaAs transistors, are suitable as high-frequency power amplifiers via high operating voltage and working temperatures [2]. Strong self-heating is typical for similar devices that give rise to thermal properties investigation of this material since the temperature stability is critical for effective and reliable work in many electronic devices and systems.

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Thermal simulation can help to manage temperature mode, define the main reason for heating and estimate the wide spectrum of alternative variants for construction optimization. Heat transfer simulation in the device structure consists in solving the heat flow equation. The main parameter of this equation is thermal conductivity [3].

Discrepancies both in experimental and theoretical values given in the literature motivated our investigation. The empiric values of GaN and AlN thermal conductivities differ from each other significantly which is mostly associated with the difference in purity and microstructure of samples [4-9]. Theoretical models of thermal conductivity consist of a combination of the first-principle calculations and the solution of the linearized Boltzmann transport equation for phonons. They also have distinction, although less significant [10-15].

Furthermore, AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ have C_{6v}^{4}-$P6_{3}mc$ symmetry space group that corresponds to hexagonal syngony [16]. Thus, anisotropy manifestation of the thermodynamic properties (including thermal conductivity) is typical for these materials. In this case, λ is introduced as a second rank tensor. However, in many papers, the thermal conductivity coefficient is considered a constant value [4-7,9,11,12]. Therefore the thermal conductivity models which take into consideration both temperature dependence and anisotropy are necessary for applied aims.

The main task of the presented work is the temperature dependence calculation of thermal conductivity of AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ for different crystallographic directions via first-principal methods. Moreover, a comparative analysis of our results and those of other authors, where the results were obtained by both theoretical and experimental methods, is given.

2. Methodology of thermal conductivity calculation

For the thermal conductivity calculation, we take into account interactions at some physical levels. The first level is the atomic one (~ 10^{-9} m or some nanometers). The main objects on this level are recognized to be electrons. The calculations of structural and electronic properties of the systems studied are performed through the use of quantum-mechanics methods [17]. For the result verification, the obtained physical properties were compared with the experimental data of other authors. On the basis of the crystal structure got, the phonon spectra were determined by the methods [18,19]. We ignore electron contribution to the thermal conductivity since in the case of wide band gap gallium nitride GaN, aluminum nitride AlN, and gallium nitride – aluminum nitride alloy $Al_xGa_{1-x}N$, the contribution of electrons to the heat transfer is negligibly small compared to phonons. Really, according to [20], electron contribution to the thermal conductivity is about 1000 times less than phonon contribution for bulk crystal GaN sample (dopant concentration ~10^{16}-10^{18} cm^{-3}).

The next physical level is microscopic (~ 10^{-6} m or some micrometers), at which the interaction of objects of study (ions and valence electrons) can be described via classic interatomic potentials. On this level calculation of the lattice thermal conductivity of the material is performed using the software *Phono3py* [21,22]. In this case, the lattice thermal conductivity of a material is defined by solving the linearized Boltzmann equation (LBTE) for the phonons with the one-mode approximation of relaxation time [23] on the basis of calculated second rank harmonic interatomic force constants (IFC) and third rank anharmonic IFC.

The last physical level is macroscopic (~ 10^{-2} m or some centimeters), which is of interest for technology applications. Interactions in the system are usually described by the phenomenological theories on the macroscopic scale [24]. On this level, the crystal anisotropy and geometric dimensions are taken into account.

3. Results of the thermal conductivity calculations

First-principle calculation. Choice of the parameter set (computational grid for k-points, cutoff energy, etc.), exchange-correlation energy calculation methods, and pseudopotential set was performed based on convergence criteria of test calculation. During calculations of the structure properties, the energy difference between two iterations must not exceed 10^{-6} eV; during calculations of the phonon properties; the analogous value must not exceed 10^{-8} eV. The obtained numerical values of structural properties (crystal elementary cell characteristics) with setting calculation parameters must be close to experimental values (difference less than 5%). The supercells for further phonon dispersion calculation and for evaluating thermal conductivity were created by the elementary cell in the ground state.

To perform a series of first-principle calculations we used VASP software. PBE functional was used as exchanged-correlation functional. For all investigated structures, the cutoff energy of the plane waves was equal to 520 eV. The valence electron configurations for nitrogen N, aluminum Al, and gallium Ga were taken as $[He]2s^2 2p^3$, $[Ne]3s^2 3p^1$, and $[Ar]4s^2 3d^{10} 4p^1$, respectively. Non-self-consistent calculations were performed along the contour "M-K-Γ-A" between high symmetry points of the first Brillouin zone.

In Table 1 calculated crystal structure characteristics of GaN, AlN, and $Al_{0.5}Ga_{0.5}N$ are compared with the experimental data [25,26].

Table 1. Structure properties of the investigated crystals

Crystal	Symmetry group	Lattice constants, Å		Dispersion, %
		Calculated	Experimental	
GaN	C_{6v}^4-$P6_3mc$	a = 3.164 c = 5.114 a/c = 0.618	a = 3.189 c = 5.186 a/c = 0.615 [25]	1.388
AlN	C_{6v}^4-$P6_3mc$	a = 2.983 c = 4.933 a/c = 0.605	a = 3.112 c = 4.982 a/c = 0.624 [25]	4.145
$Al_{0.5}Ga_{0.5}N$	C_{6v}^4-$P6_3mc$	a = 3.135 c = 4.917 a/c = 0.637	a = 3.149 c = 5.079 a/c =0.621 [26]	3.189

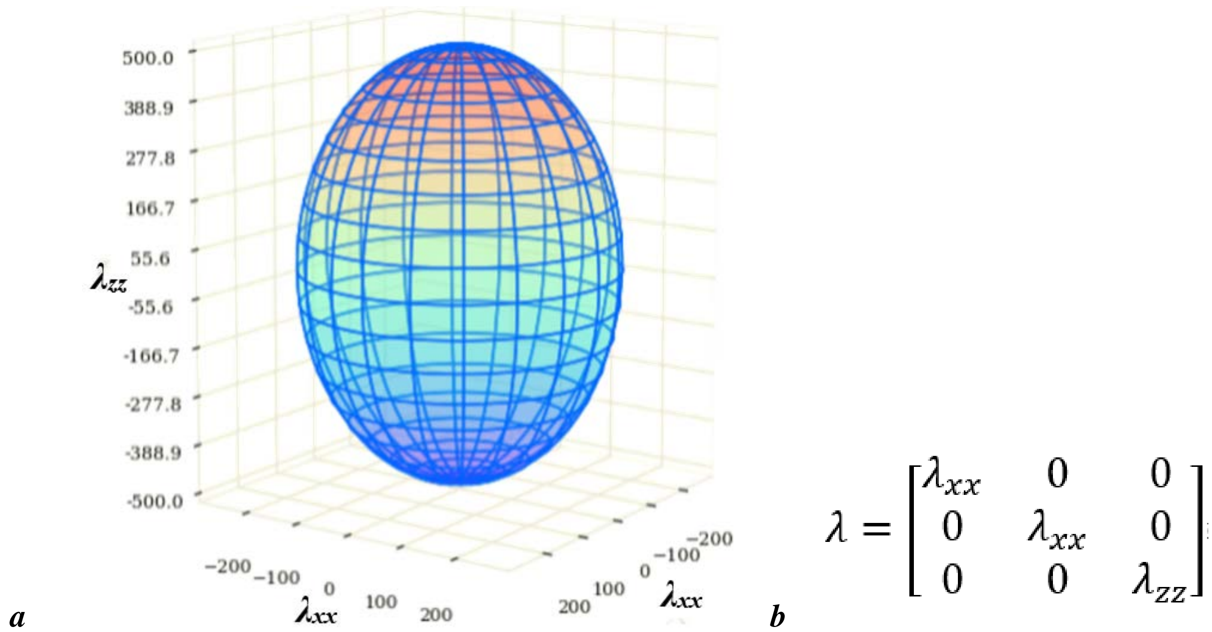
For calculating the harmonic-second-rank-interatomic-force constants, 2×2×2 supercells were created. The 3×3×3 supercells with atom displacement of 0.01 Å were used for anharmonic IFC calculations. We considered the phonon-phonon interaction with the three closest atoms inside the supercell. The necessary information for supercell building was taken from the calculations of the structure properties.

Based on the harmonic and anharmonic interatomic force constants calculated with quantum-mechanics methods, the thermal conductivity coefficients were determined in the main crystallographic directions [100], [010], and [001] for GaN, AlN, and $Al_{0.5}Ga_{0.5}N$ in the temperature range from 0 to 1000 K with the help of software *Phono3py*. The hexagonal syngony of the crystals under investigation points on thermal conductivity characteristic features in crystallographic directions: $\lambda_{[100]} = \lambda_{[010]} = \lambda_{[110]}$, and also $\lambda_{[101]} = \lambda_{[011]} = \lambda_{[111]}$.

The obtained values of calculated thermal conductivity coefficients at 300 K are $\lambda_{[100]}$ = 259.28 and $\lambda_{[001]}$ = 335.96 W/(m·K) for GaN crystal; $\lambda_{[100]}$ =396.06 and $\lambda_{[001]}$ = 461.65 W/(m·K) for AlN crystal; $\lambda_{[100]}$ = 186.74 and $\lambda_{[001]}$ = 165.24 W/(m·K) for $Al_{0.5}Ga_{0.5}N$ crystal.

Anisotropy of the thermal conductivity. Using calculated values of the thermal conductivity coefficients in the crystallographic directions [100], [010], and [001], it is possible to define numerical values of thermal conductivity coefficients for crystallographic direction [u v w].

For some physical properties described by the second rank symmetric tensor (electrical conductivity, electrical dielectric permittivity, dielectric susceptibility, diffusion, thermal conductivity, thermal expansion, deformation), there is the simple geometric method of their presentation in quadric view. The thermal conductivity quadric for hexagonal syngony represents the spheroid generated by the rotation of an ellipse about the Z-axis with semi-axes λ_{xx}, λ_{xx}, and λ_{zz} (Fig. 1a). Form of the thermal conductivity tensor for crystals with hexagonal syngony is presented in Fig. 1b. Conversion from Cartesian coordinate system to spherical was performed for quadric presentation of thermal conductivity.



$$\lambda = \begin{bmatrix} \lambda_{xx} & 0 & 0 \\ 0 & \lambda_{xx} & 0 \\ 0 & 0 & \lambda_{zz} \end{bmatrix}$$

Fig. 1. Crystals with hexagonal syngony:
a) thermal conductivity quadric; b) form of thermal conductivity tensor

According to the Fourier law, heat flow q is associates with the temperature gradient and material thermal conductivity λ in the following way:

$$q = -\lambda \cdot \nabla T, \quad (1)$$

where q is the local heat flow density, W/m^2, λ is the thermal conductivity of the material, W/(m·K), ∇T is the temperature gradient, K/m.

Since the thermal conductivity in the anisotropic materials appears to be a second-rank tensor, then the thermal-conductivity Fourier law (1) can be presented in a tensor form when transiting to a spherical coordinate system through the use of the following ratio:

$$q(\theta,\varphi) = -[\sin\theta \cdot \cos\varphi \quad \sin\theta \cdot \sin\varphi \quad \cos\theta] \begin{bmatrix} \lambda_{xx} & \lambda_{xy} & \lambda_{xz} \\ \lambda_{yx} & \lambda_{yy} & \lambda_{yz} \\ \lambda_{zx} & \lambda_{zy} & \lambda_{zz} \end{bmatrix} \frac{\partial T}{\partial r} \begin{bmatrix} \sin\theta \cdot \cos\varphi \\ \sin\theta \cdot \sin\varphi \\ \cos\theta \end{bmatrix} = -\lambda(\theta,\varphi)\frac{\partial T}{\partial r}, \quad (2)$$

where θ is a polar angle, φ is an azimuth angle.

Eq. (2) allows determining the material thermal conductivity in any crystallographic direction, taking into account that for this direction relevant θ and φ angles are defined.

For the definition of the thermal conductivity coefficient in crystal directions of interest with hexagonal syngony ($\lambda_{xx} = \lambda_{yy} \neq \lambda_{zz}$), inserting numeric values of thermal conductivity tensor in the main directions [100] and [001] reduces equation (2) to the simpler form:

$$\lambda(\theta, \varphi) = \lambda_{xx} \cdot \sin^2\theta + \lambda_{zz} \cdot \cos^2\theta. \quad (3)$$

The polar angle θ for crystallographic direction [111] can be defined using the ratio:

$$\theta = arctg\left(\frac{\lambda_{[100]}}{\lambda_{[001]}}\right). \quad (4)$$

For visualizing the thermal conductivity coefficients of the material having hexagonal syngony, it is convenient to use an isotherm instead of a bulk quadric. This connected with the fact that according to eq. (3) the value of the thermal conductivity coefficients does not change at any value of azimuth angle φ. To set the isotherm, we need to know the numerical values of the thermal conductivity coefficients in the [100] and [001] directions.

Figure 2 presents the calculated isotherms of the thermal conductivities for AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ crystals at a temperature of 300 K and the values of the polar angle θ in the range from 0 to 360 degrees.

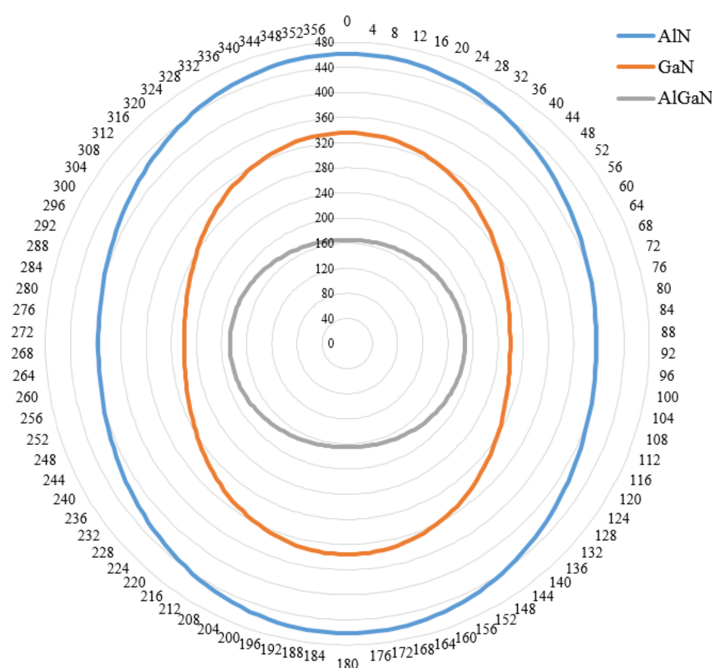


Fig. 2. Isotherms of the thermal conductivity dependencies of AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ crystals on the polar angle θ (at 300 K)

As one can see in Fig. 2, the maximum of the thermal conductivity coefficient for AlN and GaN refers to the [001] direction and equals 461.65 and 335.96 W/(m·K), respectively. The minimum is directed along the [100] direction and equals 396.06 and 259.28 W/(m·K), respectively. For $Al_{0.5}Ga_{0.5}N$ crystal maximum λ = 186.74 W/(m·K) lies in the [100] direction, and minimum λ = 165.24 W/(m·K) is in the [001] direction.

Temperature dependence of the thermal conductivity. For traditional silicon technology, the electronic devices usually are limited by work temperatures less than 380 K. In GaAs and GaN technologies work temperatures can reach 770 K. Thereby the range from 250 to 750 K was chosen for investigating the temperature dependence of the thermal conductivity of AlN, GaN, and $Al_{0.5}Ga_{0.5}N$. Figure 3 shows for AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ compounds the dependence of the thermal conductivity on temperature along the crystallographic directions. The temperature dependence of the lattice thermal conductivity of the material can be expressed as follows:

$$\lambda(T) = \lambda_{300} \cdot \left(\frac{T}{300}\right)^{\delta}, \quad (5)$$

where λ_{300} is the thermal conductivity of material at 300 K, δ is a temperature changing coefficient.

The dot lines represent the smoothing power functions derived from eq. (5). Calculated constants of the thermal conductivity equations for materials under investigation are presented in Table 2.

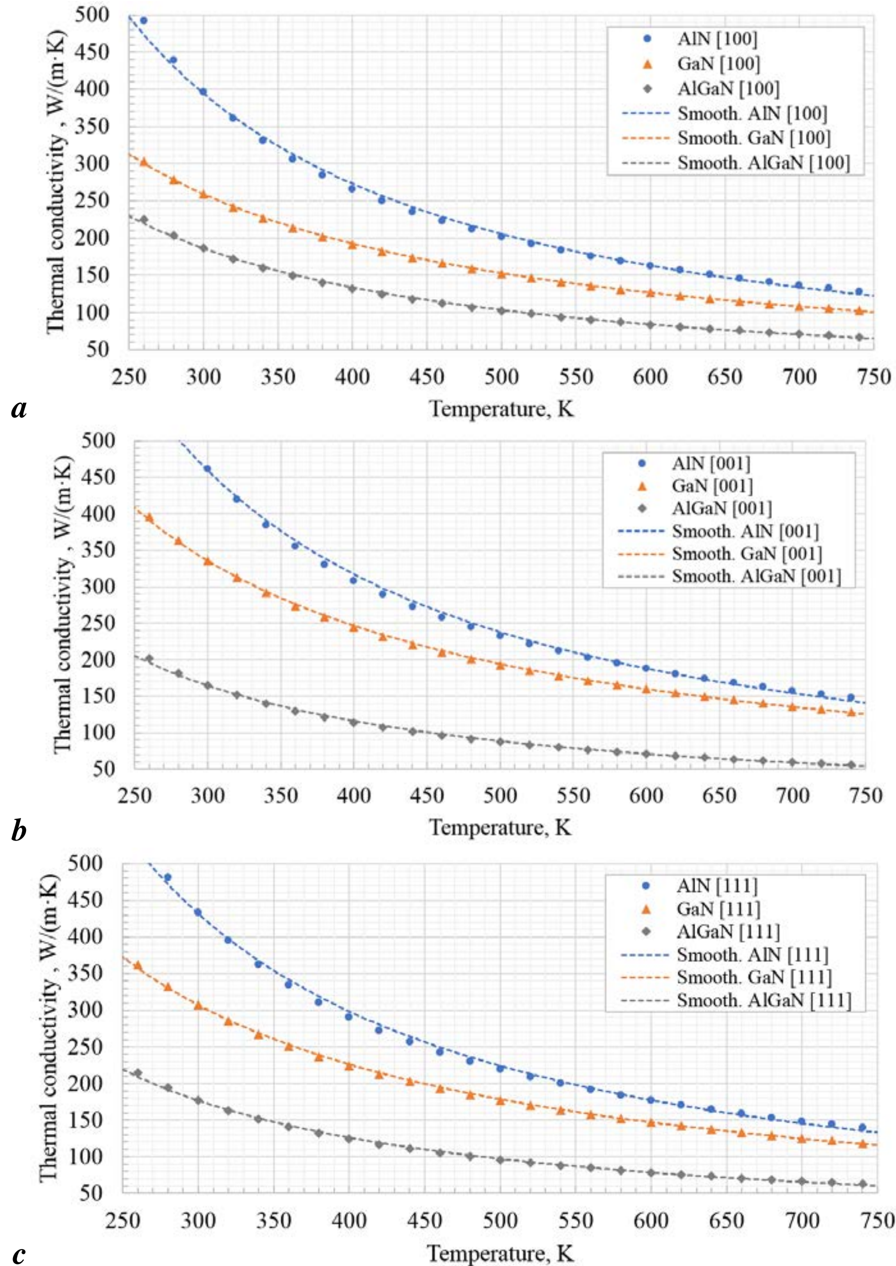


Fig. 3. Dependencies of the thermal conductivity for AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ on temperature along the directions: *a* – [100], *b* – [001], and *c* – [111]

Reliability values of approximations R^2 are calculated. The closer R^2 value to 1, the more reliable the power function is. Since numeric values R^2 are in the range from 0.997 (for AlN in the [001] direction) to 1.000 (for GaN in the [111] direction), it can be concluded that the reliability level of the power equations obtained for the thermal conductivity is very high.

Table 2. Constants for the thermal conductivity power equations

Structure	Direction	λ_{300}, W/(m·K)	δ	R^2
AlN	[100]	394.4	-1.28	0.997
	[001]	459.5	-1.29	0.997
	[111]	431.9	-1.28	0.997
GaN	[100]	259.2	-1.03	1.000
	[001]	335.7	-1.07	0.999
	[111]	307.2	-1.06	1.000
$Al_{0.5}Ga_{0.5}N$	[100]	186.3	-1.15	0.999
	[001]	164.6	-1.21	0.998
	[111]	176.8	-1.17	0.998

4. Analysis of results

We have compared the calculated thermal conductivity of GaN with the data of other authors who used both first-principle calculation methods and experimental ones. The values from the first data published by Sitchel and Pankov in 1977 to the results obtained by us in 2021 are presented in Fig. 4. The quantum-mechanical results differ from the experimental values.

For comparison, we accepted the following assumptions. If the thermal conductivity of material was presented with one numerical value without pointing the crystallographic direction, we assumed that this value refers to the [001] direction. In the case when the thermal conductivity was given as a range of values (without designation of the crystallographic direction), it was recognized that the smallest value refers to the [100] direction, and the largest to the [001] direction. The temperature of measurements was not specified, it is assumed to be equal to 300 K.

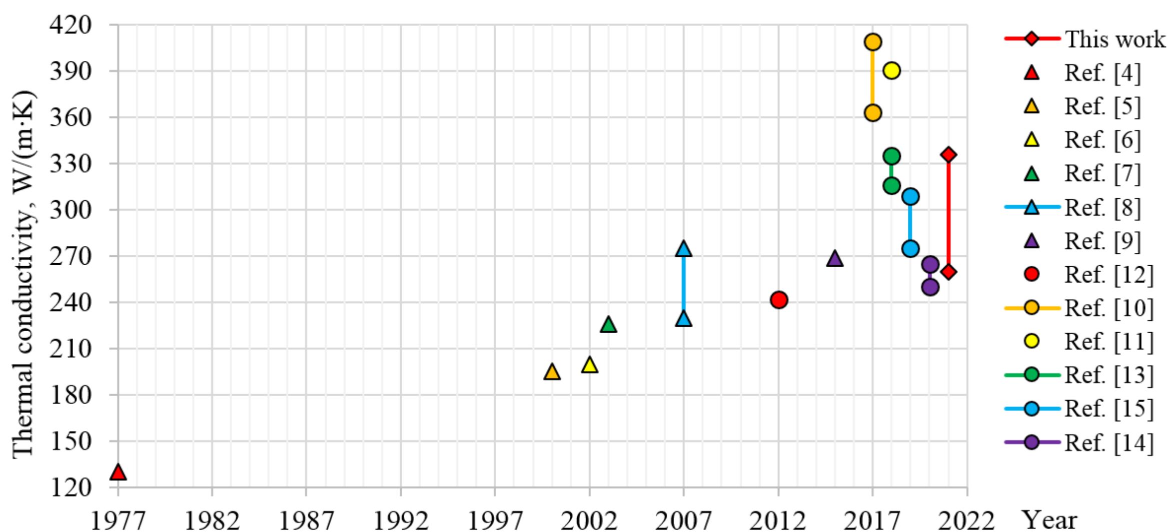


Fig. 4. GaN thermal conductivity investigations over the years (theoretical data are displayed as circles, experimental ones as triangles, and our data as rhombuses)

Comparison to theoretical works. In [10] the highest thermal conductivity values were obtained. The distinction from other works can be explained by the fact that crystal structure parameters had been taken right from experiments, i.e. structural relaxation had not been performed. Unlike other works the authors [11] calculated using different software. In [12] GaN lattice thermal conductivity and its dependence on isotopic composition were

investigated. The thermal conductivity value corresponding to a natural isotope concentration was in good agreement with experimental values in a wide range of temperatures. The authors have shown that rising of the gallium isotope concentration leads to a large frequency gap between acoustic and optic phonon branches. The gap produces unusually weak anharmonic phonon-phonon scattering that enters into the heat transfer mechanism of the material.

The remaining works gave values which are close to ours. Some different model parameters used by other authors, e.g. supercell size, cutoff energy, etc. lead to minor inconsistencies in the numerical values of lattice thermal conductivity [13-15].

Comparison to experimental works. The tendency of increasing the numeric value of thermal conductivity obtained experimentally from the earliest to the last works was noticed. This fact can be explained by the improvement of methods of crystal growing and sample preparation, betterment of measuring equipment, and mathematical treatment of the results obtained. Experimental results depend on the crystal orientation of a sample, its thickness, point defects presence (impurities or vacancies), and the substrate on which the sample is placed.

In all experimental works, GaN samples were grown by chloride-hydride gas-phase epitaxy (HVPE). Unlike the liquid phase, epitaxy HVPE allows controlling of crystal growth. Thermal conductivity values in the experimental works correspond to room temperature. One of the first studies on GaN thermal conductivity is [4]. The authors investigated a bulk GaN sample of thickness of 400 μm on the sapphire substrate, roughly rectangular shape with sizes 5×2.65×0.31 mm. The thermal conductivity was equal to 130 W/(m·K) along the [001] direction. As it will be shown further, the thermal conductivity of a monocrystal exceeds this value significantly. Up to 2000, Sichel-Pankov's work was the only one on GaN thermal conductivity when progress in the synthesis of this material allowed create high-quality crystals. That led to comprehensive research of its properties with application perspectives in electronics.

In [5] GaN films were grown on sapphire (0001) substrate in a vertical type reactor. Film thermal conductivity was about 195 W/(m·K) at a gallium concentration of $N = 6.9\times10^{16}$ cm^{-3} in the sample. The authors [6] have got GaN monocrystal samples on the sapphire substrate. The thermal conductivity value of 200 W/(m·K) was obtained for GaN sample with the impurities of oxygen ($N = 2.1\times10^{16}$ cm^{-3}) and silicon ($N = 0.37\times10^{16}$ cm^{-3}). According to [7] GaN thermal conductivity is equal to 226 W/(m·K). The samples under investigation had the following impurities: oxygen ($N = 1\times10^{20}$ cm^{-3}), silicon ($N = 1\times10^{17}$ cm^{-3}), hydrogen ($N = 7\times10^{17}$ cm^{-3}), carbon ($N = 1\times10^{19}$ cm^{-3}) and magnesium ($N = 1\times10^{18}$ cm^{-3}). Concentration of Ga vacancies was equal to $N = 1\times10^{18}$ cm^{-3}.

It is known that the heat properties of a gallium monocrystal are very sensitive to structure defects, but the authors [8] managed to get an almost perfect GaN crystal with the minimum number of point defects. GaN monocrystal thermal conductivity had been measured by the vertical type laser flash method at room temperature and was equal to 253 ± 8.8 % W/(m·K). There is the experiment [9] where the measured value of thermal conductivity is equal to 269 W/(m·K) at room temperature with high oxygen impurity concentration. The authors explained it by the fact that at this oxygen impurity concentration phonon scattering on free charge carriers is negligible, which leads to thermal conductivity increases.

The distinction between the results of theoretical investigation and experimental data can be explained as follows. *Phono3py* determines all possible variants of atomic displacements in the supercell under study. Depending on atom number in the supercell and crystal symmetry, the number of atomic-pair configurations can be large enough and exceed computation resources. To reduce computation time and the number of supercells with displacements, the "cutoff-pair" parameter is used which limits the distance between cutoff

pairs in the supercell. Thereby, some amount of the supercells with displacements could be not taken into account.

The large variety of defects arises during material layer formation. For example, the presence of impurities and dislocations significantly reduces the thermal conductivity of GaN films [27,28]. The measured thermal conductivity for GaN thin films [29] is significantly less than the thermal conductivity for bulk GaN crystal at room temperature [6].

The type of defects and their number depends on the synthesis method, subsequent thermal processing, substrate materials, etc. Receiving the result that will represent the real picture by using quantum-mechanical calculations is impossible because of the huge number of possible defect variants.

The supercell method lets us evaluate point defects' impact on properties of a material under investigation, in particular, structural and electron properties. However, in the case of thermal conductivity calculations huge computing resources are needed. For this reason for a wide range of materials, heat properties calculations are performed for idealized structures. It is worth noting that the influence of crystal grain boundaries and surface is not taken into account in quantum-mechanical calculations. So the periodic boundary conditions, which assume that the crystal under study has quasi-infinite size, are used.

Methodology of thermal conductivity experimental measurements gives values without many factors accounting: 1) contribution of heat exchange to the substrate, on which the film of the material under investigation is applied; 2) significant contribution of the heat exchange with the environment; 3) technical difficulties of measurements associated with small sample size. Thereby the thermal conductivity data taken from the literature and obtained experimentally are not ideal. In its turn, computer simulation at the atomic level does not allow taking into account all the factors described above.

5. Conclusions

The thermal conductivity along the [100], [010], and [001] main crystallographic directions for GaN, AlN, and $Al_{0.5}Ga_{0.5}N$ materials have been calculated in the temperature range from 250 to 750 K. An equation is presented for determining the thermal conductivity of a material in the required crystallographic direction.

The maximum values of the thermal conductivity coefficients of AlN and GaN are in the [001] direction and equal to 461.65 and 335.96 W/(m·K), respectively, while the minimum values are along the [100] direction and equal to 396.06 and 259.28 W/(m·K), respectively. For the $Al_{0.5}Ga_{0.5}N$ crystal, the maximum λ = 186.74 W/(m·K) is in the [100] direction, and the minimum λ = 165.24 W/(m·K) is in the [001] direction.

Models are presented that describe changes in the lattice thermal conductivity of materials with temperature. The calculated constants (the temperature change coefficient and the thermal conductivity of material at 300 K) are given for the power-law heat conduction equations along the [100], [001], and [111] crystallographic directions for the studied AlN, GaN, and $Al_{0.5}Ga_{0.5}N$ materials. The values of the reliability approximations R^2 are in the range from 0.996 (for AlN in the [001] direction) to 0.9996 (for GaN in the [111] direction). It means that the level of reliability of the obtained power-law equations of heat conduction is quite high.

A comparative analysis of the GaN thermal conductivity studies has been carried out. The peculiarities of determining the thermal conductivity of GaN were established for experimental studies and theoretical calculations.

The technical complexity of measurements in the experiment is associated with a small size of sample. Besides, the measuring technique for thermal conductivity of materials neglects the contribution of substrate and environment. Thus, the experimental data of the numerical values of thermal conductivity taken from the literature are not ideal, since they

include a number of shortcomings in the measurement methods. At this moment it is impossible to obtain a result that reflects the real picture due to limitations on the power of computing equipment and time resources for quantum mechanical simulation. The atomic level of computer simulation does not allow taking into account the influence of most structural defects (impurities, dislocations, crystal grain boundaries, surface effects). Therefore, calculations of the thermal properties of materials are carried out for an idealized structure.

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