Effect of built-in-polarization field on mean free path of phonons in binary nitrides

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In this paper, the built-in-polarization field effect on mean free path of acoustic phonons in bulk wurtzite binary nitrides (GaN, AlN) has been theoretically investigated. Due to the modification of elastic constant of the material by the effect of polarization field, there is a corresponding enhancement in group velocity and Debye frequency of phonons. The scattering rate of phonons also affected by this field, as it is a function of velocity or/and Debye frequency. The result shows that polarization field suppresses various scattering rates as well as combined scattering rate of phonons. This implies an increased combined relaxation time of phonons. Hence, the mean free path of phonons increases. Thus, phonons travel freely for a longer distance between two successive scatterings. It is found that, the mean free path of low frequency phonons are significantly affected by the built-in-polarization field. This can enhance thermal transport properties of the material, when built-in-polarization field in a desired way, which can be considered in addressing thermal management issues in nitride based optoelectronic devices to minimize self-heating effects.

Keywords: Binary nitrides, Built-in-polarization field, Phonon relaxation time, Phonon mean free path

1 Introduction

In the field of optoelectronic and high power devices, binary nitride semiconductors (GaN, AlN, InN) have dominated the other contemporary materials. The wide and direct band gap covering from ultraviolet to infrared energy range ($E_{g,GaN} = 3.4$ eV, $E_{g,AIN} = 6.2 \text{ eV}$, $E_{g,InN} = 0.64 \text{ eV})^1$ is the important reason for their broad applications. Although the performance of nitride based optoelectronic devices is reliable but the main drawback is self-heating effect². It reduces the performance and lifetime of the devices. Poor heat dissipation at the active region is the basic cause of self-heating. Again the heat dissipation from the active region is directly dependent on the thermal transport properties of the material. If the thermal transport of the material can be enhanced by any means then the self-heating effect can be minimized. As a result the efficiency as well as the lifetime of nitride based devices can be further improved. Thus, there should be a proper investigation of the properties in the material that can enhance thermal transport.

III-V nitride semiconductors have superior properties over Si, Ge, GaAs, etc., and promising

materials for optoelectronic devices. They have manifested their feathers like high mobility, high saturation velocity, high sheet carrier concentration, high breakdown field, high absorption coefficient and high radiation tolerance. Gallium nitride (GaN) is the next important semiconductor material after silicon, which can be operated at high temperatures and the key material for the next generation of high frequency and high power transistors. Aluminum nitride (AlN) is used as a heat-sink substrate for semiconductor devices³. Since the room temperature thermal conductivity of pure AlN is about 80% of that of copper, it has important role in addressing thermal management issues in device applications. Extremely narrow band gap and low electron effective mass of Indium nitride (InN) makes it a promising material for optoelectronic devices¹. The alloy of InN and GaN has been used as the active material in light-emitting diodes and laser diodes⁴⁻⁷. The high absorption coefficient and high radiation tolerance make these semiconductors suitable for solar cell application⁸.

Existence of intrinsic built-in-polarization field in the unit cell is one of the unique and peculiar properties of binary nitrides^{9,10}. This field is a common feature of wurtzite structures and has significant influence on their optical, thermal and

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electrical properties^{9,10}. The existence of this field in wurtzite nitrides has been verified by first-principle calculations as well as experiments¹¹⁻¹⁸. The emission efficiency reduces due to the presence of this field in InGaN/GaN quantum well structures¹⁹. The effect of polarization field has been observed in the efficiency of light-emitting diodes and laser diodes²⁰. As per their report, although the cause of efficiency drop is due to several internal mechanisms but built-inpolarization field is one of them. The performance of solar cells has also been studied on the basis of the effect of polarization field^{21,22}. The effect of this field in wurtzite nitrides has been also studied for ultraviolet and visible light emitters, solar cells and detectors. However, the role of built-in-polarization field in thermal transport properties of binary nitrides has not been properly investigated. Recently, Sztein co-workers²³ have reported and that. the thermoelectric efficiency as well as figure of merit increases in the materials those having intrinsic builtin-polarization field. They have studied the electron transport properties only taking the built-inpolarization field into account and calculated the electrical properties of alloys. However, with respect to phonon transport properties the role of built-inpolarization field has not been addressed²⁴.

To the best of our knowledge, the effect of built-inpolarization field on mean free path of phonons in binary nitrides during thermal energy transport has not been addressed so far. So a thorough theoretical understanding of the role of built-in-polarization field deserves attention for the better performance and further improvement of the devices. In this work, using Callaway's and Klemens's model, various phonon scattering processes are computed and the corresponding combined relaxation time has been calculated. Exploiting the built-in-polarization field in binary nitrides, we have predicted a model how to enhance the mean free path of acoustic phonons.

2 Theoretical Models

2.1 Built-in-polarization field

The existence of strong built-in-polarization field is an important and useful property of wurtzite structures. In semiconductors this field is defined by the relation $P = D - \varepsilon_0 \varepsilon_r E$, where *D* is electric flux density (C m⁻²), *E* is electric field (V m⁻¹), ε_0 is permittivity of free space and ε_r is relative permittivity of the medium. The origin of such polarization field is from two sources: (i) Spontaneous polarization (P^{sp}) and (ii) piezoelectric polarization (P^{pz}). Spontaneous polarization is an intrinsic property of the material; it arises due to lack of symmetry in the structure of wurtzite unit cell. Since this polarization exists in the lattice at equilibrium state at zero strain, it is known as spontaneous polarization¹¹. The value of spontaneous polarization along z-axis of the unit cell of crystal is given by $\vec{P}^{sp} = P^{sp}\hat{z}$; here \hat{z} is the unit vector along z-direction¹⁵. In binary nitrides family, this value increases from GaN to InN to AlN¹¹. Piezoelectric polarization generates due to strain in the material. During the growth of binary nitrides on a substrate, strain is generated due to lattice mismatch and external stress. This strain produces piezoelectric polarization in the material¹⁴⁻¹⁶.

Thus built-in-polarization field is then given by:

$$P = P^{sp} + P^{pz} \qquad \dots (1)$$

For the application of external stresses σ_{jk} the deformation in the crystal \mathcal{E}_{lm} according to Hooke's can be described by^{9, 16}:

$$\sigma_{jk} = \sum_{l,m} C_{jklm} \varepsilon_{lm} \qquad \dots (2)$$

Here C_{jklm} is the elastic tensor. Due to spatial symmetry this fourth-rank tensor can be reduced to a 6×6 matrix using the Voigt notation: $xx \rightarrow 1$, $yy \rightarrow 2$, $zz \rightarrow 3$, yz, $zy \rightarrow 4$, zx, $xz \rightarrow 5$, xy, $yx \rightarrow 6$. The elements of the elastic tensor can be rewritten as $C_{jklm} = C_{pq}$, where *j*, *k*, *l*, m = x, *y*, *z* and *p*, q = 1,..., 6. According to this notation, Hooke's law can be written in a simplified form as:

$$\sigma_j = \sum_k C_{jk} \, \varepsilon_k \qquad \dots (3)$$

For the crystals with wurtzite structures, this 6×6 matrix of the elastic constants C_{ik} is given by:

$$C_{jk} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(C_{11} - C_{12}) \end{pmatrix} \dots (4)$$

The piezoelectric polarization as a function of strain can be written as 16 :

$$P_l^{p_z} = \sum e_{lm} \mathcal{E}_m \qquad \dots (5)$$

where, l = 1, 2, 3 and $m = 1, \dots, 6$

The piezoelectric constants e_{lm} describe the piezoelectric properties of wurtzite nitrides. The piezoelectric tensor for wurtzite nitrides can be explicitly written as²:

$$e_{lm} = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & 0 \\ 0 & 0 & 0 & e_{24} & 0 & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & 0 \end{pmatrix} \qquad \dots (6)$$

The strain tensor is given by 16 :

$$\boldsymbol{\varepsilon}_{m} = \begin{bmatrix} \boldsymbol{\varepsilon}_{1}, & \boldsymbol{\varepsilon}_{2}, & \boldsymbol{\varepsilon}_{3}, & \boldsymbol{\varepsilon}_{4}, & \boldsymbol{\varepsilon}_{5}, & \boldsymbol{\varepsilon}_{6} \end{bmatrix}^{T} \dots (7)$$

Here $e_{32} = e_{31}$ and $e_{24} = e_{15}^{16} \cdot \mathcal{E}_l$ is a column matrix. For convenience it is written in a row matrix form with transpose. In Eq. (7), $\mathcal{E}_4 = \mathcal{E}_1$; $\mathcal{E}_5 = \mathcal{E}_2$; $\mathcal{E}_6 = \mathcal{E}_3^{9}$. When biaxial stresses such as σ_1 and σ_2 are applied to the basal plane of unit cell of the crystal with $\sigma_1 = \sigma_2$ and if there is no stress along perpendicular direction of unit cell, i.e., $\sigma_3 = 0$, then biaxial strain \mathcal{E}_1 and \mathcal{E}_2 is generated with $\mathcal{E}_1 = \mathcal{E}_2$. The relation between the strain along the z-axis (\mathcal{E}_3) and the strain along the basal plane (\mathcal{E}_1) is given by:

$$\varepsilon_3 = -2(C_{13} / C_{33})\varepsilon_1 \qquad \dots (8)$$

The strain ε_1 and ε_3 are calculated by $\varepsilon_1 = \frac{a - a_0}{a_0}$ and $\varepsilon_3 = \frac{c - c_0}{c_0}$. Here a_0 and c_0 are the lattice constants of the unit cell at zero strain. Under this condition and assuming the shear stresses to be negligible ($\sigma_4 = \sigma_5 = 0$), the piezoelectric polarization has only one non-vanishing component, i.e., P_3^{pz} . This component of polarization is directed along the growth direction (i.e., z-axis). From Eqs (5)

and (8), it can be written as:

$$P_3^{pz} = e_{31} \varepsilon_1 + e_{32} \varepsilon_2 + e_{33} \varepsilon_3 = 2\varepsilon_1 e_{31} + \varepsilon_3 e_{33}$$

$$= 2\left(\frac{a-a_0}{a_0}\right) \left[e_{31} - e_{33}\left(C_{13}/C_{33}\right)\right] \qquad \dots (9)$$

The built-in-polarization field in the z-direction is $P = P^{sp} + P^{pz}$. As $P_1^{pz} = P_2^{pz} = 0$, hence Eq. (1) becomes:

$$P = P^{sp} + P^{pz} = P^{sp} + 2\left(\frac{a - a_0}{a_0}\right) \left[e_{31} - e_{33}\left(C_{13}/C_{33}\right)\right]$$
... (10)

Since in wurtzite binary nitrides the piezoelectric coefficient e_{31} is always negative, while e_{33} , C_{13} and C_{33} are always positive, the term $[e_{31} - e_{33}(C_{13}/C_{33})]$ is always negative¹¹. As a consequence for the layers under tensile stress in wurtzite nitrides, the piezoelectric polarization is always negative as $a > a_0$ and it is positive for layers under compressive stress as $a < a_0$. As spontaneous polarization in wurtzite nitrides is always negative, hence for the layers under tensile stress, spontaneous and piezoelectric polarizations are parallel to each other whereas the two polarizations are anti-parallel for the layers under compressive stress.

2.2 Elastic constant of material

In nitride semiconductors the phonon dynamics is influenced by the built-in-polarization field. Due to this field, the coupling between the elastic strain and electric field induces additional electric polarization which modifies the elastic constant of the material²⁶⁻²⁸. As a result the effective elastic constant of the material becomes:

$$\overline{C}_{44} = C_{44} + \left[\left(e_{15}^{2} + e_{31}^{2} + e_{33}^{2} + P_{SP}^{2}\right) / (\mathcal{E}_{0}\mathcal{E})\right].$$
... (11)

Here C_{44} be the elastic constant of the material when built-in-polarization field is not taken into account, \mathcal{E} is the dielectric constant and e_{15} is related to the polarization induced by shear strain. The additional term as given in the square bracket represents the contribution of built-in-polarization field. Hence, it is clear that polarization field enhances the value of elastic constant of binary nitride materials.

2.3 Group velocity and Debye frequency of phonons

The phonon group velocity (v) is dependent on the direction as well as magnitude of the phonon wave vector and is specific to a given phonon polarization type. As per Callaway's model, the average velocity (v) along a specified crystallographic axis is given by²⁹:

$$v = \left[\frac{1}{3}\left(\frac{1}{v_{T1}} + \frac{1}{v_{T2}} + \frac{1}{v_L}\right)\right]^{-1} \dots (12)$$

where, v_L is the longitudinal component and v_{T1} , v_{T2} are the transverse components of velocity. The two transverse branches are degenerate and have the same velocity along [0001] direction, which is given by $v_{T1} = v_{T2} = v_T = (C_{44} / \rho)^{1/2}$, whereas the longitudinal phonon velocity given is by $v_L = \sqrt{C_{33}/\rho}$. When built-in-polarization field is taken into account, the transverse velocity becomes $\overline{v}_{T} = (\overline{C}_{44} / \rho)^{1/2}$. Hence the transverse velocity is modified due to the effect of polarization field while the longitudinal velocity does not change. Thus the (\overline{v}) average velocity along а specified crystallographic axis in the presence of built-inpolarization field can be written as:

$$\overline{v} = \left[\frac{1}{3}\left(\frac{1}{\overline{v_T}} + \frac{1}{\overline{v_T}} + \frac{1}{v_L}\right)\right]^{-1}$$
$$= \left[\frac{1}{3}\left(\frac{2}{\overline{v_T}} + \frac{1}{v_L}\right)\right]^{-1} \qquad \dots (13)$$

The Debye frequency in terms of phonon group velocity is given by the expression:

$$v_D = v (3N/4\pi V_0)^{1/3}$$
 ... (14)

Here, N is the number of atoms presents in volume V_0 of the unit cell and v be the phonon group velocity. The above expression shows that Debye frequency is directly dependent on phonon group velocity; hence it is expected to be modified due to the effect of built-in-polarization field.

2.4 Scattering rates of phonons

Mostly the thermal energy is carried by acoustic phonons in semiconductors. These phonons get scattered from other phonons, electrons, impurities and defects; due to which thermal energy carried by them gets lost. The processes in which phonons scatter may be normal or resistive. During normal scattering processes the momentum of phonons gets conserved, whereas it is not conserved in resistive scattering processes. Hence, scattering of phonons and corresponding relaxation time are the major factors for the thermal transport properties of the material. According to Klemens's formulation³⁰, the combined scattering rate of phonons is the sum of normal and resistive scattering probabilities:

$$\frac{1}{\tau_C} = \frac{1}{\tau_N} + \frac{1}{\tau_R} \qquad \dots (15)$$

The phonon-phonon scattering process is known as normal scattering in which momentum of phonons is conserved²⁴:

$$\frac{1}{\tau_{N}} = \frac{k_{\beta} \gamma^{2} V_{0}}{M \hbar^{2} v^{5}} \omega^{2} T^{3} \qquad \dots (16)$$

where γ (=0.50) is the Gruneisen anharmonicity parameter, $V_0 = (\sqrt{3}/8)a^2c$ is the volume per atom, k_{β} is the Boltzmann constant and M is the molecular mass of binary nirtides (GaN, AlN). The momentum of phonons does not conserve in resistive scattering processes and thus these processes have major role in controlling the transport properties of the material. The resistive scattering processes such as three phonon Umklapp scattering, point defect scattering, scattering due to dislocation and phononelectron scattering are taken into account in this work. Three phonon Umklapp scattering is a process of phonon-phonon scattering, where momentum is not conserved and is given by the following expression³¹:

$$\frac{1}{\tau_{u}} = 2 \gamma^{2} \frac{k_{\beta}T}{\mu V_{0} \omega_{D}} \omega^{2} \qquad \dots (17)$$

where $\mu = v_T^2 \rho$ is the shear modulus and ω is the phonon frequency. The phonon scattering rates due to differences in mass (point defect) is given by 31 :

$$\frac{1}{\tau_{p}} = \frac{V_{0} \Gamma \omega^{4}}{4 \pi v^{3}} \dots (18)$$

where, $\Gamma = \sum_{i} f_{i} [1 - (M_{i} / \overline{M})]^{2}$ the measure of strength of the mass-difference scattering is, f_i is the fractional concentration of the impurity atoms, $\overline{M} = \sum f_i M_i$ is the average atomic mass. The scattering of phonons due to dislocation is given as follows³²:

$$\frac{1}{\tau_d} = \eta \, N_D \, \frac{V_0^{4/3}}{v^2} \, \omega^3 \qquad \dots (19)$$

Here N_D is the density of the dislocation lines of all types, and $\eta = 0.55$ is the weight factor to account for the mutual orientation of the direction of the temperature gradient and the dislocation line.

The scattering rate when acoustic phonons are scattered by electrons at low doping levels can be expressed as³¹:

$$\frac{1}{\tau_{ph-e}} = \frac{n_{e} \varepsilon_{1}^{2} \omega}{\rho v^{2} k_{\beta} T}$$

$$\sqrt{\frac{\pi m^{*} v^{2}}{2 k_{\beta} T}} \exp\left(-\frac{m^{*} v^{2}}{2 k_{\beta} T}\right) \dots (20)$$

where, n_e is the concentration of conduction electrons, ε_1 is the deformation potential, ρ is the mass density and m^* is the effective mass of electron.

The resistive phonon scattering rate $(1/\tau_R)$ is the summation of all the scattering rates as given in Eqs (17-20) and is given by³²:

$$\frac{1}{\tau_{R}} = \frac{1}{\tau_{u}} + \frac{1}{\tau_{p}} + \frac{1}{\tau_{d}} + \frac{1}{\tau_{ph-e}}$$
...(21)

2.5 Combined relaxation time of phonons

The combined relaxation time (τ_c) of phonons can be obtained using Eqs (15) and (21) as follows:

$$\tau_{C} = \left[\frac{1}{\tau_{N}} + \frac{1}{\tau_{R}}\right]^{-1}$$
$$= \left[\frac{1}{\tau_{N}} + \frac{1}{\tau_{u}} + \frac{1}{\tau_{p}} + \frac{1}{\tau_{d}} + \frac{1}{\tau_{ph-e}}\right]^{-1}$$
...(22)

Hence from the above expression it is expected that, the value of combined relaxation time of phonons would be modified by the effect of built-in-polarization field.

2.6 Mean free path of phonons

The average distance travelled by phonons between two successive scatterings is known as mean free path. In this work, taking the combined relaxation time and group velocity of phonons we have calculated the mean free path as follows:

$$l = v \times \tau_C \qquad \dots (23)$$

Since both group velocity and combined relaxation time of phonons are enhanced by the effect of built-inpolarization field, hence the mean free path becomes longer. That is phonons travel freely for a longer distance between two successive scatterings due to the effect of polarization field. Again longer the mean free path, higher will be the ability of the phonons to transport thermal energy. It indicates that, built-inpolarization field enhances the thermal transport properties of the material.

3 Results and Discussion

3.1 Effect of built-in-polarization field in GaN

3.1.1 Modified parameters

The elastic constant of GaN has been calculated with and without built-in-polarization field using Eq. (11). The material parameters and polarization constants of binary nitrides are presented in Table 1. Then the transverse components of phonon velocity have been calculated considering the above values of elastic constant. Taking into account Eqs (12) and (13), the average velocity of phonons without and with polarization field has been computed. Then Debye frequency is computed using Eq. (14) taking the average velocities of phonons from above calculation. The values of elastic constant, phonon group velocity and Debye frequency with and without polarization field along with their percentage of increase have been shown in Table 2. Taking the values of phonon group velocity and Debye frequency, various scattering rates have been computed with and without polarization field

Table 1 — Material parameters and polarization constants of binary nitrides ^{9,10,16,25}				
Parameters	GaN	AlN		
$\alpha(\text{\AA})$	3.189	3.122		
_c (Å)	5.185	4.982		
$P^{SP}(Cm^{-2})$	-0.0842	-0.081		
e_{31} (Cm ⁻²)	-0.55	-0.82		
e_{33} (Cm ⁻²)	1.12	2.1		
e_{15} (Cm ⁻²)	-0.30	-0.48		
C_{13} (GPa)	103	108		
C ₃₃ (GPa)	398	388		
<i>C</i> ₄₄ (GPa)	105	125		
ε	9.5	8.5		
ρ (kg m ⁻³)	6150	3266		

Table 2 — Elastic constant, phonon velocity and Debye frequency of GaN

Parameters	Without polarization	With polarization	% Increase
C ₄₄ (GPa)	105	125	19
v (ms ⁻¹)	4931	5283	7.1
$v_{\rm D} ({\rm s}^{-1})$	7.8×10 ¹³	8.4×10 ¹³	7.6

using the Eqs (16)–(20). The values of parameters used in this calculation are $\Gamma = 1.3 \times 10^{-4}$, $N_D = 1.5 \times 10^{10}$ cm⁻², $n_e = 2.6 \times 10^{18}$ m⁻³, $\varepsilon_1 = 7.1$ eV and $m^* = 0.22m_0^{25,33,34}$. The combined relaxation time of phonons is computed using Eq. (22). It is found that, at a particular frequency, the combined relaxation time with built-in-polarization field is longer compared to the time without polarization field. Taking into consideration the values of group velocity and combined relaxation time with and without polarization field, the mean free path of phonons is computed from Eq. (23) as a function of frequency. Figure 1 shows the variation of mean free path with phonon frequency at room temperature.

3.1.2 Mean free path of phonons

In the figure, the solid line with filled stars represents the mean free path with built-inpolarization field, whereas the dashed line with empty stars corresponds to the mean free path without builtin-polarization field. It is manifested from the figure that, at a particular phonon frequency, the mean free path with polarization field is longer than that of without polarization field. Again it is clearly seen from the figure; the effect is significant for low frequency phonons. It indicates that high frequency phonons are less influenced by the polarization field.

3.2 Effect of built-in-polarization field in AlN *3.2.1 Modified parameters*

Using Eq. (11) the elastic constant of AlN has been calculated with and without built-in-polarization field.



Fig. 1 — Mean free path of phonons in GaN as a function of frequency at room temperature

After calculating the transverse components of phonon velocity, the average velocity has been calculated taking into account Eqs (12) and (13). The Debye frequency is computed using Eq. (14), taking the average velocity of phonons with and without polarization field from above calculation. The values of elastic constant, phonon group velocity and Debye frequency are found to be enhanced due to the effect of polarization field. The values of elastic constant, phonon group velocity and Debye frequency with and without polarization field along with the percentage of increase have been shown in Table 3. Various scattering rates of phonons have been computed with and without polarization field using the values of phonon group velocity and Debye frequency taking into account the Eqs (16)-(20). The values of parameters used in this work are $\Gamma = 3.2 \times 10^{-4}$, $N_D = 1.5 \times 10^{10}$ cm⁻², $n_e = 4.1 \times 10^{18}$ cm⁻³, $\varepsilon_1 = 9.5$ eV and $m^*=0.30m_0^{25,33,34}$. Analysis shows that the combined scattering rate of phonons is suppressed by built-inpolarization field. The combined relaxation time of phonons has been calculated using Eq. (22). It is found that at a particular frequency, the combined relaxation time with built-in-polarization field is longer than that of without polarization case. The mean free path of phonons has been computed using Eq. (23) as a function of frequency. Figure 2 shows the variation of mean free path with phonon frequency at room temperature.

3.2.2 Mean free path of phonons

In Fig. 2, the solid line with filled squares and dashed line with empty squares corresponds to the mean free path of phonons in AlN with and without built-in-polarization field, respectively. It is seen from the figure that the mean free path with polarization field is longer in comparison to without polarization field at a particular phonon frequency. Again it can be observed from the figure that the effect on mean free path is significant for low frequency phonons and is least for high frequency phonons. It is an indication that the high frequency phonons are influenced less in

Table 3 — Elastic constant, phonon velocity and Debye frequency of AlN					
Parameters	Without polarization	With polarization	% Increase		
C ₄₄ (GPa)	125	195.7	56.56		
$v ({\rm ms}^{-1})$	7243	8587	18.55		
$v_{\rm D} ({\rm s}^{-1})$	1.28×10^{14}	1.52×10^{14}	18.75		



Fig. 2 — Mean free path of phonons in AlN as a function of frequency at room temperature

comparison to the low frequency phonons by the polarization field.

4 Conclusions

In this work, the effect of built-in-polarization field on mean free path of phonons in wurtzite binary nitrides has been investigated theoretically. The values of elastic constant of the material, group velocity of phonons and Debye frequency are found to be enhanced when polarization field taken into account. However, the scattering rates of phonons are suppressed by the effect of polarization field. As a result the combined relaxation time of phonons increases. Since group velocity as well as combined relaxation time of phonons is enhanced by the polarization field, phonons travel freely for a longer distance between two successive scatterings as the mean free path becomes longer. Hence, during the transport of energy in the material, phonons will be less frequently scattered. Again it is found that, the mean free path of low frequency phonons is longer than that of the high frequency phonons. It indicates that, low frequency phonons are significantly influenced by built-in-polarization field. Analysis shows that the increase in mean free path due to builtin-polarization field is highest in AlN and is least in GaN, i.e., AlN has highest response to polarization field. Enhancement in the mean free path of phonons leads to an improvement in the thermal transport property of nitride semiconductors. This can minimize the self-heating effect of the devices fabricated from wurtzite nitrides. The predicted model may be useful for device simulations in thermal management issues in future.

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References

- 1 Wu J, J Appl Phys, 106 (2009) 011101.
- 2 Liu W & Balandin A A, Appl Phys Lett, 85 (2004) 5230.
- 3 Kuramoto N & Taniguchi H, J Mater Sci Lett, 3 (1984) 471.
- 4 Nakamura S, *Science*, 281 (1998) 956.
- 5 Schubert E F, *Light emitting diodes*, (Cambridge University Press, New York), 2006.
- 6 Nakamura S & Fasol G, *The blue laser diode: The complete story*, (Springer, Berlin), 2000.
- 7 Piprek J, Farrell R, Den Baars S P & Nakamura S, *IEEE Photon Technol Lett*, 18 (2006) 1041.
- 8 Brown G F, Ager III J W, Walukiewicz W & Wu J, Solar Energy Mater Solar Cells, 94 (2010) 478.
- 9 Wood C & Jena D, Polarization effects in semiconductors: From Ab initio theory to device applications, (Springer Science + Business Media, New York), 2000.
- 10 Morkoc H, Handbook of nitride semiconductors and devices, (Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim), 2008.
- 11 Bernardini F, Fiorentini V & Vanderbilt D, *Phys Rev B*, 56 (1997) R10024.
- 12 Bernardini F & Fiorentini V, Appl Surf Sci, 166 (2000) 23.
- 13 Bernardini F & Fiorentini V, Phys Rev B, 64 (2001) 08520.
- 14 Bernardini F, Fiorentini V & Ambacher O, *Appl Phys Lett*, 80 (2002) 1204.
- 15 Ambacher O, Smart J & Shealy J R, *J Appl Phys*, 85 (1999) 3222.
- 16 Ambacher O, Majewski J & Miskys C, J Phys Condens Matter, 14 (2002) 3399.
- 17 Zhang H, Miller E J, Yu E T, Poblenz C & Speck J S, *Appl Phys Lett*, 84 (2004) 4644.
- 18 Feneberg M & Thonke K, J Phys Condens Matter, 19 (2007) 403201.
- 19 De S, Layek A & Bhattacharya S, *Appl Phys Lett*, 101 (2012) 121919.
- 20 Verzellesi G, Saguatti D & Meneghini M, J Appl Phys, 114 (2013) 071101.
- 21 Wierer J J, Fischer A J & Koleske D D, *Appl Phys Lett*, 96 (2010) 051107.
- 22 Kuo Y K, Tsai M C, Yen S H, Hsu T C & Shen Y J, *IEEE J Quantum Electron*, 46 (2010) 1214.
- 23 Sztein A, Bowers J E, Denbaars S P & Nakamura S, Appl Phys Lett, 104 (2014) 042106.
- 24 Sztein A, Haberstroh J, Bowers J E, Denbaars S P & Nakamura S, *J Appl Phys*, 113 (2013) 183707.
- 25 Rumyantsev S L, Shur M S & Levinshtein M E, Materials properties of nitrides: Summary, www.ecse.rpi.edu/shur/ NitrideParameters.pdf.
- 26 Balkanski M & Wallis R F, *Semiconductor physics and application*, (Oxford University Press, New York), 2000.
- 27 Sahoo B K, J Mater Sci, 47 (2012) 2624.

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- 28 Sahoo B K, Sahoo S K & Sahoo S, *J Phys Chem Solids*, 74 (2013) 1669.
- 29 Callaway J, Phys Rev, 113 (1959) 1046.
- 30 Klemens P G, Chemistry and physics of nanostructures and related non equilibrium materials, edited by E Ma, B Fultz, R Shall, J Morral & P Nash, (Minerals Metals and Materials Society, Warrendale, PA), 1997.
- 31 Zou J & Balandin A A, J Appl Phys, 89 (2001) 2932.
- 32 Zou J, Kotchetkov D, Balandin A A, Florescu D I & Pollak F H, *J Appl Phys*, 92 (2002) 2534.
- 33 Guy I L, Muensit S & Goldys E M, *Appl Phys Lett*, 75, 4133 (1999).
- 34 Muensit S, Goldys E M & Guy I L, Appl Phys Lett, 75 (1999) 3965.

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