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Piezoelectric polarization effect and phonon relaxation rates in binary wurtzite nitrides

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ABSTRACT

The piezoelectric (PZ) polarization property present in the wurtzite nitrides modifies the group velocity of phonons. As a result, the relaxation rates of phonons are changed. In this paper, we have calculated the relaxation rate of phonons as functions of the phonon frequency in binary wurtzite nitrides (GaN, AlN and InN) using the modified phonon group velocity. Different scattering mechanisms such as Umklapp, point defect, dislocation, boundary and phonon-electron scattering processes have been considered. The percentage change in phonon relaxation rates is found to be maximum for InN and minimum for GaN. This result can be used to study the effect of PZ polarization property on thermal conductivity of these materials. Copyright © 2014 VBRI press.

Keywords: Binary wurtzite nitrides; piezoelectric polarization; group velocity of phonons; phonon relaxation rates.

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Introduction

The wurtzite nitride semiconductors (GaN, AlN, InN and their alloys) are promising materials for the next generation of high-power optoelectronics devices. One of the important issues for further development of wurtzite nitrides is self-heating. Self-heating strongly affects the performance of the device. Recently, wurtzite nitride LEDs suffer from the problem of efficiency droop which resulted from the PZ polarization effect **[1]**. The material in the active layer and the substrate material generally determine the thermal resistance of the device structure. For the above reason, it is important to know the value of thermal conductivity, κ of corresponding material.

The recent experimental value of κ as reported by S. Adachi for GaN films is 1.95 W/cm K **[2]**. For some samples with lower dislocation density, the thermal conductivity value $\kappa = 2.1$ W/cm K has also been reported. The theoretical studies of the thermal conductivity of bulk GaN, conducted by Zou and co-workers **[3]**, on the basis of the Callaway - Klemens approach **[4, 5]**, have reported κ value from 3.36 to 5.40 W/cm K. by taking two sets of material parameters for GaN. They have also demonstrated the effect of impurities and dislocations on thermal conductivity **[6]**. The PZ polarization effect on thermal conductivity, so far in our knowledge has not been considered. As nitride wurtzites are strong PZ polarized materials **[7]**, the effect should be taken to study the change in the thermal conductivity.

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In the earlier work, Sahoo **[8]** studied the group velocity of the phonons by adding PZ polarization property and found an enhancement in the phonon group velocity **[9]**. Using modified phonon group velocity, calculations have been performed for Debye temperature and frequency for both binary and ternary wurtzite nitrides **[8]**. In this present work, we have calculated the change in phonon relaxation rates using the PZ polarization property of wurtzite nitrides. Different relaxation processes such as Umklapp, point defect, phonon boundary, dislocation and phonon-electron scattering have been considered in the calculation.

Photon relaxation rates

According to Callaway model, the thermal conductivity k is given by **[4, 5]-**

$$k(T) = \left(\frac{k_B}{\hbar}\right)^3 \frac{k_B}{2\pi^2 v} T^3 \int_0^{\theta_D/T} \frac{\tau_c x^4 e^x}{(e^x-1)^2} dx \qquad (1)$$

where θ_D is the Debye temperature, k_B is the Boltzmann constant, v is the phonon group velocity, $x = \hbar\omega/k_B T$, ω is the phonon frequency, and τ_c is the combined phonon relaxation time. The two important parameters influencing k are the phonon group velocity v and the combined relaxation time τ_c **[10]**. The polarization-averaged phonon group velocity along a specified crystallographic direction is

$$v = \left[{}^1/_3\left({}^1/_{v_{T1}} + {}^1/_{v_{T2}} + {}^1/_{v_L}\right)\right]^{-1}, \qquad (2)$$

v_L and $v_{T1,2}$ are the longitudinal and transverse phonon velocities, respectively. The longitudinal velocity is defined as $v_L = (C_{33}/\rho)^{1/2}$ and when piezoelectric polarization property of the wurtzite is not accounted the transverse velocity of phonons is $v_T = (C_{44}/\rho)^{1/2}$. But when piezoelectric polarization property is considered the transverse phonon velocity becomes **[9]** $v_{T,P} = [(C_{44} + (e_{15}^2/\varepsilon_0\varepsilon_{11}))/\rho]^{1/2}$, where e_{15} is PZ polarization constant, ε_0 is permittivity and ε_{11} is dielectric constant of the material along x direction. Along [0001] direction, two transverse branches are degenerate and have the same velocity given by $v_{T1} = v_{T2} = v_{T,P}$. Here C_{ij} are the elastic constants of the crystal **[11, 12]**. The material parameters and constants of GaN, AlN and InN are given in **Table1**.

The major phonon relaxation processes which limit κ of a solid are: three-phonon Umklapp (τ_u), point-defect (τ_m), dislocation (τ_d), boundary (τ_b), and phonon-electron scattering (τ_{ph-e}). The scattering rate for Umklapp processes at high temperature (T= 300 K and above) is given by **[7]-**

$$\frac{1}{\tau_u} = 2\gamma^2 \frac{k_B T}{\mu V_0 \omega_D} \omega^2, \qquad (3)$$

where γ is the Gruneisen anharmonicity parameter, $\mu = v_T^2.\rho$ is the shear modulus, $V_0 = \frac{\sqrt{3}}{8} a^2 c$ is the volume per atom, and ω_D is the Debye frequency. The phonon relaxation on mass-difference is **[6]-**

$$\frac{1}{\tau_m} = \frac{V_0 \Gamma \omega^4}{4\pi v^3} \qquad (4)$$

where $\Gamma = \sum_i f_i (1 - \frac{M_i}{\bar{M}})^2$ is the measure of the strength of the mass-difference scattering, f_i is the fractional concentration of the impurity atoms, M_i is the mass of the ith impurity atom, $\bar{M} = \sum_i f_i M_i$ is the average atomic mass. The phonon scattering rate at the core of the dislocation is proportional to the cube of the phonon frequency and is given by **[7]-**

$$\frac{1}{\tau_d} = \eta N_D \frac{V_0^{4/3}}{v^2} \omega^3, \qquad (5)$$

where 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.

Table 1. Material parameters and constants of GaN, AlN and InN **[9, 11, 12]**.

Parameter	GaN	AlN	InN
a_0 (in A^0)	3.189	3.112	3.54
c_0 (in A^0)	5.185	4.982	5.705
e_{15} (C/m^2)	-0.40	-0.48	-0.40
$\varepsilon_{11} (= \varepsilon_{xx})$	9.0	9.5	15.3
C_{33} (in GPa)	405	373	224
C_{44} (in GPa)	95	116	48
v(m/s) (Without PZ effect)	4746	6999	3234
v(m/s) (with PZ effect)	4768	7067	3290
ω_D (rad/sec) Without PZ effect	1.707818×10^{13}	2.041050×10^{13}	1.374585×10^{13}
ω_D (rad/sec) With PZ effect	1.715530×10^{13}	2.060766×10^{13}	1.402005×10^{13}
ρ(Kg/m^3)	6150	3257	6810
Deformation Potential (eV)	8.3	9.5	7.1

The boundary scattering relaxation rate is given in the Casimir limit as-

$$\frac{1}{\tau_b} = \frac{v}{L}, \qquad (6)$$

where L is the dimension of the sample. At low doping levels, the relaxation time for acoustic phonons scattered by electrons can be expressed as **[13]-**

$$\frac{1}{\tau_{ph-e}} = \frac{n_e \epsilon_1^2 \omega}{\rho v^2 k_B T} \sqrt{\frac{\pi m^* v^2}{2 k_B T}} \, exp\left(-\frac{m^* v^2}{2 k_B T}\right), \quad (7)$$

where n_e is the concentration of conduction electrons, ϵ_1 is the deformation potential, ρ is the mass density, and m^* is the electron effective mass. The combine phonon relaxation time can be obtained by the summation of the inverse relaxation times for these scattering processes and is given by

$$\frac{1}{\tau_c} = \frac{1}{\tau_u} + \frac{1}{\tau_m} + \frac{1}{\tau_d} + \frac{1}{\tau_b} + \frac{1}{\tau_{ph-e}}. \qquad (8)$$

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Results and discussion

The combine relaxation rate as functions of phonon frequency is calculated using equation (8) for GaN, AlN and InN. For the calculation we use materials parameters shown in **Table 1**. **Fig. 1** shows the variation of combine scattering rates for GaN at room temperature. Here $\Gamma = 1.3 \times 10^{-4}$, $N_D = 1.5 \times 10^{10}$ cm^{-2}, $n_e = 2.6 \times 10^{18}$ cm^{-3}, $\epsilon_1 = 10.1$ eV, $m^* = 0.22\ m_0$, and L= 22nm are used **[14]**.The dashed curve in **Fig. 1** corresponds to combine scattering rates of phonons where PZ polarization property of the material is not considered.

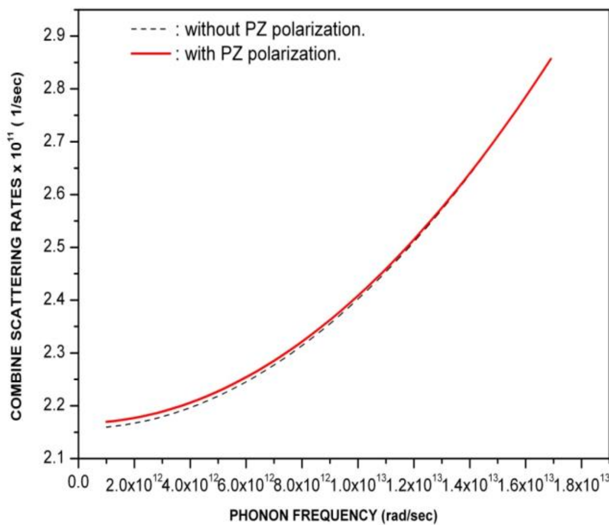

Fig. 1. The combine scattering rates with and without PZ polarization property in GaN at T= 300K due to different scattering mechanisms as functions of the phonon frequency.

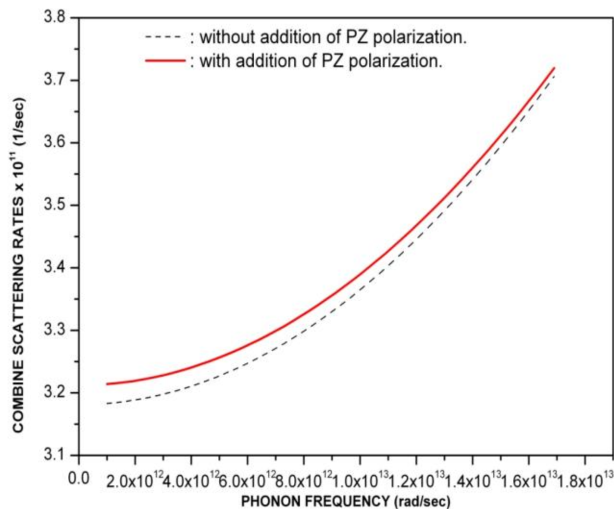

Fig. 2. The combine scattering rates with and without PZ polarization property in AlN at T= 300K.The result takes into account of the three phonon Umklapp, mass-difference, dislocation, boundary and phonon-electron scattering rates.

The solid curve is for the combine relaxation rates where PZ polarization property is taken into account. The difference between these two curves is not large but it can be seen that combine scattering rate for low frequency phonons are changed by PZ polarization property and, it is higher than the combine relaxation rates when PZ polarization property is not considered. As frequency of phonons increases, the separation between these two curves decreases. Finally, the two curves become one indicating that the combine relaxation rate of high frequency phonons are not altered by PZ polarization property of the material. In **Fig. 2**, we present the variation of combine scattering rates as functions of phonon frequency in AlN at room temperature. The dashed curve represents relaxation rates of phonons without addition of PZ polarization property while solid line denotes relaxation rates of phonons when PZ polarization property is added.

Here $\Gamma = 3.2 \times 10^{-4}$, $N_D = 1.5 \times 10^{10}$ cm^{-2}, $n_e = 4.1 \times 10^{18}$ cm^{-3}, $\epsilon_1 = 8.2$ eV, $m^* = 0.30\ m_0$, and L= 22nm are used **[12, 15]**. It can be observed from the **Fig. 2** that the difference between the two curves, in comparison to GaN case, is noticeable. The addition of PZ polarization property in AlN enhances the scattering rates of low frequency phonons and as the frequency of phonons increases the enhancement gradually decreases. Unlike the case of GaN, the combine relaxation rates of high frequency phonons of AlN are altered because of PZ polarization property. This change in combined relaxation rate can enhance the lattice thermal conductivity **[16]**. **Fig. 3** shows the variation of combine phonon relaxation rates in InN as functions of phonon frequency at room temperature. Here $\Gamma = 3.2 \times 10^{-4}$, $N_D = 5 \times 10^{10}$ cm^{-2}, $n_e = 3.3 \times 10^{18}$ cm^{-3}, $\epsilon_1 = 7.1$ eV, $m^* = 0.14 m_0$, and L= 22nm are used **[15, 17]**.

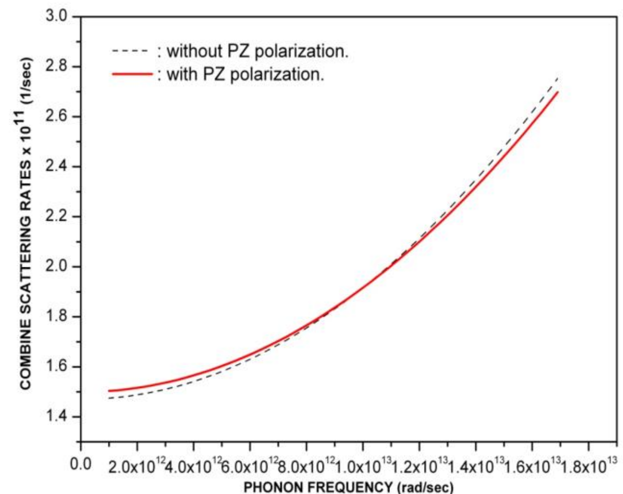

Fig. 3. The combine scattering rates with and without PZ polarization property in InN at T= 300K.The results are shown for three phonon Umklapp, mass-difference, dislocation, boundary and phonon-electron scattering rates.

The dashed curve in **Fig. 3** corresponds to the combine relaxation rates when PZ polarization property is not added. The combine relaxation rates with the addition of PZ polarization is represented by the solid curve. The difference between these two curves is clearly noticeable both for low frequency and high frequency phonons. Comparing the dashed and solid curves, it can be understood that because of addition of PZ polarization property the combine relaxation rates of low frequency phonons are enhanced and there is a decrease of combine relaxation rates for high frequency phonons. At frequency

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around 1.0 x 10^{13}(rad /sec) there is a crossover of the both curves. This result indicates that the combine relaxation rates of phonons of frequency around 1.0 x 10^{13}(rad /sec) remain unaltered by PZ polarization property. This result is a new finding in our work. **Fig. 4** shows the percentage change in relaxation rates of phonons due to addition of PZ polarization property in the materials. This gives a straight forward comparison among GaN, AlN and InN. In **Fig. 4**, the solid curve corresponds to percentage change in combine relaxation rate of phonons in GaN. The dashed curve represents percentage change in AlN and dotted curve denotes for InN. From **Fig.4**, it can be seen that the change in phonon relaxation rate is maximum in case of InN and it is minimum in GaN.

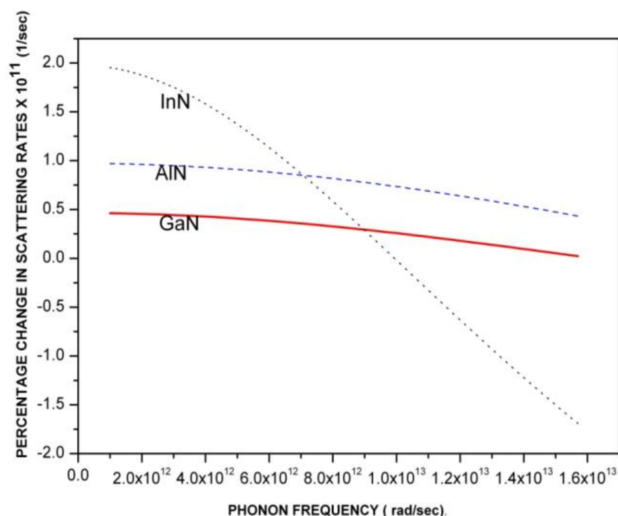

Fig. 4. Percentage change in combine scattering rates in GaN, AlN and InN. Maximum change occurs in InN and minimum occurs in GaN.

Conclusion

The phonon relaxation rates have been investigated theoretically by counting the PZ polarization property of the binary wurtzite nitrides. It is found that the phonon relaxation rate is changed. In case of GaN, the addition of PZ polarization property enhances the combine relaxation rates of low frequency phonons only. The relaxation rates of high frequency phonons are not altered by the addition of PZ polarization property. For AlN, the relaxation rates due to the addition of PZ polarization property is higher than the relaxation rates of phonons without addition of PZ polarization for both low and high frequency phonons. For InN, the combine relaxation rate is increased by PZ polarization at low frequency while at high frequency combine relaxation rate decreases from the combine relaxation rate without PZ polarization. This result can be used for evaluating the PZ polarization effect on thermal conductivity of binary wurtzite nitrides at room temperature. A noticeable change is expected in thermal conductivity of III-nitrides due to addition of PZ polarization property with maximum change in InN and minimum in case of GaN.

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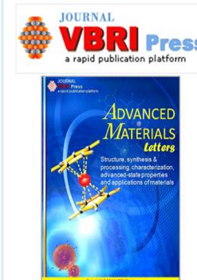

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