Role of polarization electric field on thermal conductivity of GaN/In$_{0.9}$Ga$_{0.1}$N/GaN superlattices

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Abstract. Enhancement in thermoelectric efficiency of GaN/In$_{0.9}$Ga$_{0.1}$N/GaN superlattice (SL) needs higher electrical conductivity ($\sigma$) and Seebeck coefficient ($S$); but lower thermal conductivity ($k$). Both $S$ and $\sigma$ are improved due to the presence of polarization electric field (PEF) of this SL. In this work, the role of PEF on $k$ of SL has been investigated and found that cross-plane and in-plane $k$ are reduced due to PEF up to a certain temperature. Both cross-plane and in-plane thermal conductivities in the presence of PEF show cross over temperature termed as transition temperature ($T_c$). It is noted that $T_c$ for cross-plane and in-plane thermal conductivity of GaN/In$_{0.9}$Ga$_{0.1}$N superlattice (SL) are 510K and 530K, respectively, which depends on In contents. Thus, the preferred value of $S$, $\sigma$ and $k$ of GaN/In$_{0.9}$Ga$_{0.1}$N SL can be achieved as per requirement by changing In content; making it suitable for TE module for maximum power production at room temperature and above.

Keywords: Indium gallium nitride; Superlattice; Thermoelectric efficiency; Polarization electric field.

1. Introduction

Currently GaN/In$_x$Ga$_{1-x}$N/GaN superlattice (SL) is an important structure for the manufacture of laser diodes (LD), light-emitting diodes (LED) and thermoelectric (TE) devices [1]. It is reported that the SL may be a good candidate for TE equipment due to high thermal stability and low thermal conductivity. Thermoelectric (TE) efficiency of a device is directly proportional to the coefficient of seebeck effect and electrical conductivity; but inversely proportional to thermal conductivity ($k$) of the material. A smaller reduction in $k$ will generate significant improvement in TE efficiency. For high temperature TE device GaN/InGaN/GaN SLs are promising structures as it has good thermal stability and low thermal conductivity. Thus, reducing $k$ further, device efficiency can be improved. Chen, Z. et al. reported that $k$ of InGaAs/InGaAsP SL of thicknesses 10, 20, 30 and 40nm were 6.63, 2.09, 4.42 and 5.30 W/m-K at room temperature, respectively [2]. Scott T. Huxtable et al. reported that $k$ of 3500nm thick Si/Si$_{0.5}$Ge$_{0.5}$ at room temperature, respectively [3]. Saha et al. reported that the thermal conductivity due to cross-plane of the Ti$_{0.3}$W$_{0.7}$/Al$_{0.7}$Si$_{0.3}$/S$_{0.3}$/25N SL decreases from 4.5 to 1.7W/m-K as period thickness of SL decreases from 240nm to 4nm, respectively [4]. GaN/In$_x$Ga$_{1-x}$N/GaN SL has a unique property called as polarization property. This polarization property produces electric field known as built in electric field. A. Szein, et al. [5] reported that polarization field increases electrical conductivity and SL seebeck coefficient, although their work lacks the study of polarization effects on thermal conductivity. In this work, we have studied role of polarization field on $k$ of this SLs.
2. Theoretical Development
GaN/InGaN/GaN SL has strain which generates piezoelectric polarization(pz). The pz polarization is calculated by $P_{pz} = \left[ e_{31} \varepsilon_1 + e_{32} \varepsilon_2 + e_{33} \varepsilon_3 \right] \text{C/m}^2$. The constituent material has spontaneous (sp) polarization. The sp polarization is computed by $P_{sp} = \left[ -0.042x - 0.034(1-x) + 0.037(1-x)x \right] \text{C/m}^2$. Here $x$ is In fraction, $e_{ij}$ is piezoelectric coefficient and $\varepsilon_i$ is strain. Total polarization is $P = P_{sp} + P_{pz}$. The material parameters of In$_x$Ga$_{1-x}$N are taken from ref. [2]. In this SL, GaN acts as barrier whereas InGaN acts as well. The electric field due to total polarization in well $E_w$ (or $E_b$ in barrier) semiconductor layers are:

$$E_w = L_b (P_b - P_w) / (\varepsilon_0 \varepsilon_r w_b)$$  \text{ and }  
$$E_b = L_w (P_w - P_b) / (\varepsilon_0 \varepsilon_r w_w).$$

Here $L_w$ ($L_b$), $P_w$ ($P_b$) and $\varepsilon_r$ ($\varepsilon_r$) are respectively thickness of well (barrier) layer, polarization in well (barrier) layer and dielectric constant of well (barrier) material.

Figure 1. GaN/ In$_x$Ga$_{1-x}$N/GaN SL

The field is of the order of $\sim 10^9 \text{ V/cm}$. According to Heckmann principle Coupling of polarization electric (PE) field and strain modifies thermal properties of SL via elastic constant as constituents are piezoelectric materials. The elastic constant of In$_x$Ga$_{1-x}$N including polarization field has been found as, $C_{44,p}^{\text{InGaN}} = C_{44}^{\text{InGaN}} + \left[ \left( e_{15}^2 + e_{31}^2 + e_{33}^2 + p_{ap} \right) / \varepsilon_0 \varepsilon_r \right] ^{\text{InGaN}}$, where $C_{44}^{\text{InGaN}}$ is elastic constant of In$_x$Ga$_{1-x}$N absence of polarization mechanism. Modified elastic constants tailor the phonon velocity, phonon scatterings in the presence of polarization field effect. Phonon velocity has been computed by $v = \sqrt{C_{44,p}^{\text{InGaN}} / \rho}$. The Debye frequency depends on phonon group velocity as $\omega_D = \sqrt{3N / 4\pi V_0}$, where $N$ is atoms number in the volume $V_0$, and Debye temperature depends on Debye frequency as $\theta_D = h \omega_D / k_B$, where $k_B$ is Boltzmann’s constant and $h$ is Planck’s constant. It has been seen that polarization electric field not only enhances thermal parameters of In$_x$Ga$_{1-x}$N but also contributes their bowing constants.

In semiconductors, the heat energy is transported by acoustic phonons. The thermal conductivity is the sum of both phonon and electron thermal conductivity as $k = k_{ph} + k_e$, where $k_{ph}$ is phonon
thermal conductivity and \( k_e \) is electron thermal conductivity. Experiments reported that \( k_e \approx 10^{-3} k_{ph} \). \( k_e \) can therefore be ignored and for a semiconductor \( k \approx k_{ph} \). Callaway formula is used to determine \( k \) of each layer \( (x = h_\omega / k_{ph}T) \)

\[
k(x) = \frac{k_{ph}}{2\pi^2 h^3 v} \int_0^1 \frac{x^4 e^x}{(e^x - 1)^2} dx.
\]

Interfaces generate thermal boundary resistance (TBR) due to different materials. TBR can be computed by using the transmission coefficient of the materials expressed as \([6]\)

\[
\Gamma_{ij} = p \Gamma^s_{ij} + (1-p) \Gamma^d_{ij}
\]

Where \( p \) is specularity parameter taking values from 0 to 1; \( \Gamma_{ij}^s \) is specular transmission coefficient and \( \Gamma_{ij}^d \) is diffuse transmission coefficient. Specular transmission coefficient and diffuse transmission coefficient calculated by

\[
\Gamma_{ij}^s = (4 \rho_i \rho_j v_i v_j \cos \theta_i \cos \theta_j \left(\rho_i v_i \cos \theta_i + \rho_j v_j \cos \theta_j\right))^2 \quad \text{and} \quad \Gamma_{ij}^d = (C_j v_j (C_i v_i + C_j v_j)^{-1})
\]

respectively;

where \( \rho \) density of the material , \( v \) phonon group velocity, \( \theta \) angle of incidence, \( C \) specific heat of the material. By estimating all above terms, it is easy to calculate TBR of the material \( i \) to \( j \) and it is computed by\([7]\);

\[
R_{ij} = \left[ \frac{4\pi^2 h^3 v_i^2}{k_i^3 \Gamma_{ij}^s} \right] \int_0^1 x^4 e^x / (e^x - 1)^2 dx
\]

First, every surface thermal conductivity \( k_{ph} \) is computed in the same way as the bulk material’s thermal conductivity. Then TBR is computed. SL’s in-plane and cross-plane thermal conductivity for a period of two layers can be determined by using measured layer thermal conductivity and TBR \([8]\);

\[
k_{\text{in-plane}} = (L_1 k_1 + L_2 k_2) / (L_1 + L_2)
\]

\[
k_{\text{cross-plane}} = (L_1 + L_2) \left\{ (L_1 / k_1) + (L_2 / k_2) + (R_1 + R_2) \right\}
\]

Where \( L \) is thickness of first material and \( L_2 \) is thickness of second material, while \( k_1 \) and \( k_2 \) are the corresponding surface thermal conductivities. \( R_1 \) and \( R_2 \) are the TBRs from first layer and second layer, respectively.
3. Results and Discussion

![Thermal boundary resistance of GaN/In$_x$Ga$_{1-x}$N/GaNSL(x=0.9)](image)

**Figure 2.** Thermal boundary resistance of GaN/In$_x$Ga$_{1-x}$N/GaNSL(x=0.9).

The elastic constants, group velocity due to phonon, Debye temperature of GaN/In$_x$Ga$_{1-x}$N/GaNSL have been calculated including and excluding the effect of polarization field. It has been investigated that due to this interfacial polarization electric field all above parameters are significantly enhanced. Since all these parameters are used to estimate layer’s thermal conductivity given by Callaway formula, thermal conductivity of each layer is modified. TBR in between the interfaces is also calculated through the equation 3. From fig.2 it is found that there is no significant variation between the TBRs induced by PEF and without PEF in low temperature limit. Below 200K temperature TBR without PEF is slightly smaller than TBR with PEF; however, above 200K temperature PEF reduces TBR further. Therefore, it is concluded in the high temperature limit TBR with PEF decreases than TBR without PEF.
Figure 3. In plane and cross plane thermal conductivity of GaN/InxGa1-xN/GaNSL(x= 0.9).

From figure 3, it can be seen, due to the influence of polarization electric field; in plane thermal conductivity of GaN/In0.9Ga0.1N SL decreases significantly up to the temperature 530K then above 530K in plane thermal conductivity increases due to PEF, whereas due to both the effect of interfacial polarization electric field and TBR, reduction of cross plane thermal conductivity occurs within the temperature range 60-510 K, when the In content of SL is maintained 0.9 unit and thickness of both well and barrier are maintained 10nm and 15nm respectively. Above 510K cross plane thermal conductivity with PEF exceeds than without PEF. In plane thermal conductivity with and without PEF show cross over temperature at 530K called as transition temperature(Tc) of in plane thermal conductivity, whereas cross plane thermal conductivity with and without PEF show cross over temperature at 510K called as transition temperature of cross plane thermal conductivity of GaN/In0.9Ga0.1N SL.

4. Conclusion
The interfacial polarization electric field effect on thermal properties of GaN/InGaN/GaN SL has been theoretically explored. The change in thermal conductivity ($k$) with temperature presence of polarization field and the effect of TBR predicts both in plane as well as cross plane thermal conductivity decrease with in temperature range 200K to 600K. This reduced thermal conductivity of GaN/InGaN/GaN SL significantly enhances the TE efficiency. Therefore, GaN/InGaN/GaN SLs are the best structures for the TE device preparations at room temperature and above.

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