Thermal and electrical properties of In$_x$Al$_{1-x}$N alloy

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Abstract. In$_x$Al$_{1-x}$N is a promising semiconducting material due to its wide range of potential applications in optoelectronics, bio sensing and in thermoelectric power generation. It has a tunable band gap (6 to 0.7eV), high electron saturation velocity, mobility (290 cm$^2$/Vs) and non-toxic nature. Due to this, the material’s electrical and thermal properties require further study in detail to explore more potential applications. In this work, we have investigated theoretically the thermal and electrical properties of In$_x$Al$_{1-x}$N alloy to predict thermoelectric (TE) figure of merit and performance to identify the most promising composition and carrier densities for optimum power generation at room temperature and above.

1. Introduction

III-nitride semiconductors are very useful materials for high-power and high temperature opto-electronics and thermoelectric (TE) devices. In addition to their wide band gap, nitride materials also demonstrate excellent electronic and thermal properties. III-nitride based materials are increasingly used in a wide variety of application such as laser diodes, LEDs and solar cells with a number of commercial products already available [1,2]. Thermoelectric effect is a phenomenon in which heat energy is converted into electrical energy and vice versa [3]. In order to improve efficiencies, new materials with high TE figure of merit (ZT) must be developed. The efficiency of a TE device is directly related to ZT. Figure of merit is given by

$$ZT = \frac{S^2 \sigma T}{k_{\text{lattice}} + k_{\text{electron}}}$$

Here, $\sigma$ is electrical conductivity, $S$ is Seebeck coefficient, $k$ is thermal conductivity due to the lattice vibration ($k_p$) and electron conduction ($k_e$), and $T$ is the absolute temperature. The ZT value of the best commercial TE material such as III-nitride semiconductors (GaN, AlN and InN) has attracted attention as potential system for optical and electrical devices. Liu et al investigated ZT value for bulk GaN at T=300K, is about 0.0017 while it can reach 0.2 in the thermally resistive Al$_{0.4}$Ga$_{0.6}$N alloy at 1000K [4]. Taylor and Francies investigated ZT for InN/AlN heterojunction is 0.014 at 8K and then decreases up to 40K. Recently, ternary nitrides (InAlN etc) are promising materials for high ZT. InGaN alloy have been shown to have high ZT at room temperature [5,6]. Sztein et al predicted ZT of 0.57 at 1200K for AlGaN. The TE properties of AlInN alloy experimentally investigated by Tong et al [15]. Experimental result has been motivated to
research to explore theoretically. In this work, we present the theory of thermal, electrical properties and ZT of In$_x$Al$_{1-x}$N alloy.

2. Electrical and thermal Transport properties

2.1 Electron transport model

The TE characteristics, electrical conductivity ($\sigma$), Seebeck coefficient ($S$), and $k_e$ are derived from the solution of the Boltzmann transport equation.

$$\sigma = \frac{-2q^2}{3m} \int_{E=0}^{E} \frac{\delta f_o D(E) E \tau dE}{\partial E}$$

(2)

$$S = \frac{1}{qT} \left\{ \int_{E=0}^{E} \frac{\delta f_o D(E) E (E - \mu) \tau dE}{\partial E} \right\}$$

(3)

$$k_e = \frac{2}{3mT} \left\{ \int_{E=0}^{E} \frac{\frac{\delta f_o}{\delta E} D(E) E^2 \tau dE}{\partial E} - \int_{E=0}^{E} \frac{\delta f_o}{\partial E} D(E) E \tau dE \right\}$$

(4)

Here, $q$ is charge of electron, $E$ is electron energy, $D(E)$ is density of state, $\mu$ is chemical potential and $f_0(k)$ is the Fermi - Dirac distribution function which is expressed by

$$f_o(k) = \frac{1}{\exp \left( \frac{E(k) - \mu}{k_BT} \right) + 1}$$

(5)

The energy dependent electron relaxation time $\tau_{el}(E)$ as per relaxation time approximation (RTA) is given by [14]

$$\tau_{el}^{-1}(E) = \sum \tau_{i}^{-1}$$

(6)

Here, the index $i$ describes different scattering term. The scattering mechanism is combination of piezoelectric scattering, impurity scattering, alloy scattering, polar optical phonon scattering, deformation potential scattering, and charge dislocation scattering.

2.2 Phonon transport model

The phonon component of thermal conductivity is first proposed by Callaway [7]. The Thermal conductivity of a material can be expressed by $k = k_{ph} + k_e$ where $k_{ph}$ is the thermal conductivity due to phonons and $k_e$ is thermal conductivity due to electrons. Florsecu et al. [8] experimentally found that $k_e = 10^{-3} k_{ph}$. So, $k_e$ is neglected and for a medium doped semiconductor $k = k_{ph}$. The Callaway model for $k_{ph}$ InAlN can be written by

$$k = \frac{k_{ph}T^3}{2\hbar^2 \pi^2 \nu} \int_0^{\theta_d} \tau_{C}(x) \frac{x^4 e^x}{(e^x - 1)^2} dx$$

(7)

Here $\nu$ is average group velocity, $\theta_d$ is Debye temperature and $\tau_C$ represent the combined scattering time due to both normal and resistive processes. The variable of $x$ is connected to the phonon frequency($\omega$), is defined by
The phonon normal scattering \((\tau_N^{-1})\) represent phonon-phonon scattering where momentum is conserved and in resistive scattering \((\tau_R^{-1})\), the momentum is not conserved \([10-13]\). The key resistive rates are three phonon Umklapp scattering \((\tau_U^{-1})\), dislocation scattering \((\tau_D^{-1})\), phonon-electron scattering \((\tau_{e-p}^{-1})\) and boundary scattering \((\tau_B^{-1})\), virtual atomic mass \(M\) describes by alloy components

\[
M = y_A M_A + (1 - y_A) M_B,
\]

\(y_A\) is mass fraction of alloy constituent \(A\); and \(M_A\) and \(M_B\) represent atomic masses of constituents \(A\) and \(B\) respectively.

The normal scattering is given by

\[
\tau_N^{-1} = \frac{k_B T}{\hbar \omega} e^{-\omega/3T} \tag{8}
\]

Here \(\gamma\) is Gruneisen parameter, \(V\) volume per unit atom, phonon-phonon scattering events where momentum is not conserved called Umklapp scattering and given by \([13]\).

\[
\tau_U^{-1} = \frac{\hbar^2 \omega^2 T}{M \nu \theta_f} e^{-\omega/3T} \tag{9}
\]

Point defect scattering is a very important scattering which having due to heavily doped atoms. It is also known as mass defect scattering following the approach of Liu et al. \([14]\).

\[
\tau_{e-p}^{-1} = \frac{V_0 \Gamma \omega^4}{4\pi^3} \tag{10}
\]

Here, \(\Gamma\) is point defect scattering factor \([14]\). The phonon scattering rate at the core of the dislocation is proportional to the cube of the phonon frequency and is given by.

\[
\tau_D^{-1} = \eta N_D \frac{V_0^4/3}{V^2} \omega^3 \tag{11}
\]

Here, \(N_D\) is density dislocation lines, and \(\eta\) is weight factor to account for the mutual orientation of the direction of the temperature gradient and the dislocation line. The average value of \(\eta = 0.55\), at low doping levels, electron-phonon scattering is given by,

\[
\tau_{e-p}^{-1} = \frac{n e_i^2 \omega}{\rho v^2 k_B T} \sqrt{n m^* v^2} \exp \left( - \frac{m^* v^2}{2k_B T} \right) \tag{12}
\]

Here \(n\) is electrons concentration, \(e_i\) is deformation potential, and \(m^*\) is electron effective mass. The boundary scattering is,

\[
\tau_B^{-1} = \frac{\nu}{L} \tag{13}
\]

Here \(L\) is the dimension of the sample. The combined phonon relaxation time is given by.

\[
\tau = \frac{1}{\tau_N} + \frac{1}{\tau_U} + \frac{1}{\tau_p} + \frac{1}{\tau_D} + \frac{1}{\tau_B} + \frac{1}{\tau_{p-e}} \tag{14}
\]
3. Results and discussion

We have computed combined relaxation time for phonons in In$_x$Al$_{1-x}$N at room temperature, which is shown in figure 1. It can be found that combine relaxation time ($\tau$) decreases with phonon frequency at room temperature. It has been observed that point defect scattering is the dominant mechanism due to which phonon relaxation time decreases. It is important to keep in mind that the relaxation time affects thermal conductivity. Material parameter values have been taken from ref. [9,10].

![Figure 1](image1.png)

**Figure 1.** Combine relaxation time for In$_x$Al$_{1-x}$N alloy at room temperature.

We have computed thermal conductivity of InAlN at 300K. Figure 2 shows the $k$ of InAlN alloy. It can be seen that when Al-content varies from $x=0.1$ to 0.5, thermal conductivity ($k$) of InAlN decreases initially and attains minima at $x=0.5$ and when Al content varies from $x=0.5$ to 0.9, $k$ increases and finally catches thin film limit. The simulated $k$ is compared with available experimental results. It can be observed that simulated $k$ is close to experimental results.

![Figure 2](image2.png)

**Figure 2.** Thermal conductivity for In$_x$Al$_{1-x}$N alloys with various Al-contents.
The thermoelectric property of InAlN is experimentally investigated by Tong et al and found that n-type In$_{0.17}$Al$_{0.83}$N film ($n$= 5.1x10$^{18}$ cm$^{-3}$) has thermal conductivity $k$ equal to 4.87 W/(m-k), electrical conductivity $\sigma$ equal to 2.38x10$^4$ (Ω-m), and Seebeck coefficient $S$ equal to -6.012x10$^{-4}$ (V/K). The power factor ($P$) for the n- In$_{0.17}$Al$_{0.83}$N was measured as 0.864x10$^{-2}$ W/(mK$^2$) and the TE figure of merit ($ZT$) value of 0.532 was measured at room temperature [$T$=300K]. The result shows InAlN alloy exhibits excellent material for thermoelectric application.

4 Conclusions
Thermal and electrical properties In$_{x}$Al$_{1-x}$N alloy are studied. Thermal conductivity is calculated by Callaway model for phonon transport. III-V nitride semiconductors are one of the good choices due to medium range of carrier concentration (5.1x10$^{18}$ cm$^{-3}$), high carrier mobility, high Seebeck coefficient and low thermal conductivity, which is relevant for improving thermodynamic efficiency. The accuracy of theoretical result is confirmed through comparison to experimental data.

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