

High Temperature Transport Properties of AlGaN/GaN Heterostructures

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Abstract—High temperature transport properties of the two-dimensional electron gas (2DEG) in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures are investigated theoretically. An overview of previous high temperature investigations of the 2DEG mobility and density is provided. A one-dimensional Schrodinger-Poisson solver is used to determine the 2DEG sheet concentration as a function of temperature. A method of calculating the polar optical phonon scattering rate is shown.

Index Terms—AlGaN, GaN, phonon scattering, temperature, transport.

I. INTRODUCTION

Electronic devices based on $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures have shown promise as high temperature and high power devices due to the large energy band gaps of the materials involved. It is known that a two dimensional electron gas (2DEG) is formed at the interface of an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure even without intentional doping, due to the spontaneous and piezoelectric polarizations. To understand device operation, it is thus important to understand the 2DEG carrier density, mobility, and the scattering mechanisms at high temperatures. In this report, we provide a review of prior art studies of the temperature dependence of the 2DEG properties. In addition, we provide our own theoretical study of the 2DEG carrier density as a function of temperature using a one dimensional self consistent Schrodinger-Poisson solver. Finally, we provide an overview of scattering processes in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures and outline a method to calculate the polar optical phonon scattering rate.

II. PRIOR ART

Figure 1 shows the 2DEG mobility and density as a function of temperature for an $\text{Al}_{0.18}\text{Ga}_{0.82}\text{N}/\text{GaN}$ heterostructure [1]. High temperature Hall measurements were performed from room temperature up to 500°C on this structure, consisting of a 20 nm unintentionally doped AlGaN layer grown on a $2.2\ \mu\text{m}$ thick unintentionally doped GaN layer. It can be seen that the 2DEG density decreases with increasing temperature up to approximately 250°C and then begins increasing with increasing temperature above this. This behavior can be explained with the aid of figure 2 [1]. Figure 2 shows the temperature dependence of mobility and electron

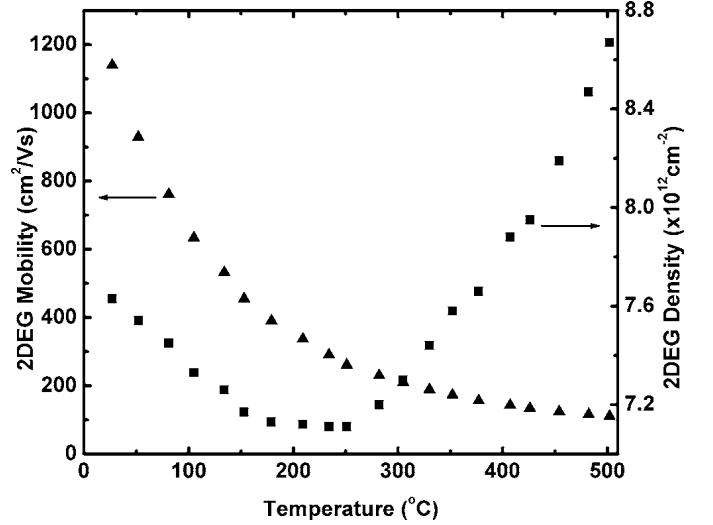


Fig. 1. Temperature dependence of the 2DEG mobility and density in an $\text{Al}_{0.18}\text{Ga}_{0.82}\text{N}/\text{GaN}$ heterostructure [1].

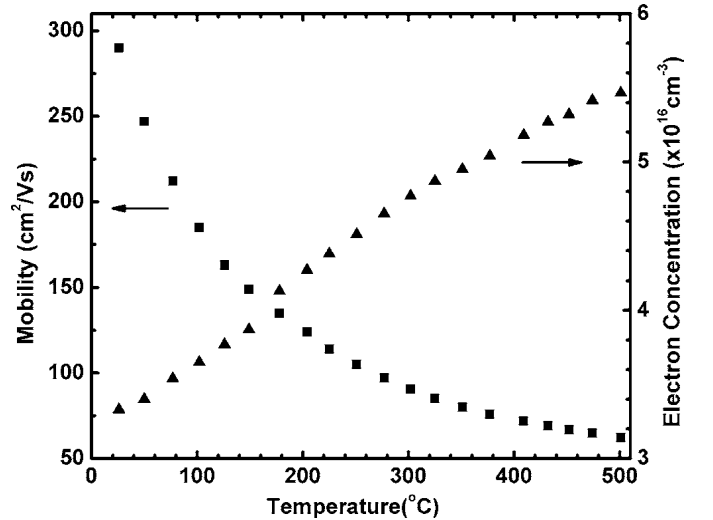


Fig. 2. Temperature dependence of the mobility and electron concentration of unintentionally doped GaN layer [1].

concentration in the i-GaN layer of the heterostructure. In the temperature range below 250°C , the 2DEG mobility is large in comparison with the bulk GaN mobility. Now, the measured 2DEG density and mobility can be expressed as

$$n_M \mu_M = n_{2DEG} \mu_{2DEG} + n_{GaN} \mu_{GaN} \quad (1)$$

where n_M and μ_M are the measured density and mobility,

$n_{2\text{DEG}}$ and $\mu_{2\text{DEG}}$ are the actual sheet density and mobility, and n_{GaN} and μ_{GaN} are the actual carrier concentration and mobility of the i-GaN layer. Thus, the measured 2DEG density is in fact the true 2DEG density below 250°C. The decrease in 2DEG density with temperature can be attributed to the decrease in the conduction band offset with temperature and hence a decreasing quantum well depth.

Above 250°C the 2DEG mobility and bulk GaN mobility become comparable. Thus, the measured density will contain a contribution from the bulk GaN density. As seen in figure 2, this concentration increases with temperature due to the increase in background electron concentration with temperature. Thus, the increase in 2DEG density with temperature can be attributed to this increase in background electron concentration.

It is well established, that the intrinsic carrier concentration (n_i) in GaN is low compared to the donor concentration [2]. Even at 1000K, n_i is about 10^{12} cm^{-3} whereas the donor concentration of an unintentionally doped GaN layer is about 10^{16} cm^{-3} . This allows GaN based devices to operate at a very high temperature without entering the intrinsic temperature region.

Having said that, it is essential to examine the scattering mechanisms and mobility variation at high temperature. But S. B. Lisesivdin [3] showed evidence that the dominant scattering mechanism at very high temperature is polar optical phonon scattering. In the following sections, the effect of temperature on bandstructures, 2 DEG carrier density and how they affect the polar optical phonon dominated mobility have been investigated.

III. 1D POISSON 2DEG DENSITY SIMULATIONS

In order to investigate the temperature dependence of 2DEG sheet density in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, a theoretical calculation has been performed using a 1D Poisson solver [4]. This solver uses the method of finite differences to find the one-dimensional band diagram of a semiconductor structure. Figure 3 shows the heterostructure we have used for the simulation.

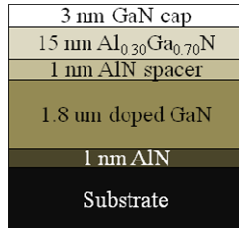


Fig. 3. The AlGaIn/GaN heterostructure used for simulation.

The band gap of GaN, AlN and AlGaIn alloys depends on temperature [5]. So to incorporate this effect in the Poisson solver we have calculated the bandgap of GaN, AlN, $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ and their respective conduction band offset at

different temperature. The band gap of GaN and AlN was calculated using the Varshni equation.

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{\beta + T} \quad (2)$$

Where $E_g(0)$, α and β are suspected to be 3.5 eV, 0.94 meV/K, 791 K and 6.2 eV, 2.63 meV/K, 2082 K for GaN and AlN, respectively [5]. The band gap of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ is calculated using the commonly known compositional dependence

$$E_g(x, T) = (1 - x) E_{g\text{GaN}}(T) + x E_{g\text{AlN}}(T) - b x (1 - x) \quad (3)$$

Where b is about 1 eV. The conduction band offset of the heterostructure is assumed to be 70% of the total band gap difference. Figure 4 and 5 show the temperature dependence of the bandgap of GaN, AlN, $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ and their respective conduction band offset.

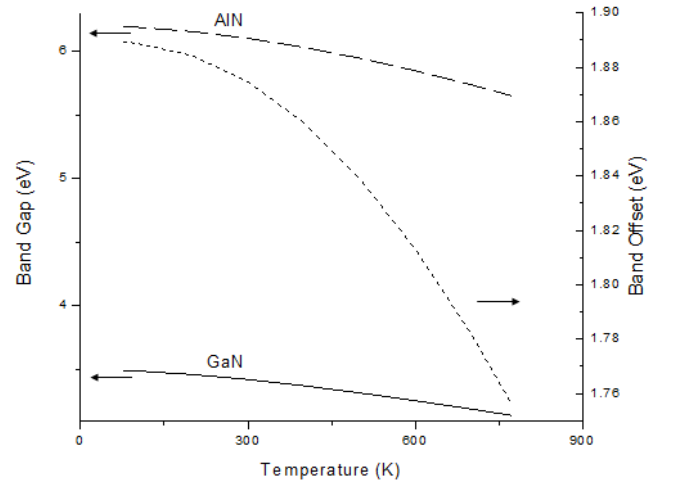


Fig. 4. Temperature dependence of AlN and GaN bandgap and their respective conduction band offset.

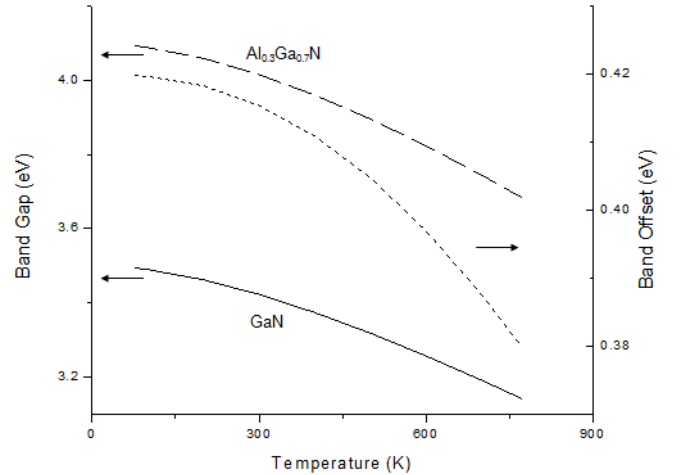


Fig. 5. Temperature dependence of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ and GaN bandgap and their respective conduction band offset.

Deep-level defects in AlGaIn/GaN heterostructures at 0.21 eV and 0.23 eV below the conduction band have been reported [6]. 0.21 eV defect is due to point defects such as nitrogen vacancies, while the 0.23 eV defect is related to extended

defects due to the interface between the GaN and AlGaIn layers. In our simulation we have considered the deep level defect in AlGaIn/GaN heterostructures at 0.21 eV.

Figure 6 and 7 show the calculated conduction band edge with respect to temperature. From figure 7 it is evident that the well depth reduces with the increase of temperature.

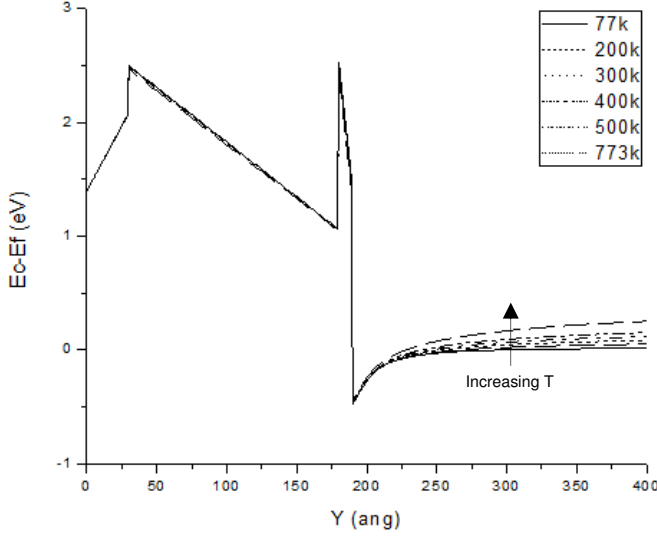


Fig. 6. Calculated conduction band edge along the growth direction with respect to temperature.

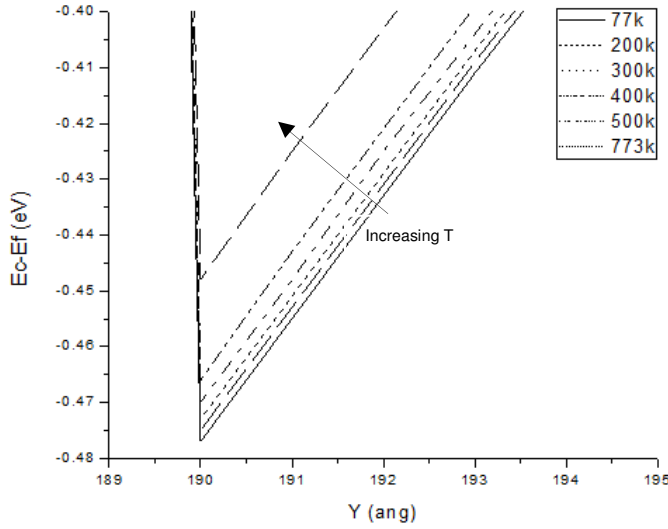


Fig. 7. Calculated conduction band edge inside the well with respect to temperature.

Figure 8 and 9 show the sheet density in GaN layer and in 2D well with respect to temperature. From the figure it is found that although the overall bulk sheet density in GaN increases with temperature it decreases in 2D well. We think that, the decrease of the 2DEG density with the increase in temperature is caused by the reduction of the well depth with temperature. On the other hand the increase in bulk sheet density with temperature is due to the ionization of the deep level defects. At low temperature overall sheet density is dominated by 2D well but at higher temperature it is dominated by bulk sheet density. Although the overall sheet

charge density decreases with temperature initially, it increases with temperature afterwards. Published data [1] shows the similar temperature dependency of sheet charge in AlGaIn/GaN heterostructure.

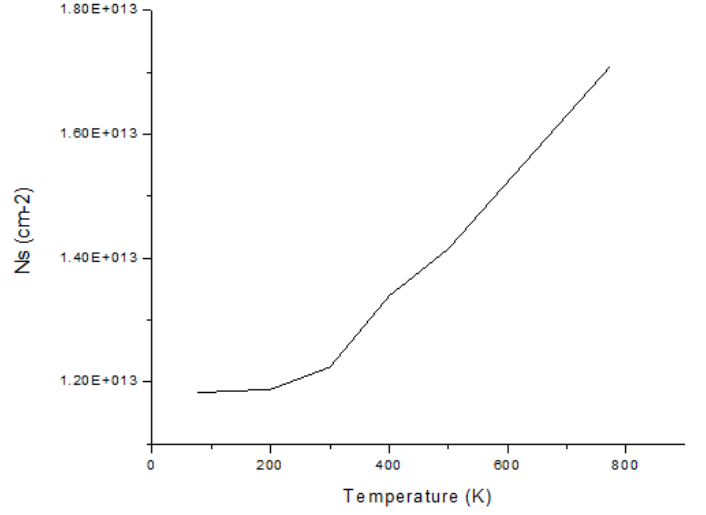


Fig. 8. Calculated sheet charge density in GaN layer with respect to temperature.

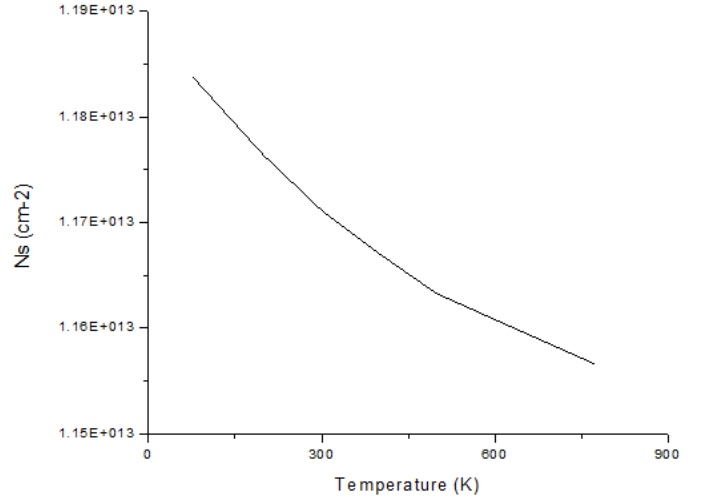


Fig. 9. Calculated sheet charge density inside the 2D well with respect to temperature.

IV. PHONON SCATTERING RATE

In AlGaIn/GaN heterostructure, 2D quantum well is formed. So scattering rate should consider bound states in the 2DEG if electrons occupy only in the well. According to our simulation, lowest 2 subbands are full. Therefore the bottom two subbands will be taken into account when the scattering rate is calculated.

Scattering rate for polar optical phonon in 2DEG is calculated on the basis of the following matrix element.

$$H_{p'p} = \int_{-\infty}^{\infty} F_f^*(z) \frac{e^{-ip_y \cdot \rho / \hbar}}{\sqrt{A}} (A_\beta K_\beta e^{i\beta_1 \cdot \rho} e^{i\beta_2 z}) F_i(z) \frac{e^{ip_y \cdot \rho / \hbar}}{\sqrt{A}} dz d\rho$$

Where A_β and K_β are related to the amplitude of oscillation/vibration and scattering potential respectively. A_β and K_β are given by the following equations.

$$|K_\beta|^2 = \left(\frac{\rho q^2 \omega_0^2}{\beta^2 \kappa_0 \epsilon_0} \right) \left(\frac{\kappa_0}{\kappa_\infty} - 1 \right)$$

$$|A_\beta|^2 = \frac{\hbar}{2(2\pi)\rho\Omega\omega_\beta} (N_{\omega_\beta})$$

The scattering time from initial to final state is defined as,

$$\frac{1}{\tau_{fi}} = \sum_{p_i} \frac{2\pi}{\hbar} \left\{ \sum_{p_z} |I_{fi}(\beta_z)|^2 |K_\beta|^2 |A_\beta|^2 \right\} \delta_{p_i, p_i \pm \hbar\beta_i} \delta(E' - E \mp \hbar\omega)$$

Where $I_{fi} = \int_{-\infty}^{\infty} F_f^*(z) F_i(z) e^{\pm\beta_z z} dz$ and F_n is envelope function. Subscript i and f denote initial and final state. In our case we will only consider intraband scattering since the probability of interband scattering is low compared to intraband one.

V. CONCLUSION

The 2 DEG electron density of AlGaN/GaN heterostructure has been calculated for a range of very high temperature incorporating the effect of band offset variation and deep level defects. The next step is to match the calculated 2DEG density closely with the experimental results. An appropriate relationship between the calculated carrier density and the mobility of the 2DEG channel will be formulated considering polar optical phonon scattering. The mobility of 2 DEG will also be compared with bulk GaN mobility at very high temperature to see if they have significant difference.

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