

A quantitative study of nitrogen content influence on the carrier mobility in GaN_xAs_{1-x} ($0.008 < x < 0.022$)

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In this article we report our theoretical analysis of the electrical transport properties for experimental data on three Si-doped dilute nitride GaN_xAs_{1-x} ($0.008 < x < 0.022$) samples. Our analysis is based on effective electron scattering mechanisms including acoustic, piezoelectric and polar optical phonons, ionized and neutral impurities, dislocations and random and cluster alloys. Our analytical results show that: (a) As the nitrogen concentration increases, both the dislocation and the trap density increase, in the range $(3-7) \times 10^9 \text{ cm}^{-2}$ and $(0.5-4) \times 10^{17} \text{ cm}^{-3}$ respectively. (b) In the sample with the lowest N-content ($x=0.8\%$) the cluster alloy dominates throughout temperature range 77-300 K. For other samples with $x=1.7$ and 2.2% , gradually the dislocation and neutral impurity scattering dominate the cluster alloy scattering up to 200 K.

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1. Introduction

In the last decade, investigations and researches have been widely focused on III-V dilute nitride (less than 5%) compound semiconductors. It has been revealed that there are anomalous behaviours including appreciable reductions in their band gap [1-3] as well as reductions in electrons mobilities and concentrations [4-8]. There is also a drastic increase in the bowing parameter [3, 9, 10] and the electron effective mass (m_e) [3, 11, 12] in these materials.

In this paper, we are interested in a quantitative description of the electrical transport properties in bulk Si-doped GaN_xAs_{1-x} ($0.008 < x < 0.022$), as reported by Ishikawa et al. [13]. All these samples were grown on semi-insulating $GaAs$ (001) substrates using the molecular-beam epitaxy (MBE) method, at 450°C . The thickness of the layers ranged from 500 to 700 nm. The samples were Si doped with a concentration (N_{Si}) of about $1 \times 10^{18} \text{ cm}^{-3}$. The electron concentration (n) and the mobility were obtained from Hall effect measurements on samples in the van der Pauw geometry. This research group presented a data analysis related to the temperature dependence of the resistivity in their samples. In interpreting the data, they focused on the influence of potential fluctuations and the resulting carrier localization. According to this model, depending on the electron concentration and the N content in their as-grown samples (i.e. sample labelled 082, with $x=0.8\%$) a metallic conductivity, and in samples labelled 172 with $x=1.7\%$ and 222 with $x=2.2\%$ a thermally activated conductivity from localized to delocalized states has been suggested.

Here our analysis, which can be complementary to the source paper, gives an explanation for the reduction in the electron mobility and their concentration, regarding the creation of an inhomogeneous N distribution, dislocations and neutral impurity and trap centres, by increasing the

nitrogen content in the material. This work is mainly based on mobility data analysis using various scattering processes: phonon limited mobilities including acoustic, piezoelectric and polar-optical phonons, plus ionized and neutral impurities, dislocations, random alloys and cluster in the framework of Matthiessen's rule.

2. Theory of scattering processes

Here, the mobility limit due to each individual scattering process is calculated independently, using their average relaxation time $\langle\tau_i(x)\rangle$ given elsewhere [14], or by their corresponding analytical expressions (μ_i).

2.1 Phonon scattering mechanisms

a. deformation acoustic potential scattering

The mobility limited by acoustic-mode deformation potential scattering is [15]:

$$\tau_{ac}(x) = \frac{2.4 \times 10^{-20} C_1 (\text{dyn/cm}^2) \left(\frac{m_0}{m_e^*} \right)^{3/2}}{E_{ac}^2 (eV) T^{3/2}} x^{-1/2} \quad (1)$$

The material parameters involved in the scattering mechanisms are introduced in Table 1.

b. piezoelectric scattering

The mobility limited by piezoelectric scattering is given by [16]:

$$\tau_{pe}(x) = \frac{9.54 \times 10^{-8} C_1}{h_a^2 (V/cm) (3/C_1 + 4/C_2)^{1/2}} \left(\frac{m_0}{m_e^*} \right)^{1/2} x^{1/2} \quad (2)$$

c. polar optical phonon scattering

Ehrenreich has derived an analytical expression for the mobility limit due to polar optical scattering as follows [17]:

$$\tau_{po}(x) = \frac{9.61 \times 10^{-15} \epsilon_s \epsilon_\infty [\exp(\theta/T) - 1] \left(\frac{m_0}{m_e^*} \right)^{1/2}}{[\epsilon_s - \epsilon_\infty] \theta^{1/2} (\theta/T)} x^r \quad (3)$$

where $\theta (= \hbar \omega_{LO}/k_B)$ is the longitudinal optical (LO) phonon temperature and r varies with θ/T . For simplicity, we have considered $r = 0.3$ as an average value for $T > 100\text{K}$.

2.2 Extrinsic Scattering Mechanisms:

d. ionized impurity scattering

The mobility limited by ionized impurity has been formulated by Brooks and Herring after taking into account the screening effect of both the free carriers and the impurity ions, and has the following expression [18]:

$$\tau_n(x) = \frac{0.414 \epsilon_s^{2/3} T^{3/2}}{N_i (cm^{-3}) g(n, T, x)} \left(\frac{m_e^*}{m_0} \right)^{1/2} x^{3/2} \quad (4)$$

where

$$g(n, T, x) = \ln(1+b) - \frac{b}{1+b}, \quad b = 4.31 \times 10^{13} \frac{\epsilon_s T^2}{n} \left(\frac{m_e^*}{m_0} \right) x$$

e. neutral impurity scattering

The neutral impurity mobility has been modeled by Erginsoy [19] as:

$$\tau_n(x) = \frac{8.16 \times 10^6 (m_e^*/m_0)^2}{N_n (cm^{-3}) \epsilon_s} \quad (5)$$

where N_n is the neutral impurity concentration $[(1-\varphi)N_{Si} - n]$, and φ is the compensation ratio, as described in section 3.

f. dislocation scattering

Podor [20] used a screened potential and found the dislocation scattering limited mobility as:

$$\mu_{dis} = \frac{30\sqrt{2}\pi\epsilon_s^2 e_0^2 d^2 (k_B T)^{3/2}}{q^3 N_{dis} f^2 L_D n^{1/2}} \quad (6)$$

where the quantities d , N_{dis} , f , and L_D are the distance between the defect centers along the dislocation line ($\sim 5 \text{ \AA}$ in GaN), the dislocation density, the occupation rate of these sites (assuming a value of unity), and the Debye screening length ($\sqrt{\epsilon_s \epsilon_0 k_B T / q^2 n}$), respectively.

g. random and cluster alloy scattering

Due to the fact that the spatial distribution of nitrogen atoms are not all completely random and form clusters around Ga atoms, as suggested by Suzuki et al. [21]; Fahy, Lindsay and O'Reilly [22, 23] have tried to model these effects, i. e. the random alloy (μ_{rand}) and cluster alloy mobility (μ_{cl}) as a function of nitrogen composition and temperature in dilute nitride $GaN_{x}As_{1-x}$ materials. Fig. 1 shows the results of their calculations at temperatures of 30 and 300K. In these results, it is noticeable that the formation of nitrogen clusters drastically (by about one order of magnitude) decreases the electron mobility for nitrogen mole fractions of $x > 0.005$. It should be noted that in our calculations we have used a linear approximation for our temperature range of interest of 77 to 300 K, at a given x .

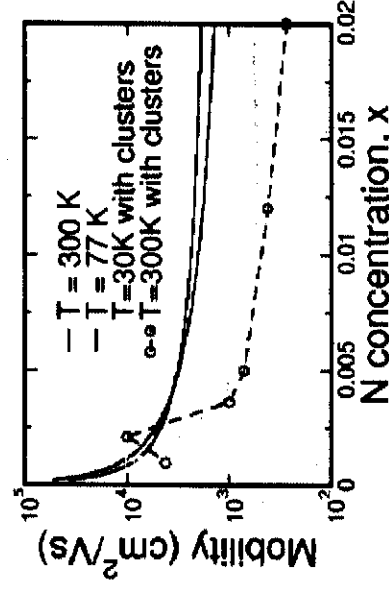


Fig. 1. Calculated electron mobility of GaN_xAs_{1-x} assuming independent scattering by individual N atoms (solid lines) and allowing for interaction between N atoms in clusters (dashed lines and symbols) [23].

3. Results and discussion

The temperature dependences of the electron mobility and concentration in three samples of GaN_xAs_{1-x} with different nitrogen contents (0.8%, 1.7%, 2.2%) are shown in Fig. 1 [13]. As is obvious, the temperature dependences of the mobility and concentration of electrons are weak for all samples. Also, in samples with higher nitrogen contents both the mobility and carrier density are reduced. This is more noticeable in the density of free electrons; giving a variation of about one order of magnitude for each percentage increase in the nitrogen mole fraction.

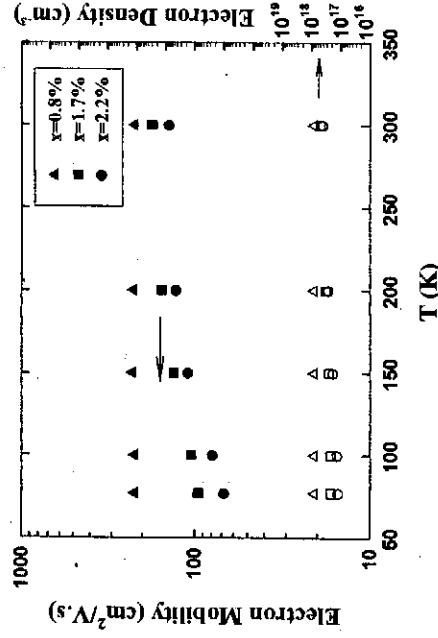


Fig. 1. Temperature dependence of electron mobility and density in Si-doped $\text{GaN}_x\text{As}_{1-x}$ samples [13].

To explain these behaviours quantitatively, we have studied the electron mobility data in each sample separately. Figs. 2 (a, b, c) show our theoretical calculations, by considering the effect of various important carrier scattering mechanisms including: polar-optical phonons, ionized and neutral impurity scattering, dislocations, random and cluster alloys, in samples with nitrogen mole fractions of $x=0.8$, 1.7 and 2.2 %. In these analyses, we have considered a electronic effective masses of 0.094 m_0 , 0.103 m_0 and 0.106 m_0 , for these samples, respectively [3], where m_0 is the free electron mass ($=9.1 \times 10^{-31}$ kg) and other parameters used in our calculations are approximated mainly based on GaAs material parameters given in Table 1.

Table 1. Values of the material parameters used in the calculations [14].

High frequency dielectric constant	$\epsilon_{\infty} = 10.90$
Static dielectric constant	$\epsilon_s = 12.53$
LO-phonon temperature (K)	$\theta = 423$
Deformation potential energy (eV)	$E_{ac} = 6.3$
Longitudinal elastic constant (10^{12} dyn/cm ²)	$C_l = 1.44$
Piezoelectric constant (10^{-3} V ² /dyn)	$\frac{h^2}{14(C_l + 4C_t)}$ $= 2.04$

Through our analysis, two quantities are considered as fitting parameters, the compensation ratio, $\phi (=N_t/N_d)$ and the dislocation density, N_{dis} , where N_t is the trap density, related to the nitrogen atoms in the crystal, and N_d is the donor density (here equal to the Si concentration (N_{Si}) of about 1×10^{18} cm⁻³). The results of our analysis are given in Table 2.

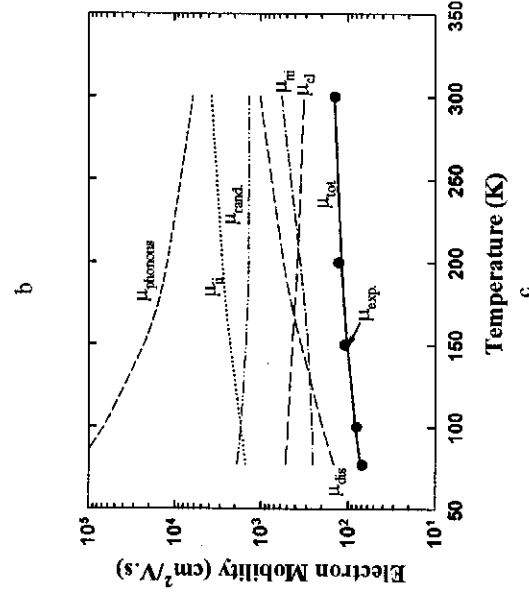
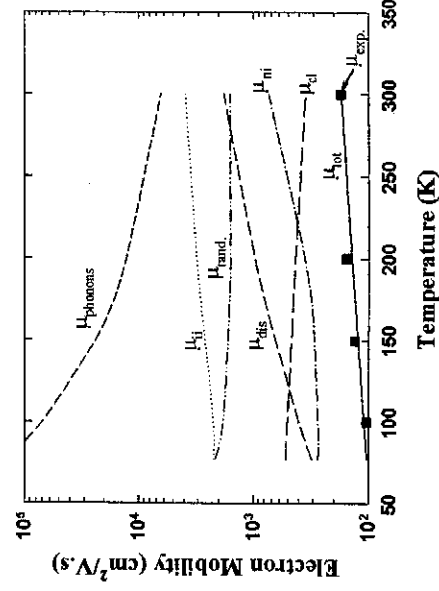
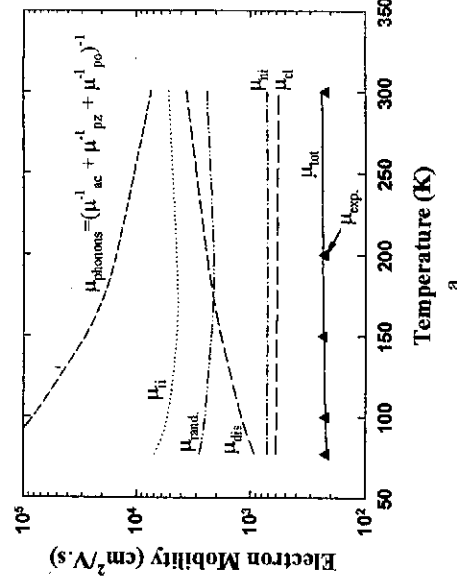


Fig. 2. Temperature dependence of the electron mobility for Si-doped $\text{GaN}_x\text{As}_{1-x}$ samples with different nitrogen mole fractions, x , (a) 0.8%, (b) 1.7%, (c) 2.2%. As x increases, the role of dislocation and neutral impurity scattering gradually becomes more dominant than the cluster alloy towards higher temperatures. (see the text).

Table 2. The fitting parameters of our calculations in Si-doped $\text{GaN}_{1-x}\text{As}_x$ samples with different nitrogen mole fractions, x .

$x(\%)$	$N_{\text{dis}} (\times 10^9 \text{ cm}^{-3})$	$N_t (\times 10^{17} \text{ cm}^{-3})$
0.8	3.0	0.5
1.7	4.5	3.5
2.2	7.0	4.0

4. Conclusions

Our analytical method shows a reasonable fit to the experimental data shown in Figs. 2 (a, b, c). According to our modelling in these figures and fitting parameters (Table 2) we conclude that:

(a) As x increases from 0.8 to 2.2%, the dislocation density and trap density increases by factors of about 2 and 8, respectively. The keys to the understanding of these unusual properties are the large difference in size as well as electronegativity of As and N atoms [24, 25]. The difference in size may lead to more lattice disturbances in the crystal potential at the N sites and therefore a higher dislocation density in the crystal. A relatively high increment in the trap density can be due to the fact that N is much more electronegative than As, the Si-N bond is expected to be much stronger than the Si-As bond [26]. Therefore, any one of the four nearest-neighboring Ga sites of the N_{As} atoms becomes an effective trap for the Si atoms. As a result of the $\text{Si}_{\text{Ga}}\text{-}N_{\text{As}}$ pair formation, the fourth valence electron of the Si atom is locally bound to the N atom, as opposed to being donated to the conduction band. The effect of these parameters, together with the increase in the effective mass of the carriers in samples with more nitrogen content, are the main reasons for the reduction of the mobility and density of the carriers.

(b) As is clear in Fig. 2 (a), for sample with the lowest nitrogen concentration (i.e. $x=0.8\%$) the cluster alloy scattering is the main controlling mechanism of the electrons mobility throughout the temperature range of 77-300 K. Figs. 2 (b and c) show that by increasing the nitrogen content to 1.7 and 2.2%, dislocations and neutral impurities gradually become more effective in limiting the electron mobilities.

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