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The applicability of α model to the degenerate InN

S GÖKDEN[*], A TEKE, R BARAN
Balikesir University, Faculty of Art & Science, Department of Physics, Balıkesir-Turkey

This paper presents a theoretical study of the carrier mobility in Indium Nitride (InN) material system. We used a model, referred to as α-model, based on a simplified relationship between the donor and dislocation densities, $N_D=\alpha(N_{dis}/c)$. It has been shown that this model correctly predicts the low temperature mobilities in InN/sapphire lattice mismatched system with high concentrations of impurities, point defects, and dislocations. It yields important information on the donors and dislocations in the InN/Al_2O_3 interface region. The donor and dislocation concentrations were calculated and compared favorably with the recently reported Hall mobility data. The specific α value was calculated for InN and its validity was confirmed. The predicted and experimental results also suggested that the potential candidate for dominant donor in InN is hydrogen.

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1. Introduction

Over the more than 20 years, nearly all electronic and optoelectronic devices have been realized using alloys of III-V nitrides, AlN, GaN, and InN [1-3] because of new developments in blue/UV LEDs, and laser diodes, and also high-frequency transistors operating at high powers and temperatures [4]. While both AlN and GaN have been extensively studied [5-6], InN remains the most mysterious compound, due mainly to difficulty in growing high-quality crystals because of the extremely high equilibrium vapour pressure of nitrogen [7]. Wurtzite InN permits photonic devices in the red (band gap ≈0.8 eV), and much faster electronic devices, because of higher mobility and peak velocity than those of most other III-N materials. Lattice-mismatched epitaxial growth (e.g. InN, GaN, ZnO, GaAs on Al_2O_3) is of high technological importance. The principal problem encountered in this growth is a high dislocation density N_{dis} in a narrow region between the substrate (e.g. Al_2O_3) and the epilayer (e.g. InN). This region is often highly conductive due to donor (N_D) contents of the dislocations. Moreover, these dislocations can promote impurity diffusion, leading to clustering of the impurities around the dislocations. If these impurities are O_N, Si_{In} and possibly interstitial H, then a thin, degenerate, donor-impurity band can form in the substrate/layer interface region. Since degenerate electrons are temperature-independent, they can dominate the low temperature electrical properties. Thus dislocations will exhibit a wide variety of effects that can have a significant impact on the mechanical, electrical and optical properties of lattice-mismatched materials.

The analytical model (called the α model) was proposed for comparison with the low-temperature mobilities for a number of various technologically important material systems, such as GaN [8], ZnO and GaAs [9, 10] in order to predict the dislocation density and donor concentration. However, no work has been done on another mysterious and equally important material system, InN. In the current study, we have applied this simple model, $N_D=\alpha(N_{dis}/c)$, where N_D is the donor concentration, c is the lattice constant and α may be thought of as the average number of donor atoms loading each dislocation-core lattice site. Additional support for the applicability of the α model comes from the study of Czochralski-grown deformed Si [11]. Thus, the α model appears to be applicable to bulk dislocated semiconductor materials.

This study is an area of interest to the device applications and very worthy of investigation. We predict for the first time the specific α value, the donor and dislocation concentrations for degenerate InN/sapphire with high concentrations of impurities, point defects and dislocations. The result is compared with recently published data [12] and GDMS (glow discharge mass spectroscopy) measurements [13] and shows a reasonable correlation. This good correlation indicates that the calculated α value is acceptable and the model is applicable [8] for the InN grown on sapphire as well. Theoretical calculations also indicate that the high values of N_D could possibly be explained by H impurity rather than O or Si as will be discussed in details later.

2. Theory and results

In lattice-mismatched systems, the mismatches in lattice constant and thermal expansion coefficient between the substrate (e.g.Al_2O_3) and epilayer (e.g. InN) are expected to generate high densities of threading edge, screw, and mixed dislocations. Thus, the band extremes (conduction band minimum, valance band maximum) shift under the influence of the strain fields existed around interface region. Thus, the imperfections which cause scattering of electrons will also change the transport properties.

The scattering theory for degenerate electrons at low temperatures has been investigated under the following assumptions [8]:

1- In a degenerate material, n is simply related to the Hall coefficient R, i.e., $n=1/eR$.

2- Phonon scattering is negligible at low temperatures, and the only important mechanisms are dislocation scattering and ionized point-defect/impurity scattering.

3- The degeneracy of the electrons allows the application of Matthiessen's rule:

$$\mu_{TOT}^{-1} = \mu_{ion}^{-1} + \mu_{dis}^{-1}.$$

4- The relaxation time approximation holds for these two elastic scattering mechanisms.

5- For the edge-dislocation, the parabolic approximation is used.

For edge- dislocation scattering the relaxation time is given by [14],

$$\tau_{dis}(E) = \frac{\hbar^3\varepsilon^2c^2}{N_{dis}m^*e^4}\frac{\left(1+8\lambda^2m^*\,E/\hbar^2\right)^{3/2}}{\lambda^4} \qquad (1)$$

where $E=\hbar^2k_\perp^{\,2}/2m^*$, c is the c-lattice constant (=5.71 Å), ε is the static dielectric constant (=15.3 ε_0), N_{dis} is the dislocation density. Also λ is the Debye screening length which is given by:

$$\lambda^2 = \frac{eE_F}{3e^2n_{3D}} \qquad (2)$$

where E_F is the Fermi energy and n_{3D} is the three dimensional carrier concentration. The quantities n_{3D} and E_F can be related in the usual way:

$$n_{3D} = \frac{2\left(2\pi\ m^*k_BT\right)^{3/2}}{\hbar^3}\int_0^\infty \frac{2x^{1/2}}{\pi^{1/2}\left(1+e^{x-U(n,T)}\right)}dx \qquad (3)$$

where $U(n,T)$ is the reduced Fermi energy. Solving this equation in the degenerate limit leads to $E_F=\left(\hbar^2/2m^*\right)\left(3\pi^2n_{3D}\right)^{2/3}$. Finally, if we combine Eqs. (1)- (3), mobility can be written as,

$$\mu_{dis} = \frac{e\tau_{dis}}{m^*} = \frac{4\times 3^{2/3}ec^2n_{3D}^{\ \ 2/3}}{\pi^{8/3}\hbar N_{dis}}\left[1+\gamma(n_{3D)})\right]^{3/2} \qquad (4)$$

where

$$\gamma(n_{3D}) = \frac{2\times 3^{1/3}\pi^{8/3}\hbar^2\varepsilon\ n_{3D}^{\ \ 1/3}}{e^2m^*} \qquad (5)$$

where m^* is the effective mass (=0.11 m_0).

Also, the degenerate form of μ_{ion} is written as [14]

$$\mu_{ion} = \frac{24\pi^3\varepsilon^2\hbar^3n_{3D}}{e^3m^{*2}N_{ion}\left[\ell n\left[1+\gamma(n_{3D})\right]-\dfrac{\gamma(n_{3D})}{1+\gamma(n_{3D})}\right]} \qquad (6)$$

where N_{ion} is the density of ionized impurities and point defects. Eq. (6) is the degenerate form of the familiar Brooks-Herring formula [15]. For $n_{3D}\rangle 10^{24}\,m^{-3}$, we can assume that an impurity band is formed, and that all donors are ionized. Thus we can approximate N_{ion} by N_D. The combined mobility is simply given by Matthiessen's rule, since the electrons are degenerate (energy independent):

$$\mu_{tot}^{-1} = \mu_{dis,\deg}^{-1} + \mu_{ion,\deg}^{-1} \qquad (7)$$

Clearly, the weak correlation between μ and n_{3D} violates the predictions of Eq. (7), unless there is a relationship between n_{3D}, N_{dis}, and N_D; indeed, the simple postulate mentioned above, i.e. $N_D=\alpha(N_{dis}/c)$, provides just the needed relationship. Another reasonable postulate is $n_{3D}=N_D - N_{dis}/c = (\alpha-1)(N_{dis}/c)$. These two postulates are known as the "α model" and we will refer to it. Implementation of the α model into Eq. (7) leads to μ as a function of α and N_{dis}.

The sample studied was grown on (0001) sapphire substrate by Moleculer Beam Epitaxy (MBE) (Look *et al.* [12]). AlN buffer layer between InN thin film and substrate were included in the sample. The low temperature mobility μ_{tot} (=0.1055 m^2/V.s at 20 K), and the carrier density n_{3D} (=3.5×10^{24} m^{-3}) are provided from the recently published Hall effect measurements [12]. In this particular sample, about 5×10^{14} m^{-2} dislocations has been found from TEM measurements.

Fig. 1 shows the low-temperature mobility as a function of α for different N_{dis} values. The high and low values of N_{dis} in the figure, 1×10^{13} m^{-2} and 1×10^{17} m^{-2} were chosen to give minimum and maximum electron concentration values about 1×10^{24} and 7×10^{26} m^{-3}, respectively. The reasoning is that about 1×10^{24} m^{-3} is required for degeneracy, and the value 7×10^{26} m^{-3} is close to the highest concentration ever measured for InN [16]. We have found the specific α value of about 5.7 by fitting the mobility with a power equation of the type $\mu = A(\alpha - 1)^{a}$ (A and a are fitting parameters) and the donor density of $N_D = 5x10^{24} m^{-3}$, and carrier concentration of $n_{3D} = 3.9x10^{24} m^{-3}$ for having $N_{dis}=5\times10^{14}$ m^{-2} .

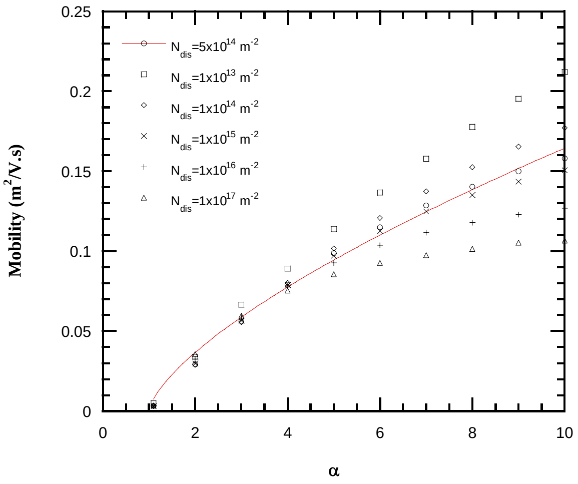

Fig. 1. Low temperature mobility as a function of α for N_{dis} *values of* 1×10^{13} m^{-2}, 1×10^{14} m^{2}, 5×10^{14} m^{-2}, 1×10^{15} m^{-2}, 1×10^{16} m^{-2} *and* 1×10^{17} m^{-2}.

Although the origin of these donors have not yet been identified in InN grown on sapphire substrate by molecular beam epitaxy, defects, such as the N vacancy, and impurities, such as O_N, Si_{In}, and possibly interstitial H have been proposed as potential candidates in the literature [17]. To compare the predicted donor density, N_D, with the concentrations of various donor type impurities, available GDMS analysis for six selected elements with the following results were considered for the currently studied sample: [C]=1×10^{21} m^{-3}, [S]=4×10^{21} m^{-3}, [Al]=2×10^{22} m^{-3}, [O]=3×10^{22} m^{-3}, [Si]=2×10^{22} m^{-3}, and [H]=9×10^{25} m^{-3}. From theoretical calculations, Stampfl *et al* [17] find that O_N and Si_{In} have lower formation energies than those of any of the native donor type defects in n-type InN. However, GDMS analysis does not find significant quantities of O and Si in the bulk of the InN layer. Hence, neither O nor Si qualifies, even though they both have lower formation energies. Noting that $N_D=5\times10^{24}$ m^{-3}, we can state that, among these elements, only H is the most likely candidate for the dominant donor in this particular InN material.

In addition, from transmission electron microscopy (TEM) measurements, Look *et al* [12] established for N_{dis} a value of 5×10^{14} m^{-2} and the donor density has been found to be 5.1×10^{24} m^{-3} for this dislocation density. This value is the same as our calculated value of $N_D=5\times10^{24}$ m^{-3}. The experimental value of n_{3D} was measured as $3.49\times10^{24}\,\mathrm{m}^{-3}$ while we have calculated it as $3.9\times10^{24}\,\mathrm{m}^{-3}$, which is in reasonable agreement with experimental result. They have been presented that oxygen would be a candidate because of its high affinity for Al first; however, GDMS measurements do not support the significant quantities of O in the bulk of the InN layer.

Fig. 2. depicts the mobility versus carrier at $N_{dis} = 5\times10^{14}$ m^{-2}. Here we assumed that the mobility is solely determined by dislocation scattering and ionized-defect/impurity scattering. It has been drawn from the equations 4 and 6. The vertical and horizontal lines here correspond to the experimental mobility of 0.1055 m^2/V.s at 20 K and the calculated electron density of $3.9x10^{24} m^{-3}$. The phonon scattering is assumed to be negligible at low temperatures. As seen in Fig. 2 the best fit to the experimental data is obtained for the dislocation density of $N_{dis} = 5 \times 10^{14}$ m^{-2} which is quite consistent with the value found using the α-model.

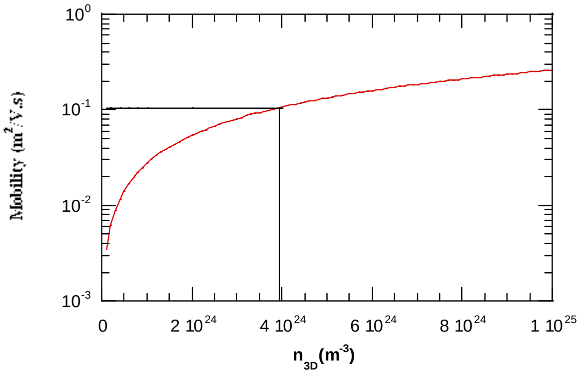

Fig. 2. The calculated low temperature mobility versus carrier density at $N_{dis} = 5\times10^{14}$ m^{-2}.

3. Conclusion

This work is the first application of the α-method to the lattice mismatched InN. By using this method, we have determined the specific α value of about 5.7, the donor density, N_D, of 5×10^{24} m^{-3} and for having $N_{dis}=5\times10^{14}$ m^{-2}. Our results are quite close to the experimental and theoretical calculations of previous authors. The GDMS measurement and theoretical calculations also promotes to offer that the dominant donor is interstitial H. In conclusion, we have shown here that the α–method can be applied to the InN grown on sapphire.

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[*] Corresponding author: sozalp@balikesir.edu.tr