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Physics Based Modeling of Intrinsic Material Parameters of III-V Nitride Semiconductors: Elevated Temperature Effects

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Abstract: ***A physics based model of temperature and field dependent electrical parameters of compound semiconductor materials such as Gallium Nitride (GaN), Aluminum Nitride (AlN) and Indium Nitride (InN) are developed exclusively. A huge number of (MC) Monte Carlo equations and experimental data results are described in this work for this model development. This paper represents the comparison of different material parameters like electron mobility, velocity, intrinsic carrier concentration and energy gap in different III-V materials like GaN, AlN and InN of Wurtzite structure using an iterative method at 300K and elevated temperature. The electron mobility dependence on doping concentration, electron mobility dependence on temperature, velocity dependence on electric field, intrinsic carrier concentration dependence on temperature and energy gap dependence on temperature for the III-V group materials are investigated thoroughly. The results obtained from this newly developed numerical device simulators can be used for RF power transistor development. To the best of authors' knowledge this is the first comprehensive report on realistic modeling of III-V Nitride family materials.***

Index Terms: Elevated temperature, energy gap dependence on doping concentration, nitride semiconductor, temperature dependent mobility, dynamic characteristics.

I. INTRODUCTION

The studies of III-V group based materials are so important because of their wide band gap properties.The band gap of GaN,AlN and InN are respectively 3.47ev, 6.026ev and 1.970ev.Due to the favorable electrical properties like high values ofcarrier mobility, saturation velocity,break down field, sheet carrier concentration high power is generated in devices developed with these semiconductors. Because of these interesting material properties, these compound materials are used in various industrial as well as biological sectors. The industrial applications such as blue, green, white light, UVemitters, traffic lightand display solid state lighting etc .It can also be used in microwave sources, high power microwave switches, wireless communication, high temperature electronics,saw and acousto-optoelectronics, pyroelectricsensors, terahertz electronics, non volatile memories etc.

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The biological application like in water, food, air sterilization and detection of biological agents, environmental protection, homeland security, surgery lighting, plant growth, capillaroscopy, visualstimuli. Phototherapy of seasonal affective disorder, monitoring and arterial oxygen, dense data storage, water and air purification, photo-bioreactors, Photo-polymerization, of dental composites etc.[1]. The band gap of GaN, AlN and InN are direct band gap and with a Wurtzite crystal structure. The Wurtzite structure is so important because each of the two atom types forms a sub-lattice which is hexagonal close pack type. When viewed together, the atomic positions are the same as in ionsdaleite (hexagonal diamond).Each atom is tetrahedrally coordinated. The Wurtzite structure is non-centrosymmetric. Due to this, Wurtzite crystals can have properties such as piezoelectricity and pyro electricity which Centro symmetric crystals lack [2].

The target of this article is to report a comprehensive and generalized modelfor the electron mobility of GaN,AlN,InN for serving in device simulators.Based on proclaimed mobility data and in addition to the belief of mobility on temperature, doping concentration, electric field the models are described.This paper described as follows.The primary knowledge of mobility modeling are represents in section II , development of the model description is described in section III discussions is presented in section IV, conclusion is given in section V, acknowledgement is given in section VI and references are given at last.

II. THE PRIMARY KNOWLEDGE OF MOBILITY MODELING

The electron transfer is naturally conducted by drift diffusion phenomena. The electron drift velocity can be calculated from electron mobility μ multiplied with electric field E [3].

$$v = \mu \times E \qquad (1)$$

It can be seen from here that it is a linear equation as far as the value of electric field and the mobility value are underneath. The lower value of mobility is called μ_0 (low-field mobility).It is a consequence of temperature and dopping concentration.The extensively used low-field mobility has been recommended by [4].

$$\mu^{L1} = \mu^{min} + \frac{\mu^{L} - \mu^{min}}{1+(\frac{C}{C^{ref}})^{\gamma 0}} \qquad (2)$$

Where μ^{L} , μ^{min} , $\gamma 0$ and C^{ref} are the applicable parameters.Where μ^{L} is the mobility of undopped material and μ^{min} is the mobility of

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the doped material and profoundly C is the total doping concentration. Mobility is the intermediate point of μ^L and μ^{min} at which the doping concentration is present and $\gamma 0$ is a calculated value at which it is showing that how rapidly the mobility improved from μ^L to μ^{min}.

To calculate the value of $\mu^L, \mu^{min}, C^{ref}$ and $\gamma 0$ some proper equations are taken [3].

$$P_{ar} = P_{ar0} \times \left(\frac{T}{300}\right)^{\gamma} \quad (3)$$

Where P_{ar0} is the parametric value of P_{ar} at 300k and γ is a constant material specific [4].

$$\mu^L = \mu_{300}^L \left(\frac{T_L}{300K}\right)^{\gamma 1} \quad (4)$$

$$\mu^{min} = \mu_{300}^{min} \left(\frac{T_L}{300K}\right)^{\gamma 2} \quad (5)$$

$$C^{ref} = C_{300}^{ref} \left(\frac{T_L}{300K}\right)^{\gamma 3} \quad (6)$$

The electron velocity is not proportional to the applied field as soon as the heavy electric field is used, that's why it is not described by field independent mobility [5].

$$\mu = \frac{\mu_0}{\left[1+\left(\frac{E}{v_{sat}}\right)\right]^{\beta}} \quad (7)$$

Where, v_{sat} is the saturation velocity and β is a constant defining of how drastically electron velocity reach into the saturation point. For generating the value of velocity-field characteristics the electric field has to be multiplied in two sides. The experimental data value of v_{sat} of GaN, AlN and InN are 1.4x107cm/sec,1.6x107cm/sec and 2.5x107cm/sec respectively which is recommended by [6].

For calculating the value of intrinsic concentration n_i and energy gap the proposed formulas are recommended by [7][8][9].

$$n_i = (N_c N_v)^{\frac{1}{2}} \exp\left(\frac{-E_g}{2k_B T}\right) \quad (8)$$

The value of N_c and N_v are given bellow of GaN.

$$N_c = 4.3x10^{14} x T^{\frac{3}{2}} cm^{-3} \quad (9)$$

$$N_v = 8.9x10^{15} x T^{\frac{3}{2}} cm^{-3} \quad (10)$$

Where,E_g is the band gap energy. In a given semiconductor material at a constant temperature, the value of n_i is a constant, and it is independent of Fermi energy. N_c is the effective density of state in the conduction band , N_v is the effective density of state in the valance band and k_B is the Boltzmann constant.

For calculating the value of energy gap E_g the proposed formula is recommended by [7].

In case of calculating the energy gap of GaN the proposed formula is[7].

$$E_g = E_g(0) - 9.39x10^{-4} x \frac{T^2}{(T+772)} \quad eV \quad (11)$$

$$E_g(0) = E_g(300K) = 3.47eV$$

In case of calculating the energy gap of AlN the proposed formula is [7].

$$E_g = E_g(0) - 1.799x10^{-3} x \frac{T^2}{(T+1462)} \quad eV \quad (12)$$

$$E_g(0) = E_g(300K) = 6.026eV \quad (13)$$

$$N_c = 1.2x\ 10^{15} x T^{\frac{3}{2}} cm^{-3} \quad (14)$$

$$N_v = 9.4x10^{16} x T^{\frac{3}{2}} cm^{-3} \quad (15)$$

In case of calculating the energy gap of InN the proposed formula is [7].

$$E_g = E_g(0) - 2.45x10^{-4} \frac{T^2}{(T+624)} \quad eV \quad (16)$$

$$E_g(0) = E_g(300K) = 1.970eV \quad (17)$$

$$N_c = 1.76x10^{14} T^{\frac{3}{2}} cm^{-3} \quad (18)$$

$$N_v = 10^{16} x T^{\frac{3}{2}} cm^{-3} \quad (19)$$

III. DEVELOPMENT OF THE MODEL

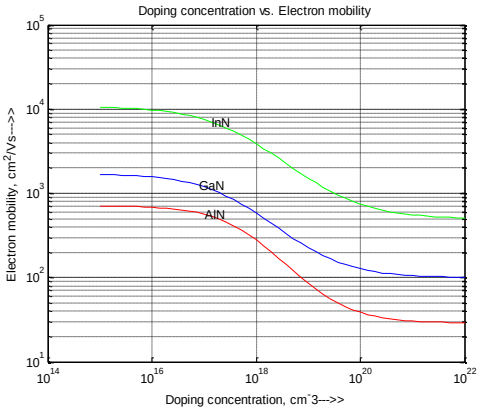

Fig.1.Low field electron mobility as a function of doping concentration in GaN, AlN and InN at T=300K.The green line indicates the nature of InN, the blue line indicates the behavior of GaN and the red line indicates the nature of AlN.

Table1: Parameters value for low field mobility [4]

material	carrier	μ_{300}^L (cm²/Vs)	μ_{300}^{min} (cm²/Vs)	C_{300}^{ref} cm⁻³
GaN	n	1600	100	3x10¹⁷
	p	175	10	2.5x10¹⁷
AlN	n	683	29	5x10¹⁷
InN	n	10200	500	3.4x10¹⁷

material	carrier	$\gamma 0$	$\gamma 1$	$\gamma 2$	$\gamma 3$
GaN	n	0.7	-1.5	-0.2	1.3
	p	1.5	-3.7	-1.5	1.0
AlN	n	0.8	-3.21	1.21	-0.18
InN	n	0.65	-3.7	2.39	-0.33

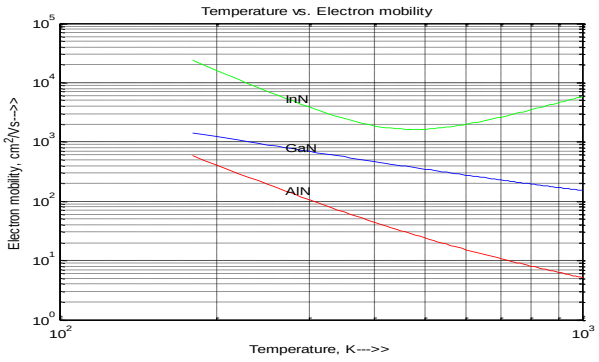

Fig.2.Low field electron mobility as a function of temperature of GaN, AlN and InN .

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The green line indicates the nature of InN, the blue line indicates the behavior of GaN and the red line indicates the nature of AlN.

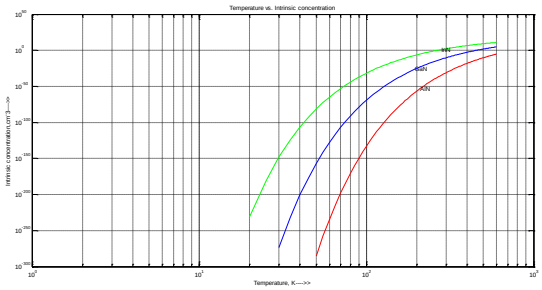

Fig.3.Intrinsic carrier concentration as a function of temperature of GaN,AlN and InN .The green line indicates the nature of InN, the blue line indicates the behavior of GaN and the red line indicates the nature of AlN.

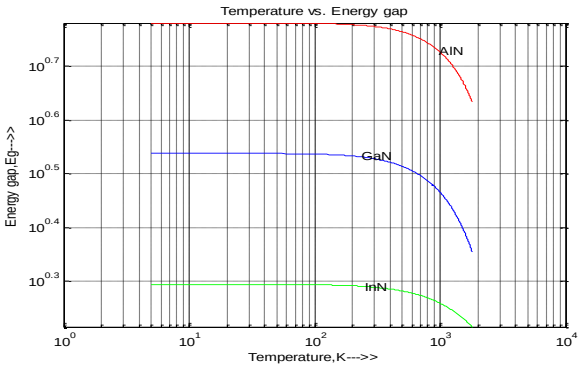

Fig.4. Energy gap as a function of GaN, AlN and InN .The green line indicates the nature of InN, the blue line indicates the behavior of GaN and the red line indicates the nature of AlN.

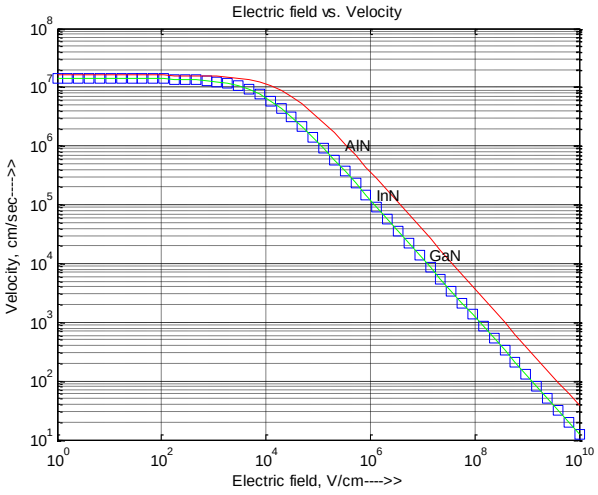

Fig.5. Electron drift velocity as a function of GaN,AlN and InN .The green line indicates the nature of InN, the blue color diamond line indicates the behavior of GaN and the red line indicates the nature of AlN.

IV. DISCUSSION

Fig.1 represents variation of electron mobility with doping concentration in GaN, AlN and InN at room temperature. Necessary input parameters data are tabulated in Table1. It is observed that for a particular doping concentration InN shows higher value of electron mobility than its counterparts. This comparative study will be useful for choosing appropriate Nitride semiconductors for developing high speed RF switches.

Fig.2 represents elevated temperature effects on electron mobility of III-V materials. It is observed that with increasing temperature electron mobility decreases in all the materials but with different slopes.Fig.3 represents effect of elevated temperature on intrinsic concentration of III-V Nitride materials. The simulation results indicates that with increasing temperature intrinsic concentration increases much in InN whereas, the rate of increase is moderate in cases of GaN and AlN. This is very interesting observation for using GaN and AlN in high temperature module.Fig.4 represents temperature dependence on energy gap in III-V materials.Fig.5 represents velocity field properties of Nitride materials. These simulations results are encouraging to select suitable material for high frequency and high power applications.

V. CONCLUSION

Electrical parameters are simulated on the for III-V materials such as GaN, AlN and InN. The numerical model is developed incorporating electric field, crystal structure and elevated temperature effects. To the best of authors knowledge this is the first report on comprehensive simulation studies of major III-V Nitride materials. The observation will find immense application possibilities in developing high power millimeter wave devices including power transistors.

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