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Computer Software for Calculating Electron Mobility of Semiconductors Compounds; Case Study for N-Gan

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Abstract**—**Computer software to calculate electron mobility with respect to different scattering mechanism has been developed. This software is adopted completely Graphical User Interface (GUI) technique and its interface has been designed by Microsoft Visual basic 6.0. As a case study the electron mobility of n-GaN was performed using this software. The behavior of the mobility for n-GaN due to elastic scattering processes and its relation to temperature and doping concentration were discussed. The results agree with other available theoretical and experimental data.

Keywords**—**Electron mobility, relaxation time, GaN, Scattering, Computer software, computation physics.

I. Introduction

IN solid-state physics, the term carrier mobility refers in general to both electron and hole mobility in semiconductors. These parameters characterize how quickly an electron and/or hole can move through a metal or semiconductor when pulled by an electric field. It is play an important role for characterizing the transport of charged carriers and formulating the current in semiconductor devices. Carriers are able to flow more quickly in materials with higher mobility; since the speed of an electronic device is limited by the time it takes a carrier to move from one side to the other, devices composed of materials with higher mobility are able to achieve higher speeds. For this reason, it is useful to maximize the mobility of materials used [1].

A great deal of attention has been paid to these parameters and many authors have measured the carrier mobility for various III–V compounds by Hall Effect measurement technique [2], [3]. Efforts have also been focused on theoretical formulation of carrier mobility in semiconductors [4]. Researchers have been forced to manually go through the calculations if they want to know what the theoretically predicted mobility of a particular semiconductor is.

This paper solves the problem by providing a Graphical User Interface (GUI) program which can specify various parameters to calculate the mobility. Also, in this study the electron mobility as a function of temperature for n-GaN has been calculated by using the program. Elastic scattering processes including acoustic phonon scattering (with the two modes deformation potential and piezoelectric), neutral impurity scattering and ionized impurity scattering are considered in this study and its relation to temperature and doping concentration were discussed.

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II. Theory

The Mobility is determined by the rate of electrons which scattered by impurities and defects within the crystal structure of the semiconductor. This rate $1/\tau$ (s^{-1}) is the reciprocal of the relaxation time τ (s), the average time between collisions. The relaxation time can be adjusted to account for the varying degrees of scattering on any given collision. A simple model gives the approximate relation between scattering time and mobility by solving Boltzmann equation in the relaxation time approximation as [5].

$$\mu = \frac{e\langle\tau\rangle}{m^*} \tag{1}$$

where, μ is the mobility, e is the electronic charge, $\langle\tau\rangle$ is the average relaxation time over the electron energies and m* is the effective mass of the electron. The expressions of relaxation time and mobility caused by different scattering mechanisms are given in the following sections.

A. Ionized Impurity Scattering

The scattering due to electrostatic forces between the carrier and the ionized impurity centers depends on the interaction time and the number of impurities. Larger impurity concentrations result in a lower mobility [6]. The standard formula for calculating the average relaxation time is given by [7].

$$\langle\tau_{ii}(\varepsilon)\rangle = \frac{e}{m^*}\frac{\int_0^\infty \tau_{ii}(\varepsilon)\in^{3/2}\frac{df_0}{d\varepsilon}d\varepsilon}{\int_0^\infty \in^{3/2}\frac{df_0}{d\varepsilon}d\varepsilon} \tag{2}$$

where, f_0 is the thermal equilibrium Fermi-Dirac distribution function and $\in$ is the static dielectric constant of the semiconductor (C^2/Nm^2).

The mobility associated with the ionized impurity scattering is calculated as:

$$\boldsymbol{\mu_{ii}} = \frac{128\sqrt{2}\pi^{1/2}\varepsilon^2 k^{3/2}}{N_i e^3 m^{*1/2}\left[\ln(1+y)-\frac{y}{1+y}\right]}\boldsymbol{T^{3/2}} \tag{3}$$

where $y=(24\varepsilon m^* k^2 T^2)/(\hbar^2 e^2 n)$, k is Boltzmann constant (m^2kg/s^2K), T is temperature (K), N_i is the concentration of the ionized impurities, $\hbar$ is the Plank's constant divided by 2π, n is the concentration of the carriers.

B. Neutral Impurity Scattering

When an electron passes close to neutral atom, momentum is transferred through a process in which the free electrons exchange with a bound electron on the atom. The relaxation time is given by [8].

$$\tau_{ni}(\varepsilon) = \frac{m^*}{20 N_n \hbar a_0} \tag{4}$$

where, a_0 and N_n are the effective Bhor radius of donor and concentration of neutral impurities, respectively.

The mobility associated with neutral impurity scattering is calculated as [9].

$$\boldsymbol{\mu_{ni}} = \frac{e^3 m^*}{80\pi N_n \hbar^3 \in} \tag{5}$$

C. Acoustic Phonon (Deformation Potential Scattering)

The acoustic mode lattice vibration induces changes in lattice spacing, which vary the band gap from point to point. Since the crystal deforms at these points, the potential is called deformation potential. The corresponding relaxation time is given by [10].

$$\tau_{dp}(\varepsilon) = \frac{\pi \hbar^4 \rho s^2}{\sqrt{2} E_1^2 m^{*3/2} kT} \varepsilon^{-1/2} \tag{6}$$

where ρ is crystal density, s is average velocity of sound and E_1 is deformation potential.

The mobility associated with deformation potential scattering is calculated as

$$\boldsymbol{\mu_{dp}} = \frac{2\sqrt{2}\pi^{1/2}\hbar^4 \rho s^2 e}{3E_1^2 m^{*5/2} K^{1/2}} \cdot \frac{\mathbf{1}}{\boldsymbol{T^{1/2}}} \tag{7}$$

D. Acoustic Phonon (Piezoelectric Scattering)

Electrons can suffer scattering with piezoelectric mode of acoustic lattice vibrations. The corresponding relaxation time is given by [7].

$$\tau_{pe}(\varepsilon) = \frac{2\sqrt{2}\pi\hbar^2 \in^3 \rho^2 s^4}{e^2 h_{pe}^4 m^{*1/2} kT} \varepsilon^{1/2} \tag{8}$$

where, h_{pe} is the piezoelectric constant and ∈ is the dielectric constant.

The mobility associated with piezoelectric potential scattering is calculated as

$$\mu_{pe} = \frac{16\sqrt{2}\pi^{1/2} \in^3 \hbar^2 \rho^2 s^4}{3 e h_{pe}^4 m^{*3/2} K^{1/2}} \cdot \frac{1}{T^{1/2}} \tag{9}$$

Finally, the drift mobility estimate by using Matthessen's rule [5].

$$\frac{1}{\mu} = \frac{1}{\mu_{ii}} + \frac{1}{\mu_{ni}} + \frac{1}{\mu_{dp}} + \frac{1}{\mu_{pe}} \tag{10}$$

III. Proposed Computer Software

According to the previous theoretical treatments, computer software has been developed to calculate electron mobility with respect to different scattering mechanism. This software is adopted completely Graphical User Interface (GUI) technique for operating in various windows-based microcomputers. The software interface has been designed using by Microsoft Visual basic 6.0. It is based on the flow chart as in Fig. 1.

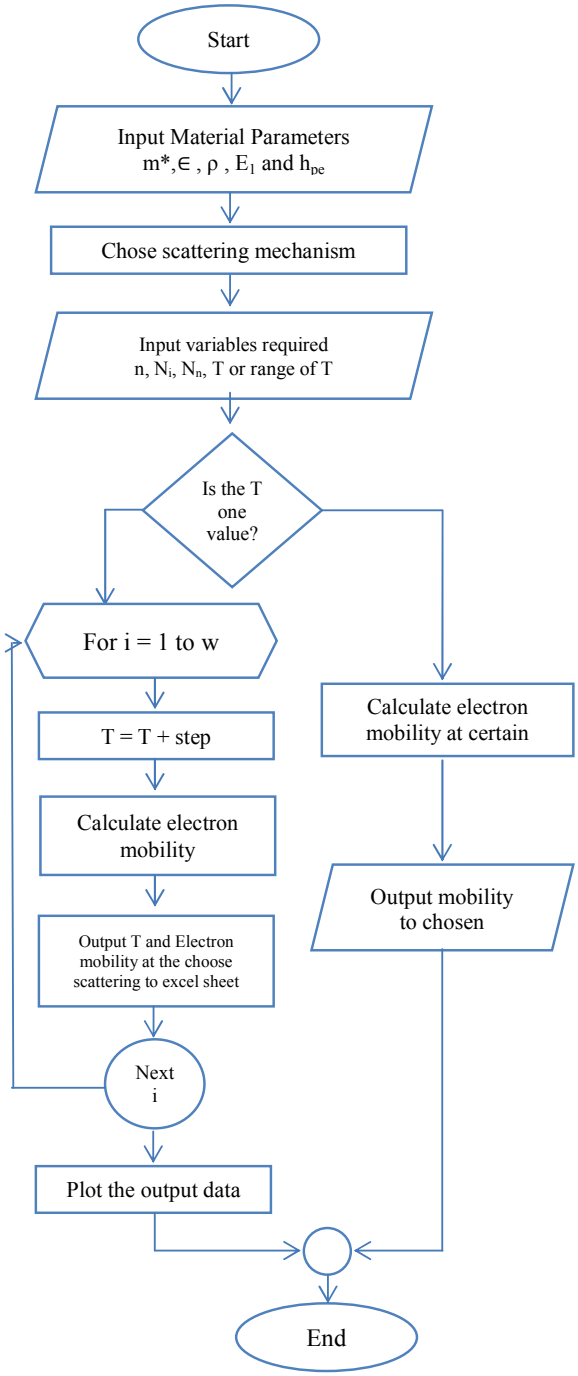

Fig. 1 Flow chart of the software

After run the software, the GUI main form will bring up, which should look like as Fig. 2. User need to input material parameters under consideration into the corresponding text

boxes on the upper left and variables such as carrier concentrations and temperature whether a single value or range of values on the lower left. User have the choice to calculate the electron mobility with respect one or more electron scattering mechanism on the upper right. The outputs electron mobility will be shown on the lower right. User can export output data in MS Excel format and plot the electron mobility verse temperature.

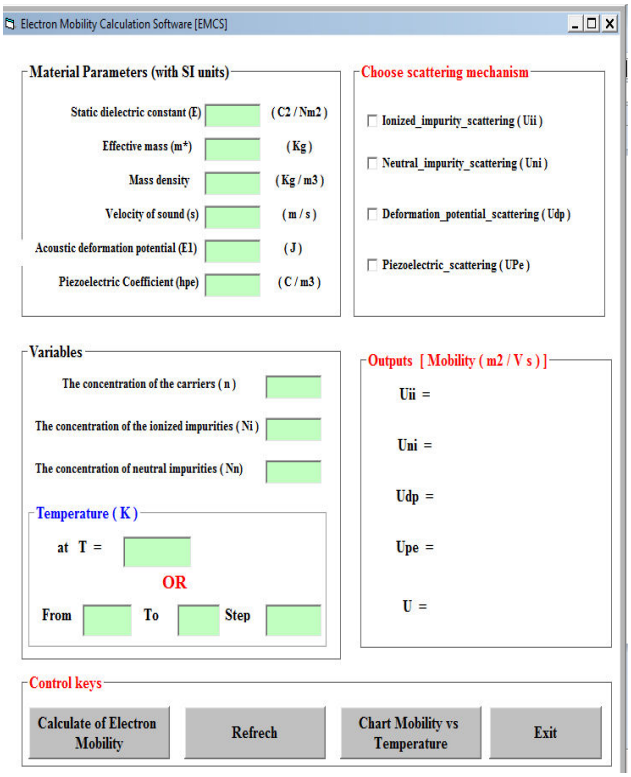

Fig. 2 Main form of the software

IV. Results and Discussions

Using previous software, Calculations of the electron mobility were carried out using the parameters of n-GaN at different temperature including different types of scattering mechanisms such as ionized impurity, neutral impurity and acoustic phonon via deformation potential and piezoelectric potential scattering. The parameters used in the calculations are shown in Table I. Also, input in the software the ionized impurity concentration, carrier density and neutral impurities equal to $6x10^{20}$ m^{-3}, $6x10^{10}$ m^{-3} and $6x10^{20}$ m^{-3}, respectively.

Fig. 3shows the mobility versus temperature for n-GaN in a temperature range from 10 K to 400 K for different types of scattering mechanisms. From the graph it is seen that calculations explored the behavior of the mobility due to elastic scattering processes by ionized impurity, neutral impurity, acoustic phonon deformation potential and acoustic piezoelectric individually.

TABLE I
The Material Parameters of GaN Compounds Used in Calculations

Parameter	Symbol	value	Unit	Reference
Effective mass	m*	0.22 m_0	Kg	[11], [12]
Static dielectric constant	∈	10.4 $∈_0$	C^2/Nm^2	[13], [14]
Mass density	ρ	6100	Kg/m^3	[15], [16]
Velocity of sound	s	6590	m/s	[15], [13]
Acoustic deformation potential	E1	$1.47x10^{-18}$	J	[14], [17]
Piezoelectric coefficient	hpe	0.5	C/m^3	[18], [19]

The mobility due to ionized impurities increased by increasing of temperature while that due to acoustic lattice vibrations decreased by raising the temperature. These results agree well with the general concepts recorded in the literatures for this system or other like III-V systems [20]. The mobility due to piezoelectric acoustic phonon scattering is noticed to be greater than that of deformation potential. Also, one can observe that the curve of mobility due to acoustic phonons is close to the curve of deformation potential scattering at higher temperatures and this may lead to ignoring the effect of the piezoelectric mode of acoustic phonons at high temperatures [21].

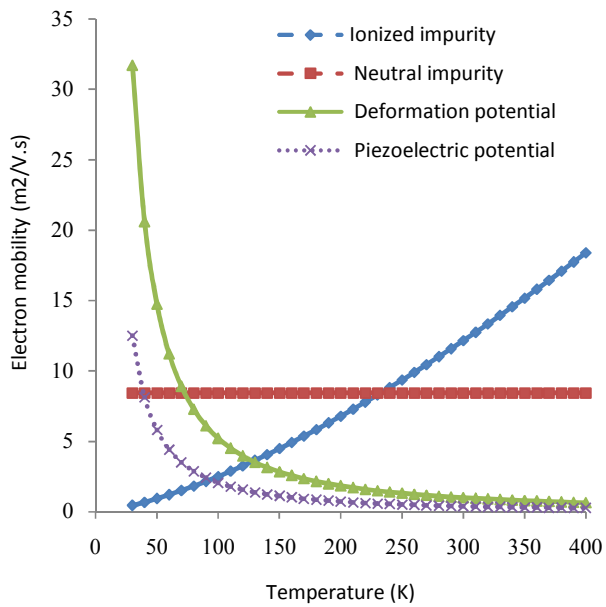

Fig. 3 The mobility versus temperature for n-GaN at different types of scattering mechanisms

The neutral impurity scattering process is a temperature independent and then the mobility associated to it is expected to be a constant through the material under consideration as shown in fig this agrees to the conclusions made by R. Karthik et al [9].

Fig. 4 shows the behavior of the electron drift mobility in temperature range at different doping concentration. We regarded that the electron concentration equals to impurity concentration. Because of this we took into account screening

by free carriers [22], [23]. From this figure, one can observe that as temperature increases the mobility increases until have a peak value (at low temperature) then mobility decreases (at high temperature). Also As impurity concentration increases the peak value of mobility decreases. These results agree well with that obtained by J. Kundu et al. [24]. The results obtained from Figs. 1 and 2 let one to notice that the ionized impurity scattering probably could be the dominant scattering process that may present in this system.

Fig. 5 shows the calculated electron drift mobility as a function of carrier concentrations at 100 K, 200 K, 300 K and 400 K. The electron drift mobility decreases as the material becomes more doped. The decrease of the electron mobility when the material becomes more doped is probably explained due to large ionized impurity scattering which limits the electron mobility particularly at low temperatures.

V. Conclusion

This paper presents development of computer software to calculate electron mobility with respect to different scattering mechanism such as ionized impurity, neutral impurity and acoustic phonon via deformation potential and piezoelectric potential scattering. This software is adopted completely GUI technique to help researchers to predicted mobility by just input the parameters of a particular semiconductor and to study of the behavior of mobility at range of temperature or carrier concentration which useful to maximize the mobility of materials used.

We have been used the software to calculate the electron mobility for n-GaN as a case study and test the outputs of the software. By using the results output from the software, the behavior of the mobility for GaN due to elastic scattering processes by ionized impurity, neutral impurity, acoustic phonon deformation potential and acoustic piezoelectric individually were discussed. Also, the drift electron mobility as a function of temperature and doping concentration were discussed. Drift mobility of the electrons in the system was found to be diminished by lowering down the temperature while by decreasing the impurity doping density the drift mobility was noticed to be increased. This may be due to the effect of the ionized impurity scattering with electrons in the material. The ionized impurity scattering probably could be the dominant elastic scattering process that may present in such system. Overall the results agree quite satisfactorily with the published theoretical and experimental results [10], [25].

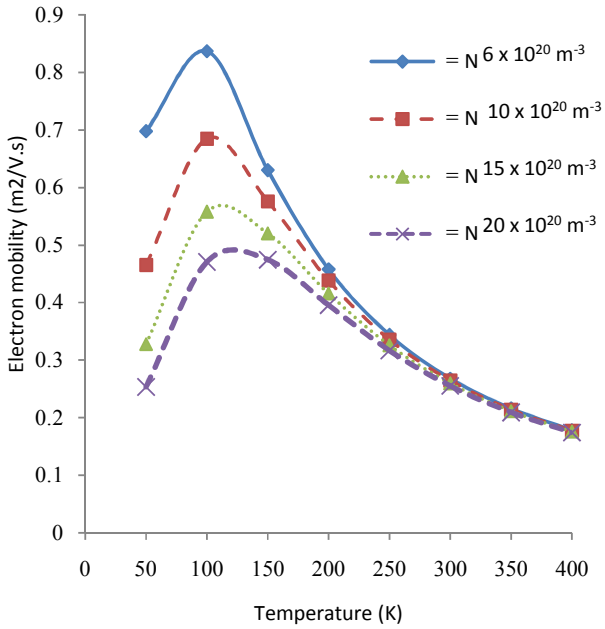

Fig. 4 The electron drifts mobility in temperature range at different doping concentration

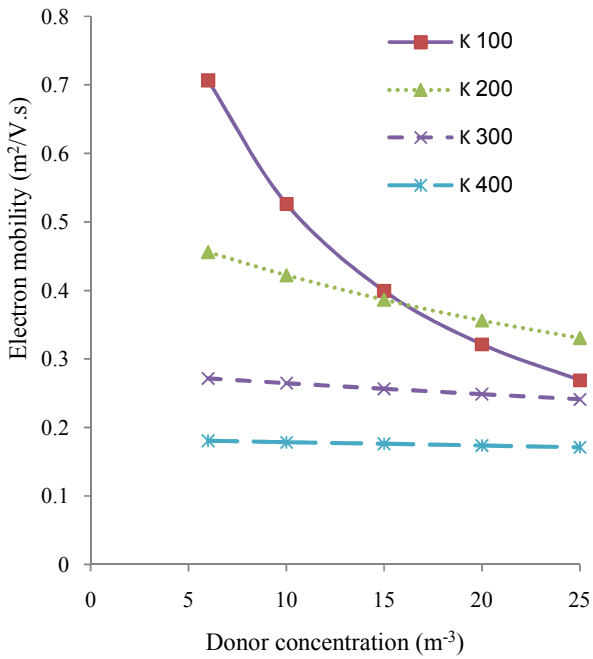

Fig. 5 The electrons drift mobility in doping concentration range at different temperature

REFERENCES

[1] C. M. Wolfe, N. Holonyak, Jr., and G. S. Stillman, *Physical Properties of Semiconductors*. Englewood Cliffs, N. J.: Prentice Hall, 1989.
[2] S. Adachi, GaAs and Related materials, "Bulk Semiconducting and Superlattice properties, *"World Scientific, Singapore*, 1994, Chap. 14.
[3] Z. Hongwei, Z. Yiping, W. Hongmei, D. Jianrong, Z. Zhanping, P. Liang and K. Meiying, "Growth and transport properties of InAs thin films on GaAs,"*J. Crystal Growth 191*, 1998, 361.
[4] M. Sotoodeh, A. H. Khalid and A. A. Rezazadeh, "Empirical low-field mobility model for III–V compounds applicable in device simulation codes,"*J. Appl. Phys*. 87, 2000, 2890.
[5] B. R. Nag, *Electron Transport in Compound Semiconductors*, Springer, New York, 1980.
[6] S. Dharand S. Ghosh, "Low field electron mobility in GaN,"*Journal of Applied Physics*, 86, 1999, 2668.
[7] S. Mallick, J. Kundu and C. K. Sarkar, "Calculation of ionized impurity scattering probability with scattering angles in GaN,"*Can. J. Phys.*, 86, 2008, 8.
[8] C. Erginsoy, "Neutral impurity scattering in semi-conductors, *"Physical Review*, 79, 1950, 1013.
[9] R. Karthik, P. Uma Sathyakam, P. S. Mallick, "Effect of dislocation scattering on electron mobility in GaN,"*Natural Science*, Vol.3, No.9, 2011, 812-815.
[10] D. A. Anderson, N. Apsley, "The Hall effect in III-V semiconductors,"*Semicond. Sci. Technol.*, 1, 1986, 187.
[11] P. Perlin, E.L. Staszewska and B. Suchanek, "Determination of the effective mass of GaN from infrared reflectivity and Hall Effect, *"Applied Physical Letters*, 68, 1996, 1114.
[12] V. Bougrov, M. E. Levinshtein, S. L. Rumyantsev and A. Zubrilov, *Properties of Advanced Semiconductor Materials GaN, AlN, InN, BN, SiC, SiGe.* Eds. Levinshtein M. E., Rumyantsev S. L., Shur M.S., John Wiley & Sons, Inc., New York,2001, 1-30.
[13] Y. J. Wang, R. Kaplan, H. K. Ng, K. Doverspike, D. K. Gaskil, T. Ikedo, H. Amano and I. Akasaki, "Magneto-optical studies of GaN and GaN/AlxGa1-xN: Donor zeeman spectroscopy and two dimensional electron gas cyclotron resonance,"*Journal of Applied Physics*, 79, 1996, 8007.
[14] H. Morkoç, *Nitride Semiconductors and Devices*, Springer–Verlag Berlin Heildelberg New York, 1999, 245.
[15] D. C. Look, J. R. Sizelove, S. Keller, Y. F. Wu, U. K. Mishra and S. P. Den Baars, "Accurate mobility and carrier concentration analysis for GaN,"*Solid State Communications*, 102, 1997, 297.
[16] D.K. Schroeder, *Semiconductor material and device characterization*. Wiley, New York, 1990.
[17] W. Shan, S. Schmidt, X.H. Yang, J.J. Song, and B. Golden-berg, "Optical properties of wurtziteGaN grown by low-pressure metal organic chemical-vapor deposition,"*Journal of Applied Physics*, 79, 1996, 3691.
[18] A.D. Bykhovski, V.V. Kaminski, M.S. Shur, Q.C. Chen, and M.A. Khan, "Piezoelectric effect in wurtzite n-type GaN,"*Applied Physical Letters*, 68, 1996, 818.
[19] J. D. Albercht, R. P. Wang, P. P. Ruden, M. Farahmand, K. F. Brennan, "Electron transport characteristics of GaN for high temperature device modeling," *J. Appl. Phys*., 83, 1998, 4777.
[20] K. Alfaramawi, "Numerical calculations of the electron mobility of n-GaN, J. Optoelectron,"*Adv. M.-Rapid Comm*., 4, 2010, 922.
[21] K. Alfaramawi and M.A. Alzamil, "Temperature-Dependent Scattering Processes of n-type Indium Antimonide,"*Optoelectron. Adv. Matr.-Rapid Comm*., 3, 2009, 569.
[22] H. Tang, W. Kim, A. Botchkarev, G. Popovici, F. Hamdani and H. Morkoç,"Analysis of carrier mobility and concentration in Si-doped GaN grown by reactive molecular beam epitaxy,"*Solid-State Electronics*, 42(5), 1998, 839-847
[23] S. Aydogu, M. Akarsu and Ö. Özba, "Numerical calculation of the electron mobility of GaN semiconductor compound,"*Rom. Journ. Phys*., Vol. 50, Nos. 9–10 ,Bucharest 2005, P. 1047–1053.
[24] J. Kundu, C. K. Sarkar and P. S Mallick, "Calculation of electron mobility and effect of dislocation scattering in GaN Semiconductor Physics,"*Quantum Electronics & Optoelectronics*, Vol. 10 Issue 12 ,2007, p1.
[25] D. Subhabrata and G. Subhasis, "Low Field Electron Mobility in GaN,"*J. Appl. Phys.*,86 (5), 1999, 2668.

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