

Calculation of Elecron Mobility in WZ-AIN and ZB-AIN at Low Electric Field

¹H. Arabshahi, ²M. Izadifard and ²A. Karimi

¹Physics Department, Payame Noor University, Tehran, Iran

²Physics Department, Shahrood University of Technology, Shahrood, Iran

Abstract

In this work the electron mobility of AlN Wurtzite and AlN Zincblende semiconductor compounds were calculated using iterative method in range of 100-600 K. We compare polar optic phonon scattering, deformation-potential acoustic phonon scattering, piezoelectric scattering and impurity scattering mechanisms. Boltzmann transport equation was solved using iterative method. In addition, we took into account the mixing of wave functions and electron screening and we investigated temperature dependence of mobility of the given compound.

Keywords-: AlN Wurtzite , AlN Zincblende ,electron mobility , iterative method , III-Nitrides.

I. INTRODUCTION

Recently ,the previous studies about III-V semiconductor compounds are considered important III-V semiconductor compounds, InN, GaN and AlN, respectively 1.8 eV, 3.4 eV, 6.2 eV, have the wide band gaps . Because of these properties III-nitrides are used in the blue and UV light emitting diodes (LED's) ,blue lasers ,UV detectors and high power , high temperature field effect transistors [2,3,4,5,6]. Aluminum nitride is a very interesting material because of it's wide band gap (6.3 eV), high decomposition temperature (2400 c) chemical stability (in air up to 700 c) and good dielectric properties . In the last decade considerable interest arose in the use of thin films of AlN for various applications , from hard coatings and overcoatings for magneto- optic media ,to thin films transducers and GHz-band surface acoustic wave devices .The bandgap of AlN is direct in the Wurtzite phase and indirect in Zincblende phase .The electronic structure around the Valence band maximum of AlN in the WZ structure around the Valence band maximum of AlN in the WZ structure is different from that of the ZB-type crystal. In WZ-AIN ,the bandgap is 4.3 eV and direct at gamma point and in ZB-AIN the conduction-band minimum (CBM) is located away from the gamma point at the X-point and in this point the bandgap is 3.2 eV. ZB-AIN is an object of the invention to prepare ZB-AIN OF sufficient quality and thickness to characterize it for its mechanical, optical and electrical properties and to be useful for device fabrication . WZ-AIN is a

III-V semiconductor with Wurtzite crystalline properties of WZ-AIN , it has a very wide bandgap ,high thermal conductivity and transparency of ultraviolet LEDs and high-power electronic devices for promising material in deep UV devices , white color LED ,high density medical laser , photolithography, photocatalytic decontamination , alternative of Hg lamp and He-Cd laser . They are also applied to high-power electronic devices and solar cells.With comparison of scattering effect in ZB-AIN and WZ-AIN structures, we result that for deformation potential scattering, the scattering of electron increased with increasing the energy. In piezoelectric scattering with increasing of energy the scattering decreased in polar optical phonon scattering, the scattering is increasing by increasing temperature however changes differ is not important and in impurity scattering, the scattering rate of electron due to impurities atom in low-temperature is more than high temperature. Thus, the scattering rate of electron in WZ-AIN is more than ZB-AIN because their bandgap and the effective mass of electron in Γ -valley is different. The Boltzmann equation is solved iteratively for our purpose, jointly incorporating the effects of all the scattering mechanisms. This paper is organized as follow as follows details of iterative model is presented in Section II and result of iterative calculations carried out on ZB-AIN and WZ-AIN structures are interpreted in Section III [3-5].

II. SOLVING THE BOLTZMANN TRANSPORT EQUATION

In principle the iterative technique give exact numerical prediction of electron mobility in bulk semiconductors. To calculate mobility, we have to solve the Boltzmann equation to get the modified probability distribution function under the action of a steady electric field . Here, we have adopted the iterative technique for solving the Boltzmann transport equation . Under application of a uniform electric field the Boltzmann equation can be written as :

$$\left(\frac{e}{\hbar}\right) E \cdot \nabla_k f = \phi [S' f (1-f) - S f (1-f)] dk$$

(1)

where $f=f(k)$ and $f'=f(k')$ are the probability distribution functions and $s=s(k,k')$ and $s'=s(k',k)$ are the differential scattering rates . If the electric field is small ,we can treat the change from the equilibrium

distribution function as a perturbation which is first order in the electric field. The distribution in the presence of a sufficiently small field can be written quite generally as:

$$f(k) = f_0(k) + g(k) \cos\theta \quad (2)$$

Where $f_0(k)$ in the equilibrium distribution function, θ is the angle between k and E and $g(k)$ is an isotropic function of k , which is proportional to the magnitude of the electric field. Boltzmann transport equation is involved in scattering mechanisms may have occurred in the material. In this work we regarded that it was taken place acoustic phonon deformation potential scattering, acoustic piezoelectric scattering, ionized impurity scattering and polar optic phonon scattering for given materials. We took acoustic phonon deformation potential scattering, acoustic piezoelectric scattering, ionized impurity scattering as elastic process (S_{ei}) and also polar optic phonon scattering as inelastic process (S_{inel}). The total elastic scattering rate will be the sum of all the different scattering rates.

$$S(k, k') = S_{ei}(k, k') + S_{inel}(k, k') \quad (3)$$

In this case, S_{inel} represents transitions from the state characterized by k to k' either by emission [$S_{em}(k, k')$] or by absorption [$S_{ab}(k, k')$] of a phonon. And polar optic phonon scattering, we have to consider scattering – in rates by phonon emission and

Parameter	WZ-AIN	ZB-AIN
Band-gap (eV)	6.25	5.4
Electron effective mass (m^*)	0.31	0.35
Static relative permittivity ϵ_0	8.5	8.07
Optical relative permittivity ϵ_∞	4.77	4.46
Density (kgm^{-3})	3230	3257
Sound velocity (ms^{-1})	9060	5740
Deformation potential (eV)	9.5	9
Optical phonon energy (eV)	0.0992	0.099

absorption.

Table 1. Important parameters used in our calculations for WZ-AIN and ZB-AIN [6-7-9].

Using Boltzmann equation and considering all differential scattering rates, the factor $g(k)$ in the perturbed part of the distribution function $f(k)$ can be given by:

$$g(k) = \frac{(-\frac{eE}{\hbar})(\frac{\partial f_0}{\partial k}) + \sum \int g' \cos\varphi [S'_{inel}(1-f) + S_{inel}f] dk}{\sum \int (1-\cos\varphi) S_{ei} dk + \sum \int [S_{inel}(1-f') + S'_{inel}f'] dk} \quad (4)$$

Note the first term in the denominator is simply the momentum relaxation rate for elastic scattering. It is interesting to note that if the initial distribution is chosen to be the equilibrium distribution, for which

$g(k)$ is equal zero, we get the relaxation time approximation result after the first iteration. We have found that convergence can normally be achieved after only a few iterations for small electric fields.

Once $g(k)$ has been evaluated to the required accuracy, it is which is given by:

$$\mu_d = \frac{\hbar}{3m^*} \frac{\int_0^\infty k^3 \frac{g(k)}{Ed} dk}{\int_0^\infty k^2 f(k) dk} \quad (5)$$

Where d is defined as $1/d = m \nabla_k E / \hbar^2 k$. We took the structure of AIN compound as Wurtzite structure and Zincblende structure And we took into account electron screening [2].

III. Results

Effective mobility parameters are such as temperature, density, coefficient of nonparabolic electron effective mass and the energy balance and so on.

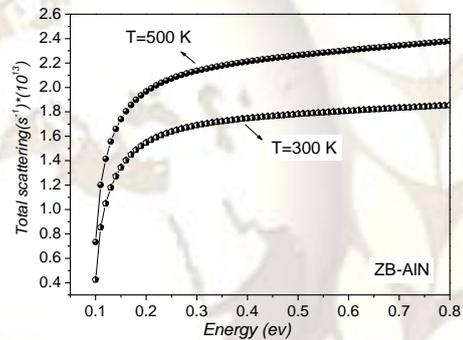


Fig 1. Changes total scattering electron function in terms of energy in bulk WZ-AIN at the different temperature.

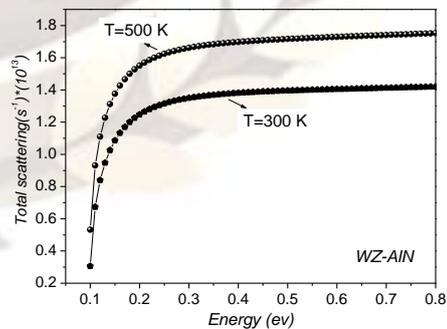


Fig 2. Changes total scattering electron function in terms of energy in bulk ZB-AIN at the different temperature.

Figure 1 and 2 show total scattering depends on energy and increasing temperature causes increasing in bulk ZB-AIN and WZ-AIN materials.

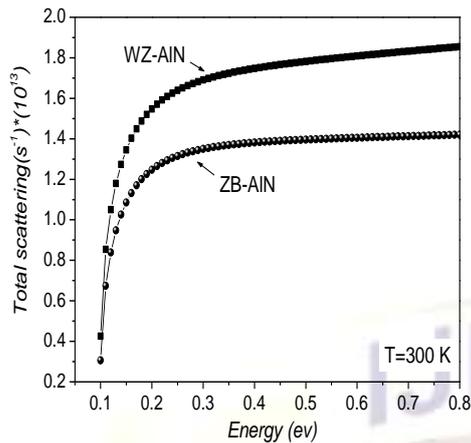


Fig 3. Changes total scattering electron function in terms of energy in bulk ZB-AIn and WZ-AIN at different temperature.

Figure 3 shows comparison of totals scattering in WZ-AIN and ZB-AIN at the different temperature .Our calculation results show that the totals scattering rate in WZ-AIN is more than ZB-AIN . Only a weak electric field the electrons in the Γ -valley electric transportation involved. Because they no longer have the energy to go to the valley .Hence transitions between valley occurs. In weak electric field piezoelectric scattering and ionized impurity scattering play an important role and they can not be ignored.

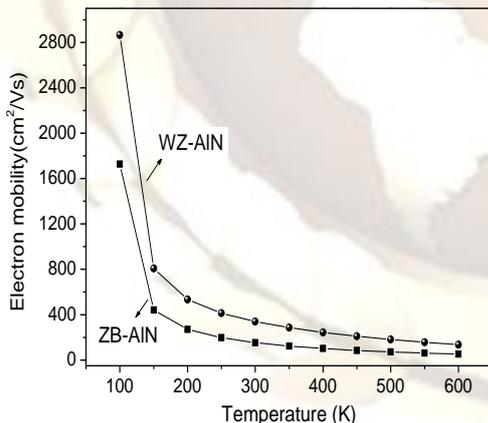


Fig 4. Changes the electron mobility function in terms of temperature in bulk ZB-AIN and WZ-AIN at different temperature.

Figure 4 shows the electron mobility of WZ-AIN is more than ZB-AIN at the different temperature . We see the electron mobility decreases with increasing temperature . Because of a phonon scattering rate increased with increasing temperature and increasing temperature also increases the energy of the phonons . Because the

effective mass of ZB-AIN is more than WZ-AIN, with increasing the effective mass , the electron mobility decreases with increasing electron effective mass increases the moment of it which reduces the electron acceleration in an electric field is uniform, which ultimately reduces mobility in an electric field is present . Increasing the non parabolic electron energy bands are meant to be paved. Smooth energy bands, effective mass of electrons and thus increase the mobility reduction in the crystal is.

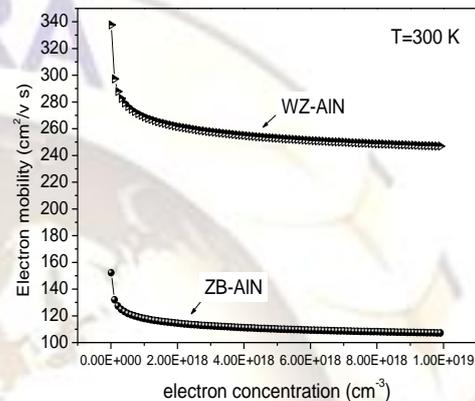


Fig 5. Changes the electron mobility function in terms of electron concentration in bulk ZB-AIN and WZ-AIN at T=300 K.

Figure 5 shows the electron mobility of WZ-AIN is more than ZB-AIN in range of electron concentration .In this case we see the electron mobility decreases with increasing the electron concentration. Because of the increasing number of electrons ionized impurity centers is also increasing the number of times that electron feels coulomb potential, therefore the ionized impurity scattering rate increases. So, electron mobility decreases.

We result that electron mobility at the definite temperature 300K for the WZ-AIN semiconductor is gained about $337.61 \text{ cm}^2 \text{ v}^{-1} \text{ s}^{-1}$ and for ZB-AIN about 152.254 and the electron mobility WZ-AIN is more than ZB-AIN. This increasing is because of small effect mass.

REFERENCES

- [1] S. AYDOĞU, M. AKARSU and Ö. ÖZBAŞ. Calculation of the electron mobility of GaN Osmangazi University, Art and Science Faculty, Department of Physics, Eskişehir, TURKEY saydogu@ogu.edu.tr, akarsu@ogu.edu.tr, oozbas@ogu.edu.tr
- [2] H. Arabshahi, Z. Moodi and A. Pourhasan International NUMERICAL CALCULATION OF THE ELECTRON MOBILITY IN GaAs SEMICONDUCTOR UNDER WEAK ELECTRIC FIELD APPLICATION Journal of Science,

- Environment and Technology, Vol. 1, No 2,
80 - 87, 2012
- [3] N. A. Masyukov and A. V. Dmitriev. Hot electrons in wurtzite indium nitride. JOURNAL OF APPLIED PHYSICS **109**, 023706_2011_
- [4] **F Litimein¹, B Bouhafs^{1,2}, Z Dridi^{1,2} and P Ruterana²**The electronic structure of wurtzite and zinblende AlN: an *ab initio* comparative study. *New Journal of Physics* **4** (2002) 64.1–64.12
- [5] H. Arabshahi. Modeling Low Field Electron Mobility in Group III Nitride Materials . COMPUTER SCIENCE AND APPLICATION, VOL. 1, NO.1, JANUARY, 2012
- [6] Fabio Bernardini and Vincenzo Fiorentini. Spontaneous polarization and piezoelectric constants of III-V nitrides . PACS: 77.65.Bn, 77.84.Bw, 77.22.Ej. 23 Jul 1997
- [7] S.Loughin and R.H.French –Electronic structure of ALN :Theory and experiment . Appl . phys , lett ,63(9),30 August 1993
- [8] P.Jonnard , N.Capron –F.Semond ,J .Massies . Electronic structure of wurtzite and zinc-blende ALN ,February 2,2008

