Research Article

Calculation of Electron Mobility in WZ-AlN and ZB-AlN at Low Electric Field

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ABSTRACT

In this work, the electron mobility of AlN Wurtzite and AlN Zincblende semiconductor compounds was calculated using iterative method in range of 100-600 K. We compared 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 have become 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-AlN, the bandgap is 4.3 eV and direct at gamma point and in ZB-AlN 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-AlN is an object of the invention to prepare ZB-AlN of sufficient quality and thickness to characterize it for its mechanical, optical and electrical properties and to be useful for device fabrication. WZ-AlN is a III-V semiconductor with Wurtzite crystalline properties of WZ-AlN, 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 the scattering effect in ZB-AlN and WZ-AlN structures, we discover 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 increases with increased temperature. However, change difference is not important and in impurity scattering, the scattering rate of electron due to impurities atom in low-temperature is more, than in high temperature. Thus, the scattering rate of electron in WZ-AlN is more than ZB-AlN because their band gap and the effective mass of electron in Γ-valley are different. The Boltzmann equation is solved iteratively for this purpose, jointly incorporating the effects of all the scattering mechanisms. This paper is organized as follow; details of iterative model is presented in Section II and results of iterative calculations carried out on ZB-AlN and WZ-AlN structures are interpreted in Section III [3-5].
II. SOLVING THE BOLTZMANN TRANSPORT EQUATION

In principle, the iterative technique gives 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 the application of a uniform electric field the Boltzmann equation can be written as:

\[
\left( \frac{e}{h} \right) E \cdot \nabla f = \int \left[ S' f'(1-f') - S f (1-f) \right] \, dk
\]

(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 generally as:

\[
f(k) = f_0(k) + g(k) \cos \theta
\]

(2)

Where \( f_0(k) \) in the equilibrium distribution function, \( \theta \) 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 that 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 (\( S_{\text{el}} \)) and also polar optic phonon scattering as inelastic process (\( S_{\text{inel}} \)). The total elastic scattering rate will be the sum of all the different scattering rates.

\[S(k,k') = S_{\text{el}}(k,k') + S_{\text{inel}}(k,k')\]  

(3)

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

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>WZ-AlN</th>
<th>ZB-AlN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band-gap (eV)</td>
<td>6.25</td>
<td>5.4</td>
</tr>
<tr>
<td>Electron effective mass (m*)</td>
<td>0.31</td>
<td>0.35</td>
</tr>
<tr>
<td>Static relative permittivity ( \varepsilon_0 )</td>
<td>8.5</td>
<td>8.07</td>
</tr>
<tr>
<td>Optical relative permittivity ( \varepsilon_\infty )</td>
<td>4.77</td>
<td>4.46</td>
</tr>
<tr>
<td>Density (kgm(^{-3}))</td>
<td>3230</td>
<td>3257</td>
</tr>
<tr>
<td>Sound velocity (ms(^{-1}))</td>
<td>9060</td>
<td>5740</td>
</tr>
<tr>
<td>Deformation potential (eV)</td>
<td>9.5</td>
<td>9</td>
</tr>
<tr>
<td>Optical phonon energy (eV)</td>
<td>0.0992</td>
<td>0.099</td>
</tr>
</tbody>
</table>

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:

\[
g(k) = \left( \frac{-eE}{h} \frac{\partial f_0}{\partial k} \right) + \int \left[ g' \cos \theta \left( S_{\text{em}}(k,k') + S_{\text{inel}}(k,k') \right) \right] \, dk
\]

\[
\frac{1}{\sum [1 - \cos \theta] S_{\text{el}} \, dk + \sum [S_{\text{em}}(k,k') + S_{\text{inel}}(k,k')] \, dk}
\]

(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 \( g(k) \) equals 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 given by:

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\[ \mu_d = \frac{h}{3m^2} \int_0^\infty k^2 \frac{g(k)}{E_d} f(k) c \, dk \]  
\[ (5) \]

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

III. RESULTS

Effective mobility parameters are temperature, density, coefficient of non parabolic electron effective mass and the energy balance and so on.

Figures 1 and 2 show that total scattering depends on energy and increasing temperature causes increase in bulk ZB-AlN and WZ-AlN materials.
Figure 3 shows comparison of totals scattering in WZ-AlN and ZB-AlN at the different temperatures. Our calculation results, show that the totals scattering rate in WZ-AlN is more than in ZB-AlN. Only a weak electric field of the electrons in the Γ-valley electric transportation is involved, because they no longer have the energy to go to the valley. Hence transitions between valleys occurs. In a weak electric field, piezoelectric scattering and ionized impurity scattering play important roles and they cannot be ignored.

Figure 4 shows the electron mobility of WZ-AlN is more than ZB-AlN at the different temperatures. We see that the electron mobility decreases with increasing temperature. Due to a phonon scattering rate increased with increasing temperature; and increasing temperature also increases the energy of the phonons. Since the effective mass of ZB-AlN is more than WZ-AlN, with increase in 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.

![Graph showing electron mobility vs electron concentration for WZ-AlN and ZB-AlN at T=300 K.](image)

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

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

We discover that electron mobility at the definite temperature 300K for the WZ-AlN semiconductor is gained about 337.61 cm² v⁻¹ s⁻¹ and for ZB-AlN about 152.254 and the electron mobility in WZ-AlN is more than in ZB-AlN. This increase is due to small effect mass.

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