Electron mobility calculation for two-dimensional electron gas in InN/GaN digital alloy channel high electron mobility transistors

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The InN/GaN digital alloy is a superlattice-like nanostructure formed by periodically stacking ultra-thin InN and GaN layers. In this study, we calculate the electron mobility in InN/GaN digital alloy channel high electron mobility transistors (HEMTs) by performing a single-particle Monte Carlo simulation. The results of the simulation show that alloy-induced scatterings have little impact and the electron mobility significantly improves as the effective indium mole fraction of the channel increases. This contrasts with InGaN alloy channel HEMTs, where alloy disorder and random dipole scatterings have a strong impact and the electron mobility decreases as the indium mole fraction of the channel increases.

1. Introduction

Gallium nitride (GaN) and the related nitride semiconductors receive considerable attention because of their excellent properties, such as a wide bandgap, high carrier saturation velocity, and large breakdown electric field. In gallium nitride-based heterostructures such as AlGaN/GaN single heterostructures, a highly concentrated two-dimensional electron gas (2DEG) is formed at the heterointerface even in the absence of doping because of polarization charges. This enables us to realize a high-electron-mobility transistor (HEMT) for high-frequency and high-power applications.

We can expect further improvement in electron mobility by replacing the channel material of AlGaN/GaN HEMTs with InGaN/GaN HEMTs because the electron effective mass of InGaN is lighter than that of GaN. InGaN is, however, an alloy semiconductor with a random distribution of atoms, which introduces additional scattering mechanisms such as alloy disorder and random dipole scatterings. In the previous study, we showed that alloy disorder and random dipole scattering have a strong impact in AlGaN/InGaN/GaN HEMTs and the electron mobility significantly decreases as the indium mole fraction of the channel increases.

Recently, Ref. 20 proposed InN/GaN digital alloy (DA) structures for optoelectronic device applications. The InN/GaN DA is a superlattice-like nanostructure formed by periodically stacking ultra-thin InN and GaN layers. Since alloy-induced scatterings are absent in a DA channel, we expect the mobility improvement by replacing the channel material of AlGaN/GaN HEMTs with InN/GaN DA structures. To evaluate what extent this improvement occurs, here, we perform a single-particle Monte Carlo simulation of the electron mobility in InN/GaN DA channel HEMTs comparing with InGaN alloy channel HEMTs.

This paper is organized as follows: in Sect. 2, we describe the method of calculating the electron mobility in DA-channel HEMTs in more detail than the original abstract (Ref. 21). Numerical results for the electronic states, scattering rates, and electron mobility are presented and discussed in Sect. 3. A conclusion is given in Sect. 4.

2. Theory

Figure 1 shows a schematic diagram of the [0001] InN/GaN DA channel HEMT considered in the present study. The InN/GaN DA channel is sandwiched between the GaN buffer layer and the Al0.27Ga0.73N barrier layer. The InN/GaN DA channel consists of 10 period of InN/GaN layers, and each InN/GaN layer consists of m-monolayer (ML) GaN and n-ML InN. The thickness of 1 ML is one half of the lattice constant c, and the m-ML GaN (n-ML InN) corresponds to $m \times 2.593 \text{Å}(n \times 2.852 \text{Å}).$ We define the effective indium mole fraction as $x = n(m + n)$ for a InN/GaN DA consisting of periodic (GaN)$_m$(InN)$_n$ layers.

The InN/GaN DA can be modeled either by assuming a periodic layered structure with an effective mass approximation (periodic layer model, PLM) or by considering the whole InN/GaN DA as a single structure whose band structure is calculated with a band structure calculation method, such as density functional theory and tight-binding (TB) method (single layer model, SLM). We adopt the latter approach (see appendix for the former approach) and the band structure of InN/GaN DA calculated by semi-empirical tight-binding (TB) method.

We use the $sp^3d^5s^* $ nearest-neighbor (NN) TB parameters of Ref. 26 for wurtzite GaN. For wurtzite InN, we perform an optimization of $sp^3d^5s^* $ NN TB parameters to reproduce a widely accepted band structure. In the following calculations, we use the energy bandgap and the electron effective mass obtained from TB band structures. We obtain the energy bandgap as the energy difference between the conduction band minimum and the valence band maximum. The electron effective mass is calculated in the lowest conduction band at the $\Gamma$ point. Other parameters are set to the same values as in InGaN alloy.

We performed single particle Monte Carlo simulation to obtain low-field 2DEG mobility of HEMTs. The calculation method was already published in detail in Ref. 19, but for the sake of completeness we will briefly describe the method in the following.

The electronic states of HEMTs along the growth direction ($z$ direction) are calculated by self-consistently solving...
Fig. 1. A schematic diagram of the InN/GaN DA channel HEMT together with the coordinate axis.

the coupled Schrödinger equation,
\[
\left\{ \frac{\hbar^2}{2} \frac{d}{dz} \left[ \frac{1}{m^*(z)} \frac{d}{dz} \right] - e\phi(z) + \Delta E_c(z) \right\} \xi_{n'}(z) = \epsilon_n \xi_n(z),
\]
and Poisson equation,
\[
\epsilon_0 \frac{d}{dz} \left[ \kappa(z) \frac{d\phi(z)}{dz} \right] = -\rho(z) + \frac{dP(z)}{dz}.
\]
Here, \( n \) is the subband index \((n = 0, 1, 2, \ldots)\), \( \xi_n(z) \) is the electron wave function, \( \epsilon_n \) is the subband energy, \( \phi(z) \) is the electrostatic potential, \( \Delta E_c(z) \) represents the conduction band discontinuity, \( m^*(z) \) is the position-dependent electron effective mass, and \( \epsilon_0 \) is the permittivity of vacuum, \( \kappa(z) \) is the position-dependent static dielectric constant, \( \rho(z) \) is the charge distribution, and \( P(z) \) is the polarization. The total electron energy including the in-plane \((x-y)\) motion is given by
\[
E_{kn} = \frac{\hbar^2 k^2}{2m^*} + \epsilon_n,
\]
where \( k \) is the in-plane wavevector.

The scattering rates are evaluated with the obtained electronic states. We include acoustic deformation, \(^{32}\) polar optical phonon, \(^{33}\) alloy disorder, and random dipole scatterings. For the InN/GaN DA channel HEMT, we ignore alloy and random dipole scattering in the channel because the InN and GaN layers are periodically arranged.

The acoustic deformation potential scattering rate is given by \(^{33}\)
\[
W_{k\alpha}^{\text{ac}} = \sum \frac{1}{b_{mn}} \frac{D_{mn}^2 k_B T m^*}{\hbar^3 \rho s \kappa_0} u_0(E_{kn} - \epsilon_n),
\]
where
\[
\frac{1}{b_{mn}} = 2 \int dz \left| \xi_{n'}(z) \right|^2 \left| \xi_n(z) \right|^2.
\]

The polar optical phonon scattering rate is given by
\[
W_{k\alpha}^{\text{pop}} = \sum_{n'} \frac{e^2}{8\pi \epsilon_0} \left( \frac{1}{\kappa_\infty} - \frac{1}{\kappa_0} \right) \left( N_{LO} + \frac{1}{2} \pm \frac{1}{2} \right) \times \int dq f_B(\epsilon_{kn} - \epsilon_{k+q,nn} \pm \hbar\omega_{LO}) \times \frac{1}{q} \int d\omega e^{-\omega_{LO}^2} \xi_n(\omega) \xi_n'(-\omega) e^{-\eta_{\omega}^2},
\]
where \( N_{LO} \) is the phonon distribution function given by
\[
N_{LO} = \frac{1}{\exp(\hbar\omega_{LO}/k_B T) - 1},
\]
and \( \hbar \omega_{LO} \) is the polar optical phonon energy, \( \kappa_\infty \) is the high-frequency dielectric constant, \( \kappa_0 \) is the low-frequency dielectric constant, \( q \) is the in-plane phonon wavevector, and the upper (lower) symbol of \( \pm \) corresponds to the phonon emission (absorption) processes. Although the polar optical phonon scattering rate in heterostructures with wurtzite crystals is different from bulk semiconductors with cubic crystals, \(^{34-36}\) we assume a simple cubic approximation \(^{37,38}\) with bulk phonon modes because it has been confirmed that it has sufficient accuracy. \(^{19}\)

The alloy disorder scattering rate in an alloy semiconductor \( A_xB_{1-x}C \) is given by \(^{19}\)
\[
W_{kn}^{\text{alloy}} = \sum_n \int dz \frac{\Omega(z)}{2\pi} \left( 1 - x(z) \right) |V_A(z) - V_B(z)|^2 \times \left| \xi_n'(z) \right|^2 \left| \xi_n(z) \right|^2 \int d\omega f_B(\epsilon_{kn} - \epsilon_{k+q,nn}) \left( \frac{\delta(\epsilon_{kn} - \epsilon_{k+q,nn})}{\epsilon_{2D}(q)^2} \right),
\]
where \( \Omega(z) \) is the volume of the unit cell, \( V_A \) and \( V_B \) are the atomic potentials of cations A and B, respectively. We include the Thomas-Fermi dielectric function \( \epsilon_{2D}(q) \) to take into account the free-carrier screening. \(^{39,40}\) For the InGaN channel HEMT, the upper limit of the integration, \( z_{\text{max}} \), is set to the sum of the lengths of the AlGaN barrier and InGaN channel layer. On the other hand, for the DA-channel HEMT, \( z_{\text{max}} \) is set to the length of the AlGaN barrier layer only because we assume that the alloy-induced scatterings absent in the DA channel. Note that \( z = 0 \) is chosen to be at the location of the surface of the AlGaN barrier layer. In the present study, we use the reported alloy disorder potential \( \Delta V_{Al-Ga} = 1.5 \text{ eV}^{11} \) for AlGaN. For InGaN, we use \( \Delta V_{In-Ga} = 1.7 \text{ eV} \), which is the conduction-band discontinuity \( \Delta E_c \) between InN and GaN.

The random dipole phonon scattering is caused by a random distribution of dipoles in the III–V nitride alloys\(^{16,17}\) and its scattering rate can be written as\(^{19}\)
\[
W_{k\alpha}^{\text{dipole}} = \frac{2\pi}{\hbar} \sum_{n'} \int_0^{z_{\text{max}}} dz n_0^d(z) x(z) \left[ 1 - x(z) \right] \times \int d\omega f_B(\epsilon_{kn} - \epsilon_{k+q,nn}) \left( \frac{\delta(\epsilon_{kn} - \epsilon_{k+q,nn})}{\epsilon_{2D}(q)^2} \right),
\]
where \( f_{n',n}(q, z) \) is the form factor given by
\[
f_{n',n}(q, z) = \left[ \int dz' \xi_{n'}(z') \xi_n(z') e^{-\eta_{\omega}^2} \right]^2.
\]
and \( n_{3D} \) is the density of dipoles per unit cell volume. For an alloy semiconductor \( \text{A}_x\text{B}_{1-x}\text{C} \), the dipole moments \( p_A \) and \( p_B \) are given respectively by (7)

\[
p_A = [P_{sp}^{AC} + P_{pz}^{AC}]\Omega^{AC},
\]

\[
p_B = [P_{sp}^{BC} + P_{pz}^{BC}]\Omega^{BC},
\]

where \( P_{sp} \) is the spontaneous polarization and \( P_{pz} \) is the piezoelectric polarization.

3. Results and discussion

Table I summarizes the parameters used in the present calculation for wurtzite GaN, AlN, and InN. For the parameters of AlGaN and InGaN alloy, such as spontaneous polarizations, piezoelectric polarizations, and energy bandgaps, we use the same values of Ref. 19. Table II shows the TB parameters used in the present calculation for wurtzite GaN and InN. The values of GaN are cited from Ref. 26, and those of InN are obtained by the optimization of the TB parameters to reproduce the reported InN band structure. For other parameters, such as the reference bond length, we use the values of Ref. 26.

Figure 2 shows the calculated band structures of InN using the TB parameters of Table II. The bandgap is 0.7 eV and the electron effective mass is 0.07 \( m_0 \). Figure 3 depicts the band structures of InN/GaN DA of \( m = 4 \) and \( n = 1 \) (\( x = 0.2 \)). The bandgap and effective mass for InN/GaN DAs are given in Figs. 4 and 5, respectively. In these figures, \( m \) decreases from 5 ML to 0 ML with a 1 ML step, while \( n \) increases from 0 ML to 5 ML with a 1 ML step with keeping \( m + n = 5 \). Although the band gap shows a small bowing, the effective mass almost follows Vegard’s law.

### Table I. Parameters used in the present calculations for wurtzite GaN, AlN, and InN at 300 K. The listed properties are the lattice constants \( a_0 \) and \( c_0 \), energy gap \( E_g \), electron effective mass \( m^* \), crystal density \( \rho_s \), low-frequency dielectric constant \( \kappa_0 \), high-frequency dielectric constant \( \kappa_{\infty} \), longitudinal optical phonon energy \( \hbar\omega_{LO} \), transverse optical phonon energy \( \hbar\omega_{TO} \), deformation potential \( D_0 \), longitudinal sound velocity \( s_l \), and spontaneous polarization \( P_{sp} \).

| Parameter          | GaN   | AlN   | InN   |
|--------------------|-------|-------|-------|
| \( a_0 \) (\( \text{Å} \)) | 3.189 | 3.112 | 3.545 |
| \( c_0 \) (\( \text{Å} \)) | 5.185 | 4.992 | 5.703 |
| \( E_g \) (eV)      | 3.42  | 6.28  | 0.70  |
| \( m^* \)          | 0.20  | 0.30  | 0.07  |
| \( \rho_s \) (kg m\(^{-3}\)) | 6150  | 3230  | 6810  |
| \( \kappa_0 \)      | 8.9   | 8.5   | 13.52 |
| \( \kappa_{\infty} \) | 5.35  | 4.46  | 8.4   |
| \( \hbar\omega_{LO} \) (meV) | 92.12 | 110.35| 72.66 |
| \( \hbar\omega_{TO} \) (meV) | 69.55 | 83.16 | 59.02 |
| \( D_0 \)          | 8.3   | 9.5   | 7.1   |
| \( s_l \) (km/s)   | 6.59  | 9.06  | 6.24  |
| \( P_{sp} \) (C/m\(^2\)) | −0.034 | −0.090 | −0.042 |

### Table II. Parameters of the \( sp^3d^5s^* \) tight-binding model for GaN and InN at 300 K. The energy zero is taken at the valence-band maximum in the zincblende phase.

| Parameter          | GaN   | InN   |
|--------------------|-------|-------|
| \( E_{\sigma}^{s} \) | −8.937| −8.344|
| \( E_{\pi}^{s} \)   | 4.750 | 2.562 |
| \( E_{\sigma}^{p} \) | 28.182| 30.558|
| \( E_{\pi}^{p} \)   | 35.050| 34.264|
| \( E_{\sigma}^{p}^{*} \)| 2.062 | 1.958 |
| \( E_{\pi}^{p}^{*} \)| 11.450| 10.149|
| \( E_{\sigma}^{d} \)   | 27.943| 28.468|
| \( E_{\pi}^{d} \)   | 28.408| 26.496|
| \( E_{\sigma}^{d} \)   | 29.409| 30.683|
| \( E_{\pi}^{d} \)   | 26.989| 26.293|
Figure 6 shows the electronic states obtained by the self-consistent calculation at $T = 300$ K for a DA-channel HEMT of $m = 4$ and $n = 1 (x = 0.2)$. The 2DEG density is found to be $N_{DA} = 1.04 \times 10^{13}$ cm$^{-2}$ which is almost the same as the 2DEG density of an InGaN alloy channel HEMT of $x = 0.2$, i.e., $N_{InGaN} = 1.02 \times 10^{13}$ cm$^{-2}$ (see Fig. 7).

Figure 8 and 9 show the calculated scattering rates of the 2DEG in the DA- and InGaN-channel HEMTs, respectively. For the InGaN-channel HEMT, the alloy disorder and random dipole scatterings are the dominant scattering mechanisms. On the other hand, for the DA-channel HEMT, those alloy-induced scatterings have small impact on 2DEG. This can be attributed to the fact that the alloy-induced scatterings are absent in the DA channel region and the electron penetration into the AlGaN barrier layer is small (see Fig. 6). As for the phonon scatterings, the acoustic deformation potential and polar optical phonon scattering rates are almost the same between DA- and InGaN-channel HEMTs because of the small difference in the spatial distribution of 2DEGs in these HEMTs.

Figure 10 shows the 2DEG mobility $\mu$ as a function of the indium mole fraction $x$ of the channel, obtained by single-particle Monte Carlo simulation under a uniform electric field of 1 kV cm$^{-1}$. Open squares show the mobility of InGaN alloy channel HEMTs, $\mu_{alloy}$, and closed circles show the mobility of InN/GaN DA channel HEMTs within the single...
layer model (SLM), $\mu_{\text{SLM}}$. In Fig. 10, we also plot the mobility of InN/GaN DA channel HEMTs within the periodic layer model (PLM), $\mu_{\text{PLM}}$ for comparison (see Appendix for PLM). Note that the marks at $x = 0$ represent the results for the GaN-channel HEMT. For the InGaN alloy channel HEMT, alloy disorder and random dipole scatterings have a strong impact and 2DEG mobility $\mu$ decreases as $x$ increases, i.e., $\mu_{\text{SLM}} = 600 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ when $x = 0.2$, and $\mu_{\text{SLM}} = 570 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ when $x = 0.4$.

In contrast, for the DA channel HEMT, those alloy-induced scatterings have little impact and $\mu$ improves significantly as $x$ increases, i.e., $\mu_{\text{SLM}} = 1,800 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ($\mu_{\text{PLM}} = 1,900 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) when $x = 0.2$, and $\mu_{\text{SLM}} = 2,100 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ($\mu_{\text{PLM}} = 2,400 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) when $x = 0.4$.

4. Conclusions

We investigated the 2DEG mobility in InN/GaN DA channel HEMTs compared with InGaN alloy channel HEMTs. We find that alloy-induced scatterings have little impact and the electron mobility significantly improves as the effective indium mole fraction of the channel increases in InN/GaN DA channel HEMTs.

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Appendix

In this appendix, we present the Monte Carlo results within a periodic layer model (PLM). For the single layer model (SLM) as discussed in the main text, a DA channel is considered as a single material described with a single band-structure. For PLM, we solve the Schrödinger equation with a periodic potential profile assuming that each layer can be described with its band-structure, and obtain the electronic states. The obtained electronic states of InN/GaN DA channel HEMT are shown in Fig. A-1, in which we find that the 2DEG density is $1.02 \times 10^{13} \text{ cm}^{-2}$.

Figure A-2 shows the calculated scattering rates of a DA channel HEMT within the PLM. Note that, in this calculation, the electron effective mass of InN/GaN DA are assumed to be the same as that of InGaN alloy with a small bowing:

\[ m_{\text{InGaN}}^* = m_{\text{InN}}^* + m_{\text{GaN}}^*(1 - x) + bx(1 - x), \quad (A-1) \]

with $m_{\text{InN}}^* = 0.07 \text{ m}_0$, $m_{\text{GaN}}^* = 0.2 \text{ m}_0$, and $b = -0.07 \text{ m}_0$.

We see that the effect of the alloy scattering is smaller than that in the SLM [see Fig. 8]. This is because the penetration rate of the electrons into the AlGaN barrier layer is 5.4 % in the PLM, which is smaller than 10.6 % in the SLM (see also Fig. 6). On the other hand, the polar optical phonon scattering rate at the bottom of the lowest subband, which is the dominant scattering mechanism, is almost the same as in the SLM, i.e., $W_{\text{PLM}}^{\text{POM}} = 3.25 \times 10^{12} \text{ s}^{-1}$ and $W_{\text{SLM}}^{\text{POM}} = 3.21 \times 10^{12} \text{ s}^{-1}$.

Figure 10 shows a comparison of the 2DEG mobilities of the PLM and SLM. We see that the mobility of the PLM is slightly higher than that of the SLM. This is mainly because.
the electron effective mass of InGaN alloy used in the PLM is slightly smaller than that of the SLM, while the phonon scattering rates are almost the same with each other.

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