Monte Carlo simulation of InAs HEMTs considering strain and quantum confinement effects

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Abstract. We carried out Monte Carlo simulation of In₀.₅₃Ga₀.₄₇As/strained-InAs/In₀.₅₃Ga₀.₄₇As composite channel high electron mobility transistors (HEMTs) considering strain and quantum confinement effects in very thin InAs layer. We calculated the unstrained and the strained band structures of InAs. We also considered the self-consistent analysis of 2-dimensional electron gas (2DEG) by solving Schrödinger and Poisson equations. With considering the effect of 2DEG, the drain-source current $I_{ds}$ decreases. However, the negative threshold voltage shift due to the short-channel effects is not affected by considering 2DEG. The threshold voltage shift occurs in the region $L_g/d < ~5$ ($L_g$: gate length, $d$: sum of the barrier and channel layer thicknesses). We also obtained the cutoff frequency $f_T$ values. At a gate length $L_g$ of 20 nm, the calculated $f_T$ values were 943 GHz without 2DEG and 813 GHz with 2DEG. The trend of the $f_T$ values with $L_g$ reflects that of the electron velocities mainly. The present simulation results indicate that the record $f_T$ might be obtained by reducing $L_g$ to around 20 nm for In₀.₅₃Ga₀.₄₇As/strained-InAs/In₀.₅₃Ga₀.₄₇As channel HEMTs.

1. Introduction

InP-based In₀.₅₂Al₀.₄₈As/InₓGa₁₋ₓAs (x ≥ 0.53) high electron mobility transistors (HEMTs) are one of the most promising devices for future ultrahigh-speed applications because of their high electron mobilities, high electron velocities and high sheet-electron densities. At present, the record cutoff frequency $f_T$ of field effect transistors (FETs) is 688 GHz for a 40-nm-gate In₀.₇Ga₀.₃As channel HEMT [1]. On the other hand, the record $f_T$ value for any type of transistor is 765 GHz for a pseudomorphic InP/InGaAs heterojunction bipolar transistor (PHBT) [2]. To achieve higher-speed operations of HEMTs, using an InGaAs strained-InAs/InGaAs composite layer as a channel is one of the most effective methods [3]. In our previous work [4], we reported Monte Carlo (MC) simulation results of InGaAs/InAs/InGaAs composite channel HEMTs without considering strain and quantum confinement effects in very thin InAs layer.

In this work, we calculated the band structures of the unstrained and the strained InAs and carried out Monte Carlo simulation of In₀.₅₃Ga₀.₄₇As/strained-InAs/In₀.₅₃Ga₀.₄₇As composite channel HEMTs considering 2-dimensional electron gas (2DEG) self-consistent analysis by solving Schrödinger and Poisson equations. For In₀.₅₃Ga₀.₄₇As/strained-InAs/In₀.₅₃Ga₀.₄₇As channel HEMTs, very thin InAs layer must be used to prevent degradation of crystal quality due to the difference in the lattice constant.
between InAs and In\(_{0.53}\)Ga\(_{0.47}\)As (about 3%). Therefore, strain and quantum confinement effects are indispensable to theoretical analyses such as MC simulation for InAs layer. We examined the effect of the gate length \(L_g\) on DC and RF performances in the HEMTs with and without considering the effect of 2DEG.

2. Band structures of unstrained and strained InAs
The unstrained and the strained band structures of InAs were calculated by using all-electron full-potential linearized augmented-plane-wave (FLAPW) method in the local density approximation (LDA). The computational code ABCAP (All-electron Band-structure CAIculation Package) used was originally developed by Kodama, Hamada and Yanase [5]. Figure 1 shows the conduction band structures of the unstrained and the strained InAs. By applying -3% biaxial compressive strain to [100] and [010] directions in \(x\)-\(y\) plane, the increase of the electron effective mass in the \(\Gamma\)-valley and the decrease of the \(\Gamma\)-\(L\) and the \(\Gamma\)-\(X\) valley energy separations were observed. We obtained the electron effective mass in the \(\Gamma\)-valley along the [100] ([010]) direction to be 0.032\(m_0\) for the unstrained InAs and 0.038\(m_0\) for the -3% (compressive) strained InAs with considering nonparabolicity, where \(m_0\) is electron rest mass. The electron effective mass in the \(\Gamma\)-valley for the unstrained InAs is almost same as that calculated by the empirical pseudopotential method (0.031\(m_0\)) [6, 7]. On the other hand, the electron effective mass for the -3% (compressive) strained InAs is lighter than that by the pseudopotential method (0.043\(m_0\)) [7]. Note that the electron effective mass in the unstrained n-InAs deduced from magnetophonon resonance is 0.0219\(m_0\) at 250 K [8]. The details of the calculation results will be described elsewhere [9].

3. Monte Carlo simulation
MC simulations were carried out by using the program “COSMOS,” developed by Mizuho Information & Research Institute, Inc. [10]. Figure 2 shows a schematic cross-sectional model structure of the composite channel HEMT used in the present MC simulations. We used a three-valley model (\(\Gamma\), \(L\), \(X\)) with nonparabolicity for the conduction band structures of InAs, In\(_{0.53}\)Ga\(_{0.47}\)As, In\(_{0.52}\)Al\(_{0.48}\)As and InP layers. In\(_{0.53}\)Ga\(_{0.47}\)As and In\(_{0.52}\)Al\(_{0.48}\)As layers are lattice-matched to InP layer. InAs layer is compressively strained. We used the unstrained and the strained band structures of InAs obtained in section 2. The band parameters of AlAs, GaAs and InP were taken from the literature [6,
Figure 3 shows a schematic description of the calculation area of 2DEG. We considered the 2DEG in and near the channel layer by solving the 1-dimensional Schrödinger equation along y-axis at various x-positions [12]. The calculation slices in figure 3 were dense in the region with high electric field. We considered the lowest three quantum levels in the channel. The electrons above the highest quantum level energy were treated as 3-dimensional electrons. The electron scattering mechanisms [13, 14] considered were polar optical phonon scattering, non-polar optical phonon scattering, acoustic phonon scattering, inter-valley phonon scattering and ionized impurity scattering. We did not consider impact ionization in the present simulations since the previous MC simulation results [15] show that the influence of impact ionization is relatively small for the InGaAs/strained-InAs/InGaAs channel HEMT in the drain-source voltage $V_{ds}$ range between 0 and 0.8 V. We did not consider electron-electron interactions either. Sub-band scattering was considered for 2DEG. Dirichlet boundary conditions were applied to all metal-semiconductor interfaces, and Neumann boundary conditions (the zero normal derivative of the potential) were applied to other surfaces. The potential was calculated by
the finite difference method. The time step was set to 0.5 fs. The gate length $L_g$ was varied from 20 to 300 nm. All simulations were carried out at a lattice temperature of 300 K.

4. Results and discussion

4.1. DC performance

Figure 4 shows the drain-source current vs. gate-source voltage ($I_{ds}$-$V_{gs}$) characteristics of 30-nm-gate HEMTs with and without 2DEG. The drain-source voltage $V_{ds}$ is 0.8 V.

To clarify the short-channel effects on performances further, we obtained the threshold voltage shift in the $I_{ds}$-$V_{gs}$ curves. Figure 6 shows the channel aspect ratio $L_g/d$ dependence of the threshold voltage shift. In this work, $d$ was defined as the sum of the barrier and channel layer thicknesses. The threshold voltage shift was defined as the difference from the threshold voltage $V_{th}$ at $L_g/d = 10$ ($L_g = 300$ nm). The negative threshold voltage shift due to the short-channel effects occurs in the region $L_g/d < \sim 100$ nm. This phenomenon is similar to those for AlGaAs/GaAs [16], InAlAs/InGaAs [17] and AlGaN/GaN [18] HEMTs. The difference between with and without 2DEG is very small. Thus, the same scaling rule is valid for the InGaAs/strained-InAs/InGaAs composite channel HEMTs.

4.2. Cutoff frequency

The cutoff frequency $f_T$ values were calculated by the method presented by Kwon and Pavlidis [19]. Figure 7 shows the gate length $L_g$ dependence of the cutoff frequency $f_T$ under a $V_{ds}$ of 0.8 V. The $f_T$'s without 2DEG are higher than

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Figure 4. Drain-source current vs. gate-source voltage ($I_{ds}$-$V_{gs}$) characteristics of 30-nm-gate HEMTs with and without 2DEG. The drain-source voltage $V_{ds}$ is 0.8 V.

Figure 5. Gate length $L_g$ dependence of the maximum transconductance $g_{m,max}$ under a drain-source voltage $V_{ds}$ of 0.8 V.
those with 2DEG. At an $L_g$ of 20 nm, $f_T$ without 2DEG is 943 GHz. On the other hand, $f_T$ with 2DEG is 813 GHz. Thus, the record $f_T$ might be obtained by reducing $L_g$ to around 20 nm for InGaAs/strained-InAs/InGaAs channel HEMTs [2].

Figure 6. Channel aspect ratio $L_g/d$ dependence of the threshold voltage shift under a drain-source voltage $V_{ds}$ of 0.8 V.

Figure 7. Gate length $L_g$ dependence of the cutoff frequency $f_T$ with and without 2DEG under a drain-source voltage $V_{ds}$ of 0.8 V.

Figure 8. Electron velocity profiles in the channel layer for 30-nm-gate HEMTs with and without 2DEG. The drain-source voltage $V_{ds}$ is 0.8 V, and the gate-source voltage $V_{gs}$ is -2.0 V.

Figure 9. Gate length $L_g$ dependence of the average electron velocity in the channel layer under the gate electrode. The drain-source voltage $V_{ds}$ is 0.8 V.
To understand the trend of the cutoff frequency $f_T$ in detail, we obtained the electron velocity in the channel layer. The electron velocity was obtained by taking the average for the whole channel depth. Figure 8 compares the electron velocity profiles in the channel layer of the 30-nm-gate HEMTs with and without considering the effect of 2DEG under a $V_{ds}$ of 0.8 V and a $V_{gs}$ of -2.0 V. There is a velocity overshoot under the gate electrode. In the almost whole region, the electron velocity without 2DEG is higher than that with 2DEG. The peak electron velocities are about $5.7 \times 10^7$ cm/s without 2DEG and about $4.6 \times 10^7$ cm/s with 2DEG. Figure 9 shows the gate length $L_g$ dependence of the average electron velocity in the channel layer under the gate electrode under a $V_{ds}$ of 0.8 V. The $V_{gs}$ values are the voltages with the $g_{m,max}$ values. The average electron velocity increases with decreasing $L_g$ in the present simulation range. The increase of average electron velocity with decreasing $L_g$ results from the increase of the electric field under the gate electrode. On the other hand, the average velocity without 2DEG is higher than that with 2DEG. The trend of the $f_T$ values with $L_g$ reflects that of the electron velocities mainly.

Figure 10 shows the potential profiles of the 30-nm-gate HEMTs without and with 2DEG under a $V_{ds}$ of 0.8 V and a $V_{gs}$ of -2.0 V. There is a negligible difference in the potential profiles between with and without 2DEG. Therefore, the difference in electron velocity between with and without 2DEG does not result from the difference in electric field. Figure 11 shows the electron density distribution along $y$-axis at $x = 0$, i.e. the centre of the gate electrode (See figure 2), of the 30-nm-gate HEMTs. As clearly seen from figure 11, the electron density in the InAs layer without 2DEG is higher than that with 2DEG. The occupancy of electrons in the InAs layer is about 80% without 2DEG. On the other hand, the occupancy is about 65% with 2DEG. Therefore, the higher electron velocity without 2DEG results from the higher occupancy of electrons in the InAs layer in which the electron effective mass is lighter.

4.3. Comments on strain effects
So far, we discussed the quantum confinement effects on the performances in the InGaAs/strained-InAs/InGaAs composite channel HEMTs. In our MC simulations, the compressive strain is applied to the InAs layer. For the InGaAs/InAs/InGaAs channel HEMTs with and without the strain of the InAs layer, Machida et al. [15] reported that the maximum transconductance $g_{m,max}$ without strain is higher than that with strain for 30-nm-gate HEMTs. The cutoff frequency $f_T$ can be calculated by the equation, $f_T = g_m/(2\pi C_g)$, where $C_g$ is the gate capacitance. At each gate length, the $C_g$ value is approximately

Figure 10. Potential profiles for 30-nm-gate HEMTs with and without 2DEG.
constant. Therefore, the cutoff frequency $f_T$ without strain might be higher than that with strain. The MC simulation results of strain effects will be described elsewhere [20].

5. Summary
In summary, we carried out MC simulation of In$_{0.53}$Ga$_{0.47}$As/strained-InAs/In$_{0.53}$Ga$_{0.47}$As composite channel HEMTs considering strain and quantum confinement effects in very thin InAs layer to examine the effect of $L_g$ on DC and RF performances. We calculated the unstrained and the strained band structures of InAs by using all-electron FLAPW method in the LDA. We also considered the 2DEG self-consistent analysis by solving Schrödinger and Poisson equations. The $I_{ds}$ with 2DEG is lower than that without 2DEG due to the reductions of electron velocity and electron density. The reduction of the $g_{m,max}$ due to the short-channel effects was observed in the region $L_g < ~100$ nm. To clarify the short-channel effects, we obtained the threshold voltage shift in the $I_{ds}$-$V_{gs}$ curves. The negative threshold voltage shift due to the short-channel effects is not affected by considering 2DEG. The trend of the threshold voltage shift is similar to those of AlGaAs/GaAs, InAlAs/InGaAs and AlGaN/GaN HEMTs, i.e. the threshold voltage shift occurs in the channel aspect region $L_g/d < ~5$. We also obtained the cutoff frequency $f_T$ values by the method presented by Kwon and Pavlidis. The $f_T$ values at $L_g = 20$ nm are 943 GHz without 2DEG and 813 GHz with 2DEG. The trend of the $f_T$ values with $L_g$ reflects that of the electron velocities mainly. Thus, the record $f_T$ might be obtained by reducing $L_g$ to around 20 nm for In$_{0.53}$Ga$_{0.47}$As/strained-InAs/In$_{0.53}$Ga$_{0.47}$As channel HEMTs.

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