Simulation of Electron Transport in Atomic Monolayer Semiconductor FETs

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Abstract. In this paper, we discuss the device performance of atomic monolayer semiconductor FETs composed of Si, Ge and C elements. First, we present the performance potentials of silicene nanoribbon (SiNR), germanene nanoribbon (GeNR) and graphene nanoribbon (GNR), which all have a sufficient band gap to switch off, as a field-effect transistor (FET) channel material. We demonstrate that comparing at the same band gap of ~ 0.5 eV, GNR FET maintains the advantage over SiNR or GeNR FETs under an ideal transport situation, but SiNR and GeNR are attractive channel materials for high performance FETs as well. Next, we compute the electronic band structure and the electron mobility of germanane, which is a hydrogen-terminated Ge monolayer. We demonstrate that germanane has a band gap larger than 1 eV without a nanoribbon structure, and an effective mass smaller than bulk Ge. Therefore, germanane is also a promising two-dimensional material as a FET channel.

Keywords: graphene, silicene, germanene, germanane, tight-binding method, electron mobility

1. Introduction

Complementary metal-oxide-semiconductor (CMOS) device scaling has led to the continued improvement in high speed operation of LSI circuits. However, with downscaling of CMOS devices into the nanometer regime, we have faced several serious challenges, such as increase in the subthreshold and tunneling leakage current due to short-channel effects, and degradation in the carrier mobility owing to high doping concentration in the substrate [1]. To overcome the performance limit of CMOS technology, new device structures such as ultrathin body MOSFETs [2,3] and FinFETs [4,5] have been proposed to enhance the electrostatic gate controllability over the channel. Furthermore, new channel materials beyond silicon with

Figure 1: Schematics of (a) conventional Si MOSFET, (b) graphene FET, and (c) germanane FET. The generation of dangling bonds at the surfaces is one of the major drawback in conventional Si MOSFET.

higher mobilities have also been extensively studied.

Among the various alternative channel materials for CMOS technology, two-dimensional (2-D) materials are becoming attractive candidates because the materials possess certain properties that may provide a path towards the ultimate physical scaling limit beyond what is predicted for conventional channel materials [6]. These properties include: (1) presence of a large bandgap suitable for electronic switching and negligible band-to-band tunneling, (2) ultrathin channel structure providing excellent gate controllability, (3) absence of dangling bonds at the surface, (4) atomically flat surface, and (5) relatively high effective mass of carriers suppressing source-drain direct tunneling [7,8]. In conventional Si MOSFETs, it is very difficult to scale down bulk silicon thickness to a few nanometers, since there exist dangling bonds at the surfaces of the silicon channel, as shown in Fig. 1 (a), and as a result, the realization of atomically flat channel surfaces is impractical. In other words, channel thickness fluctuation is inevitable in Si MOSFETs, and it causes a new type of surface roughness scattering in a few nanometer thick silicon channels [9].

On the other hand, 2-D materials such as graphene [10], silicene [11] and germanene are atomically flat and have no dangling bonds at the surfaces owing to the robust sp^2 hybridization, as shown in Fig. 1 (b). However, such atomically flat materials have no bandgap themselves, and hence nanoscale processing technique such as a nanoribbon structure [12,13], shown in Fig. 1 (b), is needed to open a band gap for switching devices. In addition, alternative 2-D materials such as silicane and germanane [14] are hydrogen-terminated Si and Ge monolayers as shown in Fig. 1 (c), which have an analogous geometry to a Si/Ge(111) surface in which every Si/Ge atom is terminated with hydrogen (H) atoms above or below the layer, and thus no dangling bonds are generated at the surfaces.

Up till now, a lot of theoretical studies, in parallel with experimental efforts, have been performed to the understanding of the material properties of 2-D materials, but the device performance evaluation of 2-D material FETs is not sufficient yet. In view of practical use, 2-D materials from group IV elements may have better integration and process or materials

compatibility with the present Si-platform, although transition metal dichalcogenide 2-D materials typified by MoS₂ have also been actively researched [15,16] since it has a large band gap of about 1.8 eV. Therefore, in this paper, we intend to analyze atomic monolayer semiconductor FETs composed of Si, Ge and C elements, and to examine their upper limit performance.

2. Performance comparison of silicene, germanene and graphene nanoribbon FETs under ballistic transport

2.1. Silicene, germanene and graphene nanoribbons

The discovery of graphene [10] and the succeeding tremendous advancement in this field of research have promoted to search theoretically and experimentally for similar 2-D materials composed of group IV elements, especially silicon. The silicon equivalent of graphene, silicene, was first mentioned in a theoretical study by Takeda and Shiraishi [17] in 1994. However, silicene does not seem to exist in nature, and as a consequence, pure 2-D silicene layers cannot be generated by exfoliation method as performed initially in the case of graphene [10]. More sophisticated methods had to be searched for the growth or synthesis of silicene.

Recently, Fleurence et al. [11] have demonstrated for the first time that epitaxial 2-D silicene forms spontaneously on (0001)-oriented thin films of zirconium diboride (ZrB₂), that were grown epitaxially on Si (111) wafers. Through a detailed characterization of the structure and electronic properties, they have further shown that silicene is more flexible than graphene, which allows an engineering of the band structure through epitaxy. For instance, compared to graphene, the interatomic distance is larger in Si and Ge (*cf.* Table I), and hence the diminished π - π overlaps cannot maintain the planar stability anymore. Consequently, the sp^2 hybrid orbitals are slightly dehybridized to form sp^3 -like orbitals, and the stable structure for silicene and germanene results in a low buckled geometry, as shown in Fig. 2. Theoretical studies [17,18,19] have predicted that silicene and germanene exhibit similar linear-band dispersions near the Fermi level, and a semimetallic nature without a band gap. Therefore, experimental work on growth of silicene nanoribbon (SiNR) was performed to induce a band gap [20]. The electronic band structure of SiNR was also investigated theoretically [21].

The discovery of the reproducible method fabricating silicene mentioned above will

Figure 2: Low buckled geometry in silicene and germanene.

pave the way for the further study of practical device applications using silicene. In this section, we investigate the performance potentials of FETs with SiNR and germanene nanoribbon (GeNR) channels [22], where the electronic band structures are calculated using a tight-binding (TB) method and the electric characteristics of SiNR and GeNR FETs are evaluated using a ballistic FET model. We further compare them with graphene nanoribbon (GNR) FETs.

2.2. TB band structure calculations of group IV nanoribbons

In this study, a NR structure was adopted to create a band gap in silicene, germanene and graphene. Figure 3 shows the atomic structure of hydrogen-terminated NRs with an armchair-edge, where N represents the number of atoms in the width direction. It is well known that in graphene and its nanoribbons all atoms lie in the same plane, whereas structures of silicene and germanene are slightly buckled, as pointed out above. However, first-principles simulation has shown that the bond-length distribution is nearly uniform except a sudden decrease at the edges, which was the same as in armchair GNRs (A-GNRs) [23], and therefore, the electronic structures of hydrogen-terminated armchair SiNRs (A-SiNRs) and armchair GeNRs (A-GeNRs) have been successfully reproduced by a first nearest-neighbor TB approach with different TB parameters at the edges [21]. Accordingly, we have computed the band structures of the three NRs based on the first nearest-neighbor TB approach considering the relaxation effects of edge atoms due to the hydrogen termination explained below.

First, Fig. 4 shows (a) the unit cell and (b) the first-Brillouin zone of A-NRs. Since A-NR is a 1-D crystal, its primitive lattice vector is defined by $\mathbf{a}$ shown in Fig. 4 (a), and it is given by

$$\mathbf{a} = (3d, 0, 0), \quad (1)$$

Figure 3: Atomic structure of hydrogen-terminated NRs with an armchair-edge. N represents the number of atoms in the width direction, and d the interatomic distance. A unit cell is depicted by the dashed lines.

Figure 4: (a) Unit cell and (b) first-Brillouin zone of A-NRs. $\mathbf{a}$ in (a) represents a primitive lattice vector.

where d is the interatomic distance. Hence, the corresponding primitive reciprocal lattice vector $\mathbf{b}$ is obtained using the relation of $\mathbf{a} \cdot \mathbf{b} = 2\pi$ as

$$\mathbf{b} = 2\pi \left(\frac{1}{3d}, 0, 0 \right). \quad (2)$$

Accordingly, the first-Brillouin zone of A-NRs also becomes 1-D as shown in Fig. 4 (b). Here, the point M is a midpoint of the $\mathbf{b}$ vector, whose coordinates in the k -space are $M : \pi(1/3d, 0, 0)$.

The atom pair in the unit cell, A and B, is labeled using $C_1, C_2, \dots, C_N$ for the channel atoms (Si, Ge, C), and using H_l and H_u for the hydrogen atoms, as shown in Fig. 4 (a). The atom A and B in the C_i group are expressed as C_{iA} and C_{iB} , which are separated from the nearest-neighbor atoms by a spatial vector $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ or $-\mathbf{r}_1, -\mathbf{r}_2, -\mathbf{r}_3$. Based on the above notations, the TB Hamiltonian of A-NRs is represented below.

When the number of atoms in the width direction is N , the electron wavefunction for the unit cell is written as a linear superposition using every atomic orbitals as follows.

$$\Psi = c_{1A}\psi_{1A} + c_{1B}\psi_{1B} + c_{2A}\psi_{2A} + c_{2B}\psi_{2B} + \dots + c_{NA}\psi_{NA} + c_{NB}\psi_{NB}, \quad (3)$$

where ψ_{iX} and c_{iX} ($i=1, 2, \dots, N$; $X=A, B$) are the wavefunction of the π -electron p_z orbital and its amplitude, respectively. In this case, the TB Hamiltonian is given by

Figure 5: Edge relaxation effects in A-NRs due to hydrogen termination of the edge atoms.

Table I: TB parameters used in the present study [21,23]. d (γ_0) and d_{edge} (γ_0^{edge}) are the interatomic distances (hopping energies) in the inner region and at the edges, respectively.

	d (Å)	d_{edge} (Å)	γ_0 (eV)	γ_0^{edge} (eV)
A-GNR	1.42	1.37	2.60	2.91
A-SiNR	2.25	2.20	1.03	1.15
A-GeNR	2.37	2.32	1.05	1.13

$$H' = \begin{matrix} & |1A\rangle & |1B\rangle & |2A\rangle & |2B\rangle & \cdots & |N-1A\rangle & |N-1B\rangle & |NA\rangle & |NB\rangle \\ \begin{matrix} \langle 1A| \\ \langle 1B| \\ \langle 2A| \\ \langle 2B| \\ \vdots \\ \langle N-1A| \\ \langle N-1B| \\ \langle NA| \\ \langle NB| \end{matrix} & \begin{bmatrix} \varepsilon_{2p} & \gamma_0^{edge} p_1' & 0 & \gamma_0 p_2 & \cdots & 0 & 0 & 0 & 0 \\ \gamma_0^{edge} p_1'^* & \varepsilon_{2p} & \gamma_0 p_3^* & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & \gamma_0 p_3 & \varepsilon_{2p} & \gamma_0 p_1 & \cdots & 0 & 0 & 0 & 0 \\ \gamma_0 p_2^* & 0 & \gamma_0 p_1^* & \varepsilon_{2p} & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \varepsilon_{2p} & \gamma_0 p_1 & 0 & \gamma_0 p_2 \\ 0 & 0 & 0 & 0 & \cdots & \gamma_0 p_1^* & \varepsilon_{2p} & \gamma_0 p_3^* & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \gamma_0 p_3 & \varepsilon_{2p} & \gamma_0^{edge} p_1' \\ 0 & 0 & 0 & 0 & \cdots & \gamma_0 p_2^* & 0 & \gamma_0^{edge} p_1'^* & \varepsilon_{2p} \end{bmatrix} & \end{matrix}, \quad (4)$$

where ε_{2p} and γ_0 are the on-site energy and the hopping energy, respectively. In addition, the phase factor p_i is defined as follows.

$$p_i = \exp(i\mathbf{k} \cdot \mathbf{r}_i), \quad (i = 1, 2, 3). \quad (5)$$

According to the structure relaxation analysis based on first-principles calculation, the interatomic distance is decreased to d_{edge} at the edges as shown in Fig. 5 and the hopping energy is increased to γ_0^{edge} , to reflect that edge bonds are stronger than those in the inner bonds, in the case of hydrogen-terminated A-NRs [21,23]. In (4), the relaxation effects of the edge atoms

are taken into account by introducing γ_0^{edge} and $p_1 = \exp(i\mathbf{k} \cdot \mathbf{r}_1)$ with replacing $\mathbf{r}_1 \rightarrow \mathbf{r}_1'$ in

the x -direction. The TB parameters used in the present study are summarized in Table I, which were obtained by fitting to the first-principles results [21,23]. ε_{2p} was set to zero in this study.

Fig. 6 shows the band structures of A-GNRs with $N =$ (a) 12, (b) 13, and (c) 14, com-

Figure 6: Band structures computed for A-GNRs with $N =$ (a) 12, (b) 13, and (c) 14, using TB approach and first-principles method within local density approximation (LDA) [23].

puted using the TB approach and first-principles method [23]. The TB results exhibit very good agreement with the first-principles method, especially in the low-energy region. This is due to the first-nearest approximation that we employed. To improve the accuracy in high-energy region, it is well known that a third-nearest TB approach is necessary [24]. However, as found from Fig. 6 the first-nearest TB approach is sufficient to discuss the electron transport under a small bias condition considered in this study. Next, the variation in band gap energies with the ribbon width given in terms of N , calculated for (a) A-GNRs and (b) A-SiNRs and A-GeNRs are shown in Fig. 7. NRs having widths from $N = 3$ to 20 were investigated here. One can see three branches with decreasing behaviors for all the three NRs considered in this study, which indicates that the band gap opening originates from the quantum confinement effect. Incidentally, this decreasing behavior represents that SiNRs and GeNRs with infinite ribbon width, that is, silicene and germanene, have zero band gap, as in the case of graphene. Here, it is worth noting that comparing at the same number of N , A-SiNRs and A-GeNRs exhibit smaller band gaps than those of A-GNRs. This is due to the smaller γ_0 's in A-SiNRs and A-GeNRs as shown in Table I. Here, if the band gap is different among channel materials, an off-state leakage current due to band-to-band tunneling can be

Figure 7: Variation in band gap energies with the ribbon width given in terms of N , calculated for (a) A-GNRs and (b) A-SiNRs and A-GeNRs.

Figure 8: Band structures computed for A-GNR, A-SiNR, and A-GeNR with a band gap of about 0.5 eV. Specifically, the A-GNR has $N=15$, and the A-SiNR and A-GeNR have $N=6$. A-GNR has the smallest effective mass, $m_{\text{GNR}}^* = 0.051 m_0$, while A-SiNR and A-GeNR have almost the same and larger masses, $m_{\text{SiNR}}^* = 0.106 m_0$ and $m_{\text{GeNR}}^* = 0.100 m_0$.

exponentially changed by the bias condition used. Hence, to make a comparison of the performance potentials of FETs with NR channels considered here, we hereafter focus on three kinds of NRs with approximately the same band gap of ~ 0.5 eV [22], which is larger than an energy of the drain bias assumed in the electrical characteristics simulation described later. Specifically, they are A-GNR with $N = 15$, A-SiNR with $N = 6$, and A-GeNR with $N = 6$, where we adopted $N = 3m$ group (m : a positive integer) in this study since it was reported to be more suitable for high-performance use due to its smaller effective masses than those of $N = 3m + 1$ group [25,26]. Figure 8 shows the band structures computed for those NRs. It can be seen that when the band structures are compared under the same band gap of ~ 0.5 eV, the A-GNR has the smallest effective mass, $m_{\text{GNR}}^* = 0.051 m_0$, while the A-SiNR and A-GeNR have almost the same and larger ones, $m_{\text{SiNR}}^* = 0.106 m_0$ and $m_{\text{GeNR}}^* = 0.100 m_0$. This is because the effective masses are qualitatively related to $(\gamma_0 \times d)^{-1}$, which gives smaller effective masses for A-GNRs. Accordingly, A-GNR FET is expected to provide better device performance than A-SiNR and A-GeNR FETs under the ballistic transport, which will be discussed in detail next.

2.3. Top-of-the-barrier model

To evaluate the performance potentials of FETs composed of A-GNR, A-SiNR, and A-GeNR, we employ a top-of-the-barrier (ToB) model [27]. This model assumes ballistic transport and thus can assess an upper limit performance of atomic-scale FETs. Quantum tunneling is not considered in this model, so the model was shown to be valid for the Si-MOSFET structure if the channel length is equal to or larger than 10 nm [28]. Since the model provides significant insight into the importance of atomistic band structures with greatly reduced computational

Figure 9: (a) Schematic device structure assumed in the simulation. The gate insulator is SiO₂ with thicknesses of 3 and 0.5 nm. (b) ToB model represented using three capacitances, C_S , C_G and C_D . Perfect electrostatic gate control over the channel was assumed.

time compared to a full self-consistent quantum simulation, the model is suitable for a systematic study comparing the performance limits of various atomistic transistors. In this section, we discuss the electrical characteristics of the three A-NR FETs using the ToB model. Figures 9 (a) and (b) show the schematic device structure assumed in the present simulation, and the ToB model represented using three capacitances, C_S , C_G and C_D , respectively. We describe a brief summary of the ToB model below.

When we assume ballistic transport, the drain current of NRs is represented by the Landauer-Büttiker formula as follows.

$$I_D = -q \sum_n \frac{1}{\pi} \int_0^\infty \frac{1}{\hbar} \nabla_k E_n(k) [f(E_n(k) + U_{scf} - E_{F1}) - f(E_n(k) + U_{scf} - E_{F2})] dk. \quad (6)$$

In (6), $f(E_n(k) + U_{scf} - E_{F1})$ and $f(E_n(k) + U_{scf} - E_{F2})$ are the electron distribution functions of source and drain, respectively, and they are usually given by Fermi-Dirac distribution function assuming thermal distribution of electrons in the electrodes. $E_n(k)$ represents the dispersion relation of carriers, which are given by the electronic band structures obtained in the section 2.2. Consequently, we need to define the channel potential U_{scf} , to calculate the drain current using (6). Although we usually solve the 2-D or 3-D Poisson's equation and transport equations self-consistently to obtain U_{scf} , the ToB model expressed using the three capacitances shown in Fig. 9 (b) provides U_{scf} by self-consistently solving the following equations.

$$U_{scf} = -q (\alpha_G V_G + \alpha_D V_D + \alpha_S V_S) + \frac{q^2}{C_G + C_D + C_S} \Delta N, \quad (7)$$

and

$$\Delta N = (N_1 + N_2) - N_0. \quad (8)$$

Here, N_0 is the channel electron density at thermal equilibrium without any biases, and

$$\alpha_i = \frac{C_i}{C_G + C_D + C_S}, \quad (i = G, D, S). \quad (9)$$

N_1 and N_2 in (8) are the channel electron densities injected from the source and drain under a biased situation, and given by the following equations, respectively.

$$N_1 = \sum_n \frac{1}{\pi} \int_0^\infty f(E_n(k) + U_{scf} - E_{F1}) dk \quad (10)$$

$$N_2 = \sum_n \frac{1}{\pi} \int_{-\infty}^0 f(E_n(k) + U_{scf} - E_{F2}) dk \quad (11)$$

Note the difference in the integration ranges of (10) and (11). As mentioned above, the self-consistent calculation is needed to obtain the channel electron density, because the electron density depends on U_{scf} .

In this study, the gate insulator is assumed to be SiO₂ with thicknesses (T_{ox}) of 3 and 0.5 nm. The source and drain donor concentration is given as $3.35 \times 10^{12} \text{ cm}^{-2}$, and the channel is assumed to be undoped. Here, to clarify the band structure effects, we assumed perfect electrostatic gate control over the channel, i.e., zero capacitive couplings between the source-drain and the channel ($C_D / C_G, C_S / C_G = 0$), which gives ideal subthreshold swing. The drain voltage V_D is set at 0.4 V, which is sufficiently small so that band-to-band tunneling leakage current at the off-state bias can be neglected.

2.4. Comparison of device performances

Figure 10 shows the $I_D - V_G$ characteristics computed for $T_{ox} =$ (a) 3 and (b) 0.5 nm, where the vertical axis denotes the drain current density divided by the ribbon width W which was calculated by $W = (N-1) \times \sqrt{3}d/2$. The off current density I_{off} was set as $I_{off} = 0.01 \text{ } \mu\text{A}/\mu\text{m}$.

Figure 10: $I_D - V_G$ characteristics computed for $T_{ox} =$ (a) 3 and (b) 0.5 nm. The vertical axis denotes the drain current density divided by the ribbon width W . $V_D = 0.4 \text{ V}$, and the off current density I_{off} was set as $I_{off} = 0.01 \text{ } \mu\text{A}/\mu\text{m}$.

First of all, it is found that the A-GNR FET exhibits the largest drain current density, while the A-SiNR and A-GeNR FETs have almost the same drain current densities, as expected from the band structures shown in Fig. 8. Here, we may add that the largest drain current flowing through a piece of NR is also obtained with the A-GNR FET, because of its larger ribbon width $W_{\text{GNR}} = 1.722$ nm, as compared with $W_{\text{SiNR}} = 0.974$ nm and $W_{\text{GeNR}} = 1.026$ nm. However, in Fig. 10 note that the difference between the A-GNR FET and the A-SiNR or A-GeNR FET clearly decreases as T_{ox} reduces to 0.5 nm. This is considered to be due to the influence of a quantum capacitance (C_Q) of the channels, which is known to strongly appear in scaled FETs with light effective masses such as III-V nanowire FETs [29,30].

Then, the gate voltage dependences of C_Q calculated for the three A-NR FETs are shown in Fig. 11, where C_Q was calculated by $C_Q = \partial(qN) / \partial(-U_{\text{scf}} / q)$ using the channel sheet electron density $N = N_1 + N_2$ and the channel potential U_{scf} [27]. The horizontal dashed lines represent the oxide capacitances calculated from $C_{\text{ox}} = \epsilon_{\text{ox}} / T_{\text{ox}}$. ϵ_{ox} is the permittivity of the gate oxide. C_Q is basically proportional to the density-of-states (DOS) for carriers near the Fermi energy, which has a close relationship with the effective mass of carriers m^* , i.e.

$\text{DOS} \propto \sqrt{m^*}$. Consequently, in the case of $T_{\text{ox}} = 0.5$ nm shown in Fig. 11 (b), only the A-GNR FET exhibits $C_Q \approx C_{\text{ox}}$ because of its lighter effective mass. This indicates that since the total gate capacitance C_G is represented as $C_G = C_{\text{ox}} C_Q / (C_{\text{ox}} + C_Q)$ in the form of a series-connection of C_Q and C_{ox} , C_G becomes approximately $C_{\text{ox}} / 2$, that is, $C_G \approx C_{\text{ox}} / 2$ if $C_Q \approx C_{\text{ox}}$. Therefore, C_G substantially decreases from C_{ox} in the case of the A-GNR FET with $T_{\text{ox}} = 0.5$ nm, as shown in Fig. 12 where the actually calculated C_G 's were plotted for $T_{\text{ox}} =$ (a) 3 and (b) 0.5 nm. On the other hand, the influence of C_Q is found to be negligible in the case of $T_{\text{ox}} = 3$ nm, because C_Q becomes sufficiently larger than C_{ox} , as shown in Fig. 11 (a), which is called a classical capacitance limit (CCL).

Figure 11: Gate voltage dependences of quantum capacitance C_Q calculated for the three A-NR FETs. $T_{\text{ox}} =$ (a) 3 and (b) 0.5 nm.

Figure 12: Gate voltage dependences of total gate capacitance C_G calculated for $T_{ox} =$ (a) 3 and (b) 0.5 nm.

Due to the involvement of the quantum capacitance mentioned above, the channel electron density must be influenced by the decreased C_G in extremely thin T_{ox} as 0.5 nm. Accordingly, we next calculated the channel sheet electron density and the average electron velocity as a function of the gate voltage, as shown in Fig. 13, where $T_{ox} =$ (a) 3 and (b) 0.5 nm. The average electron velocity v was calculated by the equation, $I_D = qNv$. It is found that for $T_{ox} = 3 \text{ nm}$ the electron densities are nearly the same among the three NR FETs, i.e. they are in CCL, and therefore the larger drain current observed for the A-GNR FET in Fig. 10 (a) is

Figure 13: (Left column) Channel sheet electron densities and (right column) average electron velocities as a function of gate voltage computed for $T_{ox} =$ (a) 3 and (b) 0.5 nm.

simply due to the increased electron velocity as shown in the right column of Fig. 13 (a). As a result, the A-GNR FET produces the substantially larger drain current for a thick gate oxide such as $T_{\text{ox}} = 3$ nm. On the other hand, for $T_{\text{ox}} = 0.5$ nm the electron density of the A-GNR FET drastically decreases as compared to the other two NR FETs as shown in the left column of Fig. 13 (b). This is the effect from the decreased C_G owing to the quantum capacitance described in the previous paragraph, and is the cause of the relative decrease in the higher current drivability of the A-GNR FET with $T_{\text{ox}} = 0.5$ nm.

Finally, looking at Fig. 10 (b) again, A-SiNR and A-GeNR FETs have the potential to provide high current drivability beyond $2 \text{ mA}/\mu\text{m}$ at $V_{\text{DD}}=0.5 \text{ V}$ under the ballistic transport. This current level meets the requirement for the on-current value specified in the International Technology Roadmap for Semiconductors (ITRS) for 2024 [1,26], and therefore, A-SiNR and A-GeNR are also attractive channel materials for high performance FETs, though A-GNR still maintains the advantage over A-SiNR and A-GeNR under the ideal transport conditions.

2.5. Summary

In this chapter, a performance comparison between A-SiNR, A-GeNR and A-GNR FETs under the ballistic transport was performed. It was found that comparing at the same band gap of $\sim 0.5 \text{ eV}$, A-GNR FET exhibits the largest drain current even though its advantage over A-SiNR or A-GeNR FETs reduces in the quantum capacitance limit. It was also pointed out that A-GNR maintains the advantage under the ideal transport situation, whereas A-SiNR and A-GeNR are also attractive channel materials for realizing high performance FETs. In the future, we need to consider carrier scattering effects and tunneling currents to more accurately predict the device performance.

3. Performance projection of germanane FETs

3.1. Features of germanane

In this chapter, the electronic properties of germanane, such as the band structure and electron mobility, are examined using simulations. The atomic structure of germanane is depicted in Fig. 1 (c), and refer to [14] about its fabrication method based on chemical synthesis. Here, we describe the basic features of germanane.

Germanane is a 2-D material similar to graphene, but it maintains sp^3 -like orbitals rather than the sp^2 orbitals, owing to the hydrogen termination above or below the layer. As a consequence, germanane can be thought of as hydrogen-terminated isolated (111) sheets of Ge, and conveniently no dangling bonds are generated at the surfaces. According to a theoretical

Figure 14: (a) Overall view of atomic model for germanane ribbon structure used in the simulation. (b) Atomic model looking from the $\langle 11\bar{1} \rangle$ direction. The edge configuration at the ends of the width direction was assumed to be armchair. (c) Atomic model looking from the $\langle \bar{1}10 \rangle$ direction. Germanane is confirmed to have an analogous geometry to a Ge (111) surface in which every Ge atom is terminated with hydrogen atoms above or below the layer. Chair-like morphology is employed here.

calculation, germanane has a direct band gap of about 1.5 eV without a nanoribbon structure, and thus has great potential for a wide range of optoelectronic and sensing applications [14]. Furthermore, the theoretical calculation predicted a very large electron mobility of 18,195 $\text{cm}^2/\text{V}\cdot\text{s}$ in germanane, which is about 10 times larger than the bulk Si mobility for electrons.

Since ultra-scaled germanane transistors have not been fabricated yet, device simulation plays an alternative important role in exploring the characteristics of future germanane transistors and assessing their potential in advance. So far, several theoretical studies have focused on this research topic, however, the potential of germanane in ultimate transistor scaling technology is poorly understood and systematic study of germanane transistors is crucially lack. In this study, the potential of germanane as the channel material was evaluated using an atomistic simulator that combines electron band structure calculation based on the $sp^3d^5s^*$ TB approach and phonon full-band structure calculation using the Keating potential approach with the semiclassical Boltzmann transport equation [31].

3.2. Atomistic simulator

In view of the application to FET channel, channel materials have a finite width which is almost comparable to the channel length in the state-of-the-art technologies, and thus we

adopted a germanane ribbon structure with a finite width as shown in Fig. 14 (a), where the electron confinement due to the monolayer and ribbon structures occurs in the $\langle 11\bar{1} \rangle$ and $\langle \bar{1}10 \rangle$ directions, respectively, and electrons transport along the $\langle 112 \rangle$ direction. Note that the infinitely-long germanane ribbon model is considered here, because this study is intended to clarify the band structure and the electron mobility of germanane ribbon channels. As described later, the ribbon width considered here W extends from a few nanometers to a few ten nanometers, which is larger than the values chosen for SiNR, GeNR and GNR discussed in the chapter 2. The edge configuration was assumed to be an armchair-edge structure as shown in Fig. 14 (b). In particular, as found from Fig. 14 (c), germanane have an analogous geometry to a Ge (111) surface in which every Ge atom is terminated with hydrogen atoms above or below the layer, and thus no dangling bonds are generated at the surfaces. It should be added that chair-like morphology is employed here, because it is energetically more stable than other morphology, such as boat-like one [32]. Since optimized lattice parameters are presently unknown for germanan ribbon structures, so as a first step the lattic parameters such as lattice constant a and buckling distance Δz are kept the same values of bulk Ge in the present simulations: Specifically, $a = 5.66 \text{ \AA}$, $\Delta z = 0.816 \text{ \AA}$, and Ge-Ge distance = $2.449 \text{ \AA}$.

An outline of the atomic simulator is briefly summarized below. The details can be found in [31]. First, the electron band structures were computed using the $sp^3d^5s^*$ TB approach, where the following eigenvalue equation represented by the $sp^3d^5s^*$ TB orbital basis set was solved.

$$\sum_{(\eta', \kappa') \in NN(\eta, \kappa)} \sum_{\gamma'} U_{\eta\kappa, \eta'\kappa'}^{\gamma, \gamma'} e^{ik(\eta' - \eta)L} c_{\kappa', \gamma'}^n(k) - \phi_{\kappa} c_{\kappa, \gamma}^n(k) = E_n(k) c_{\kappa, \gamma}^n(k). \quad (12)$$

Here, η and κ represent the atomic index and the unit cell index, respectively, as shown in Fig. 15, and γ the $sp^3d^5s^*$ TB orbitals. NN stands for a group of nearest-neighbor atoms associated

Figure 15: Schematic diagram representing the atomic index κ and unit cells. The position of Ge atom is identified using the atomic index κ and the unit cell index η as (η, κ) . L is the length of the unit cell in the transport direction.

with the (η, κ) -th atom. In this study, spin-orbit interactions are not considered. The interatomic potential $U_{\eta\kappa, \eta'\kappa'}^{\gamma, \gamma'}$ in (12) can be formulated in terms of two-center integrals and directional cosines [33]. We used the Boykin's parameterization for the onsite energies and the two-center integrals between nearest-neighbor Ge atoms [34]. ϕ_κ is the electrostatic potential obtained from the three-dimensional Poisson equation. We assumed a zero flat-band voltage and the gate voltage was set to zero for all simulations, because the purpose of this study is to evaluate the electron mobility under a low electric field.

Phonon band structures were computed using the original Keating valence force field (VFF) approach [35], which is known to well describe the microscopic features of phonons in nanostructures. The Keating potential consists of two potential energy terms: the first is the bond-stretching term, and the other is the bond-bending term. Each term is represented as a function of the atomic coordinates, and for a diamond structure, the crystal potential energy (Keating potential energy) is given by

$$E = \frac{3}{16} \frac{\alpha}{d_1^2} \sum_{\eta, \kappa} \sum_{(\eta', \kappa') \in NN(\eta, \kappa)} (R_{\eta\kappa, \eta'\kappa'}^2 - d_1^2)^2 + \frac{3}{16} \frac{\beta}{d_1^2} \sum_{\eta, \kappa} \sum_{(\eta', \kappa') \in NN(\eta, \kappa)} \sum_{\substack{(\eta'', \kappa'') \in NN(\eta, \kappa) \\ \eta' \neq \eta'' \cap \kappa' \neq \kappa''}} \left(\mathbf{R}_{\eta\kappa, \eta'\kappa'} \cdot \mathbf{R}_{\eta\kappa, \eta''\kappa''} + \frac{1}{3} d_1^2 \right)^2. \quad (13)$$

Here, the first and the second terms correspond to the bond-stretching and bond-bending terms, respectively, and α and β are Keating's force constants. $\mathbf{R}_{\eta\kappa, \eta'\kappa'} = \mathbf{R}_{\eta'\kappa'} - \mathbf{R}_{\eta\kappa}$ indicates the relative position vector between two atoms and d_1 is the equilibrium bond length between nearest-neighbor Ge atoms. In the Keating VFF approach, the phonon band structures are calculated by introducing a harmonic perturbation approximation into (13). The final dynamical matrix equation to be solved is given by [31]

$$\sum_{(\eta', \kappa') \in NN(\eta, \kappa)} \sum_{\mu \in \{x, y, z\}} D_{\eta\kappa\mu, \eta'\kappa'\mu'}^1 [\varepsilon_{\kappa'\mu'}^\lambda(q) e^{iq(\eta' - \eta)L} - \varepsilon_{\kappa\mu}^\lambda(q)] + \sum_{(\eta', \kappa') \in NN(\eta, \kappa)} \sum_{\substack{(\eta'', \kappa'') \in NN(\eta', \kappa') \\ \eta' \neq \eta'' \cap \kappa' \neq \kappa''}} \sum_{\mu'' \in \{x, y, z\}} D_{\eta\kappa\mu, \eta'\kappa', \eta''\kappa''\mu''}^2 [\varepsilon_{\kappa''\mu''}^\lambda(q) e^{iq(\eta'' - \eta)L} - \varepsilon_{\kappa\mu}^\lambda(q)] = \omega_\lambda^2(q) \varepsilon_{\kappa\mu}^\lambda(q), \quad (14)$$

where ε and ω are eigenvectors and eigenvalues for the phonons. $D_{\eta\kappa\mu, \eta'\kappa'\mu'}^1$ and $D_{\eta\kappa\mu, \eta'\kappa', \eta''\kappa''\mu''}^2$ are matrix elements between the first nearest-neighbor and the second nearest-neighbor Ge atoms, respectively, of which expressions were derived in [31]. We note that the bond-stretching term is involved only in $D_{\eta\kappa\mu, \eta'\kappa'\mu'}^1$, while the bond-bending term is involved in both $D_{\eta\kappa\mu, \eta'\kappa'\mu'}^1$ and $D_{\eta\kappa\mu, \eta'\kappa', \eta''\kappa''\mu''}^2$. By solving (14), the phonon band structure can be obtained.

Finally, we describe a methodology to compute the electron mobility determined by the electron-phonon interaction. When the electron-phonon interaction Hamiltonian is represented by the $sp^3d^5s^*$ orbitals and is expanded to a first-order spatial derivative term [36], then the transition matrix element from a state (n, k) to a state (n', k') is given by

$$M^{n,n'}(k, k') = \sum_{q, \lambda} \sqrt{\frac{\hbar}{2MN\omega_\lambda(q)}} \sum_{\kappa} \sum_{(\eta', \kappa') \in NN(\eta, \kappa)} \sum_{\gamma} \sum_{\gamma'} \frac{\partial U_{\eta\kappa, \eta'\kappa'}^{\gamma, \gamma'}}{\partial(\mathbf{R}_{\eta'\kappa'} - \mathbf{R}_{\eta\kappa})} \Big|_0 \quad (15)$$

$$\times \begin{bmatrix} \varepsilon_{\kappa', \lambda}(\pm q) c_{\kappa, \gamma}^{n'}(k') c_{\kappa', \gamma'}^n(k) e^{ik'(\eta' - \eta)L} \\ - \varepsilon_{\kappa, \lambda}(\pm q) c_{\kappa, \gamma}^{n'}(k') c_{\kappa', \gamma'}^n(k) e^{ik(\eta' - \eta)L} \end{bmatrix} \delta_{k-k' \pm q, G} e^{-i[E_n(k)/\hbar - E_{n'}(k')/\hbar \pm \omega_\lambda(q)]t}.$$

M denotes the mass of Ge atom, and N the number of Ge atoms. In practical calculations, solutions for the electron wavefunctions $c(k)$, the phonon eigenvalues $\omega(q)$ and polarization vectors $\varepsilon(q)$, which have been derived above, are substituted into (15). The electron eigenenergies are implicitly considered in the term $\partial U_{\eta\kappa, \eta'\kappa'}^{\gamma, \gamma'} / \partial(\mathbf{R}_{\eta'\kappa'} - \mathbf{R}_{\eta\kappa})$, which is numerically calculated using analytical formulae given by the Slater-Koster table [31]. Note that G denotes the reciprocal lattice vector, and thus both normal ($G = 0$) and umklapp ($G \neq 0$) processes are automatically included in the present calculation.

Next, the scattering rates from the state (n, k) to the state (n', k') are represented by applying Fermi's golden rule as follows.

$$S^{n,n'}(k, k') = \frac{2\pi}{\hbar} \left[\left| M^{n,n'}(k, k') \right|^2 g(\hbar\omega_\lambda(k' - k)) \delta(E_n(k) - E_{n'}(k') + \hbar\omega_\lambda(k' - k)) \right. \\ \left. + \left| M^{n,n'}(k, k') \right|^2 [1 + g(\hbar\omega_\lambda(k - k'))] \delta(E_n(k) - E_{n'}(k') - \hbar\omega_\lambda(k - k')) \right], \quad (16)$$

where $g(\hbar\omega_\lambda(q))$ is the equilibrium Planck distribution function, and the Dirac delta function represents the energy conservation law. Here, as found from (16), the final states (n', k') after the scattering events need to be searched by imposing momentum and energy conservations. To perform accurate detection of the final states over the whole first Brillouin zone, we introduced quadratic spline interpolations of the electron and phonon band structures between discretized points [31].

Generally, by assuming that the electron distribution function $f_n(k)$ can be represented by the sum of the equilibrium Fermi-Dirac function $f_0(E_n(k))$ and a first-order perturbation component $\delta f_n(k)$ driven by an electric field F , the Boltzmann transport equation is transformed into the following equation.

$$-\frac{e}{k_B T} F v_n(k) f_0(E_n(k)) [1 - f_0(E_n(k))] = \hat{C} \{ \delta f_n(k) \}, \quad (17)$$

where $v_n(k)$ is the group velocity of the electrons, which is calculated using the electron band structure. We represented the collisional integral in the right-hand side of (17) using the

scattering rate $S^{n,n'}(k,k')$ and applying detailed balance conditions. As a result, the following expression for the collisional integral was obtained.

$$\hat{C}\{\delta f_n(k)\} = \frac{NL}{2\pi} \sum_{n'} \int_{-\pi/L}^{\pi/L} dk' S^{n,n'}(k,k') \left[\delta f_{n'}(k') \frac{f_0(E_n(k))}{f_0(E_{n'}(k'))} - \delta f_n(k) \frac{1-f_0(E_{n'}(k'))}{1-f_0(E_n(k))} \right]. \quad (18)$$

Here, L denotes the length of the unit cell in the transport direction and N is the number of unit cells. The first and second terms correspond to the in-scattering process from (n', k') to (n, k) and the out-scattering process from (n, k) to (n', k') , respectively. Here, we introduce a relaxation time approximation,

$$\hat{C}\{\delta f_n(k)\} = -\frac{\delta f_n(k)}{\tau_n(k)}. \quad (19)$$

Then, by substituting (19) into (18), we can derive an equation for determining a relaxation time $\tau_n(k)$ as follows.

$$\frac{NL}{2\pi} \sum_{n'} \int_{-\pi/L}^{\pi/L} dk' S^{n,n'}(k,k') \frac{1-f_0(E_{n'}(k'))}{1-f_0(E_n(k))} [v_n(k)\tau_n(k) - v_{n'}(k')\tau_{n'}(|k'|)] = v_n(k). \quad (20)$$

Once the relaxation time was obtained, the electron mobility μ_n for n -th mode can be calculated using the following equation [31].

$$\mu_n = \frac{4e}{2\pi n_n k_B T} \int_0^{\pi/L} dk \left(\frac{\partial E_n(k)}{\hbar \partial k} \right)^2 f_0(E_n(k)) [1-f_0(E_n(k))] \tau_n(k). \quad (21)$$

The total electron mobility is calculated by $\mu = \sum_n^{N_{sub}} \mu_n n_n / \sum_n^{N_{sub}} n_n$, where N_{sub} is the number of subbands considered in the mobility calculation. In the following sections, the calculated results using the methods described above will be shown.

3.3. Band gap and effective masses

Figure 16 shows the band structures computed for germanane ribbons with $W =$ (a) 4, (b) 11.6, and (c) 20 nm. As in the first-principles calculation for germanane [14], the present TB calcu-

Figure 16: Band structures computed for germanane ribbons with $W =$ (a) 4, (b) 11.6, and (c) 20 nm. Note that germanane ribbons are a direct band gap material.

Figure 17: Ribbon width dependence of band gap energy of germanane ribbons.

lation suggests that germanane ribbons are a direct band gap material. This is due to the k -space projection of bulk L valleys into the $\langle 11\bar{1} \rangle$ plane, and they has a smaller subband energy than the Γ and X valleys similarly projected into the $\langle 11\bar{1} \rangle$ plane. Figure 17 shows the ribbon width dependence of the band gap energy of germanane ribbons. It is clearly found that the band gap drastically increases if W becomes narrower than about 10 nm, and it is due to the quantum confinement effect in the width direction. Furthermore, since the band gap decreases to converge on about 1.4 eV with increasing W , the germanane ribbons are found to be always semiconducting. The smaller band gap compared with the result in [14] may be due to the fact that we have employed the lattice parameters at the same values of bulk Ge, whereas the lattice structure was optimized in [14].

Next, we evaluated the electron effective masses of the germanane ribbons. Figure 18 shows the conduction band structures for germanane ribbons with $W =$ (a) 4, (b) 11.6, and (c) 20 nm, where the effective mass in the lowest subband is indicated in each figure. It is found that the germanane ribbons have lighter effective mass than that of bulk Ge ($0.082 m_0$)

Figure 18: Conduction band structures for germanane ribbons with $W =$ (a) 4, (b) 11.6, and (c) 20 nm, where the effective mass in the lowest subband is indicated in each figure.

Figure 19: Ribbon width dependence of electron effective mass in germanane ribbons.

[32,37]. This may be partially due to a residual biaxial tensile strain to the germanane ribbons because of the employment of the bulk lattice parameters, which are known to be larger than the optimized ones using first-principles simulation for germanane 2D planes [37]. As W decreases, the effective mass increases similarly to the band gap result. The detailed ribbon width dependence of the effective mass is shown in Fig. 19, which reconfirms that the effective mass increases when $W < \sim 10$ nm. The increase in the effective mass may be due to the band nonparabolicity of the conduction band L valleys. Here, we observe a characteristic behavior in the conduction band structure owing to the ribbon width narrowing in Fig. 18. That is, the closely-spaced dispersion curves at the conduction minimum in the case of $W = 20$ nm becomes less-crowded with decreasing W , and the energy spacing between the lowest and the first excited states finally becomes larger than severalfold thermal energy at room temperature for $W < 11.6$ nm. This means that the intersubband phonon scattering decreases as W decreases, and therefore we can expect a mobility enhancement due to the ribbon width narrowing. This speculation will be examined in the next section.

3.4. Electron mobility

Finally, we computed the electron mobility of the germanane ribbons. Before showing the result, the phonon band structures in a low energy regime are presented in Fig. 20 for $W =$ (a) 4, (b) 11.6 nm, and (c) 20 nm. There are many modes exhibiting $\omega \propto q^2$ dispersions, which represents a mixed state of transverse and longitudinal acoustic modes [31]. Aside from those mixed modes, pure transverse and longitudinal acoustic modes with $\omega \propto q$ dispersion also exist in a long wavelength regime, i.e., $q \approx 0$. Considering the interactions between those phonon modes and the electron modes shown in Fig. 18, we obtained the electron mobility of the germanane ribbons as a function of W , as shown in Fig. 21 (a). The temperature is 300 K. Here, note that the solid and the dashed lines correspond to the results obtained considering

Figure 20: Phonon band structures computed for germanane ribbons with $W =$ (a) 4, (b) 11.6, and (c) 20 nm.

multisubbands with energy up to 0.2 eV higher than the lowest subband minimum and considering only the lowest subband, respectively. This is to highlight the influence of the inter-subband phonon scattering, as discussed later. From the solid line results, the electron mobility increases with decreasing W from 28 to 11.6 nm, which agrees with our speculation described in the previous section. In Figs. 21 (b), (c) and (d), the conduction band structures corresponding to $W = 28$, 11.6, and 4 nm are plotted, respectively, and the number of subbands, N_{sub} , locating within the energy range of about $3k_B T$ from the lowest subband minimum are also indicated in each figure. In accordance with our expectation, the electron mobility increases with decreasing N_{sub} . On the other hand, when W further becomes smaller than 11.6 nm, the electron mobility turns to decline as shown in Fig. 21 (a). This is due to the fact that the electron-phonon interaction becomes stronger by decreasing W [31], and also the effective mass increases in the sub-10 nm ribbons, as shown in Fig. 19.

Here, it is interesting to compare between the solid and the dashed lines in Fig. 21 (a), which reveals that when $W > 11.6$ nm, i.e., when the multisubbands are involved, the electron mobility substantially decreases from the results considering only the lowest subband, as shown in the solid line. This suggests that the intersubband phonon scattering significantly decreases the electron mobility, and as a result, it produces the characteristic ribbon width dependence of the electron mobility, especially producing the maximum electron mobility at $W = 11.6$ nm. The maximum electron mobility is 1,332 $\text{cm}^2/\text{V}\cdot\text{s}$ in the present simulation, which is much smaller than the value reported in [14]. However, it is about 10 or 100 times larger than that of MoS_2 monolayer transistors [15,16]. Accordingly, germanane channels are found to have the potential outperforming the transition metal dichalcogenide 2-D materials.

Figure 21: (a) Computed electron mobility of germanane ribbons as a function of W . The temperature is 300 K. Note that the solid and the dashed lines correspond to the results obtained considering multisubbands with energy up to 0.2 eV higher than the lowest subband minimum and considering only the lowest subband, respectively. (b) Conduction band structures with $W = 28$ nm, (c) $W = 11.6$ nm, and (d) $W = 4$ nm, also indicated with the number of subbands, N_{sub} , locating within the energy range of about $3k_B T$ from the lowest subband minimum.

3.5. Summary

In this chapter, the electronic properties of germanane ribbon channels were examined using the atomistic simulator. First, it was shown that the germanane ribbons are a direct band gap semiconductor with a band gap energy larger than about 1.4 eV. Next, the germanane ribbons were shown to have lighter effective mass than that of bulk Ge, but when the ribbon width decreases to less than about 10 nm, the effective mass increases along with the band gap. Finally, the electron mobility of germanane ribbons was computed, and it was shown to be significantly decreased by the intersubband phonon scattering. As a result, the electron mobility strongly depends on the ribbon width, i.e. the number of subbands, which produced the

maximum electron mobility at $W = 11.6$ nm. It is important to note that this ribbon width is approximately one order of magnitude greater than those for SiNR, GeNR and GNR with a reasonable band gap. Therefore, practical fabrication will become far less difficult in germanane FETs.

4. Conclusion

Over the past decade, the most widely researched of 2-D materials is graphene, but it is just one material from an entire group categorized into van der Waals bonded structures. Although graphene is a semimetal, other 2-D materials can have a band gap which changes from indirect to direct depending on their structures. Limiting our interest to the integrated switching device application in LSI circuit, the opening of a band gap and ultrathin channel structure are indispensable; thus atomic monolayer semiconductors such as SiNR/GeNR/GNR, germanane, silicane, transition metal dichalcogenide, and so on, are expected subject of research.

Turning our attention to the outside world, there are several applications where 2-D materials can provide a significant advantage. The loosely-bonded sheets and large surface area make these materials attractive for energy storage applications. In addition, their 2-D nature enhances performance in sensor applications, since surface adsorbate induces drastic change in electronic properties.

We add lastly that theoretical studies such as material design and device simulation are expected to lead the way in the advancement of 2-D material researches, especially in an early stage of the investigation. In this regard, a lot of modeling techniques, for instance, analytical band structure representation, establishment of scattering parameters, development of tunneling model and interaction model with substrates and gate insulators, etc. is highly required to be developed swiftly.

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