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High Thermoelectric Power Factor of High-Mobility 2D Electron Gas

Hiromichi Ohta,* Sung Wng Kim, Shota Kaneki, Atsushi Yamamoto, and Tamotsu Hashizume*

Thermoelectric conversion is an energy harvesting technology that directly converts waste heat from various sources into electricity by the Seebeck effect of thermoelectric materials with a large thermopower \( S \), high electrical conductivity \( \sigma \), and low thermal conductivity \( \kappa \). State-of-the-art nanostructuring techniques that significantly reduce \( \kappa \) have realized high-performance thermoelectric materials with a figure of merit \( ZT = S^2 \sigma / \kappa T \) between 1.5 and 2. Although the power factor \( PF = S^2 \sigma / \kappa \) must also be enhanced to further improve \( ZT \), the maximum PF remains near 1.5–4 \( mW \ m^{-1} K^{-2} \) due to the well-known trade-off relationship between \( S \) and \( \sigma \). At a maximized PF, \( \sigma \) is much lower than the ideal value since impurity doping suppresses the carrier mobility. A metal-oxide-semiconductor high electron mobility transistor (MOS-HEMT) structure on an AlGaN/GaN heterostructure is prepared. Applying a gate electric field to the MOS-HEMT simultaneously modulates \( S \) and \( \sigma \) of the high-mobility electron gas from \(-490 \mu V \ K^{-1}\) and \(10^{-1} \ S \ cm^{-1}\) to \(-90 \mu V \ K^{-1}\) and \(10^{-5} \ S \ cm^{-1}\), while maintaining a high carrier mobility \((=1500 \ cm^2 \ V^{-1} \ s^{-1})\). The maximized PF of the high-mobility electron gas is \(=9 \ mW \ m^{-1} K^{-2} \), which is a two- to sixfold increase compared to state-of-the-art practical thermoelectric materials.

Currently, more than 60% of the energy produced from fossil fuels is lost as waste heat. Consequently, thermoelectric energy conversion has attracted much attention as an energy harvesting technology since thermoelectric devices can directly convert waste heat from various sources such as electric power plants, factories, and automobiles into electricity.[1] The energy conversion efficiency is generally evaluated using the dimensionless figure of merit, \( ZT = S^2 \sigma / \kappa T \), where \( Z \) is the figure of merit, \( T \) is the absolute temperature, \( S \) is the thermopower (=Seebeck coefficient), \( \sigma \) is the electrical conductivity, and \( \kappa \) is the sum of the electronic \( (\kappa_{el}) \) and lattice thermal conductivities \( (\kappa_{lat}) \) of a thermoelectric material. To date, state-of-the-art nanostructuring techniques, which can reduce \( \kappa_{lat} \) significantly through phonon scattering by nanosized structural defects,[2] have realized high-performance thermoelectric materials showing a large \( ZT \) of 1.5–2. However, \( \kappa_{lat} \) reduction techniques generally deteriorate \( \sigma \) due to the significant decrease in carrier mobility \( (\mu) \), leading to a moderate net benefit in the maximized \( ZT \), which is determined by the ratio of \( \mu / \kappa_{lat} \) (quality factor).[3]

On the other hand, the product \( S^2 \sigma \), which is called the power factor (PF), is also used to evaluate a thermoelectric material. Although a low \( \kappa \) is strongly required when the material is placed in a thermally isolated atmosphere such as space (in a vacuum), a high PF is more critical than a low \( \kappa \) when the surrounding atmosphere heats and cools the material. In fact, Yamamoto et al. experimentally demonstrated that thermoelectric devices with large \( \kappa \) metals composed of Constantan (N-leg) and Chromel (P-leg) sheets efficiently generate electric power in a butane gas flame.[4] In this case, heat transfer is governed by convection heat flow, which cancels the conduction in the material. Thus, a high PF is necessary for efficient power generation rather than low \( \kappa \) when a material is not in a thermally isolated atmosphere.

The PF must be optimized due to well-known trade-off relationships between \( S \) and \( \sigma \) in terms of the volume carrier concentration \( (n_v) \); as \( n_v \) increases, \( \sigma \) increases, whereas \( |S| \) decreases. Optimized PF values of state-of-the-art bulk thermoelectric materials range between 1.5 and 4 \( mW \ m^{-1} K^{-2} \) at room temperature, without exception of recently reported \( Nb_{1-x}Ti_xFeSb \) half-Heusler (10.6 \( mW \ m^{-1} K^{-2} \)).[5] Examples include SnSe (\( PF = 4 \ mW \ m^{-1} K^{-2} \)),[6] Bi$_5$Sb$_3$Se$_3$,
(PF ≈ 4 mW m⁻¹ K⁻²),[2b,c] AgPb₃SbTe₂⁺m (3.6 mW m⁻¹ K⁻²),[2a] CsBi₄Te₆ (3.4 mW m⁻¹ K⁻²),[7] SiGe alloy (1.5 mW m⁻¹ K⁻²),[8] Na₀.₈₈CoO₂ (3.4 mW m⁻¹ K⁻²),[9] Nb-doped SrTiO₃ (~2.5 mW m⁻¹ K⁻²),[10] PbTe-SrTe (1.4 mW m⁻¹ K⁻²),[11] and rough Si nanowire (PF ≈ 3 mW m⁻¹ K⁻²).[12] Thus, the PF enhancement is limited by difficulties realizing a simultaneous increase in S and σ. Additionally, there is another trade-off relationship between the carrier mobility (μ) and n; σ at the maximized PF is much lower than the ideal value since impurity doping significantly suppresses μ (Figure 1a). In a typical semiconductor, μ decreases ≈1/10 by conventional impurity doping.[13]

Herein we propose that a high-mobility 2D electron gas (2DEG) at a semiconductor heterointerface is a viable solution to overcome the bottleneck in thermoelectric trade-off relations. In 2DEG, μ is not suppressed since the high-mobility channel lacks an impurity (Figure 1b). Furthermore, the PF by the electric field carrier concentration modulation can be optimized by the metal-oxide-semiconductor (MOS) structure on such a 2DEG. In this study, we investigate the PF of a 2DEG, which is induced at an AlGaN/GaN heterointerface by the electric field thermopower modulation method.[14] The maximized PF of the 2DEG is ≈9 mW m⁻¹ K⁻² at room temperature, which is an order magnitude greater than that of the doped GaN bulk and two- to sixfold greater than those of state-of-the-art thermoelectric materials, while maintaining a higher σ (≈ 6030 S cm⁻¹) than state-of-the-art thermoelectric materials (σ = 1000–2500 S cm⁻¹).

Figure 1. Schematic illustration of thermoelectric power generation in an n-type semiconductor. a) Conventional impurity doped n-type semiconductor. Carrier electron flow from the hot to the cold side due to the Seebeck effect. Low mobility of the carrier electron originates from ionized impurity scattering. b) Electric field induced high-mobility 2DEG. Larger electric power can be obtained compared with (a).

Figure 2. Electric field thermopower modulation measurement of AlGaN/GaN-MOS-HEMT. a) Schematic energy band diagram of 2DEG confined at an AlGaN/GaN heterointerface. CBM and VBM denote the conduction band minimum and the valence band maximum, respectively. Thermoelectric properties can be modulated by applying a gate voltage (∆T). b) Schematic illustration of the AlGaN/GaN MOS-HEMT. c) Photograph of the electric field thermopower modulation measurement of AlGaN/GaN-MOS-HEMT. MOSHEMT is placed between the gap (2 mm) of two Peltier devices. During a gate voltage application, temperature differences (∆T) are introduced between both ends of the channel using the Peltier devices.

We fabricated an Al₂O₃/AlGaN/GaN metal-oxide-semiconductor high electron mobility transistor (MOS-HEMT)[15] and measured the thermoelectric properties of the 2DEG by
introducing a temperature difference during a gate voltage ($V_g$) application to modulate the Fermi energy ($E_F$) (Figure 2a). We used a commercially available Al$_{0.24}$Ga$_{0.76}$N (20 nm)/GaN (900 nm)/Fe-doped GaN (300 nm) heterostructure film, which was grown on a semi-insulating (0001) SiC substrate by metal organic chemical vapor deposition (Figure 2b). The sheet resistance ($R_s$), Hall mobility ($\mu_{\text{Hall}}$), and sheet carrier concentration ($n_s$) were 423 $\Omega$ sq$^{-1}$, 1730 cm$^2$ V$^{-1}$ s$^{-1}$, and $8.53 \times 10^{12}$ cm$^{-2}$, respectively, at room temperature. The gate length ($L$) and width ($W$) of the MOS-HEMTs were 800 $\mu$m and 400 $\mu$m, respectively. Details of our MOS-HEMT preparation are described in the Experimental Section and elsewhere.$^{[15]}$

Figure 2c shows the carrier transport properties at room temperature. The transistor characteristics were measured using a semiconductor device analyzer (B1500A, Agilent). For the $S$ measurements, we used two Peltier devices placed under the MOS-HEMT with a 2 mm gap to induce a temperature difference between the source and drain electrodes ($\Delta T$, 0–1 K), which was monitored via two thermocouples (K-type, 150 $\mu$m diameter, SHINNETSU Co.) mechanically attached at both edges of the 2DEG channel. The thermo-electromotive force ($\Delta V$) and $\Delta T$ were simultaneously measured at room temperature. Then the slope of the $\Delta V$–$\Delta T$ plots yielded the $S$-values. Details of our electric field modulated $S$ measurement are described elsewhere.$^{[14b–d]}$

Figure 3 summarizes the carrier transport properties of the MOS-HEMT at room temperature. Applying a gate voltage ($V_g$) from $-9$ to $+4$ V at a constant drain voltage ($V_d$) of $+10$ V dramatically modulates the drain current ($I_d$) from 7 nA to 7 mA ($I_{\text{on}}$ to $I_{\text{off}}$ current ratio $\approx 10^6$) (Figure 3a). The gate leakage current ($I_g$) is $\approx 300$ pA when $V_g$ is less than $+2$ V, while the $I_{d0.5}$ versus $V_g$ plot indicates that the threshold gate voltage ($V_{\text{th}}$) is $-7.98$ V. The gate capacitance per unit area ($C_i$) is 166.3 nF cm$^{-2}$ (Figure 3a, inset). The output characteristic curves clearly show the pinch-off behavior and the current saturation of $I_d$ (Figure 3b), indicating that the characteristic of the MOS-HEMT obeys the standard transistor theory.

The $n_s$ value was calculated as $n_s = C_i \cdot (V_g - V_{\text{th}}) \cdot e^{-1}$. At $V_g = 0$ V, its value is $8.32 \times 10^{12}$ cm$^{-2}$, which agrees well with that obtained from the Hall measurement ($n_s = 8.53 \times 10^{12}$ cm$^{-2}$).
(Figure 3c). In the present MOS-HEMT, $n_e$ can be modulated from $\approx 10^{11}$ cm$^{-3}$ up to $1.25 \times 10^{13}$ cm$^{-3}$. The field effect mobility ($\mu_{\text{FE}}$) was calculated as

$$\mu_{\text{FE}} = \frac{g_m \cdot L}{C_m \cdot (V_g - V_a) \cdot W}$$  \hspace{1cm} (1)$$

where $g_m$ is the transconductance, $dI_d/dV_g$. $\mu_{\text{FE}}$ drastically increases from $\approx 10^{-1}$ to $\approx 10^3$ cm$^2$ V$^{-1}$ s$^{-1}$ around $V_g \approx -7$ V, and is almost saturated at $\approx 1500$ cm$^2$ V$^{-1}$ s$^{-1}$ when $-7$ V $< V_g < +2$ V, similar to that of the original value ($1730$ cm$^2$ V$^{-1}$ s$^{-1}$) obtained from the Hall measurement (Figure 3c). These results clearly demonstrate that the 2D carrier concentration can be modulated without suppressing the mobility in the MOS-HEMT.

Next, we measured $S$ of the MOS-HEMT as a function of $V_g$ (Figure 3d). The observed $S$ values are always negative, indicating that the channel is an n-type semiconductor. As $V_g$ increases, the $|S|$ monotonically decreases from 490 to 90 $\mu$V K$^{-1}$. The observed $S$ values reflect a bulk-like energy derivation of the parabolic shaped density of states (DOS) of the conduction band near the Fermi energy. The observable $S$ is roughly expressed as $S_{\text{obs}} = (\sigma_{2\text{DEG}} - \sigma_{\text{bulk,}0})/\sigma_{2\text{DEG}} + \sigma_{\text{bulk,}0}$, where $\sigma_i$ is the sheet conductance of each layer. In the present case, $S_{2\text{DEG}}$ dominates $S_{\text{obs}}$ due to the relation of $\sigma_{2\text{DEG}} \gg \sigma_{\text{bulk}}$.

Since the energy dependence of the DOS near the conduction band bottom for GaN is parabolic, the $n$ dependence of $S$ for electron-doped GaN bulk can be theoretically calculated using the following equations (2)–(4)\cite{16}

$$n_e = 4\pi \left(\frac{m^* T}{\hbar^2}\right)^{3/2} F_{1/3}(\xi)$$  \hspace{1cm} (2)$$

$$F_{1/3}(\xi) = \int_0^\infty \frac{x e^{-x}}{1 + e^{-x}} \, dx$$  \hspace{1cm} (3)$$

$$S = -k_b T \frac{e}{r} \frac{(r + 2) F_{5/3}(\xi) - \xi}{(r + 1) F_{2/3}(\xi) - \xi}$$  \hspace{1cm} (4)$$

where $m^*$, $T$, $h$, $\xi$, $F_r$, and $r$ are the DOS effective mass, Boltzmann constant, absolute temperature, Planck constant, chemical potential, Fermi integral, and scattering parameter of relaxation time, respectively. We used 0.19 $m_0$\cite{17} as $m^*$ of GaN, where $m_0$ is the free electron mass. Figure 4 shows the calculated $S$ of bulk GaN as a function of the volume carrier concentration ($n_e$) at 300 K. For comparison, several reported $S$ values of electron-doped GaN are also plotted (Brandt\cite{18}, Sztein\cite{19}, Nagase\cite{20}). The calculated line completely reproduces these reported values. Thus, we used this $S$–$n$ relationship to calculate the PF of the 2DEG layer.

The PF of the AlGaN/GaN 2DEG was calculated using the observed $S$, $n_e$ obtained from Figure 4, and the observed $\mu_{\text{FE}}$ (Figure 5a). A high PF of $\approx 9$ mW m$^{-1}$ K$^{-2}$ with $n_e = 2.5 \times 10^{10}$ cm$^{-3}$ is calculated in high-mobility 2DEG at the AlGaN/GaN interface at room temperature, which is an order magnitude greater than that of doped GaN bulk\cite{19} and a two- to sixfold increase compared to those of state-of-the-art practical thermoelectric materials (1.5–4 mW m$^{-1}$ K$^{-2}$).
of 2–6 compared to those of state-of-the-art practical thermoelectric materials (1.5–4 mW m\(^{-1}\) K\(^{-2}\)). Although the present AlGaN/GaN cannot be used as the thermoelectric generator because of its narrow thickness, the present high-mobility electron gas approach should open an avenue to further improve the thermoelectric performance of state-of-the-art thermoelectric materials.

**Experimental Section**

Preparation of Al\(_2\)O\(_3\)/AlGaN/GaN MOS-HEMT: An Al\(_{0.24}\)Ga\(_{0.76}\)N (20 nm)/GaN (900 nm)/Fe-doped GaN (300 nm) heterostructure film grown on a semi-insulating (0001) SiC substrate via metal organic chemical vapor deposition was used. The sheet resistance, Hall mobility, and sheet carrier concentration were 423 \(\Omega\) sq\(^{-1}\), 1730 cm\(^2\) V\(^{-1}\) s\(^{-1}\), and \(8.53 \times 10^{12}\) cm\(^{-2}\), respectively, at room temperature. As an ohmic electrode, a multilayer consisting of Ti/Al/Ti/Au was deposited on the AlGaN surface and subsequently annealed at 830 \(^\circ\)C for 1 min in N\(_2\) ambient. A 20 nm thick SiN\(_x\) film was used as a surface protection layer to mitigate damage to the AlGaN surface during ohmic annealing.\(^{[15,23]}\) After forming the ohmic electrode, the SiN\(_x\) layer was removed in a buffered HF solution. An Al\(_2\)O\(_3\) layer with a nominal thickness of 30 nm was then deposited on the AlGaN surface at 300 \(^\circ\)C using an atomic layer deposition (ALD) system. Trimethylaluminum and water vapor were introduced into an ALD reactor in alternate pulse form as the aluminum and oxygen precursors, respectively. The deposition rate was 0.11 nm cycle\(^{-1}\). Finally, a Ni/Au (20/50 nm) gate electrode was formed on the Al\(_2\)O\(_3\) layer. To improve the Al\(_2\)O\(_3\)/AlGaN interface properties, the sample was annealed at 300 \(^\circ\)C for 3 h in air under a reverse bias of \(-10\) V.\(^{[24]}\)

The gate length \(L\) and width \(W\) of the MOS-HEMTs were 800 \(\mu\)m and 400 \(\mu\)m, respectively.

**Measurements:** The transistor characteristics of the AlGaN/GaN MOS-HEMT were measured using a semiconductor device analyzer (B1500A, Agilent) at room temperature in air. The 5 measurements, two Peltier devices were used, which were placed under the MOS-HEMT, to generate a temperature difference between the source and the drain electrodes. Two thermocouples (K-type, 150 \(\mu\)m diameter, SHINNETSU Ti/Al/Ti/Au was deposited on the AlGaN surface and subsequently annealed at 830 \(^\circ\)C for 1 min in N\(_2\) ambient. A 20 nm thick SiN\(_x\) film was used as a surface protection layer to mitigate damage to the AlGaN surface during ohmic annealing.\(^{[15,23]}\) After forming the ohmic electrode, the SiN\(_x\) layer was removed in a buffered HF solution. An Al\(_2\)O\(_3\) layer with a nominal thickness of 30 nm was then deposited on the AlGaN surface at 300 \(^\circ\)C using an atomic layer deposition (ALD) system. Trimethylaluminum and water vapor were introduced into an ALD reactor in alternate pulse form as the aluminum and oxygen precursors, respectively. The deposition rate was 0.11 nm cycle\(^{-1}\). Finally, a Ni/Au (20/50 nm) gate electrode was formed on the Al\(_2\)O\(_3\) layer. To improve the Al\(_2\)O\(_3\)/AlGaN interface properties, the sample was annealed at 300 \(^\circ\)C for 3 h in air under a reverse bias of \(-10\) V.\(^{[24]}\) The gate length \(L\) and width \(W\) of the MOS-HEMTs were 800 \(\mu\)m and 400 \(\mu\)m, respectively.
Co.), which were mechanically attached at both edges of the 2DEG channel, monitored the temperature difference ($\Delta T$, 0–1 K). The thermo-electromotive force ($\Delta V$) and $\Delta T$ values were simultaneously measured at room temperature, and the slope of the $\Delta V$–$\Delta T$ plots yielded the $S$-values. The error of $S$ should be less than 5%. Details of electric field modulated $S$ measurement are described elsewhere.[14b–d]

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

2D electron gas, AlGaN/GaN-MOS-HEMT, thermoelectric power factor

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