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科研費 KAKENHI

科学研究費助成事業　　研究成果報告書

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研究課題名（和文）Searching new operation area for QCL by Gain Mapping using NEGF

研究課題名（英文）Searching new operation area for QCL by Gain Mapping using NEGF

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交付決定額（研究期間全体）：（直接経費）　　3,400,000円

研究成果の概要（和文）：1. GaN/AlGaN 超格子の双極子散乱自己エネルギーがモデル化され、NEGF に基づくキャリア輸送の調査に利用されました。 この研究により、0.3 から 0.7 の間の組成 Al 比が、レベルの広がりに大きく影響することが確認されました。
2. GaN/AlGaN 多重量子井戸 (MQW) の界面での粗さ誘起電荷によるランダム電界の生成が報告されています。この研究により、GaN/AlGaN MQWのAl組成比が0.1の場合でも、界面品質が悪い場合には、1MV/cm以上のRMSランダム電界を発生できることが明らかになりました。

研究成果の学術的意義や社会的意義
We step forward to clarify the carrier transport in AlGaN-based superlattices through this project's analytical and numerical calculations. Continuous research stemming from this project will help realize the unexplored frequency's terahertz laser device and high-efficiency deep-UV emitter.

研究成果の概要（英文）：1. Dipole scattering self-energy for GaN/AlGaN superlattices were modeled, and it was utilized to investigate carrier transport based on the NEGF. By this study, it was confirmed that compositional Al ratios between 0.3 and 0.7 can highly influence the level broadening.
2. Generation of random electric field due to the roughness induced charge at the interfaces of GaN/AlGaN multiple quantum well (MQW) is reported. By this study, it is revealed that even for the 0.1 Al compositional ratio of GaN/AlGaN MQW can generate RMS random electric field over 1 MV/cm for the case of bad interface quality.

研究分野：Optoelectronics

キーワード：QCL　AlGaN　NEGF　Alloy disorder　Radom field

1．研究開始当初の背景

GaN-based quantum cascade laser (QCL) has been regarded as a strong candidate for realizing forbidden pure lasing frequencies of 5 ~ 12 THz over room temperature. The reason as the strong candidate comes from the relatively high longitudinal optical (LO) phonon energy of about 90 meV, which is higher than the case of GaAs having LO phonon energy of about 32 meV. In our previous investigation, simulation results by Nextnano.QCL considering two quantum wells, three levels, interface roughness scattering, charged impurity scattering (CIS), the lowest level of electron-electron scattering, and LO-phonon scattering based on the NEGF framework have shown high optical gain over 180 /cm at 300 K at 12.5 THz. Based on the extracted results, we started this project with the hope of realizing the efficient GaN-based QCL soon.

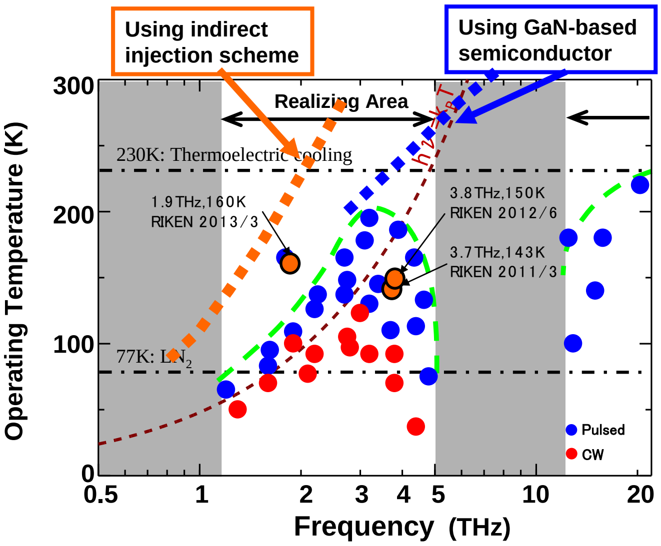

Fig. 1. Recent status and future prospects of the operation temperature and lasing frequency of THz-QCL

2．研究の目的

(1) Construction of gain-mapping as functions of lasing mechanisms, applied voltage per period, and energy for GaN/AlGaN QCL.

(2) Realization of lasing at unexplored frequency range at high temperature based on GaN/AlGaN material system.

3．研究の方法

(1) Design and investigation by non-equilibrium Green's function NEGF and analytical calculation

(2) MBE (Molecular beam epitaxy) growth and experimental measurements

4．研究成果

By utilizing commercial software, we found an AlGaN-based QCL structure consisted of two quantum wells (QWs) per period, which shows optical gain over 180 cm^{-1}. Therefore, we proposed this project and started. However, during the performance of this project, we recognize that several factors originated from the properties of GaN/AlGaN must be additionally considered for accurate simulation and gain-mapping. Since the commercial tool did not consider such factors yet, it was inevitable to calculate related effects by developing the NEGF simulator and related self-energy to describe carrier transport more accurately. The factors are as below.

(1) In the AlGaN material system, Al and Ga sites can be randomly distributed like a partially amorphous material. Due to such alloy disorder, dipole scattering happened for the carrier transport.[1)–3)]

(2) The scattering effect due to the roughness-induced charge near the GaN/AlGaN interface in the polarization material should be considered.[4)–7)]

Without considering at least the two important factors mentioned above, extracted simulation results for GaN/AlGaN QCL are very suspicious. Therefore, after developing 1D NEGF software based on the well-known algorithm written by Prof. Kubis, we started to

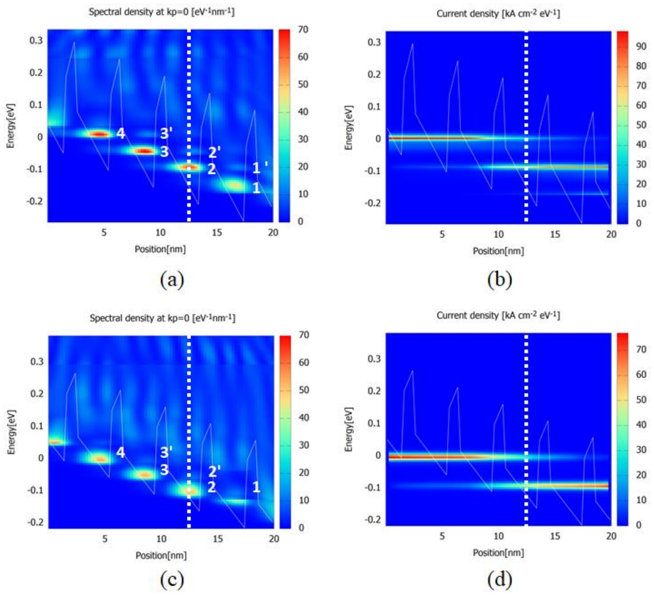

Fig. 2. Heatmap plots of (a) the spectral function A(z,E) of SL1, (b) the current density of SL1, (c) the spectral function of SL2, and (d) the current density of SL2 as functions of position and energy.

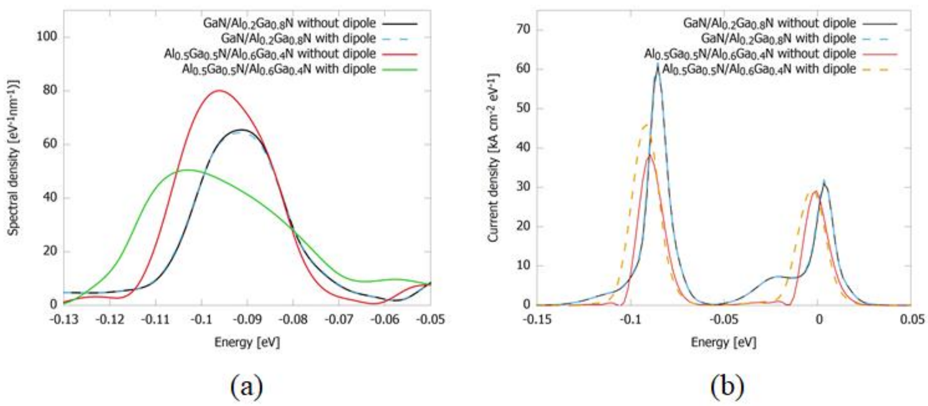

Fig. 1. (a) Cross-sectional view of the spectral density at $\boldsymbol{k}_{\parallel} = \mathbf{0}$ before and after dipole scattering for SL1 and SL2 structures at z=12.75 nm. (b) Cross-sectional view of the current density before and after dipole scattering for SL1 and SL2 structures at z=12.75 nm.

investigate the averaging effect for the two scattering sources mentioned above.[8),9)]

As a first step, we investigated level broadening by dipole scattering and its influence on carrier transport in $Al_xGa_{1-x}N/Al_yGa_{1-y}N$ superlattice structures. For this study, we derived the dipole self-energy within the self-consistent Born approximation. Using the NEGF method and dipole scattering self-energy, we extracted the spectral density and current density as functions of energy, applied voltage, and position before and after adopting the dipole self-energy. The underlying scattering mechanisms for this investigation were polar optical phonon and interface roughness scattering. The results obtained from this study clearly showed that dipole scattering due to microscopic disorder in the AlGaN structure has a significant effect on level broadening and carrier transport in AlGaN-based devices when Al composition of both well and barrier is quite high, as shown by Fig. 2 and 3.[10),11)] In Fig. 2 and 3, SL1 and SL2 mean $GaN/Al_{0.2}Ga_{0.8}N$ and $Al_{0.5}Ga_{0.5}N$ /$Al_{0.6}Ga_{0.4}N$ repetitive superlattices, respectively. The thicknesses of the wells and barriers in the samples were fixed to 3 and 1 nm, respectively. However, extracted results based on this averaged dipole scattering could not explain the difficulty of spontaneous photon emission by ISBT (intersubband transition) in GaN/AlGaN QWs since the distinctive energy levels of states are confirmed as shown in Fig. 2.

As the second, we investigated random electric field induced by interface roughness in $GaN/Al_xGa_{1-x}N$ multiple-quantum wells analytically before modeling the related self-energy.[12)] Extracted results showed that even with 0.1 Al composition of barrier, generated RMS random electric field due to the polarization-induced interface roughness can be over 1

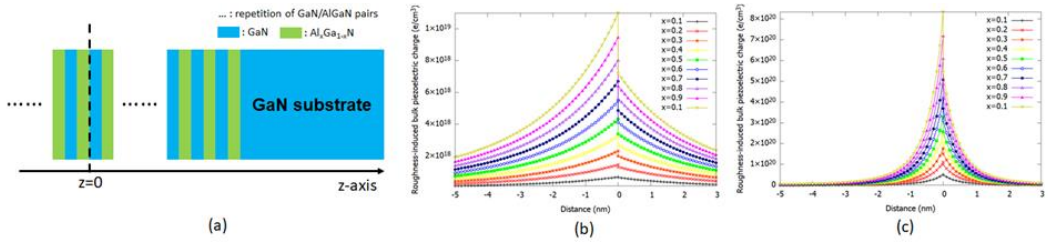

Fig.4. (a) A schematic of GaN/AlGaN MQW considered in this study. (b) RMS roughness-induced bulk piezoelectric charge $\overline{\boldsymbol{\rho}}_{\boldsymbol{\lambda}}(\mathbf{z})$ with Δ= 0.3 nm and $\boldsymbol{\Lambda}$= 8.0. (c) $\overline{\boldsymbol{\rho}}_{\boldsymbol{\lambda}}(\mathbf{z})$ with Δ= 0.8 nm and $\boldsymbol{\Lambda}$= 1.5 nm.

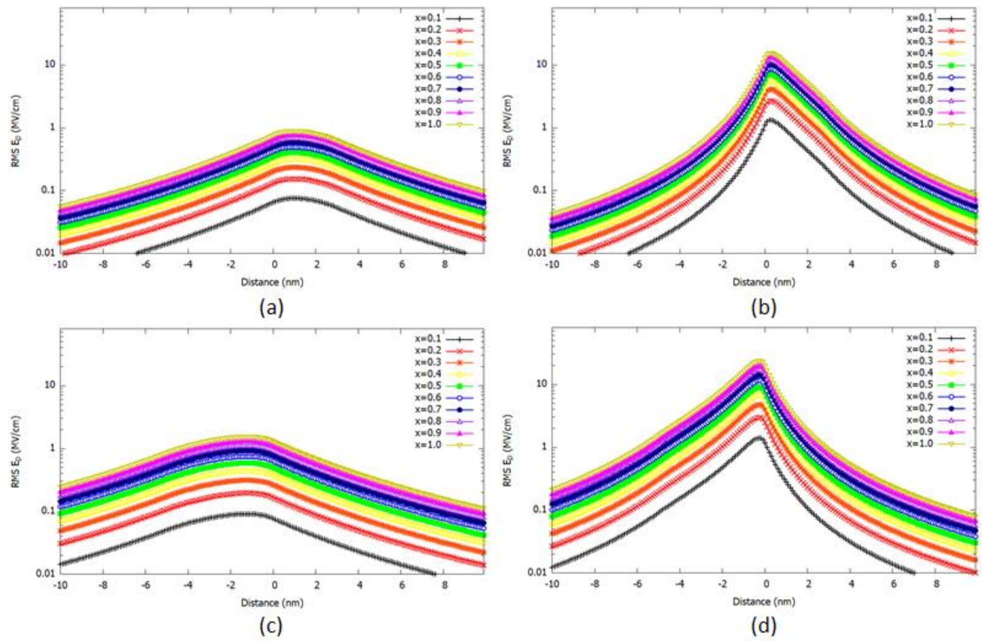

Fig.**5**. (a) Parallel RMS electric field $\overline{E_p^w}(z)$ due to $\bar{\rho}_w(z)$ with Δ= 0.3 nm and Λ= 8.0 nm. (b) $\overline{E_p^w}(z)$ with Δ= 0.8 nm and Λ= 1.5 nm. (c) Parallel RMS electric field $\overline{E_p^b}(z)$ due to $\bar{\rho}_b(z)$ with Δ= 0.3 nm and Λ= 8.0 nm. (d) $\overline{E_p^b}(z)$ with Δ= 0.8 nm and Λ= 1.5 nm.

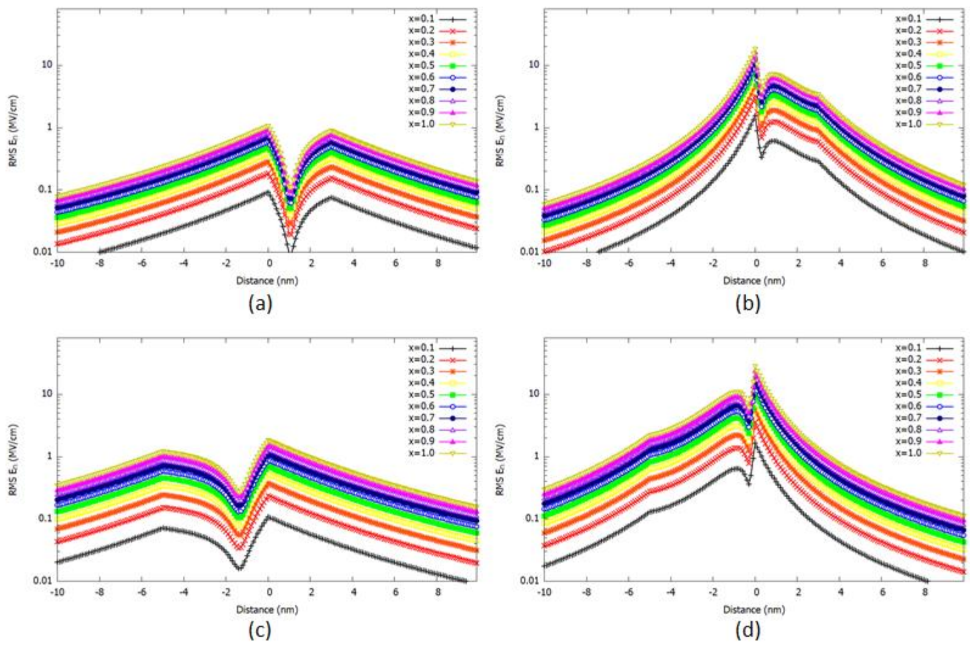

Fig. 6. (a) Normal RMS electric field $\overline{E_n^w}(z)$ due to $\bar{\rho}_w(z)$ with Δ= 0.3 nm and Λ= 8.0 nm. (b) $\overline{E_n^w}(z)$ with Δ= 0.8 nm and Λ= 1.5 nm. (c) Normal RMS electric field $\overline{E_n^b}(z)$ due to $\bar{\rho}_b(z)$ with Δ= 0.3 nm and Λ= 8.0 nm. (d) $\overline{E_n^b}(z)$ with Δ= 0.8 nm and Λ= 1.5 nm.

MV/cm when interface condition is bad. The structural geometry used for this study is shown in Fig. 4(a). Figure 4(b) shows $\bar{\rho}_\lambda(z)$ as functions of Al compositional ratio of AlGaN barrier and distance from the origin when Δ= 0.3 nm and Λ= 8.0 nm, which describe a relatively good interface. Here, $\bar{\rho}_\lambda(z)$, Δ, and Λ mean RMS roughness-induced bulk piezoelectric charge, roughness height, and correlation length, respectively. In the good case, the $\bar{\rho}_\lambda(0)$ varies from 6.83×10^{17} to $1.10 \times 10^{19}\ e/cm^3$ gradually as a function of Al ratio. Figure 4(c) shows the $\bar{\rho}_\lambda(z)$ when Δ= 0.8 nm and Λ= 1.5 nm describing a relatively bad interface. In this case, the $\bar{\rho}_\lambda(0)$ changes from 5.18×10^{19} to $8.33 \times 10^{20}\ e/cm^3$ as a function of Al ratio. Results in Fig. 4(b) and (c) imply that a rougher interface induces higher $\bar{\rho}_\lambda(z)$. Figure 5 and 6 show $E_p^\lambda(z)$ and $E_n^\lambda(z)$, respectively, which are generated by the $\bar{\rho}_\lambda(z)$ in Fig. 4(b) and (c). About ten-times larger $E_p^\lambda(0)$ and $E_n^\lambda(0)$ are observed in the case of the worse interface when compared with the better one in Fig. 5 and 6. For the calculation of Fig. 5 and 6, we fixed the thicknesses of well/barrier as 3nm/5nm. Since these random fields can play a role as a strong scattering source, which can disturb ISBT of QCL and radiative recombination in AlGaN-based light-emitting devices, we should find a way to overcome such a high RMS field.

For both studies above, we only investigated the average effect. When 2D or 3D randomness of interface roughness and alloy disorder in AlGaN are considered, the problems for realizing high-efficiency GaN/AlGaN QCL may be more severe than estimated by our methods. Therefore, we are currently developing 3D NEGF and related self-energies to investigate related scattering phenomena more deeply.

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５．主な発表論文等

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１．著者名 Joosun Yun, Dong-Pyo Han, and Hideki Hirayama	４．巻 12
２．論文標題 Random electric field induced by interface roughness in GaN/AlGaN multiple quantum wells	５．発行年 2019年
３．雑誌名 Applied Physics Express	６．最初と最後の頁 124005
掲載論文のDOI（デジタルオブジェクト識別子） 10.7567/1882-0786/ab548a	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

１．著者名 Wang Ke、Grange Thomas、Lin Tsung-Tse、Wang Li、Jehn Zoltan、Birner Stefan、Yun Joosun、Terashima Wataru、Hirayama Hideki	４．巻 113
２．論文標題 Broadening mechanisms and self-consistent gain calculations for GaN quantum cascade laser structures	５．発行年 2018年
３．雑誌名 Applied Physics Letters	６．最初と最後の頁 061109～061109
掲載論文のDOI（デジタルオブジェクト識別子） 10.1063/1.5029520	査読の有無 有
オープンアクセス オープンアクセスではない、又はオープンアクセスが困難	国際共著 該当する

〔学会発表〕　計5件（うち招待講演　0件／うち国際学会　3件）

１．発表者名 Joosun Yun and Hideki Hirayama
２．発表標題 Influence of Dipole Scattering to Level Broadening and Carrier Transport in AlGaN-based Superlattice Structures
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４．発表年 2019年

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３．学会等名 the 7th RAP symposium
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２．発表標題 Design and analysis of DUV-LEDs and QCLs by utilizing HOKUSAI
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１．発表者名 Ke Wang, Tsung-Tse Lin, Li Wang, Joosun Yun, Wataru Terashima, Hideki Hirayama, Thomas Grange, Zoltan Jehn, and Stefan Birner
２．発表標題 Broadening mechanisms and self-consistent gain calculations for GaN quantum cascade laser structures
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４．発表年 2018年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

Design of high performance THz-QCL and DUV-LED http://i.riken.jp/download/Q18381.pdf

６．研究組織

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７．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

８．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関