

Quasi-Bound State Tunneling in GaN Devices using 2D NEGF with Supercell Mode-Space Method

Heonseok Oh, Phil-Hun Ahn, Jooseok Kim, and Mincheol Shin
School of Electrical Engineering, Korea Advanced Institute of Science and Technology
 291 Daehak-ro, Daejeon, 34141, Republic of Korea
 E-mail: mshin@kaist.ac.kr

Abstract—This work proposes a computationally efficient two-dimensional (2D) non-equilibrium Green's function (NEGF) framework based on the supercell mode-space (Super MS) method to analyze quasi-bound-state (QBS) gate leakage tunneling in GaN devices. Unlike the one-dimensional (1D) optical potential (OP) method, the proposed 2D NEGF framework explicitly includes source, drain, and gate contacts. The OP method requires empirical fitting of the broadening parameter for different potential profiles, gate biases, or device geometries, whereas the 2D NEGF approach describes these effects through physical contact coupling. Therefore, QBS formation, carrier injection, and state broadening can be described in a physically consistent manner without adjustable parameters. The proposed framework accurately captures QBS-assisted tunneling under varying gate bias and device thickness, providing an efficient and predictive platform for gate leakage analysis and structural optimization of GaN devices.

Index Terms—2D NEGF, Gate leakage current, Optical potential

I. INTRODUCTION

GaN-based devices currently have played a pivotal role in communication systems and power electronics owing to their excellent material properties, such as high breakdown field, high electron mobility, and high-frequency operation capability [1]–[3]. In particular, AlGaIn/AlN/GaN heterostructures can form a high-density two-dimensional electron gas (2DEG) through strong spontaneous and piezoelectric polarization effects, enabling high-performance high-electron-mobility transistors [4]. However, as device dimensions are scaled and gate controllability becomes increasingly important, gate leakage current becomes a critical factor that limits device reliability and performance [5].

Forward gate leakage in GaN devices is strongly influenced by tunneling from the channel toward the gate. In addition to direct tunneling through the barrier, electrons confined in the quantum well near the GaN-side interface can contribute to leakage through quasi-bound states (QBS). Therefore, an accurate treatment of QBS formation, broadening, and carrier injection is essential for quantitatively evaluating gate leakage current and optimizing GaN device structures. A 1D NEGF approach adopting an optical potential (OP) has been proposed for QBS analysis [6], where an imaginary potential

This work was supported by the Technology Innovation Program (20026402, RS-2023-KT226402) funded by the Ministry of Trade, Industry Energy (MOTIE), Republic of Korea.

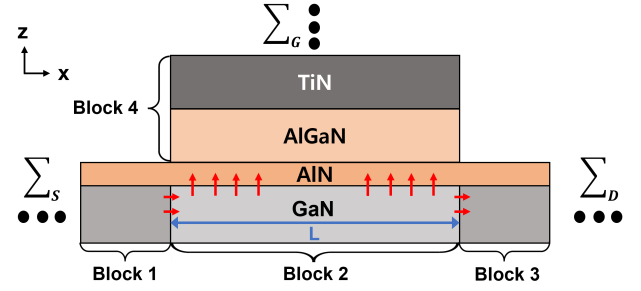


Fig. 1. Schematic illustration of the three-terminal NEGF model. The self-energies corresponding to the source, drain, and gate are indicated, representing blocks 1, 3, and 4, respectively.

is introduced to emulate the finite lifetime and broadening of QBS. Although this approach is computationally simple, the OP parameter must be empirically adjusted depending on device geometry and bias conditions, limiting its predictive capability. By contrast, a multi-terminal 2D NEGF approach can explicitly include source, drain, and gate contacts, allowing QBS broadening and carrier injection to be described more rigorously without empirical fitting parameters [7], [8]. However, the application of 2D NEGF to QBS gate leakage analysis in GaN devices has rarely been explored because of its high computational cost.

In this work, we present a three-terminal 2D NEGF framework for GaN devices, enabling rigorous calculation of gate leakage current including QBS effects. To overcome the computational burden, the supercell mode-space (Super MS) method and the coupled recursive Green's function algorithm are employed [9]. Based on the proposed 2D NEGF framework, we investigate QBS-assisted tunneling characteristics under different gate bias and device thickness conditions for GaN gate leakage analysis.

II. METHOD

The QBS tunneling current is evaluated using the NEGF formalism within the effective mass approximation, based on the potential profile obtained from a self-consistent solution of the Schrödinger–Poisson equations. The retarded Green's function is calculated as

$$G^r = (EI - H - \Sigma)^{-1}, \quad (1)$$

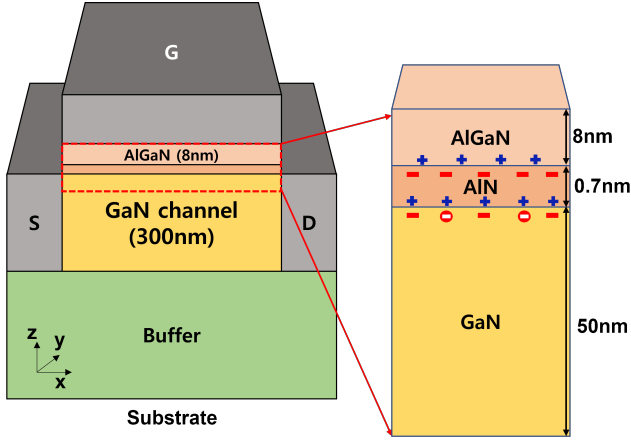


Fig. 2. Schematic of the GaN-based device structure. The enlarged region on the right represents the active simulation domain used in this work. Polarization charges at the heterointerfaces are also indicated.

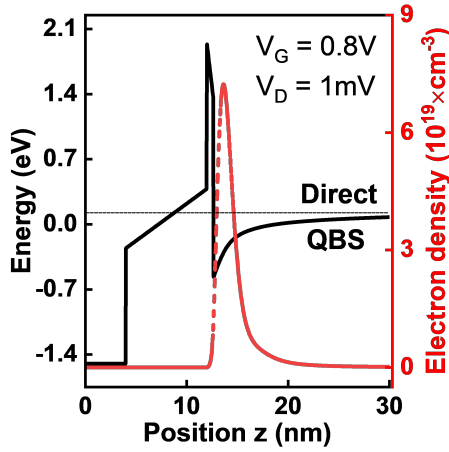


Fig. 3. Band profile of the GaN device. The black solid line represents the band structure, while the red dashed line indicates the electron density.

where the self-energy for 1D NEGF approach is given by

$$\Sigma = \Sigma_{\text{gate}} + \Sigma_{\text{channel}}. \quad (2)$$

For the 2D NEGF calculation, the self-energy is expressed as

$$\Sigma = \Sigma_{\text{source}} + \Sigma_{\text{drain}} + \Sigma_{\text{gate}}. \quad (3)$$

The 2D NEGF therefore explicitly accounts for carrier injection from the source into the QBS region [8], while in the 1D NEGF, the OP term, $-i\eta$, is added to the on-site energies of the Hamiltonian in the QBS region [6].

The coupled RGF method is applied for the three-terminal 2D NEGF calculation. The Schur complement method is applied to block 2 in Fig. 1. The effective matrix of block 2 is given by

$$\tilde{A}_{22} = A_{22} - A_{21}G_{11}^0A_{12} - A_{24}G_{44}^0A_{42} - A_{23}G_{33}^0A_{32}, \quad (4)$$

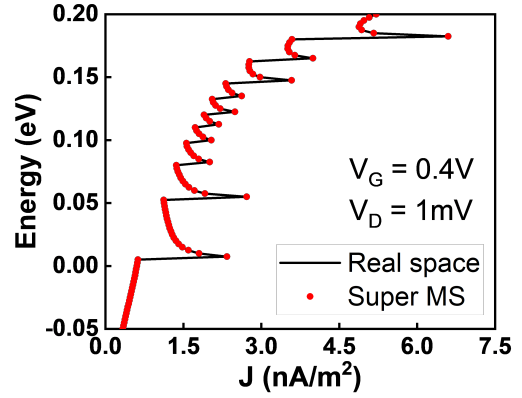


Fig. 4. Comparison of the current density spectra between real-space and mode-space approaches at $V_G=0.4V$. The black line represents the real-space result, while the red dots denote the Super MS result.

where G_{ii}^0 denotes the retarded Green's function of the isolated i -th block [7]. By inverting $\tilde{A}_{22}$, the retarded Green's function of block 2 is obtained as

$$G_{22} = \tilde{A}_{22}^{-1}. \quad (5)$$

Subsequently, the Green's functions of the adjacent blocks, namely blocks 1, 3, and 4, are updated using the Dyson equation:

$$G_{ii} = G_{ii}^0 + G_{ii}^0 A_{i2} G_{22} A_{2i} G_{ii}^0, \quad i = 1, 3, 4. \quad (6)$$

A key advantage of our approach lies in the application of the Super MS method [9]. Using this method, the Hamiltonian matrix of the channel block is reduced from approximately $10,000 \times 10,000$ in real space to approximately 100×100 in mode space, enabling efficient calculation of the gate leakage current.

III. NUMERICAL RESULTS

Three-terminal 2D NEGF simulations are performed for the GaN device structure shown in Fig. 2. The potential profile and electron density are first obtained from a self-consistent Schrödinger–Poisson calculation, where polarization-induced charges at the AlGaIn/AlN and AlN/GaN heterointerfaces are included in the Poisson equation. The parabolic effective mass theory (PEMT) Hamiltonian is then constructed using the calculated potential profile and employed in the NEGF transport calculation. Material parameters, including polarization charge, conduction-band offset, dielectric constant, and effective mass are adopted from previous studies [10], [11]. As shown in Fig. 3, strong band bending occurs near the GaN-side interface due to polarization discontinuity, resulting in the formation of a triangular quantum well and a high-density electron gas. These confined electrons can contribute to gate leakage through QBS-assisted tunneling in addition to direct tunneling through the barrier.

To verify the numerical accuracy of the proposed mode-space approach, the current density spectrum obtained from the Super MS method is compared with that from the full

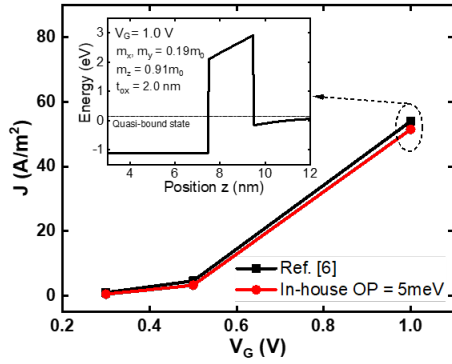


Fig. 5. Comparison of the 1D NEGF results with previous work. The black line represents the previous study, while the red line corresponds to the results obtained from our code. The optical potential is set to 5 meV. The inset shows the band profile at $V_G=1.0V$.

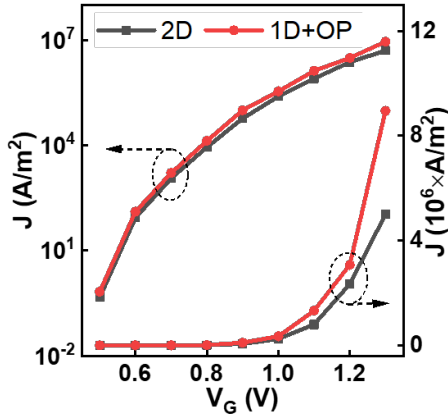


Fig. 6. Comparison of the 2D and 1D NEGF results for the GaN device. The optical potential is set to 5 meV. The black line represents the 2D NEGF result, while the red line corresponds to the 1D NEGF result.

real-space calculation, as shown in Fig. 4. The excellent agreement in the current density spectrum indicates that the Super MS method can accurately describe both direct tunneling and QBS-assisted tunneling while significantly reducing the computational cost.

Figs. 5 and 6 compare the QBS analysis obtained from the proposed 2D NEGF simulation and the conventional 1D NEGF method. For validation of the developed 1D NEGF code, our result was compared with a previous silicon-device study, as shown in Fig. 5 [6]. The agreement confirms that the OP implementation can reproduce previously reported results when an appropriate η value is selected. However, as shown in Fig. 6, the 1D NEGF result with a single fixed η shows noticeable deviation from the 2D NEGF result for the GaN device, where a drain bias of $V_D = 1mV$ was applied in the 2D simulation. This discrepancy originates from the fact that the OP parameter artificially represents QBS broadening and carrier injection, whereas the actual broadening depends on the

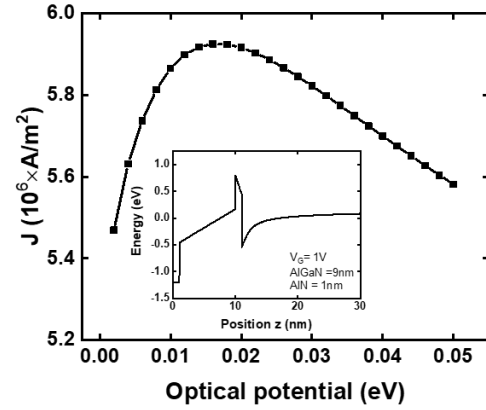


Fig. 7. Variation of the current density with the OP value for the GaN device. The inset shows the band profile at $V_G = 1V$

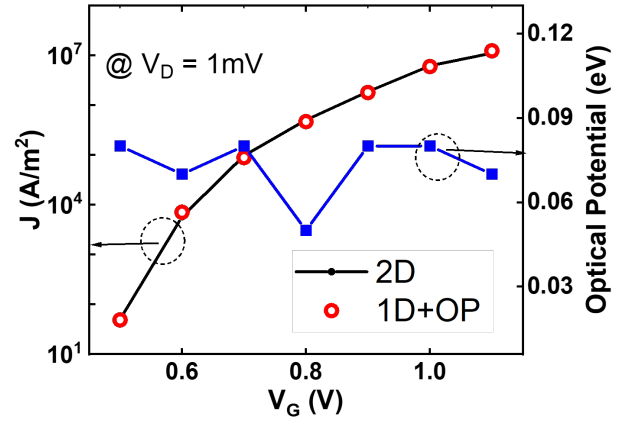


Fig. 8. 2D NEGF results for the case of a 9 nm AlGaIn layer, along with the OP values used to tune the 1D NEGF results to match the 2D results.

potential profile, gate bias, and device geometry. In the 2D NEGF framework, these effects are naturally determined by the source, drain, and gate self-energies, without introducing an empirical fitting parameter. For example, Fig. 7 shows the variation in current density with respect to the OP value for the GaN device.

Fig. 8 shows that the OP parameter required for the GaN device differs from that used for the silicon device. In addition, different η values are needed to reproduce the 2D NEGF reference results depending on the gate bias and AlGaIn thickness. This indicates that a single OP parameter cannot universally describe QBS tunneling in GaN devices. In particular, because the energy position and spatial extent of QBS change with bias-induced band bending, the effective coupling between the QBS region and the contacts also changes. Therefore, the OP method must be recalibrated for each potential profile, while the 2D NEGF approach provides a parameter-free and physically consistent description of the same process.

IV. CONCLUSION

In this work, a three-terminal 2D NEGF framework is developed for the rigorous analysis of QBS-assisted gate leakage current in GaN devices. The proposed approach explicitly includes the source, drain, and gate contacts. Therefore, carrier injection into QBS and the corresponding state broadening are determined by physical contact coupling, rather than by empirically fitted optical-potential parameters. This feature makes the framework applicable across different potential profiles, gate biases, and device geometries compared with the 1D NEGF method. The simulation results show that QBS tunneling becomes increasingly dominant as the gate bias increases, while direct tunneling mainly contributes at lower gate bias. In addition, the gate leakage current is found to be strongly affected by the barrier thickness, indicating that geometrical optimization is essential for suppressing leakage while maintaining channel charge density. This framework can be further extended to other device structures where quasi-bound-state-assisted leakage plays an important role.

REFERENCES

- [1] J. W. Chung, W. E. Hoke, E. M. Chumbes, and T. Palacios, "AlGaIn/GaN HEMT with 300-GHz f_{max} ," *IEEE Electron Device Letters*, vol. 31, no. 3, pp. 195–197, Mar. 2010.
- [2] M. Akita, S. Kishimoto, and T. Mizutani, "High-frequency measurements of AlGaIn/GaN HEMTs at high temperatures," *IEEE Electron Device Letters*, vol. 22, no. 8, pp. 376–377, 2002.
- [3] K. H. Teo, Y. Zhang, N. Chowdhury, S. Rakheja, R. Ma, Q. Xie, E. Yagyu, K. Yamanaka, K. Li, and T. Palacios, "Emerging GaN technologies for power, RF, digital, and quantum computing applications: Recent advances and prospects," *Journal of Applied Physics*, vol. 130, no. 16, 2021.
- [4] O. Ambacher, "Polarization induced effects in AlGaIn/GaN heterostructures," *Acta Physica Polonica A*, vol. 98, no. 3, pp. 195–201, 2000.
- [5] J. W. Chung, J. C. Roberts, E. L. Piner, and T. Palacios, "Effect of gate leakage in the subthreshold characteristics of AlGaIn/GaN HEMTs," *IEEE Electron Device Letters*, vol. 29, no. 11, pp. 1196–1198, Nov. 2008.
- [6] S. Muraoka, S. Souma, and M. Ogawa, "Analysis of direct tunneling current from quasi-bound states in n-MOSFET based on non-equilibrium Green's function," in *Proc. 2008 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*, 2008, pp. 221–224.
- [7] M. Shin, "Large-scale quantum simulations enabled by real-space-equivalent SuperMS method," in *Proc. 2025 IEEE International Electron Devices Meeting (IEDM)*, 2025, pp. 1–4.
- [8] S. Muraoka, R. Mukai, S. Souma, and M. Ogawa, "2D quantum mechanical simulation of gate-leakage current in double-gate n-MOSFETs," in *Proc. 2009 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*, 2009, pp. 1–4.
- [9] M. Shin, "Hetero-structure mode space method for efficient device simulations," *Journal of Applied Physics*, vol. 130, no. 10, 2021.
- [10] Y. Zhang, I. P. Smorchkova, C. R. Elsass, S. Keller, J. P. Ibbetson, S. Denbaars, U. K. Mishra, and J. Singh, "Charge control and mobility in AlGaIn/GaN transistors: Experimental and theoretical studies," *Journal of Applied Physics*, vol. 87, no. 11, pp. 7981–7987, Jun. 2000.
- [11] L. S. Yu, D. J. Qiao, Q. J. Xing, S. S. Lau, K. S. Boutros, and J. M. Redwing, "Ni and Ti Schottky barriers on n-AlGaIn grown on SiC substrates," *Applied Physics Letters*, vol. 73, no. 2, pp. 238–240, Jul. 1998.