Integrated TCAD Methodology for Simulating Ion Implantation and Device Isolation in GaN ICs

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Abstract— **This study proposes an integrated TCAD (Technology Computer-Aided Design) model to predict and optimize the isolation performance of GaN integrated circuits through ion implantation. Unlike existing studies, which fail to quantitatively integrate ion implantation process simulations with device-level isolation characteristics, this research incorporates the implantation damage profiles obtained from ion implantation simulations into device simulations. This enables to reflect the key mechanisms such as stress relaxation at the heterojunction interface and trap formation related with ion implantation damage. The proposed model predicts the band structure near the heterojunction interface based on the interaction of these mechanisms and explains the experimental results quantitatively. Validation using argon-implanted TLM (Transmission Line Method) structures demonstrates precise predictions of the isolation characteristics, with a 77% reduction in stress at heterojunction interface, and trap contributions from gallium vacancies (V_{Ga}) and nitrogen interstitials (N_I) to be 0.1% and 99.9%, respectively. Additionally, the VRH (Variable Range Hopping) mechanism is incorporated to describe the electron transport through defect states, ensuring an accurate prediction under low and high bias conditions. This approach provides precise predictions of the leakage characteristics across various implantation conditions and establishes a robust framework to optimize GaN IC designs and to implement high-performance power electronics and RF systems.**

Keywords—GaN, TCAD, Argon, Ion-implanted Isolation, TLM (Transmission Line Method), VRH (Variable Range Hopping), Gallium vacancies (V_{Ga}), Nitrogen interstitials (N_I)

I. Introduction

Gallium nitride (GaN) is a promising compound semiconductor for high-performance power devices. GaN-based high-electron-mobility transistors (HEMTs) provide lower on-resistance and higher power conversion efficiency compared to silicon MOSFETs. The main reasons for these advantageous properties are its material properties, such as high critical breakdown due to its wide bandgap and 2-dimensional electron gas (2DEG) formed by hetero junctions, which reduce the die size and internal capacitance significantly. However, there is one crucial requirement to fully utilize the advanced properties of GaN – the isolation process. Since the 2DEG channel is formed across the entire wafer as soon as the GaN epitaxy is completed, active areas must be defined using appropriate isolation techniques, such as ion implantation. Insufficient isolation can lead to a signal degradation in RF systems and performance issues in power devices due to increased leakage currents and reduced breakdown voltage. Currently, ion implantation is preferred for device isolation over mesa isolation processes. It is because it has advantages in providing stable isolation in complex patterns through a non-destructive process, as well as reducing substrate damage due to low-temperature compatibility [1], [2]. Moreover, ion implantation is also utilized to engineer resistivity in GaN devices [3]. In these applications, it is crucial to control and optimize the implantation condition.

However, a robust framework integrating process simulations and device simulations has not been proposed for the effective utilization of ion implantation techniques. While process simulation tools, such as TRIM (Transport of Ions in Matter), are effectively used to model impurity distribution and lattice damage profiles, they are not directly utilized in device simulations [4].

To address these challenges, this study proposes an integrated TCAD (Technology Computer-Aided Design) methodology that incorporates the ion implantation process simulations with device simulations to predict the isolation characteristics of GaN devices. As shown in Figure 1, the defect distributions induced by ion implantation are simulated, and physical models, including trap generation [5] and stress relaxation [6] caused by these defects, are incorporated into the device simulations. This integration enables an accurate prediction of the isolation performance under various ion implantation conditions. Furthermore, by adopting the model of electron transport through the defects [7] in the ion-implanted region, the proposed approach demonstrates an effective predictive capability even at high voltages. This study quantitatively analyzes the isolation leakage current characteristics under various voltage and temperature conditions by applying the methodology to the TLM structures implanted with argon ions. The purpose of this research is to predict the isolation performance based on ion implantation conditions, thereby providing an accurate resource for the design of GaN-based discrete switches and high-density circuits.

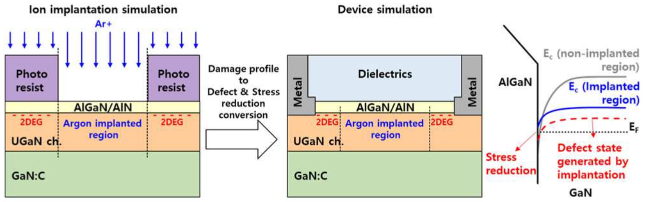

Figure.1 Concept of proposed TCAD Methodology. Damage profiles obtained from process simulation are converted into trap profiles in device simulation.

II. Methodology

The physical mechanisms to describe the electrical isolation in GaN devices through ion implantation were analyzed. Based on the understanding, a simulation model was proposed. To validate the effectiveness of the model, experimental data from the argon implanted TLM structure were compared.

A. Physical model of isolation using ion implantation

In the AlGaN/AlN/GaN heterojunction, spontaneous and piezoelectric charges, whic5h is resulting from lattice constant mismatch-induced stress, induce a high-density 2-

dimensional electron gas (2DEG). Argon implantation into the heterojunction causes a disruption of the lattice bonding between the two layers, leading to a reduction in stress within the system. This stress relief decreases the density of the 2DEG and consequently enhances the electrical isolation characteristics between active areas with 2DEG. Moreover, the argon atoms collide with gallium and nitrogen atoms in the GaN layer, creating multiple Gallium vacancies (V_{Ga}) and Nitrogen interstitials (N_I). Most argon atoms remain in interstitial states and are chemically inert, not directly forming trap states within the bandgap [8]. In contrast, the generated V_{Ga} and N_I induce trap states within the bandgap at Ev+1.0 eV [9], [10] and Ec-0.76 eV [11], respectively. These traps, particularly the acceptor-type traps, reduce the number of electrons in the conduction band by capturing electrons. The traps can also emit electrons under a strong electric field, which means they become scattering centers, resulting in significantly reduced mobility within the GaN structure. As the strength of the electric field increases, the frequency of capture and emission events decreases, leading to an increase in mobility. The mobility reduction can be modeled using Poole-Frenkel model or the Variable Range Hopping (VRH) model. These models describe that the defects can hinder carrier transport pathways and limit the conductivity of the carriers. In summary, argon ion implantation induces stress relaxation and lattice damage in the AlGaN/AlN/GaN structure, reducing the 2DEG density and electron mobility to turn the active channel to be highly resistive.

B. Experiments Method

The device isolation experiment by ion implantation was conducted using the TLM (Transmission Line Method) structure, which is an appropriate configuration to evaluate the electrical isolation characteristics between devices within GaN ICs. As shown in Figure 2, a 280 nm thick u-GaN layer is deposited on top of Carbon-doped GaN. On top of the u-GaN, 15 nm thick AlGaN and 0.5 nm thick AlN layers were subsequently grown by MOCVD (metal organic chemical vapor deposition). The test structures include two electrodes with a 0.5μm active area with 2DEG and isolated regions between the electrodes. The isolation distance between the two electrodes (L_{iso}) lengths are 2 μm, 4 μm, 6 μm, and 8 μm. Three steps of Ar+ isolation implantation processes were applied to define the isolation region. All four samples were measured at various temperatures (300 K to 425 K) and the voltage applied between two electrodes was up to a voltage of 600 V. As the leakage current toward the buffer layer is very small, the vertical leakage components were ignored in this experiment. Figure 3 shows the main experimental results. The leakage currents at the closest distance (L_{iso}: 2 μm) at room temperature, with 10 V and 200 V between isolation, are approximately 0.82 nA/mm and 80 nA/mm, respectively. These values are sufficiently low for typical GaN ICs operating from 5 V to 200 V. From the measured results with different isolation distances, it was found that the isolation region has a lateral (surface and channel) resistance of approximately 6.159 x 10^{12} Ohm/sq at 300 K and 10 V bias. When the temperature is elevated at 10V bias, the current increases by one orders of magnitude for every 62.5 K. In the Arrhenius plot of the experimental results at 10 V, the activation energy (E_a) of Eq. (1) was determined to be approximately 0.414 eV:

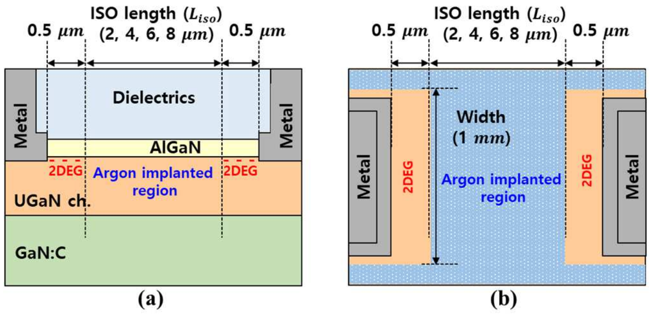

Figure.2 (a) Cross section and (b) top view of experiment structure. Argon ions are implanted on the middle of TLM structures.

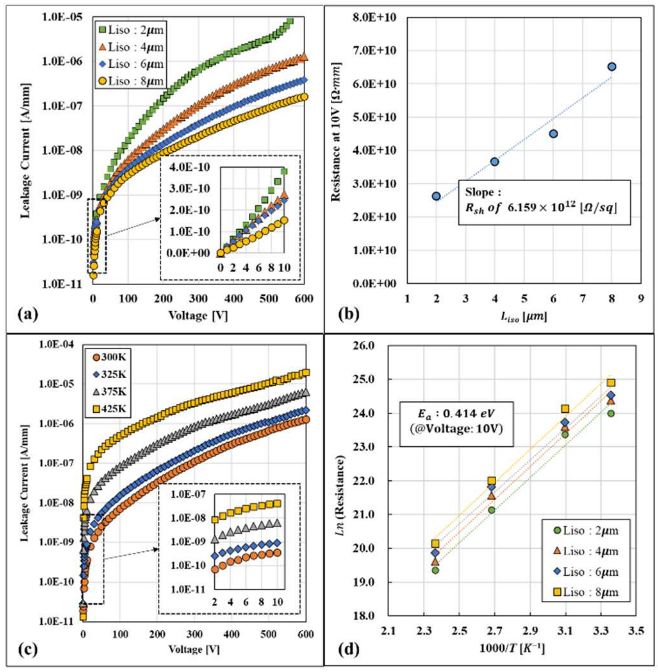

Figure.3 (a) Leakage current for L_{iso} : 2, 4, 6, and 8 μm at 300 K. (b) Resistance plot at 10 V for L_{iso} : 2, 4, 6, and 8 μm at 300 K. (c) Leakage current for various temperature from 300 K to 425 K. (d) Arrhenius plot at 10 V for L_{iso} : 2, 4, 6, and 8 μm.

$$R_{sh} = Aexp\left(-\frac{E_a}{kT}\right) \quad (1)$$

Where k and T are the Boltzmann constant and temperature, respectively. At voltages above 100 V, the current is not linear, and the rate of increase also shows a significant rise with voltage.

III. IMPLEMENTATION OF TCAD MODEL

A. TCAD simulation about Argon implantation

Argon ion implantation process simulations, as described in Section II.A, are conducted on the TLM structure using the Sentaurus Monte Carlo (M.C) implantation simulation model. Since this approach is an atomistic simulation of the ion implantation, not only the profile of implanted argon but also the quantified damage induced in the GaN lattice are presented.

The black solid line data in Figure 4 illustrates the simulated argon atom profile, which exhibits similar trends to the measured argon profile (black circles) obtained from SIMS (Secondary Ion Mass Spectroscopy). The simulation reveals that the concentration of argon atoms is distributed in the range of approximately ~10^{18} to ~10^{20} cm within the undoped

GaN channel (UGaN ch.), penetrating sufficiently into the Carbon-doped GaN (GaN:C) layer. The blue dashed line in Figure 4 displays the implantation damage profile, indicating the defect densities exceeding ~10^{21} cm^{-3} within the GaN lattice, peaking at ~10^{22} cm^{-3} at the AlGaN/AlN/GaN interface. This confirms the formation of sufficient defects to achieve electrical isolation.

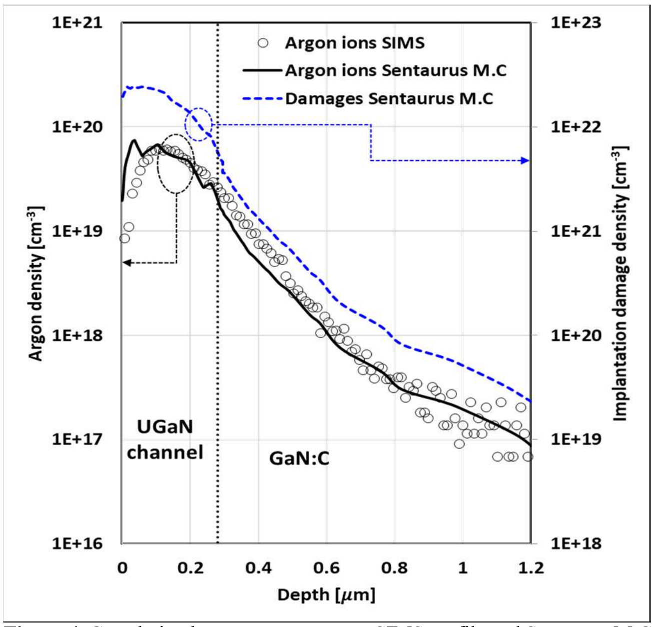

Figure 4. Correlation between argon atoms SIMS profile and Sentaurus M.C simulation results, with implantation damage profile.

B. Implmentation of isolation mechanism in TCAD model

Experimentally quantifying the amounts of V_{Ga} and N_I traps from the damage profile, as well as the degree of stress relaxation between the hetero junction (AlGaN/AlN/GaN) layers, is not straightforward. These unknown parameters must be inferred indirectly from the electrical experiment data. First, in the context of an Arrhenius plot, the activation energy of 0.414 eV implies that the electron concentration in the conduction band increases by an order of magnitude with every 62.5 K rise in temperature. This observation suggests that the conduction band rises relative to the Fermi level due to ion implantation.

This behavior can be attributed to the following factors: 1) Stress relaxation at the heterojunction interface reduces the original band bending effect. 2) Acceptor traps (V_{Ga}: $E_t = E_v+1.0$ eV) created by the implantation capture electrons and elevate the band. 3) Donor traps (N_I: $E_t = E_c-0.76$ eV) that release electrons partially lower the band. Therefore, the following parameters are defined as fitting parameters for the simulation:

1) Reduced ratio of the piezoelectric charge at the heterojunction interface: r_{str}.

2) Scaling factor of V_{Ga} trap concentration based on the damage profile: R_{Ga}.

3) Scaling factor of N_I trap concentration based on the damage profile: R_N.

The piezoelectric charge at the hetero junction interface is calculated to be decreased by a factor of r_{str} compared to the original value. The amount of traps in V_{Ga} and N_I are multiplied by R_{Ga} and R_N, respectively, as indicated in the damage profile shown in Figure 4.

C. Results and Discussion

At first, the band characteristics and the temperature dependence of the leakage currents are analyzed with respect to r_{str}, R_{Ga}, and R_N. Figure 5 describes the conduction band and the electron concentration at the heterojunction interface under equilibrium conditions simulated with various conditions of r_{str}, R_{Ga}, and R_N. Under high stress conditions in non-implanted region, the conduction band aligns closer to the Fermi level. However, as the stress is reduced and the concentration of acceptor-type traps due to V_{Ga} increases, the conduction band shifts upward from the Fermi level.

The experimental data of the isolation leakage and activation energy in Arrhenius plot showed the best agreement under conditions of a 77% reduction (r_{str} = 0.77) in stress at the heterojunction interface with 99.9% of donor traps associated with N_I activated (R_N = 0.999) and only 0.1% of acceptor traps associated with V_{Ga} activated (R_{Ga} = 0.001). The acceptor trap is a critical factor to make the isolation in GaN devices. The electrons in the conduction band, which is formed by these factors, are drifted by the electric field under bias.

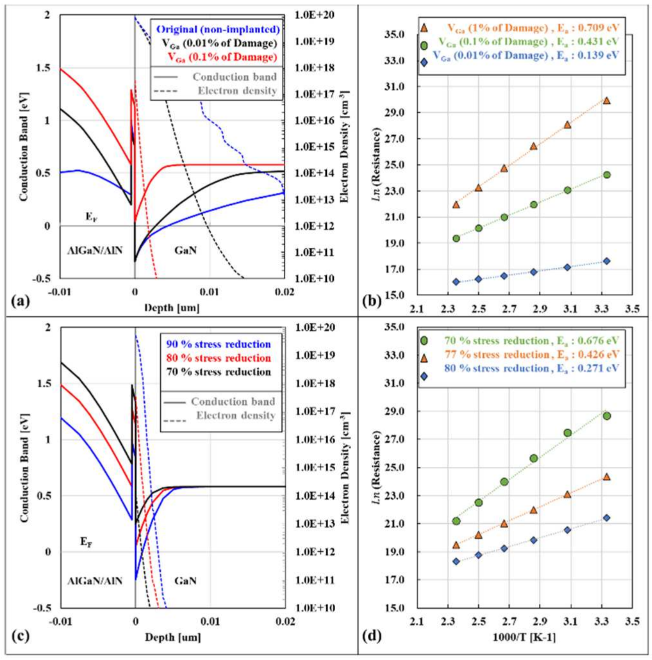

Figure 5. (a) Band diagram of solid lines, electron density of dash lines, and (b) Arrhenius plot for different V_{Ga} portion (R_{Ga}) cases. (c) Band diagram of solid lines, electron density of dash lines, and (b) Arrhenius plot for different stress reduction (r_{str}) cases.

At low voltages, the resistance exhibits Ohmic characteristics. At higher voltages, however, the resistance (=ΔV/ΔI) decreases as electrons from the non-implanted 2DEG source region begin to migrate into the isolation region, increasing the electron concentration. These electrons, which are trapped by defects, are subsequently released by the electric field, effectively increasing mobility. This phenomenon can be modeled using the following VRH mobility model in Eq. (2):

$$\mu = \frac{v_0 b}{2F} exp\left(-\frac{\sigma^2}{(kT)^2}\right)\left[exp\left(\frac{qbF}{kT}\right)-1\right] \quad (2)$$

Where, b is the hopping site distance of 5.0×10^{-8} cm, estimated from the defect density (~10^{22} cm^{-3}) created by argon implantation at the hetero junction. v_0 represents the hopping frequency, determined to be approximately

1.21×10^{11} Hz based on the experimental results. This value is ~10 × smaller than the VRH model transition time of about 1.0×10^{12} Hz at the given hopping distance. σ, the Gaussian distribution width of hopping traps, is set to 0.05 eV. q is the electron charge. F is the electric field, which is calculated during the simulation.

With these calibrated parameters, the leakage currents for the various isolation lengths ranging from 2 μm to 8 μm were tested under different bias conditions. The simulation results based on this physical model align well with the measured values as shown in Figure 6. The proposed TCAD model for isolation by an ion implantation explains the leakage characteristics under various implantation conditions, making it a valuable tool for analyzing and optimizing the isolation performance of GaN processes. It also means that our methodology can be utilized to resistivity engineering in GaN IC. Furthermore, this model can be extended to predict the isolation characteristics of other ions by incorporating their specific trap formation mechanisms.

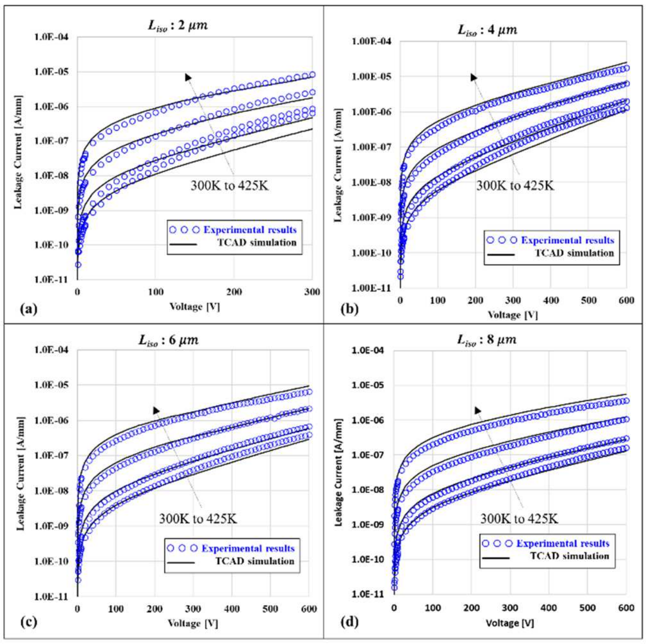

Figure 6. Comparison of simulation and experimental results of the leakage in the isolation regions with distances of 2, 4, 6, and 8 μm at temperature of 300, 325, 375, and 425 K.

IV. Conclusion

In this study, a TCAD simulation methodology has been proposed to investigate the mechanisms of ion implanted isolation between devices in gallium nitride integrated circuits. The proposed approach represents an integrated TCAD methodology capable of simulating ion implantation and the isolation characteristics between devices. As a case study, the proposed methodology is applied to a TLM structure isolated by argon ion implantation. This structure serves as a representative model of the isolation regions in GaN devices. The results successfully demonstrate the effectiveness and applicability of the proposed approach. The lattice damage profile due to argon ion implantation is predicted using the Monte Carlo simulator in the TCAD tool Sentaurus. The ratios of the damage profile to the trap densities induced by gallium vacancies (V_{Ga} : $E_t = E_V+1.0$ eV) and nitrogen interstitials (N_I : $E_t = E_c-0.76$ eV) were employed as calibration factors in the device simulation process. The extent of stress relaxation at the heterojunction interface, induced by ion implantation, is also incorporated as a calibration parameter in the device simulation process. In this study, the isolation region exhibited a sheet resistance of approximately 6.159×10^{12} [Ohm/sq]. The Arrhenius plot revealed an activation energy of 0.414 eV. In the TCAD simulation, 99.9 % conversion from damage profile to the nitrogen interstitials donor trap, 0.1 % to the gallium vacancy acceptor trap, and 77% reduction in the stress relaxation at the heterojunction interface are applied as calibration parameters. It yields results that closely aligned with the experimental data. By utilizing the calibration methodology, the isolation or resistance characteristics between devices under different ion implantation conditions can be predicted. This study proposes an integrated TCAD methodology to simulate isolation between devices by ion implantation processes. The proposed approach can be applied to further develop future GaN IC processes.

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