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Correlation between experimental and modeled capacitance-voltage characteristics of Ga_2O_3 Schottky barrier diode in temperature range of 300–673 K

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ABSTRACT

The experimental and modeling results of the capacitance-voltage characteristics of a Pt/Ga_2O_3 Schottky barrier diode (SBD) are correlated in the temperature range of 300–673 K, where the modeling is conducted using technology computer-aided design (TCAD) simulations. The Pt/Ga_2O_3 SBD displays well-behaved diode performance and a rectification ratio of about 10^6 at $\pm$1.5 V, which correlates well with the TCAD modeling. The temperature-independent behavior of the reverse current as temperature increases is attributed to the high-quality depletion layer, which prevents the presence of additional free charges. The capacitance value increases slightly with temperature due to the reduction of the depletion width, which also correlates well with the TCAD modeling.

1. Introduction

Wide bandgap semiconductors (WBSs) have been used in various applications such as power electronics and ultraviolet detectors [1–3]. Among WBSs, gallium oxide (Ga_2O_3) stands out due to its exceptionally large bandgap of about 5.0 eV [4] and excellent thermal stability compared to other WBSs such as SiC (3.26 eV for 4H-SiC) [2] and GaN (3.44 eV) [5]. The wider energy bandgap characteristics of Ga_2O_3 when compared to conventional WBSs lead to a higher theoretical breakdown field of 8 MeV/cm [6,7], which is advantageous for power devices. Recently, various types of Ga_2O_3-based Schottky barrier diodes (SBDs) have been examined experimentally for power device applications [8–12]. While the results have been impressive, correlation with modeling techniques such as technology computer-aided design (TCAD) is an indispensable tool in the design of SBDs using new semiconductors [13]. TCAD's ability to predict performance, minimize costs and development time, evaluate material properties, and validate new designs make it essential for the development of innovative electronic devices. While a large number of experimental results have been reported [14–16], only a few modeling studies have been conducted, particularly in high temperature ranges [17,18]. In this work, we have observed the capacitance-voltage (C-V) of a Pt/Ga_2O_3 single crystal SBD in the temperature range of 300–673 K for the first time. Using TCAD simulations, the C-V results have been correlated with experimental results.

2. Experimental and modeled

Monoclinic gallium oxide (β-Ga_2O_3) semiconductors, consisting of an 11.1-μm thick Si-doped n-type β-Ga_2O_3 epitaxial layer via hydride vapor phase epitaxy on a Sn-doped n-type β-Ga_2O_3 single-crystal substrate (100), were commercially purchased from Novel Crystal Technology. The carrier concentration of the epitaxial layer was 1.9×10^{16} cm^{-3}, while that of the single-crystal substrate was 5.0×10^{18} cm^{-3}. On the back side (single-crystal substrate), Ti/Au (20/100 nm) was deposited using electron beam evaporation. The sample was then annealed with a rapid thermal process at 500 °C for 60 s in a N_2 atmosphere, processing in order to form the Ohmic contact. To form a Schottky contact with the

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epitaxial layer (front side), a Pt/Ti/Au (20/10/100 nm) metal electrode was formed via electron beam evaporation followed by conventional photolithography and a lift-off process. The capacitance-voltage (C-V) and current-voltage (I-V) were characterized using a Keithley 4200 SCS semiconductor analyzer. The device was placed on a ceramic heater inside a sealed chamber in a Nextron Micro Probe System (Republic of Korea) with a HiCube 300H Neo Pfeiffer vacuum system. Temperatures ranging from room temperature (300 K) to 400 °C (673 K) were precisely controlled to within ±1 °C using the Nextron temperature controller. Modeling parameters such as the dielectric constant, thermal conductivity, and constant mobility were obtained from the database provided by SILVACO [19]. The thermal conductivity was set to 0.147 W/(Kcm), corresponding to the (001) direction. The electron density of state to 300 K was set at 4.97×10^{18} cm^{-3}, which was calculated from the electron effective mass of β-Ga_2O_3 $m_e = 0.34m_o$ [7].

3. Results and discussion

A schematic drawing of the cross section of the Pt/Ga_2O_3 SBD is presented in Fig. 1(a), in which a circular electrode with a diameter of 270 μm is formed. Fig. 1(b) shows the semilog I-V characteristics of the Pt/Ga_2O_3 SBD in the temperature range from 300 to 673 K, 20 K step. At each temperature step, the device was held for 3 min to ensure thermal stabilization prior to I-V and CV measurements. The results indicated well-behaved diode performance and a rectification ratio of about 10^6 at ±1.5 V. The forward voltages of the SBD were determined by the built-in voltages and were as low as 1.25 V at room temperature. Thermionic emission current equation is used to describe the current in this SBD and is given by [5].

$$I = I_0\left[\exp\left(\frac{qV}{nkT}\right) - 1\right] \tag{1}$$

where I, I_0, n, K, T, q, and V are current through the Schottky barrier, reverse current, ideality factor, Boltzmann constant, electronic charge, and applied voltage, respectively. The ideality factor (n) provides insight into the quality of the depletion region and Schottky contact. The SBD exhibited a low ideality factor of only 1.05 at room temperature, and its value was comparable to that of the commercially available Si-based SBD (IN5819), which had a value of 1.03 [5]. This indicated that high-quality Ga_2O_3 semiconductors had been formed, as it suggested minimal recombination and an efficient charge carrier transport. As shown in Fig. 1(b), the reverse current was found to be almost constant over the specified temperature ranges, indicating that the formed Ga_2O_3-based SBD exhibited excellent thermal stability up to at least 673 K. This was presumably due to the high-quality depletion width and the absence of additional free carriers due to the wide bandgap characteristics. It has been reported that the Schottky barrier quality can be further evaluated by observing the depletion region using capacitance-voltage measurements [8].

Fig. 2(a) shows the measured reverse bias C-V characteristics and the corresponding modeling results of the Pt/Ga_2O_3 SBD in the temperature range from 300 to 673 K step 20 K at 2 MHz; data points of 300 K, 373 K, 473 K, 573 K, and 673 K are shown. The results demonstrated that the capacitance decreased with increasing reverse bias voltage because the depletion width expanded with the reverse bias voltage. As was seen in Fig. 1(b) when the current in the I-V curves was depicted within the temperature range, the capacitance in the C-V curves also increased slightly with temperature. In semiconductors, capacitance increases with temperature due to several reasons related to the behavior of charge carriers and the depletion layer width. In the present study, the increased charge carrier density in the Pt/Ga_2O_3 SBD was initially negligible in the temperature range from 300 to 673 K due to the wide bandgap properties. Thus, the effect of the increased charge carrier density according to temperature was ruled out. Next, the reduction in depletion region width could be considered. The results in Fig. 2 revealed that the Pt/Ga_2O_3 SBD demonstrated excellent thermal stability up to at least 673 K. The experimental results were compared with the modeling results in the temperature range from 300 to 673 K. The two sets of results correlated well with one another. Depletion width in a semiconductor junction typically decreases with increasing temperature, as was seen in Fig. 2(b) [20,21]. This reduction occurs because of the significant enhancement in the minority carrier concentration. A narrower depletion width results in higher junction capacitance.

Fig. 3(a) shows the experimental and modeling results of the Pt/Ga_2O_3 SBD $(A/C)^2$-V capacitance-voltage characteristics in the temperature range from 300 to 673 K at 2 MHz. An analysis of the A^2/C^2 plot, often referred to as a Mott-Schottky plot, provides critical information about the built-in potential (V_{bi}) and the majority carrier concentration (N_d) [5,22]. The V_{bi} can be determined from the intercept of the extrapolated linear portion of the plot on the voltage axis. The V_{bi} is essential for understanding the electrostatic properties of the SBD junction. The slope of the plot is inversely proportional to the electron carrier concentration in this work. By analyzing the slope, the concentration of majority carriers (electrons in this work) can be quantified. In this regression analysis, the R-square values ranged from 99.93 % to 99.98 % regardless of different conditions, suggesting that the extracted V_{bi} and N_d values were highly reliable. The dependence of V_{bi} and N_d on the temperature ranges from 300 to 673 K is shown in Fig. 3(b), revealing that V_{bi} was inversely proportional to the temperate in the range of 300–673 K, which was consistent with theoretical expectations.

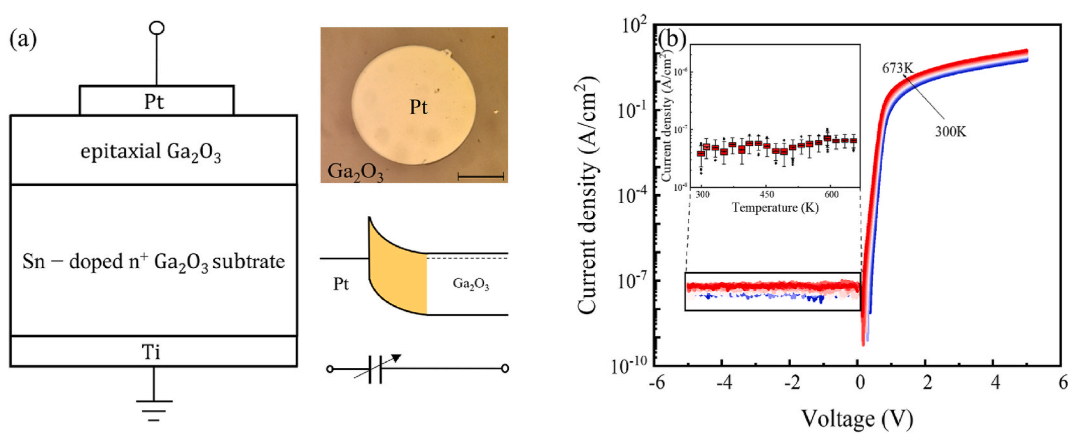

Fig. 1. (a) Schematic drawing of the cross section of the Pt/Ga_2O_3 SBD in which a circular electrode with a diameter of 270 μm is formed (scale bar 100 μm). (b) Semilog current-voltage (I–V) characteristics in the temperature range from 300 to 673 K. The inset shows the current density as a function of the measured temperatures. These data points were obtained in the range of 0 to −5 V.

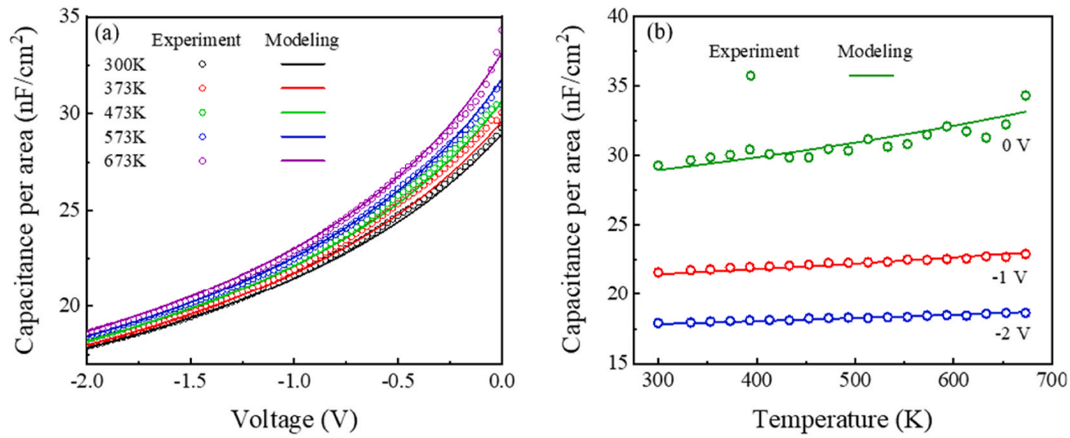

Fig. 2. Experimental and modeling results of the Pt/Ga_2O_3 SBD in the temperature range from 300 to 673 K at 2 MHz. (a) Capacitance-voltage (C–V) characteristics; data points of 300 K, 373 K, 473 K, 573 K, and 673 K are shown here for the sake of simplicity. (b) Capacitance as a function of temperatures at different reverse voltages.

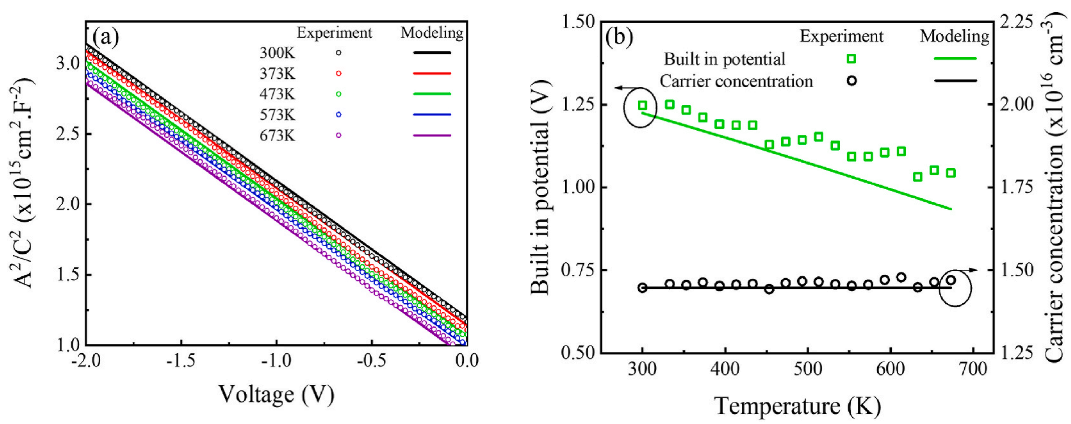

Fig. 3. Experimental and modeling results of the Pt/Ga_2O_3 SBD in the temperature range from 300 to 673 K at 2 MHz. (a) $(A/C)^2$-V capacitance-voltage characteristics 300 K, 373 K, 473 K, 573 K, and 673 K are shown here for the sake of simplicity. (b) Built-in potential and carrier concentration as a function of temperatures.

The slight discrepancies observed between the simulation and experimental results may have arisen from simplifications in the model or deviations in the experimental conditions. Nonetheless, the overall consistency between the two provides confidence in the modeling approach and offers valuable insights into device behavior under varying conditions. Fig. 3(b) also showed that the electron carrier concentration remained almost constant in the temperature range of 300–673 K, which was consistent with the results in Fig. 1(b).

TCAD simulations can provide detailed information about the energy band diagram, which helps to understand the electronic properties and performance of a device under various operating conditions. Fig. 4(a) exhibits a comparison of the energy band diagram of the Pt/Ga_2O_3 SBD and Pt/Si SBD at both 300 K and 673 K. The results showed that the depletion width of the Ga_2O_3 SBD decreased slightly at 673 K compared to that at 300 K, while the reduction was significant for the conventional Si SBD. With both the Si and Ga_2O_3-based SBDs, the charge carrier density at 300 K was dominated by the dopant density. However, at 673 K, the charge carrier density was primarily affected by the intrinsic carrier density; $ni_{Ga2O3} = 10^3 cm^{-3}$ while $ni_{Si} = 10^{16}\ cm^{-3}$ at 673 K. This indicated that the Si-based SBD lost its rectifying characteristics, whereas the Ga_2O_3-based SBD maintained its diode behavior effectively. The depletion width can be obtained from equation (2) [22].

$$C = \frac{\varepsilon\varepsilon_0 A}{W} \tag{2}$$

where C is the capacitance (F), A is the diode area cm^2, ε_0 is the permittivity of the free spaces $8.85 \times 10^{-14}\ F\ cm^{-1}$ and ε is the dielectric constant of Ga_2O_3. The experimental and modeling results of the depletion width were compared at the 0 V bias voltage in the temperature range of 300–673 K, as shown in Fig. 4(b). The slight reduction of the depletion width was satisfactorily captured in the TCAD modeling. For comparison, the charge carrier concentration of the Ga_2O_3 according to temperature was compared to concentrations of Si, GaAs, and SiC. This revealed that the Ga_2O_3-based SBD was able to sustain its device performance up to at least 673 K, whereas the conventional Si-based SBD degraded performance at 673 K.

4. Conclusion

This work showed that the Pt/Ga_2O_3 SBD maintained its diode performance up to at least 673 K, which was correlated with the TCAD modeling. The enhancement of the intrinsic carrier concentration was insignificant for the Ga_2O_3 SBD due to its wide bandgap properties. In addition, the C-V characteristics of the Ga_2O_3 SBD also correlated well with the TCAD modeling in the temperature range of 300–673 K. The capacitance value increased slightly with temperature due to the reduction of the depletion width, which also correlated well with the TCAD modeling.

CRediT authorship contribution statement

Thanh Huong Vo: Validation, Investigation. **Sunjae Kim:**

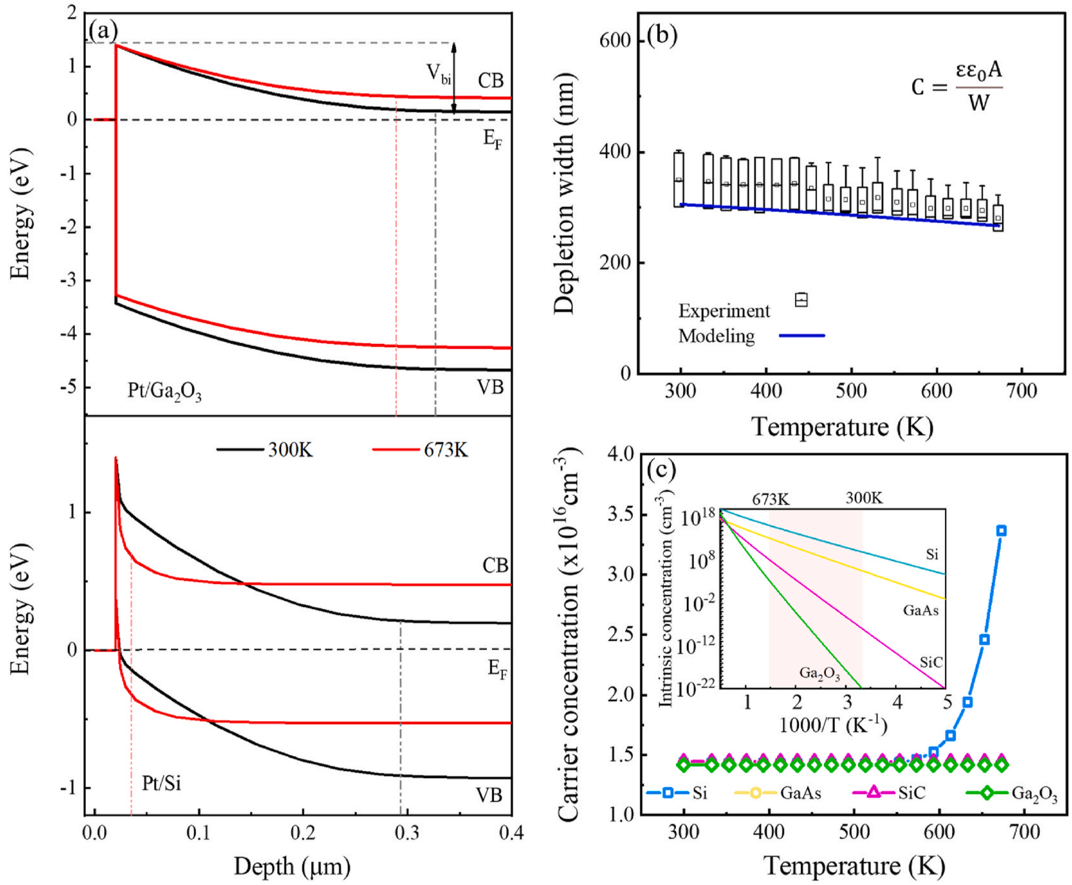

Fig. 4. (a) Energy band diagram of Pt/Ga_2O_3 SBD and Pt/Si SBD at both 300 K and 673 K, highlighting that the depletion width at 673 K is significantly reduced compared to that at 300 K. (b) Experimental and modeling results of the depletion width at 0 V bias voltage in the temperature range of 300–673 K. (d) Carrier concentration of different semiconductors (Si, GaAs, SiC, and Ga_2O_3) according to temperature. Inset: intrinsic carrier concentration of Ga_2O_3 compared to that of other materials according to temperature.

Validation, Investigation. **Heejoong Ryou:** Software, Methodology. **Dae-Woo Jeon:** Writing – original draft, Resources. **Jinyoung Hwang:** Writing – review & editing. **Wan Sik Hwang:** Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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