Research on the Negative Resistance Characteristics of Silicon-based Trench MOS Barrier Schottky Diodes

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Abstract. The negative resistance characteristics of Trench MOS Barrier Schottky (TMBS) diodes were studied by simulation and theoretical calculation. A reasonable simulation model was established according to the experimental results of Schottky Barrier Diodes (SBD), which were utilized to simulate the TMBS diodes. A theoretical calculation model of TMBS diodes under forward bias was constructed based on existing SBD theoretical analysis to systematically understand the simulation results. Both simulation and theoretical calculation demonstrate that the negative resistance characteristics of TMBS diodes under forward bias are caused by the accumulation of minority carriers at the epitaxial region and the accumulation of majority carriers at the epitaxial region and oxide layer.

Keywords: Negative differential resistance, semiconductor device simulation, trench MOS barrier Schottky diode.

1. Introduction

The structural component of Trench MOS Barrier Schottky (TMBS) diodes was proposed by Mehrotra and Baliga for the first time in 1995. Follow-up studies mainly focus on the further performance improvement of TMBS diodes by changing their parameters. Several studies explore the influences of material parameters on device performance. For example, Baliga and Mahalingam improved the breakdown voltage of the device by improving the doping distribution in the active region; however, this approach increased the reverse leakage current. Juang et al. improved the electric field distribution at the trench bottom by introducing a p–n junction, which increased the breakdown voltage successfully. Khemka et al. designed the 4H-SiC-based TMBS diodes and analyzed their performance. Other studies focus on the influences of structural parameters on device performance. For example, Li Weiyi et al. designed TMBS diodes with trapezoid trench structures. Zhai et al. analyzed TMBS diodes with fillet trench and trapezoid trench structures. Several studies emphasize the construction of a TMBS analysis model.

Although TMBS diodes have attained much progress, almost all studies focus on how to increase the reverse blocking voltage, decrease the reverse leakage current, and decrease the forward turn-on voltage. No research has dealt with the negative differential resistance, which is another important device performance index. TMBS diodes are developed based on Schottky Barrier Diodes (SBDs). Utilizing theoretical and experimental studies, Yamamoto and Miyanaga produced negative resistance under a moderate barrier height and high injection, which are caused by the accumulation of minority carriers at the epitaxial region. The present study investigates the negative resistance characteristics of TMBS diodes through simulation and theoretical calculation. A reasonable model was established according to SBD experimental results, which were applied to simulate the TMBS diodes. Section 2 introduces the SBD and TMBS diode parameters for simulation.
and calculation. Section 3 establishes the simulation model based on a comparison with the SBD experimental results and simulates the negative resistance characteristics of TMBS diodes. Section 4 presents a theoretical calculation model of the TMBS diodes under forward bias. Section 5 explains the causes of the negative resistance characteristics of TMBS diodes by a contrast analysis between the simulation and theoretical calculation results.

2. Basic Device Parameters
The SBD employed in this study has the same parameters with the experimental samples of Yamamoto and Miyanaga[17].

Under the same parameters with the SBD epitaxial region, MOS trenches were added to the left and right sides, and the substrate was widened to form the TMBS diodes. The cross-sections of the SBD and TMBS diodes employed in this study are shown in figure 1. The structure of the traditional SBD is shown in figure 1(a), whereas the structure of TMBS diodes is shown in figure 1(b). The x-axis (X) is the device width, whereas the y-axis (Y) is the device thickness.

The concentration of the donor impurity phosphorous at the epitaxial region is $5 \times 10^{15} \text{cm}^{-3}$. The thickness of the epitaxial layer is $h = 1.5 \mu \text{m}$. The Schottky junction area at the top of the epitaxial layer is $S = a \times a = 5 \times 5 \mu \text{m}^2$. The thickness and phosphorous concentration of the substrate are $h_{\text{sub}} = 250 \mu \text{m}$ and $5 \times 10^{19} \text{cm}^{-3}$, respectively. The trench width for the TMBS diodes is $t = 1 \mu \text{m}$, and the thickness of the oxide layer is $t_{\text{ox}} = 0.2 \mu \text{m}$. These geometric and technological parameters were applied in the follow-up simulation and theoretical calculations.

![Figure 1](image.png)

**Figure 1.** Cross-sections of devices utilized in the experiment, simulation, and theoretical calculation. (a) SBD structure; (b) TMBS structure.

3. Construction of the Simulation Model and TMBS Simulation
The 2D numerical simulation of the silicon-based SBD and TMBS diode was conducted in this study by the device generation tool MYDRAW and device simulation tool DESSIS in the technological and device simulation platform ISE-TCAD[18]. The SBD in figure 1(a) was simulated to determine the simulation model. Simulation results were compared with the experimental results of Yamamoto and Miyanaga[17]. The thermodynamics model was determined by adjusting the simulation model and parameters continuously.

The model comprises three basic equations of the semiconductor that control the carrier transport, current density equation of the electron and hole, and equation of heat conduction, respectively. The three basic equations are the Poisson’s equation, the electron continuity equation, and hole continuity equation. The following is the Poisson’s equation:

$$\nabla^2 \psi = -\frac{q}{\varepsilon} \left[ p - n + N_D^+ - N_A^- \right]$$  (1)
where $\varepsilon$ is the permittivity, $q$ is the elementary charge, $p$ and $n$ are the hole and electron concentrations, and $N_D^+$ and $N_A^-$ are the ionized donor and acceptor concentrations, respectively. The electron and hole continuity equations are as follows:

$$\nabla \cdot J_e = qR + q \frac{\partial n}{\partial t}$$  \hspace{1cm} (2)

$$-\nabla \cdot J_h = qR + q \frac{\partial p}{\partial t}$$  \hspace{1cm} (3)

where $R$ is the electron-hole net recombination rate, and $J_e$ and $J_h$ are the current densities of the electrons and holes. The thermodynamics model considers the temperature gradient contributions to the current density based on the drift–diffusion model. The modified equations of the electron and hole current densities are as follows:

$$J_e = -n q \mu_e (\nabla \phi_e + P_e \nabla k)$$  \hspace{1cm} (4)

$$J_h = -p q \mu_h (\nabla \phi_h + P_h \nabla k)$$  \hspace{1cm} (5)

where $\mu_e$ and $\mu_h$ are the electron and hole mobility values; $\phi_e$ and $\phi_h$ are quasi-Fermi potentials of the electrons and holes; and $P_e$ and $P_h$ are the absolute thermoelectric powers of the electrons and holes. The following heat conduction equation must be solved first to calculate the internal temperature distribution of the device based on the self-heating effect:

$$c \frac{\partial T}{\partial t} - \nabla \cdot (\kappa \nabla T) = -\nabla \cdot [(P_e T + \phi_e) J_e + (P_h T + \phi_h) J_h]$$

$$- \left( E_e + \frac{3}{2} k_B T \right) \nabla \cdot J_e - \left( E_h + \frac{3}{2} k_B T \right) \nabla \cdot J_h + qR(E_e - E_h + 3k_B T)$$  \hspace{1cm} (6)

where $c$ is the heat capacity of the lattice, $\kappa$ is the thermal conductivity, $k_B$ is the Boltzmann constant, and $E_e$ and $E_h$ are the minimum conduction and maximum valence band energies, respectively. These six equations form the thermodynamics model for simulation analysis. The calculation of the model parameters is introduced as follows. Considering the influences of the doping concentration and velocity saturation of the high electrical field on carrier mobility, $\mu_e$ and $\mu_h$ were calculated utilizing the default Masetti and Canali models. The calculation of $R$ considers the doping and temperature-dependent SRH indirect recombination model. The narrowing of the energy gap caused by doping and the resulting changes in the energy band and carrier concentration were calculated by the OldSlotboom model.18

The boundary and initial conditions were set as follows. The anode on the upper surface of the epitaxial layer of the diodes in figure 1 is the Schottky contact, whereas the cathode on the lower surface is the ideal Ohmic contact. The initial voltages are 0, and other boundaries are the Neumann electrical boundary conditions. The lower surface is connected to the 293K ideal heat sink, but the other boundaries have no thermal contact and are processed as the Neumann thermal boundary conditions. A load resistance is connected in series between the anode and positive electrode of the DC power supply ($R = 1$ kΩ).

All of the parameters of the aforementioned thermodynamics model utilized the default values of the ISE–TCAD system, except for the barrier height of the Schottky electrode ($\phi_B$), which was employed as the simulation variable.

The simulated IV characteristic curves of the SBD under four different barrier heights are shown in figure 2. Simulation results show the following conditions when high current is injected into the region: the SBD represents characteristics of the traditional rectifier diodes if the barrier height of the Schottky electrode is high; the SBD represents the characteristics of parasitic resistance if the barrier height is small; and the SBD represents the negative resistance characteristics if the barrier height is moderate. The simulation results basically conform to the experimental results in figure 4 of Ref. 17, which indicates that the established simulation model is feasible.

The TMBS diodes with different Schottky barrier heights under forward bias were simulated by the same SBD thermodynamics model. The results are shown in figure 3. Similar to the SBD experimental
and simulation results, the simulated IV curves of the TMBS diodes represent the rectifier diodes, parasitic resistance, and negative resistance with the change in barrier height. This study focused on the negative resistance characteristics of devices. A comparison of the simulation results of the IV characteristics between the SBDs and TMBS diodes under forward bias and the same barrier height $\phi_B = 0.68$V is shown in figure 4. The results show that although both the SBDs and TMBS diodes have negative resistance characteristics in the high current region, the threshold voltage of the TMBS diodes when negative resistance starts is higher than that of the SBDs. This condition is related to the effect of the MOS trench. The reasons for this phenomenon will be further analyzed in the following section.

Figure 2. Simulated IV curves of the SBD under different barrier heights and forward bias.

Figure 3. Simulated IV curves of the TMBS diodes under different barrier heights and forward bias.

Figure 4. Simulated IV curves of the SBD and TMBS diodes under $\phi_B = 0.68$V and forward bias.
4. Theoretical Calculation of TMBS

The mathematical analysis model of the TMBS diodes was established by combining the equivalent circuit of Schottky diodes and the fundamental principle of the MOS capacitor. This model can comprehend the negative resistance characteristics of the TMBS diodes in the high-current region under forward bias. Yamamoto and Miyanaga conducted a theoretical analysis and mathematical process of SBDs based on an equivalent circuit of Schottky diodes. The mathematical analysis model in the current study is an improved model that considers the electron accumulation effect of the MOS capacitor under forward bias.

The equivalent circuit model of SBDs is shown in figure 5. One SBD can be viewed as a series connection of one Schottky junction \( D \) and one parasitic resistance \( R_s \). The parasitic resistance mainly comes from the low-conductivity epitaxial region. \( V \) is the bias voltage, \( I \) is total current, \( V_D \) is the voltage drop on \( D \), and \( V_R \) is voltage drop on \( R_s \) in figure 5. The current–voltage relationship of an ideal Schottky junction is as follows:

\[
I = I_s \cdot e^{\frac{qV_D}{kT}}
\]

where \( I_s \) is the SBD saturation current.

\[
I_s = A \cdot T^2 \cdot S \cdot e^{\frac{q\phi_B}{kT}}
\]

where \( A \) is the effective Richardson constant, \( T \) is the environment temperature of the device, \( S \) is the Schottky junction area in figure 1, and \( \phi_B \) is the Schottky barrier height. The said figure shows that the relationship between the bias voltage (V) and current (I) of SBD is as follows:

\[
V = V_D + V_R = \frac{kT}{q} \cdot \ln \left( \frac{I}{I_s} \right) + R_s \cdot I
\]

\( R_s \) can be calculated approximately according to the average concentrations of the electrons and holes at the epitaxial region. Thus,

\[
R_s = \frac{1}{q\mu_n \bar{n} + q\mu_p \bar{p}} \cdot \frac{h}{S}
\]

where \( \mu_n \) and \( \mu_p \) are the mobility values of the electrons and holes at the epitaxial region. Given Scharfette and Gummel’s method, the mobility was calculated as the function of the average electrical field and doping concentration of the epitaxial region. \( \bar{n} \) and \( \bar{p} \) are the average concentrations of the electrons and holes in the epitaxial region. \( h \) is the thickness of the epitaxial region in figure 1. The \( \bar{n} \) and \( \bar{p} \) calculations are introduced in the following section. Yamamoto and Miyanaga stated that the average hole concentration of the minority carrier can be calculated as follows:

\[
\bar{p} = \frac{q \cdot \tau_p}{q \cdot S \cdot h} = \frac{l_p \cdot \tau_p}{q \cdot S \cdot h} = \frac{\gamma \cdot l_p \cdot \tau_p}{q \cdot S \cdot h}
\]
where $Q_p$ is the total hole change in the epitaxial region, $I_p$ is hole current of the epitaxial region, $\tau_F$ is the hole lifetime, and $\gamma$ is the injection efficiency of the hole of the minority carrier. Scharfette and Gummel\cite{16} stated that $\gamma$ is as follows:

$$
\gamma = \frac{I_p}{I_n} \approx \frac{I_p}{I_n} \left( \frac{n_i}{N_D} \right)^2 \frac{I}{I_s}
$$

where $I_n$ is the electron current of the epitaxial region, $n_i$ is the intrinsic carrier concentration of silicon, and $N_D$ is the donor impurity concentration in the epitaxial region.

The average electron concentration in the epitaxial layer for SBD is approximately equal to the donor impurity concentration:

$$
\bar{n} \approx N_D
$$

One MOS plate capacitor is added to two sides of the SBD epitaxial region of the SBD for the TMBS diodes (figure 1b). Given the forward voltage, each MOS capacitor is at the accumulation state of $n$ type Si-based semiconductor. The capacitance is as follows:

$$
C = \frac{\varepsilon A_G}{t_{ox}}
$$

where $\varepsilon = K_o \varepsilon_o$ is the dielectric constant of SiO$_2$; $A_G = \pi \sqrt{S}$ is the area of the MOS plate capacitor; and $t_{ox}$ is the thickness of SiO$_2$. The average electron concentration can then be calculated as follows:

$$
\bar{n} = \frac{2Q_n}{q \cdot S \cdot h} \approx \frac{2e \cdot V}{q \cdot S \cdot h} = \frac{2e}{q \cdot \sqrt{S} \cdot t_{ox}} \cdot V
$$

Combining Eqs. (7) to (15) derives the implicit functional model between the injection current ($I$) and forward voltage ($V$) of the SBD and TMBS diodes. The model parameters are as follows:

Unit charge $q = 1.60218 \times 10^{-19}$ C; Bolzmann constant $k = 1.38066 \times 10^{-23}$ J/K; environment temperature $T = 293$ K; dielectric constant of vacuum $\varepsilon_0 = 8.85418 \times 10^{-12}$ F/m; relative dielectric constant of SiO$_2$ $K_o = 3.9$; intrinsic carrier concentration of silicon $n_i = 1.6 \times 10^{10}$ cm$^{-3}$; hole lifetime of the minority carrier $\tau_F = 7.0 \times 10^{-9}$ s; effective Richardson constant $A = 110$ A/(cm$^2$ K$^2$).

The calculated IV results of the SBD under a forward bias by utilizing the aforementioned model and parameters are shown in figure 6. The results of the present study conform to the experimental results in figure 4 of Ref. 17. Therefore, the proposed calculation model is reasonable.

The theoretical calculation results of the TMBS diodes under different barrier heights are shown in figure 7. The TMBS diode in the high current regions is a traditional rectifier diode when $\phi_B = 0.85$ V but changes to parasitic resistance when $\phi_B = 0.48$ V and negative resistance when $\phi_B = 0.72$ V – 0.68 V. The theoretical calculation results of the TMBS diodes conform to the simulation results in figure 3.

![Figure 6. Theoretically calculated IV curves of the SBD under different barrier heights and forward bias.](image_url)
Figure 7. Theoretically calculated IV curves of the TMBS diodes under different barrier heights and forward bias.

Figure 8. Theoretically calculated IV curves of the SBD and TMBS diodes when $\phi_B = 0.68$ V under forward bias.

Figure 9. Relationship between the total average carrier concentration of the epitaxial layer of the SBD and TMBS and the injection current when $\phi_B = 0.68$ V.
Figure 10. Relationship between the parasitic resistance of the epitaxial layer of the SBD and TMBS and injection current when $\phi_B = 0.68 \, V$.

The IV calculated results of the SBD and TMBS diodes when $\phi_B = 0.68 \, V$ are shown in figure 8 to compare the theoretical calculation results of the negative resistance characteristics between the SBD and TMBS diodes. The theoretical calculation results are consistent with the simulation results. The threshold voltage of the TMBS diodes when the negative resistance starts is higher than that of the SBDs.

5. Cause Analysis and Discussion of the Negative Resistance Characteristics of the TMBS Diodes

Unlike the SBDs, TMBS diodes have one additional MOS plate capacitor at each side. Although electron accumulation occurs in the semiconductor and SiO$_2$ boundaries under the forward voltage, the average electron concentration in the epitaxial layer of TMBS diodes becomes lower than that in SBDs. The theoretical calculation results of the total average electron and hole concentrations in the epitaxial layer of the SBD and TMBS diodes are shown in figure 9. The existence of MOS capacitors changes the average electron concentration as well as the distribution of the total average carrier concentration in the epitaxial layer. Given that the total average carrier concentration of the TMBS diodes is smaller than that of SBD, the parasitic resistance of TMBS is higher than that of SBD (figure 10). Therefore, the threshold voltage of the TMBS diodes when the negative resistance starts is higher than that of SBD due to the high parasitic resistance.

6. Conclusion

The experimental research on SBDs reveals that SBDs possess the traditional rectifier diode characteristics in the high current region under large barrier heights. Results show the negative resistance characteristics under moderate barrier heights and parasitic resistance characteristics under small barrier heights. The SBD simulation results based on the thermodynamics model basically conform to the experimental results. Thus, TMBS diodes were simulated to determine similar characteristics. Given the same barrier height, the threshold voltage of the TMBS diodes when the negative resistance starts is also higher than that of SBDs.

A theoretical calculation model for TMBS diodes is constructed and validated by the SBDs to explain systematically the different simulation characteristics of TMBS diodes. This model is then used for the theoretical calculation of TMBS diodes.

The theoretical calculations and analyses show that the negative resistance characteristics of the TMBS diodes are different from those of SBDs. These characteristics are the collaborative results of the hole injection and accumulation of the minority carrier at the epitaxial region as well as the overall decrease in electrons of the majority carrier. The overall decrease in electrons of the majority carrier is caused by the MOS capacitor at the trenches of the TMBS diodes.
The research results can provide a reliable simulation model to study the characteristics of TMBS diodes under a forward bias and lay a suitable theoretical foundation to improve the characteristics of TMBS diodes.

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