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The impact of trapping centers on AlGaN/GaN resonant tunneling diode

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Abstract: We report on a simulation for aluminum gallium nitride (AlGaN)/gallium nitride (GaN) resonant tunneling diode (RTD) at room temperature by introducing deep-level trapping centers into the polarized AlGaN/GaN/AlGaN quantum well. Theoretical analysis reveals that the degradations of NDR characteristics in GaN based RTDs are actually caused by the combined actions of the activation energy and the trap density. Furthermore, the trapping centers with high activation energy play a dominant role in the degradation of negative differential resistance (NDR) characteristics.

Keywords: GaN, resonant tunneling diode, trapping center, quantum well
Classification: Microwave and millimeter wave devices, circuits, and systems

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1 Introduction

Nitride based RTD is one of the promising candidates in terahertz regime because nitrides exhibit excellent properties such as high peak electron velocity, high saturation electron velocity, and thermal stability. AlGaN/GaN double-barrier RTDs grown on different substrates have been reported, from which it was observed an evident degradation in NDR characteristics with the rising scan number of bias voltage sweep [1]. It has been proved that the degradation is caused by the charge trapping effects since these trapped charges alter the dominant transport mechanism and cause an instability of NDR characteristic. So far, available terahertz

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signals of GaN RTDs have not been obtained because the terahertz oscillation is hardly generated in the case of instable NDR. In this paper, we employ a SILVACO simulator to analysis the influence of trapping center on the NDR characteristic to theoretically reveal the mechanism of the degradation in NDR characteristic.

2 Simulation parameters

The RTD structure for simulation consists of an n-type AlGaN/GaN/AlGaN active region sandwiched between two 100 nm thick GaN cathode and anode ohmic contact regions, and two 3 nm thick GaN spacers inserted between the contact region and the active region, respectively, to prevent the dopant diffusion. The ohmic contact region is heavily doped at $5\times10^{18}\,cm^{-3}$. The RTD active region is composed of 1.5 nm$Al_{0.2}Ga_{0.8}N$, 1.5 nm GaN, and 1.5 nm $Al_{0.2}Ga_{0.8}N$. The spatial mesh size is set as 0.1 Å in order to increase the accuracy of the calculation. The diode section area is set to be 25 μm^2. For the polarized AlGaN/GaN/AlGaN quantum well, we introduce interface charges into the heterostructure to exhibit the effect of the 2DEG, which originates from the spontaneous and piezoelectric polarization difference at the interface.

According to some deep level transient spectroscopy (DLTS) measurements, most of the traps are the interface electron traps located on the AlGaN side of AlGaN/GaN heterointerface. In this work, we take several of the dominant trapping centers into account to characterize the charge trapping effects [2, 3]. The location of the first trapping center is at the activation energy of 0.208 eV (E_{a1}), where the trap density and capture cross-section were determined to be $4.3\times10^{16}\,cm^{-3}$ and $1.1\times10^{-18}\,cm^2$. The location of the second one is at the activation energy of 0.493 eV (E_{a2}), where the trap density and capture cross-section were determined to be $2.6\times10^{18}\,cm^{-3}$ and $2.4\times10^{-14}\,cm^2$. The location of the third one is at the activation energy of 1.02 eV (E_{a3}), where the trap density and capture cross-section were determined to be $2\times10^{14}\,cm^{-3}$ and $2.0\times10^{-12}\,cm^2$.

3 Theoretical model

In this paper we employ the Silvaco's ATLAS simulation platform to solve the self-consistent solution of Poisson-Schrödinger equations including trapped Charge. Meanwhile, some basic equations are solved, such as the carrier continuity equation, carrier drift-diffusion model, etc. The Poisson's equations are expressed as follows:

$$div(\varepsilon\nabla\psi) = q\left(n - p - N_D^+ + N_A^-\right) - Q_T, \quad (1)$$

where ψ is the intrinsic potential, n and p are free electron and hole concentration, $N_D{}^+$ and $N_A{}^-$ are the ionized donor and acceptor impurity concentrations, and $Q_T = q\times Density\times F_{tA}$ is the charge due to traps and defects, where Density is the trap density of the trapping centers. The probability of ionization traps F_{tA} is expressed as [4]:

$$F_{tA} = \frac{n\sigma_n v_n + e_{pA}}{n\sigma_n v_n + p\sigma_p v_p + e_{nA} + e_{pA}}, \quad (2)$$

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where σ_n and σ_p are the carrier capture cross sections for electrons and holes respectively, v_n and v_p are the thermal velocities for electrons and holes. For acceptor like traps, the electron and the hole emission rates, e_{nA} and e_{pA}, are defined by

$$e_{nA} = \sigma_n n_i v_n \exp \frac{E_t - E_i}{kT} \tag{3}$$

and

$$e_{pA} = \sigma_p n_i v_p \exp \frac{E_i - E_t}{kT}, \tag{4}$$

where n_i is the intrinsic carrier concentration, E_t is the energy of the acceptor trap level, and E_i is the energy of the intrinsic level.

4 Results and discussions

At first, I-V characteristic, conduction band profile and other properties of the AlGaN/GaN RTD are investigated via the first forward- and backward-scan of bias voltage across the diode. Showing in Fig. 1 (a) is the static-state conduction band profile for the quantum well structure of 1.5/1.5/1.5 nm without external bias voltage. Where, the electric field distributions as well as the electron concentrations are given in Fig. 1 (b). The evident band bending of conduction band is due to the existence of 2DEG density and internal electric field. The electric field changes the distributions of electrons in the structure, therefore, electrons in the active region are accumulated in the spacer region near the anode side. Showing in

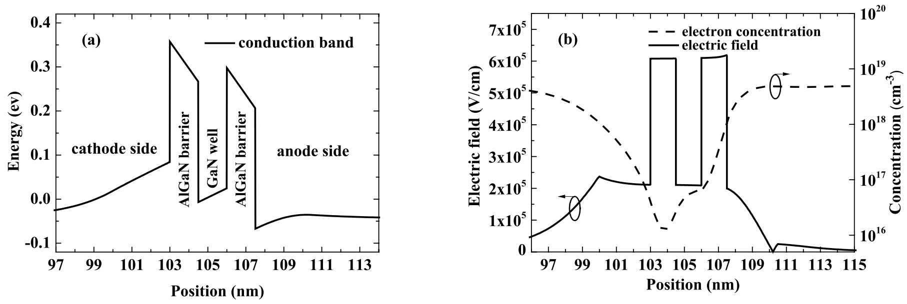

Fig. 1. (a) The conduction band profile, and (b) the electron concentrations and the electric field distributions in the AlGaN/GaN/AlGaN quantum well without external bias voltage.

Fig. 2 (a) is the simulated I-V characteristic of the AlGaN/GaN RTD, exhibiting a peak current I_P of 0.241 A and a peak-to-valley current ratio (PVCR) of 1.77. There is a large difference between the calculated result and experimental data of I_P (0.02 A) [1], which is attributed to the differences in the magnitude of doping (5×10^{18} and $6 \times 10^{16}\,\mathrm{cm}^{-3}$). It is known that the tunneling current is proportional to the electron concentration in the cathode region. Besides, the large parasitic-induced resistances in the realistic devices also have a significant impact on the tunneling current. Meanwhile, the I-V characteristic demonstrates a smaller threshold voltage V_P of around 0.348 V compared with that of 1.0 V in the

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realistic devices [1]. It is known that V_P is composed of two components including the voltage that pulls the first discrete energy level down to the conduction band edge and the voltage drop on the series resistance. We calculate the dependence of transmission coefficient on energy without external bias voltage in order to obtain a static-state distribution of discrete energy level, with the result given in Fig. 2 (b). The transmission peak at 0.163 eV corresponds to the first discrete energy level in the GaN quantum well, which is lower than that of 0.32 eV in the realistic devices [1]. The difference in the discrete energy level is a main factor of the different V_P. Besides, another part of V_P caused by the voltage drop across the parasitic resistance and the charge accumulation on the cathode and anode is taken into account in the simulation, and it is much smaller than that in realistic devices. It is also found from Fig. 2 (a) that the current hysteresis effect in the I-V characteristic of AlGaN/GaN RTD is consistent with that of the realistic AlGaN/GaN RTD [1].

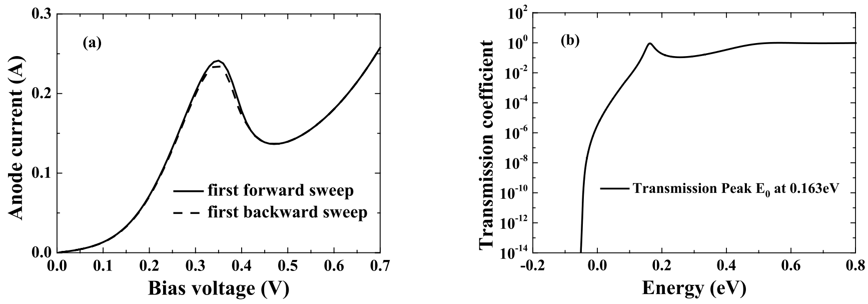

Fig. 2. (a) Simulated I-V characteristics of AlGaN/GaN RTD under the first forward- and backward-scans, and (b) static-state distribution of the transmission coefficient in the AlGaN/GaN/AlGaN quantum well.

Fig. 3 shows the simulated I-V characteristics of AlGaN/GaN RTD under the 1st, 50th, and 100th forward-scans of bias voltage by introducing the trapping centers at E_{a1}, E_{a2} and E_{a3} into the AlGaN/GaN/AlGaN quantum well. Results demonstrate that the NDR characteristics become irreproducible and the degradation is about 38% under 100th scans, in accordance with the tendency of the state-of-the-art AlGaN/GaN RTDs [1]. This degradation is mainly caused by the deep-level trapping centers with the location at the activation energy of 1.03 eV (E_{a3}). It is mainly due to that the probability of ionization F_{tA} is exponentially proportional to the activation energy. The ionized trap density increase with the rising F_{tA}, therefore do harm to the NDR characteristics with rising scan number of bias voltage sweep.

In order to quantitatively reveal the relationships among the reproducible NDR characteristics, trap density, probability of ionization F_{tA} and ionized trap density, we theoretically calculate Eq. (1-4) with an external bias voltage of 0.348 V (V_P). We firstly solve Eq. (3-4) by introducing the trap energy levels of 0.208 eV (E_{a1}), 0.493 eV (E_{a2}) and 1.02 eV (E_{a3}) in order to obtain the electron and the hole emission rates. Then we solve the Eq. (2) by introducing the electron and the hole emission rates, the carrier capture cross sections and the thermal velocities for electrons and holes in

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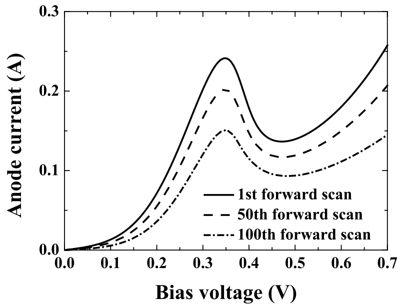

Fig. 3. I-V characteristics of AlGaN/GaN RTD under 1st, 50th, and 100th forward-scans of bias voltage.

order to obtain F_{tA1}, F_{tA2} and F_{tA3} corresponding to the trapping centers at E_{a1}, E_{a2} and E_{a3}, respectively, as shown in Table I. The ionized trap density is lower compared with the trap density which is due to the low probability of ionization F_{tA} in the active region. The total charge Q_T that is calculated by $Q_T = q \times (\text{Density1} \times F_{tA1} + \text{Density2} \times F_{tA2} + \text{Density3} \times F_{tA3})$ is subtracted from the right hand side of Poisson's equation. Then we solve the self-consistent solution of Poisson-Schrödinger equations, etc, in order to obtain the simulation result. As can be seen from Table I, the ionized trap density corresponding to the trapping center at E_{a3} is $1.2 \times 10^{13}\,\text{cm}^{-3}$ which will do harm to the NDR characteristics after numerous forward- and backward-scans.

Table I. Parameters of trapping centers.

Activation energy (eV)	0.208 (E_{a1})	0.493 (E_{a2})	1.02 (E_{a3})	1.8
Trap density (cm^{-3})	4.3×10^{16}	2.6×10^{18}	2×10^{14}	1×10^{15}
Probability of ionization	6.27×10^{-11}	1.154×10^{-7}	6.1×10^{-2}	7.63×10^{-1}
Ionized trap density (cm^{-3})	2.7×10^{6}	3×10^{11}	1.2×10^{13}	7.63×10^{14}

Note that we assume another trapping center with the activation energy at 1.8 eV in Table I, referring to the reported DLTS measurements in the AlGaN/GaN heterostructures [5]. Results show that the internal potential profile becomes irregular and the NDR characteristics are significantly affected by the trap centers at deeper activation energy. Theoretical analysis reveals the physical mechanisms that the degradations of NDR characteristics in GaN based RTDs are actually caused by the combined actions of the activation energy and the trap density. Furthermore, the trapping centers with high activation energy play a dominant role in the degradation of NDR characteristics. Therefore, it is imperative to take measures for more reliable NDR characteristic in RTD, such as fabricating GaN RTDs on homogeneous substrates, reducing Al composition of the barrier layer.

5 Conclusion

In conclusion, we have proposed a simulation for $Al_{0.2}Ga_{0.8}N$/GaN RTD by introducing deep-level trapping centers into the polarization induced AlGaN/GaN/AlGaN quantum well to reveal the mechanism of NDR degradation in RTD. Theoretical analysis reveals the physical mechanism that the degradations of NDR characteristics in AlGaN/GaN RTDs are

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actually caused by the combined actions of the activation energy and the trap density. Furthermore, the trapping centers with high activation energy play a dominant role in the degradation of NDR characteristics. Thus, it is promising that reducing Al composition of AlGaN/GaN RTD and fabricating GaN based RTDs on homogeneous substrates can lower the activation energy level of trapping centers, suppress the probability of ionization of the trapping centers so as to minimize the degradation of GaN-based RTDs in realistic applications.

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