Quantitative analysis of the trapping effect on terahertz AlGaN/GaN resonant tunneling diode

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We report on a simulation for terahertz aluminum gallium nitride (AlGaN)/gallium nitride (GaN) resonant tunneling diode (RTD) at room temperature by introducing deep-level defects into the polarized AlGaN/GaN/AlGaN quantum well. Results show that an evident degradation in negative-differential-resistance characteristic of RTD occurs when the defect density is higher than $\sim 10^6$ cm$^{-2}$, which is consistent with the measurements of the state-of-the-art GaN RTDs. At around 300 GHz, the simulation for a RTD oscillator also demonstrates evident decreases of rf power and efficiency because of the electron trapping effect. © 2011 American Institute of Physics. [doi:10.1063/1.3650253]

Nitride based resonant tunneling diode (RTD) is one of the promising candidates in terahertz regime because nitrides exhibit excellent properties such as high peak electron velocity, saturation electron velocity, and thermal stability. Alumnum nitride (AlN)/gallium nitride (GaN) and aluminum gallium nitride (AlGaN)/GaN double-barrier RTDs grown on different substrates have been fabricated in recent years.1–5 AlN/GaN RTD was expected to have higher peak-to-valley current ratio (PVCV), but the significant lattice-mismatch at AlN/GaN heterointerface raises the surface roughness and dislocations, and the large band gap of AlN reduces the tunneling probability; therefore, the diode demonstrates a low current density and a high tunneling resistance. AlGaN/GaN RTD with lower Al composition in AlGaN barrier layer was proposed to reduce the lattice-mismatch, suppress the dislocation density, and weaken the piezoelectric field at the heterointerface.1 Meanwhile, tremendous efforts have been made to reduce the defect density in GaN heterostructures, e.g., GaN epitaxial layers were grown on homogeneous or nonpolar-plane heterogeneous (silicon carbide and sapphire) substrates.1,4,7 But the performance of GaN RTDs is yet behind the expectation comparing with traditional III-V compound semiconductor RTDs.8,9 Particularly, the electrical measurements of GaN RTDs demonstrate that the PVCV of current-voltage (I-V) curve evidently degrades with a rising scan number of the bias sweep.1–5 The phenomenon is attributed to the charge trapping effect at the interface and the inner of heterostructure since the trapped charges lower the effective barrier height, alter the dominant transport mechanism, and finally, cause an instability of negative-differential-resistance (NDR) characteristic.3,4 So far, available terahertz 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 investigate the output performance of AlGaN/GaN double-barrier RTD at room temperature. The deep-level defects at AlGaN/GaN heterointerface are quantitatively analyzed to reveal the charge trapping effect on the steady state and instantaneous characteristics of RTD.

The RTD structure for simulation consists of an n-type AlGaN/GaN/AlGaN active region sandwiched between two 100-nm thick n$^+$-GaN ohmic contact regions, and two 5-nm thick GaN spacers inserted between the contact region and the active region, respectively, to prevent the dopant diffusion. The active region and the spacer are unintentionally doped at $1 \times 10^{16}$ cm$^{-3}$, and the ohmic contact region is heavily doped at $1 \times 10^{18}$ cm$^{-3}$. The specific contact resistivity of the ohmic contact region is set as low as $1 \times 10^{-6}$ $\Omega$ cm$^2$ in order to enhance the performance of active region. The AlGaN barrier layer with an Al composition of 30% is suggested to increase the output efficiency. The thickness of AlGaN barrier and GaN well ranges from 1 to 3 nm, respectively, where we put an emphasis on the AlGaN/GaN/AlGaN structure of 2/2/2 nm. The diode section area is set to be 28 $\mu$m$^2$. For the polarized AlGaN/GaN/AlGaN quantum well, we introduce interface charges into the heterostructure, where the charge density as a function of Al composition and thickness is quantitatively calculated.10,11 Concerning to the charge trapping effect in AlGaN/GaN heterostructure, numerous deep-level transient spectroscopy measurements have demonstrated that most of the dislocation induced traps seem to be the interface electron traps located on the AlGaN side of AlGaN/GaN heterointerface, where the distribution and the magnitude of traps closely depend on the Al composition of barrier layer, the configuration of quantum well, and the substrate the epitaxial grown on. In this work, we take several of the dominant traps into account, such as the activation energy ($E_a$) of 0.93 eV with a capture cross-section of $1.2 \times 10^{-13}$ cm$^2$ which is regarded to be strongly dependent on the Al composition of the AlGaN barrier,12 $E_a$ of 0.33 eV with a capture cross-section of $8.719 \times 10^{-19}$ cm$^2$ which is related to the substrate,13 and $E_a$ of 1.0 eV with a capture cross-section of $2.0 \times 10^{-12}$ cm$^2$ which is believed to be associated with threading dislocations.14

At first, we introduce a variable density of aforementioned deep-level defects into the AlGaN/GaN/AlGaN (2/2/2 nm)
quantum well to simulate $I-V$ characteristics of RTD under the forward- and backward-scans of bias sweep. Fig. 1(a) shows the simulated $I-V$ characteristics under the first forward-scan of bias voltage, and (b) shows the peak current $I_p$ and the valley current $I_v$ as a function of forward-scan number, both at the defect densities of $5 \times 10^3$–$5 \times 10^{11}$ cm$^{-2}$. It is observed that a serious degradation of $I-V$ characteristics occurs when the defect density is higher than $5 \times 10^9$ cm$^{-2}$ and even the NDR totally disappears when the defect density approaches $10^{11}$ cm$^{-2}$ under the first forward-scan (see Fig. 1(a)), which means the quantum well is not capable of generating a stable NDR characteristic at a high density of defects. With a rising scan number of the bias sweep, the degradation becomes more evident, which is consistent with previous measurements of AlGaN/GaN RTDs, and supports the proposal that the degradation is actually attributed to the action of unreleased charges in trapping center.\textsuperscript{3,4} The simulation also shows that the reproducible NDR characteristic is assured when the defect density decreases to below $10^{10}$ cm$^{-2}$ (see Fig. 1(b)), which further implies that material improvement is imperative for more reliable NDR characteristic in RTD.

Second, we investigate the performance of AlGaN/GaN RTD with a quantum well of 2/2/2 nm and a defect density of $5 \times 10^8$ cm$^{-2}$ by using steady state and instantaneous simulations. Fig. 2 shows the simulated $I-V$ characteristics under the 1st, 15th, and 20th forward- and backward-scans of bias voltage, respectively. The current hysteresis appearing on $I-V$ characteristics and the NDR degradation with increasing scan number is closely consistent with the measurements on real AlGaN/GaN RTDs,\textsuperscript{15} which implies that it hardly sustains a stable output performance at terahertz frequency. For instantaneous simulation, we first build an equivalent circuit model of RTD that includes an analytical model of NDR characteristic and a parasitic large signal capacitance ($C_s = 8 \times 10^{-14}$ F) and a parasitic resistance ($R_s = 7$ Ω) which are extracted from the steady state simulation, then mount the model to an external RLC resonant circuit ($L = 3.52$ pH, $C = 2.25 \times 10^{-14}$ F, $R_p = 15$ Ω) to form a NDR oscillator working at terahertz frequency. At a bias voltage of 1.33 V, the stable oscillation is created and the output current through the external parallel resistance $R_p$ is extracted. Under the 1st, 20th, and 50th scans, respectively, the model of degraded NDR characteristic certainly causes an evident degradation in current waveforms, as is observed in Fig. 3, in which the frequency decreases from 323 to 299 GHz, the rf power on $R_p$ decreases from 21 to 7.5 mW, and the efficiency decreases from 10.3% to 3.9%, respectively. It is also found that the calculated rf power of GaN RTD is at least two orders of magnitude larger than traditional III-V compound semiconductor RTDs, which will be a distinguished performance for application in terahertz regime if the NDR degradation is eliminated by lowering the defect density.

Third, we investigate the influence of AlGaN/GaN/AlGaN quantum well structure on the NDR characteristics of RTD, where the defect density is still set as $5 \times 10^8$ cm$^{-2}$. Fig. 4(a) shows the variation of NDR characteristic with the
In summary, we propose a simulation for terahertz AlGaN/GaN RTD by introducing quantitative deep-level defects and polarized charges into AlGaN/GaN AlGaN quantum well to reveal the mechanism of NDR degradation in RTD. Results demonstrate that the defect density of below $10^6$ cm$^{-2}$ is imperative for RTD to generate a reproducible NDR characteristic, and the defect density of $10^5$--$10^6$ cm$^{-2}$ leads to an evident NDR degradation with rising number of either forward- or backward-scans, which is mainly attributed to the trapping effect of deep-level defects. A simulation for NDR oscillator based on GaN RTD demonstrates evident decreases in rf power and efficiency at around 300 GHz. In addition, an influence of quantum well structural parameters on NDR characteristic is also investigated. All the results are consistent with electrical measurements of the state-of-the-art GaN RTDs.

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