Resonant tunneling transport in $Zn_xBe_{1-x}Se/ZnSe/Zn_yBe_{1-y}Se$ asymmetric quantum structures

Vadim P. Sirkeli*[ab], Oktay Yilmazoglu[c], Shihab Al-Daffaie[a], Ion Oprea[a], Duu Sheng Ong[d], Franko Küppers[a], and Hans L. Hartnagel[a]
[a]Institut für Mikrowellentechnik und Photonik, Technische Universität Darmstadt, Merckstraße 25, Darmstadt, 64283 Germany; [b]Dept. of Information Technologies, Mathematics and Physics, Comrat State University, Galatsan street 17, Comrat, MD-3800 Moldova; [c]Dept. of High Frequency Electronics, Technische Universität Darmstadt, Merckstraße 25, Darmstadt, 64283 Germany; [d]Faculty of Engineering, Multimedia University, Persiaran Multimedia, Cyberjaya, Selangor, 63100 Malaysia

ABSTRACT

II-VI compounds are promising materials for the fabrication of room-temperature terahertz devices due to their beneficial properties like as type-I conduction band alignment, high breakdown field strength (~331 kV/cm for ZnSe vs. ~80 kV/cm for GaAs), and higher values of the conduction band offset (1.5 eV for BeSe/ZnSe vs. 0.7 eV for AlAs/GaAs). In this paper we report on numerical study of the resonant tunneling transport in ZnBeSe/ZnSe/ZnBeSe symmetric and asymmetric resonant tunneling diodes (RTDs). The negative differential resistance feature is observed in the current-voltage characteristics of the ZnSe-based RTDs. It is found that the maximum of peak-to-valley ratio (PVR) of the current density is equal to 6.025 and 7.144 at 150 K, and to 1.120 and 1.105 at 300 K for the symmetric and asymmetric RTDs, respectively. The effect of barrier heights on the frequency and output power performance of RTD devices are studied and discussed.

Keywords: resonant tunneling diodes, negative differential resistance, terahertz emission, ZnSe, BeSe, ZnBeSe, alloy

1. INTRODUCTION

Resonant tunneling diodes (RTDs) are promising devices for applications in the radiation and detection of millimeter- and terahertz waves at room temperature.[1,2] In the last decade significant progress has been made in the design and fabrication of RTDs based on AlGaAs/GaAs, InGaAs/AlAs, InGaAs/InAs and AlGaN/GaN material systems, with a typical current density peak-to-valley ratio (PVR) of ~ 2-4 at 300 K.[3] The record oscillation frequency of 1.92 THz at 300 K was reported by Maekawa et al.[4] for InGaAs-based RTD devices with a slot antenna. To improve the characteristics of the RTDs several approaches have been proposed. Suzuki *et al.*[5] suggested InGaAs-based RTD devices with a 3-step graded emitter. Yang et al.[6] and Bouhri et al.[7] suggested the design of asymmetric AlGaN/GaN RTD structures and found that the PVR of optimized devices can reach values up to 882.

II-VI compounds are attracted attention as promising materials for fabrication of the room-temperature RTD devices since they have several advantages like a high breakdown field strength (~ 331 kV/cm for ZnSe[8] vs. ~ 80 kV/cm for GaAs[9]) and higher values of the conduction band offset (CBO), which is about 1.5 eV for the BeSe/ZnSe system in comparison to 0.7 eV for AlAs/GaAs.[10-12] Moreover, among II-VI compounds, the ZnBeSe/ZnSe and ZnMgSe/ZnSe materials systems are attractive as promising materials for the fabrication of room-temperature THz RTD devices, due to the fact that these material combinations create a type-I bandgap alignment. Recently, Maximov *et al.*[12] reported on experimentally fabricated symmetric ZnBeSe/ZnSe-based RTD devices with PVR of ~2.5 at 4 K.

In this paper we report on a numerical study of the quantum transport in symmetric and asymmetric ZnBeSe/ZnSe RTD structures with fixed and variable barrier heights. The NDR feature, observed in the current-voltage characteristics of the

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*sirkeli@imp.tu-darmstadt.de; phone +49 6151 16 28438

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ZnSe-based RTDs are considered for use in the design of devices for high-power terahertz generation at room temperature. The effect of barrier heights on the frequency and output power performance of RTD devices are studied and discussed.

2. MODEL AND METHODS

The one-dimensional Schrödinger-Poisson equation within the single-band effective mass approximation (EMA) was used to calculate the electronic conduction band diagram of the investigated THz RTDs. Along the growth direction of quantum structures (z-axis), the Schrödinger equation can be expressed as[13]:

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m(z)}\frac{\partial}{\partial z}+\left(eV(z)+\Delta E_C(z)\right)\right]\Psi(z)=E\Psi(z), \tag{1}$$

where $m(z)$ is the position-dependent electron effective mass in the growth direction, z, $V(z)$ is the electrostatic potential, $\Delta E_C(z)$ is a stepwise function due to the conduction band discontinuity, $\Psi(z)$ is the Eigen wave function. The electrostatic potential $V(z)$ is determined by solving the Poisson equation, which is given in the absence of polarization by[7]:

$$\frac{\partial}{\partial z}\left[-\varepsilon(z)\frac{\partial}{\partial z}V(z)\right]=q\left(N_D(z)-n(z)\right), \tag{2}$$

where $\varepsilon(z)$ is the position-dependent dielectric constant, $V(z)$ is the electrostatic potential, $N_D(z)$ is the ionized donor doping concentration, and $n(z)$ is the free electron concentration. This system of coupled equations (1-2) is solved numerically using nextnano MSB solver software.[14,15] This software is based on the modified non-equilibrium Green's function (NEGF) method employing the multi-scattering Büttiker probe (MSB) model for calculation of dissipative quantum transport in multilayered quantum heterostructures. The following scattering mechanisms were taken into account in the MSB model: the electron-longitudinal optical (LO) phonon scattering, electron-electron scattering, electron-longitudinal acoustic (LA) phonon scattering. It is a memory efficient method and it has successfully predicted the experimental results of AlInAs/InGaAs and GaAs/AlGaAs-based RTDs and quantum cascade lasers.[15] The CBO offset of $Zn_{1-x}Be_xSe$ used in the calculations is 1.5x eV, and the bandgap energy is 2.82+2.30x [20] for x < 0.46. The other materials parameters used were taken from Refs. [11-13, 16, 17]. The maximum of operation frequency of RTD devices was estimated using the approximation of the equivalent circuit of a tunnel-diode oscillator.[18] The temperature was varied from 100 to 300 K. The cross section area of all the investigated RTD devices is 1 μm^2.

3. RESULTS AND DISCUSSION

3.1 Structure of symmetric and asymmetric RTD devices

The conduction band diagram of investigated symmetric and asymmetric RTD structures is shown in Figs. 1(a) and 1(b), respectively. The symmetric ZnBeSe/ZnSe/ZnBeSe RTD structure consists of 10 nm thick 10^{18} cm^{-3} n-doped ZnSe emitter/5nm thick undoped ZnSe spacer/5 nm thick undoped $Zn_{0.7}Be_{0.3}Se$ quantum barrier/9 nm thick undoped ZnSe quantum well/5 nm thick undoped $Zn_{0.7}Be_{0.3}Se$ quantum barrier/5 nm thick undoped ZnSe spacer/10 nm thick 10^{18} cm^{-3} n-doped ZnSe collector. The undoped ZnSe spacers between emitter (collector) and ZnBeSe barrier are required to prevent the diffusion of doping impurity to the ZnBeSe quantum barriers. In the asymmetric RTD structures shown in Fig. 1(b) all layers have the same widths as in the symmetric RTD structure, except the composition of barrier material: the first barrier (from the emitter side) is $Zn_{0.85}Be_{0.15}Se$, and the second barrier is $Zn_{0.80}Be_{0.20}Se$.