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# Epitaxial Structure Simulation Study of In<sub>0.53</sub>Ga<sub>0.47</sub>As/AlAs Double-Barrier Resonant Tunnelling Diodes

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Abstract—In this paper, we report about an epitaxial structure simulation study of In<sub>0.53</sub>Ga<sub>0.47</sub>As/AlAs double-barrier resonant tunneling diodes (RTD) employing Atlas TCAD quantum transport simulation software developed by SILVACO Inc., which is based on the non-equilibrium Green's function formalism. We analyse how epitaxial layers design impacts the heterostructure static current density-voltage characteristic, including barriers, quantum well (QW), and lightly-doped spacer layers, as well as the employment of a high-bandgap emitter region. Our analysis shows that, while barriers and QW thicknesses have a strong impact on the current density operation of the RTD device, accurate asymmetric spacers design can trade-off between the voltage span and relative position of its negative differential resistance region. This work will guide in optimising the RTD epitaxial structure in order to maximise its RF power performance at low-terahertz frequencies ( $\sim 100-300$  GHz).

*Index Terms*—Resonant tunnelling diode, double-barrier quantum well, non-equilibrium Green's function, epitaxial structure design.

#### I. INTRODUCTION

**R** ESONANT tunnelling diodes (RTD) [1] are the fastest demonstrated solid-state semiconductor-based electronic devices operating at room temperature (RT), which makes them attractive for consumer-oriented terahertz (THz) (0.1-10 THz [2]) applications. Indeed, maximum oscillation frequencies  $f_{max}$  up to around 2 THz have been attained in indium phosphide (InP) technology [3], providing a milestone for the viability of next-generation ultra-high-speed wireless communications [4] [5]. In this context, accurate device epitaxial structure design optimisation is crucial to tailor both sources and detectors performance according to the operational requirements. However, this needs a clear and comprehensive understanding on how epitaxial structure parameters impact the electrical properties of the RTD device.

In this paper, we present an epitaxial structure simulation study of lattice-matched to InP indium gallium arsenide/aluminium arsenide (In<sub>0.53</sub>Ga<sub>0.47</sub>As/AlAs) double-barrier RTDs by making use of the approach we have demonstrated in [6], which is based on the Non-equilibrium Green's Function (NEGF) method implemented in SILVACO Inc. Atlas TCAD quantum transport simulation package. By tuning the parameters associated with epitaxial layers, including barriers, quantum well (QW), and lightly-doped spacer layers, we analysed the impact on the associated static current density-voltage (JV) characteristic in terms of peak current density  $J_p$ , peak voltage  $V_p$ , and valley-to-peak voltage difference  $\Delta V = V_v - V_p$  of the negative differential resistance (NDR) region, which are the electrical quantities that can be accurately estimated with the current release of the software. A qualitative analysis of the valley current density  $J_v$ , peak-to-valley current density difference  $\Delta J = J_p - J_v$ , and peak-to-valley current ratio PVCR =  $J_p/J_v$  in terms of both barriers and QW design was carried out based on the heterostructure transmission coefficient. The employment of a high-bandgap material at the emitter side was also studied.

### II. EPITAXIAL STRUCTURE SIMULATION STUDY

To investigate the impact of epitaxial structure design parameters on the heterostructure static JV characteristic, an *n*-type intraband In<sub>0.53</sub>Ga<sub>0.47</sub>As/AlAs double-barrier reference epitaxial structure (RES) with symmetric geometry, which is depicted in Fig. 1, was adopted, and consisted of: barriers thickness  $t_b = 1.46$  nm; QW thickness  $t_{qw} =$ 4.39 nm; emitter/collector undoped spacers thickness: 2 nm; emitter/collector lightly-doped spacers thickness  $t_{e/c,ls} =$ 100 nm and doping level  $N_{De/c,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>; emit-

n++ In <sub>0.53</sub> Ga <sub>0.47</sub> As	Collector contact: 40 nm, 2x10 <sup>19</sup> cm <sup>-3</sup>
<i>n</i> + In <sub>0.53</sub> Ga <sub>0.47</sub> As	Collector: 20 nm, 2x10 <sup>18</sup> cm <sup>-3</sup>
<i>n-</i> In <sub>0.53</sub> Ga <sub>0.47</sub> As	Lightly-doped spacer: $t_{c,ls} \simeq 50/100$ nm, $N_{Dc,ls} \simeq 2 \times 10^{16/17}$ cm <sup>-3</sup>
<i>u</i> In <sub>0.53</sub> Ga <sub>0.47</sub> As	Undoped spacer: $\simeq 2$ nm
<i>u</i> AlAs	Barrier: $t_b \simeq 1.17/1.46/1.75$ nm (4/5/6 ML)
<i>u</i> In <sub>0.53</sub> Ga <sub>0.47</sub> As	Quantum well: $t_{qw} \simeq 4.10/4.39/4.69$ nm (14/15/16 ML)
<i>u</i> AlAs	Barrier: $t_b \simeq 1.17/1.46/1.75$ nm (4/5/6 ML)
<i>u</i> In <sub>0.53</sub> Ga <sub>0.47</sub> As	Undoped spacer: ≃ 2 nm
<i>n</i> - In <sub>0.53</sub> Ga <sub>0.47</sub> As	Lightly-doped spacer: $t_{e,ls} \simeq 50/100$ nm, $N_{De,ls} \simeq 2 \times 10^{16/17}$ cm <sup>-3</sup>
n+ In <sub>0.53</sub> Ga <sub>0.47</sub> As	Emitter: 20 nm, 2x10 <sup>18</sup> cm <sup>-3</sup>
n++ In <sub>0.53</sub> Ga <sub>0.47</sub> As	Emitter contact: 40 nm, 2x10 <sup>19</sup> cm <sup>-3</sup>

Fig. 1. Reference epitaxial structure (RES) and associated parameters (in red), including the whole set of simulation study parameters.

ter/collector thickness and doping level: 20 nm,  $2 \times 10^{18}$  cm<sup>-3</sup>; emitter/collector heavily-doped contacts thickness and doping level: 40 nm,  $2 \times 10^{19}$  cm<sup>-3</sup>. This choice was made based on reported epitaxial structures employed in oscillators operating below 300 GHz [7]. Parameters associated with barriers, QW, and lightly-doped spacers were tuned, as shown in Fig. 1, and simulation results compared and discussed. Forward bias (collector positively biased with respect to the emitter) and RT (T = 300 K) operation was assumed.

## A. Barriers

The RES was simulated setting  $t_b = 1.17$  nm, 1.46 nm, and 1.75 nm (4 ML, 5 ML, and 6 ML), where ML stands for monolayer (1 ML  $\simeq$  0.293 nm). The impact of  $t_b$  on the static JV characteristic was revealed in terms of current density, while the effect on voltages was negligible ( $V_p \simeq 1.2$  V,  $V_v \simeq$ 2.7 V, and  $\Delta V \simeq 1.5$  V). Simulation results are shown in Table I. As  $t_b$  increases,  $J_p$  decreases from  $\simeq 656$  kA/cm<sup>2</sup> with 4 ML to  $\simeq 263$  kA/cm<sup>2</sup> and  $\simeq 101$  kA/cm<sup>2</sup> with 5 ML and 6 ML, respectively, revealing an exponential trend  $J_p \propto e^{-\alpha t_b}$  $(\alpha > 0)$ , which is explained by the drop of the full-width at half maximum (FWHM)  $\Gamma_1$  of the heterostructure transmission coefficient  $T_{rtd}$  associated with the QW first quasi-bound state energy level  $E_1$  resonant peak, which is shown in Fig. 2, which decreases from  $\simeq$  7.5 meV with 4 ML to  $\simeq$  2.9 meV and  $\simeq$  1.1 meV with 5 ML and 6 ML, respectively, increasing carrier confinement and narrowing the channel for electron tunnelling due to the lower associated available density of states. Although  $J_p$  increases by reducing  $t_b$ , the  $T_{rtd}(E_2)$ resonant peak FWHM  $\Gamma_2$  (where  $E_2$  is the QW second quasibound state resonant level) increases more than  $\Gamma_1$ , from  $\simeq$ 13.8 meV with 6 ML to  $\simeq$  25.1 meV and  $\simeq$  47.6 meV with 5 ML and 4 ML, respectively, where  $d\Gamma_2/dt_b \gg d\Gamma_1/dt_b$  due to the weaker electron confinement, making the valley current density  $J_v \propto e^{-\beta t_b}$  to rise more than  $J_p$  ( $\beta \ll \alpha$ ).

In summary, the analysis showed that, while both  $J_p$  and the available current density  $\Delta J = J_p - J_v$  increases reducing  $t_b$ , the peak-to-valley current ratio PVCR =  $J_p/J_v$  drops, while  $V_p$  and  $\Delta V$  are almost unchanged [8] [9].



Fig. 2. Computed resonant peak associated with the QW first quasi-bound state energy level of the heterostructure transmission coefficient energy spectrum at RT and thermal equilibrium for different barriers thicknesses  $t_b$ .

TABLE I SIMULATION RESULTS FOR DIFFERENT BARRIERS THICKNESSES

$t_b$ [nm]	$J_p  [\mathrm{kA/cm^2}]$	$V_p$ [V]	$V_v$ [V]	$\Delta V [V]$
1.17	656	1.2	2.7	1.5
1.46	263	1.2	2.7	1.5
1.75	101	1.2	2.7	1.5



Fig. 3. Computed static JV characteristic at RT for different QW thicknesses  $t_{qw}$ .



Fig. 4. Computed transmission coefficient energy spectrum at RT and thermal equilibrium for different QW thicknesses  $t_{qw}$ .

#### B. Quantum well

The RES was simulated setting  $t_{qw} \simeq 4.10$  nm,  $\simeq 4.39$  nm, and  $\simeq 4.69$  nm (14 ML, 15 ML, and 16 ML). The computed static JV characteristics are shown in Fig. 3 and the associated values in Table II, which were  $J_p \simeq 338$  kA/cm<sup>2</sup>,  $V_p \simeq 1.44$ V, and  $\Delta V \simeq 1.78$  V with 14 ML,  $J_p \simeq 263$  kA/cm<sup>2</sup>,  $V_p$  $\simeq 1.20$  V, and  $\Delta V \simeq 1.54$  V with 15 ML, and  $J_p \simeq 206$ kA/cm<sup>2</sup>,  $V_p \simeq 1.00$  V, and  $\Delta V \simeq 1.32$  V with 16 ML.

To compare and explain the results, the  $T_{rtd}$  of the heterostructures at RT was computed and analysed, which is shown in Fig. 4. Thermal equilibrium conditions were assumed to simplify the treatment. The increase in  $J_p$  and  $V_p$  with QW shrinking is

TABLE II SIMULATION RESULTS FOR DIFFERENT QW THICKNESSES

$t_{qw}$ [nm]	$J_p \ [kA/cm^2]$	$V_p$ [V]	$V_v$ [V]	$\Delta V [V]$
4.10	338	1.44	3.22	1.78
4.39	263	1.20	2.74	1.54
4.69	206	1.00	2.32	1.32

explained by the rise of  $E_1$ , which increases from  $\simeq 112 \text{ meV}$ with 16 ML to  $\simeq$  123 meV ( $\Delta E_1 \simeq 11$  meV) and  $\simeq$  135 meV  $(\Delta E_1 \simeq 23 \text{ meV})$  with 15 ML and 14 ML, respectively, and by the broadening of  $E_1$  caused by the weaker wave-function confinement, where  $\Gamma_1$  increases from  $\simeq 2.5$  meV with 16 ML to  $\simeq 2.9$  meV and  $\simeq 3.3$  meV with 15 ML and 14 ML, respectively. At the same time,  $E_2$  rises more than  $E_1$ , which shifts from  $\simeq 597$  meV with 16 ML to  $\simeq 656$  meV ( $\Delta E_2 \simeq 59$ meV) and  $\simeq 720$  meV ( $\Delta E_2 \simeq 123$  meV) with 15 ML and 14 ML, respectively. This makes  $V_v$  to shift more than  $V_p$  $(V_v \simeq 2.32 \text{ V}, \simeq 2.74 \text{ V}, \text{ and } \simeq 3.22 \text{ V} \text{ with 16 ML}, 15 \text{ ML},$ and 14 ML, respectively), making  $\Delta V$  to increase. Moreover,  $\Gamma_2$  increases more than  $\Gamma_1$ , from  $\simeq 20.6$  meV with 16 ML to  $\simeq 25.1$  meV and  $\simeq 31.0$  meV with 15 ML and 14 ML, respectively, because  $d\Gamma_2/dt_b \gg d\Gamma_1/dt_b$  due to the lower electron confinement, which makes  $J_v$  to rise more than  $J_p$ . However, the impact of  $t_{qw}$  on both  $J_p$  and  $J_v$  is weaker with respect to  $t_b$ , as reported in Section IIA.

In summary, the analysis showed that, if  $J_p$ ,  $\Delta J$ , and  $\Delta V$  increase reducing  $t_{qw}$ ,  $V_p$  rises and the PVCR drops [9] [10].

## C. Lightly-doped spacers

1) Emitter spacer: the RES was simulated setting  $t_{e,ls} = 50$  nm and 100 nm, and  $N_{De,ls} = 2 \times 10^{16}$  cm<sup>-3</sup> and  $2 \times 10^{17}$  cm<sup>-3</sup>, while the lightly-doped collector spacer thickness  $t_{c,ls}$  and doping level  $N_{Dc,ls}$  were set to 100 nm, and  $2 \times 10^{17}$  cm<sup>-3</sup> and  $2 \times 10^{16}$  cm<sup>-3</sup>, respectively. The computed static JV characteristics are shown in Fig. 5 and the associated values in Table III, which were  $J_p \simeq 265$  kA/cm<sup>2</sup>,  $V_p \simeq 1.20$  V, and  $\Delta V \simeq 1.54$  V with  $t_{e,ls} = 50$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>,  $J_p \simeq 265$  kA/cm<sup>2</sup>,  $V_p \simeq 1.20$  V, and  $\Delta V \simeq 1.54$  V with  $t_{e,ls} = 100$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>,  $J_p \simeq 215$  kA/cm<sup>2</sup>,  $V_p \simeq 1.08$  V, and  $\Delta V \simeq 1.66$  V with  $t_{e,ls} = 50$  nm and  $N_{De,ls} = 2 \times 10^{16}$  cm<sup>-3</sup>, and  $J_p \simeq 206$  kA/cm<sup>2</sup>,  $V_p \simeq 1.04$  V, and  $\Delta V \simeq 1.70$  V with  $t_{e,ls} = 100$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>. Moreover, simulations gave  $J_p \simeq 265$  kA/cm<sup>2</sup>,  $V_p \simeq 2.28$  V, and  $\Delta V \simeq 1.76$  V with  $t_{e,ls} = 50$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>, and  $J_p \simeq 265$  kA/cm<sup>2</sup>,  $V_p \simeq 2.28$  V, and  $\Delta V \simeq 1.76$  V with  $t_{e,ls} = 100$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup> assuming  $t_{c,ls} = 100$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup> assuming  $t_{c,ls} = 100$  nm and  $N_{De,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>.

To compare and explain the results, the conduction band (CB) edge energy  $E_c$  profile ( $\Gamma$  point) and electron density *n* distribution in proximity to the first barrier at RT were computed, which are shown in Fig. 6. Thermal equilibrium was assumed to simplify the treatment. In the case of symmetric



Fig. 5. Computed static JV characteristic at RT for different lightly-doped emitter spacer thicknesses  $t_{e,ls}$  and doping levels  $N_{De,ls}$ . The lightly-doped collector spacer thickness  $t_{c,ls}$  and doping level  $N_{Dc,ls}$  were set to 100 nm and  $2 \times 10^{17}$  cm<sup>-3</sup>, respectively. \*Computed assuming  $t_{c,ls} = 100$  nm and  $N_{Dc,ls} = 2 \times 10^{16}$  cm<sup>-3</sup>.



Fig. 6. Computed conduction band (CB) edge energy  $E_c$  profile and electron density *n* at RT and thermal equilibrium in the emitter region for different lightly-doped emitter spacer thicknesses  $t_{e,ls}$  and doping levels  $N_{De,ls}$ . The lightly-doped collector spacer thickness  $t_{c,ls}$  and doping level  $N_{Dc,ls}$  were set to 100 nm and  $2 \times 10^{17}$  cm<sup>-3</sup>, respectively. \*Computed assuming  $t_{c,ls} = 100$  nm and  $N_{Dc,ls} = 2 \times 10^{16}$  cm<sup>-3</sup>. The black solid line represents the Fermi level  $E_F$ .

doping between emitter and collector lightly-doped spacers, no change in the JV characteristic was revealed when  $t_{e,ls}$  was tuned, which can be explained by the weak variation in the potential barrier arising close to the QW at peak resonance, which was confirmed by the smoothness of  $E_c$  at thermal equilibrium. Similar considerations apply for the asymmetric case  $N_{De,ls} > N_{Dc,ls}$ , which was confirmed by the positive curvature of the potential profile in proximity to the first barrier at thermal equilibrium. On the other hand, if  $N_{De,ls} < N_{Dc,ls}$ ,  $J_p$  drops with increasing  $t_{e,ls}$ , which can be explained by the larger potential barrier seen by the tunnelling electrons



Fig. 7. Computed static JV characteristic at RT for different lightly-doped collector spacer thicknesses  $t_{c,ls}$  and doping levels  $N_{Dc,ls}$ . The lightly-doped emitter spacer thickness  $t_{e,ls}$  and doping level  $N_{De,ls}$  were set to 100 nm and  $2 \times 10^{17}$  cm<sup>-3</sup>, respectively.

when the equivalent voltage drop across the depletion regions at the emitter side at  $V = V_p$  is not enough to compensate for the associated intrinsic built-in potential, which is the case if the emitter contact is heavily doped (whose doping level was set to  $2 \times 10^{19}$  cm<sup>-3</sup>). This was confirmed by the negative profile of the potential at thermal equilibrium. Moreover,  $J_p$ decreases if  $N_{De,ls}$  is reduced due the lower available electron concentration, making  $E_c$  to shift towards and above the Fermi level  $E_F$ . In both cases,  $V_p$  decreases since  $E_c$  and  $E_1$  get closer because of band warping caused by the larger potential drop at the emitter side, increasing  $\Delta V$ . Generally speaking, both  $J_p, V_p(t_{e,ls}, N_{De,ls})$  are expected to depend on Thomas-Fermi screening effects caused by charge accumulation close to the first barrier. Furthermore,  $V_v$  resulted to be unaffected by both  $t_{e,ls}$  and  $N_{De,ls}$ , where the estimated  $V_v$  were  $\simeq 2.74$ V and  $\simeq 4.04$  V assuming  $N_{Dc,ls} = 2 \times 10^{17}$  cm<sup>-3</sup> and  $2 \times 10^{16}$  cm<sup>-3</sup>, respectively. However,  $J_p$ ,  $V_p$ , and  $V_v$  are expected to change as  $t_{e,ls}$  increases and/or  $N_{De,ls}$  decreases due to dissipative processes, which were not included in the simulations.

In summary, the analysis showed that, while  $J_p$ ,  $V_p$ , and  $\Delta V$  considerably change if  $N_{De,ls}$  is tuned, their dependence on  $t_{e,ls}$  turns to be relevant only if  $N_{De,ls}/N_{De,ls} \ll 1$ . In particular, both  $J_p$  and  $V_p$  decreases, while  $\Delta V$  increases, if either  $N_{De,ls}$  is reduced or  $t_{e,ls}$  increased [8].

2) Collector spacer: the RES was simulated setting  $t_{c,ls} = 50 \text{ nm}$  and 100 nm, and  $N_{Dc,ls} = 2 \times 10^{16} \text{ cm}^{-3}$  and  $2 \times 10^{17} \text{ cm}^{-3}$ , while the lightly-doped emitter spacer thickness  $t_{e,ls}$  and doping level  $N_{De,ls}$  were set to 100 nm and  $2 \times 10^{17} \text{ cm}^{-3}$ , respectively. The computed static JV characteristics are shown in Fig. 7 and the associated values in Table III, which were  $J_p \simeq 263 \text{ kA/cm}^2$ ,  $V_p \simeq 1.00 \text{ V}$ ,  $V_v \simeq 2.02 \text{ V}$ , and  $\Delta V \simeq 1.02 \text{ V}$  with  $t_{c,ls} = 50 \text{ nm}$  and  $N_{Dc,ls} = 2 \times 10^{17} \text{ cm}^{-3}$ ,  $J_p \simeq 263 \text{ kA/cm}^2$ ,  $V_p \simeq 1.20 \text{ V}$ ,  $V_v \simeq 2.74 \text{ V}$ , and  $\Delta V \simeq 1.54 \text{ V}$  with  $t_{c,ls} = 100 \text{ nm}$  and  $N_{Dc,ls} = 2 \times 10^{17} \text{ cm}^{-3}$ ,  $J_p \simeq 263 \text{ kA/cm}^2$ ,  $V_p \simeq 1.34 \text{ V}$ ,  $V_v \simeq 2.42 \text{ V}$ , and  $\Delta V \simeq 1.08 \text{ V}$  with  $t_{c,ls} = 50 \text{ nm}$  and  $N_{Dc,ls} = 2 \times 10^{16} \text{ cm}^{-3}$ , and

TABLE III SIMULATION RESULTS FOR DIFFERENT EMITTER AND COLLECTOR LIGHTLY-DOPED SPACERS THICKNESSES AND DOPING LEVELS

$t_{e,ls}$ [nm]	$N_{De,ls} \ [{\rm cm}^{-3}]$	$J_p \; [\mathrm{kA/cm^2}]$	$V_p$ [V]	$V_v$ [V]	$\Delta V$ [V]
*50	$2 \times 10^{17}$	265	1.20	2.74	1.54
*100	$2 \times 10^{17}$	265	1.20	2.74	1.54
*50	$2 \times 10^{16}$	215	1.08	2.74	1.66
*100	$2 \times 10^{16}$	206	1.04	2.74	1.70
** 50	$2 \times 10^{17}$	265	2.28	4.04	1.76
**100	$2 \times 10^{17}$	265	2.28	4.04	1.76
$t_{c,ls} \; [nm]$	$N_{Dc,ls} \ [{\rm cm}^{-3}]$	$J_p \ [kA/cm^2]$	$V_p$ [V]	$V_v$ [V]	$\Delta V [V]$
*50	$2 \times 10^{17}$	265	1.00	2.02	1.02
*100	$2 \times 10^{17}$	265	1.20	2.74	1.54
*50	$2 \times 10^{16}$	265	1.34	2.42	1.08
*100	$2 \times 10^{16}$	265	2.28	4.04	1.76

\* Computed assuming  $t_{c/e,ls} = 100$  nm and  $N_{Dc/e,ls} = 2 \times 10^{17}$  cm<sup>-3</sup>. \*\* Computed assuming  $t_{c,ls} = 100$  nm and  $N_{Dc,ls} = 2 \times 10^{16}$  cm<sup>-3</sup>.

 $J_p\simeq 263$  kA/cm<sup>2</sup>,  $V_p\simeq 2.28$  V,  $V_v\simeq 4.04$  V, and  $\Delta V\simeq$ 1.76 V with  $t_{c,ls} = 100$  nm and  $N_{Dc,ls} = 2 \times 10^{16}$  cm<sup>-3</sup>. The shift of  $V_p$  and  $V_v$  at higher voltage if  $t_{c,ls}$  is increased and/or  $N_{Dc,ls}$  decreased is explained by the larger voltage drop across the collector region. In particular,  $V_v$  shifts more than  $V_p$  since the inequality  $E_1 - E_c < E_2 - E_1$  is met, increasing  $\Delta V$ . Generally speaking, both  $V_p, V_v(t_{c,ls}, N_{Dc,ls})$ are expected to depend on the resistive nature of the collector depletion region of thickness  $l_{dc}$  through the ratio  $l_{dc}/L_{Dc}$ , where  $L_{Dc}$  is the associated Debye length. At the same time,  $J_p$  does not change by tuning both  $t_{c,ls}$  and/or  $N_{Dc,ls}$ , where the computed  $J_p$  was  $\simeq 265$  kA/cm<sup>2</sup>, unless a large potential barrier approaching  $E_1$  arises in proximity to the second barrier at  $V = V_p$  if  $N_{Dc,ls} \ll N_{De,ls}$ . However, it is expected  $J_p$ ,  $V_p$ , and  $V_v$  to change as  $t_{c,ls}$  increases and/or  $N_{Dc,ls}$  decreases due to inelastic scattering mechanisms.

In summary, the analysis showed that both  $V_p$  and  $\Delta V$  increase if  $t_{c,ls}$  is increased and/or  $N_{Dc,ls}$  is decreased, while  $J_p$  is unaffected if scattering is neglected [9] [11].

## D. High-bandgap emitter

The impact of a high energy bandgap  $E_g$  material employed at the emitter side was investigated. A quaternary  $\ln_{1-x-y}Al_yGa_xAs$  compound was assumed [11]. To show that, the RES was simulated setting  $t_{qw} = 4.10$  nm and assuming different alloy compositions  $\{x, y\} = \{0.43, 0.04\}$   $(E_g \simeq 0.93 \text{ eV}), \{0.4, 0.07\}$   $(E_g \simeq 0.98 \text{ eV}), \text{ and } \{0.37, 0.1\}$   $(E_g \simeq 1.04 \text{ eV})$  [12]. Simulations results are shown in Table IV, revealing a drop of  $V_p$  with increasing the aluminium (Al) concentration, where computed values were  $V_p \simeq 0.84$  V,  $\simeq 0.66$  V, and  $\simeq 0.52$  V with  $\{x, y\} = \{0.43, 0.04\}, \{0.4, 0.07\}, \text{ and } \{0.37, 0.1\}$ , respectively, reducing  $V_p$  up to  $\sim 3$  times if compared to an equivalent heterostructure employing



Fig. 8. Computed CB edge energy  $E_c$  profile at RT and thermal equilibrium in proximity to the first barrier for different  $In_{1-x-y}Al_yGa_xAs$  compositions. The black solid line represents the Fermi level  $E_F$ .

TABLE IV SIMULATION RESULTS FOR DIFFERENT EMITTER ALLOYS

Compound	$J_p  [\mathrm{kA/cm^2}]$	$V_p$ [V]
In <sub>0.53</sub> Ga <sub>0.47</sub> As	338	1.44
In <sub>0.53</sub> Al <sub>0.04</sub> Ga <sub>0.43</sub> As	220	0.84
In <sub>0.53</sub> Al <sub>0.07</sub> Ga <sub>0.4</sub> As	180	0.66
In <sub>0.53</sub> Al <sub>0.1</sub> Ga <sub>0.37</sub> As	145	0.52

In<sub>0.53</sub>Ga<sub>0.47</sub>As ( $E_g \simeq 0.74$  eV [13]), whose  $V_p$  was estimated to be  $\simeq 1.44$  V. At the same time,  $J_p$  drops, where computed values decrease from  $\simeq 338$  kA/cm<sup>2</sup> with y = 0 to  $J_p \simeq 220$ kA/cm<sup>2</sup>,  $\simeq 180$  kA/cm<sup>2</sup>, and  $\simeq 145$  kA/cm<sup>2</sup>, with {x, y} = {0.43, 0.04}, {0.4, 0.07}, and {0.37, 0.1}, respectively.

To explain the results, the  $E_c$  profile at RT close to the first barrier was analysed, which is shown in Fig. 8. Thermal equilibrium was assumed to simplify the treatment. As it is possible to see, the drop of  $V_p$  can be explained by the shift of  $E_c$  in both emitter and QW regions, which makes  $E_c$  and  $E_1$  to approach. However,  $J_p$  drops at the same time mainly due to the higher electron effective mass  $m_e^*$ of  $In_{1-x-y}Al_yGa_xAs$  (0.047  $\leq m_e^* \leq 0.053$ ) compared to  $In_{0.53}Ga_{0.47}As$  ( $m_e^* \sim 0.041$ ) [12].

In summary, the analysis showed that the employment of a high-bandgap emitter region lowers both  $V_p$  and  $J_p$  [11].

## **III.** CONCLUSIONS

In this work, we studied the impact of barriers, QW, and spacer layers design of  $In_{0.53}Ga_{0.47}As/AlAs$  RTD heterostructures on the associated static *JV* characteristic by employing a NEGF-based quantum transport simulator. We observed that while barriers and QW thicknesses mostly control the current density operation of the RTD device, accurate asymmetric

spacer layers design can compromise between the NDR region voltage span and relative position. Based on these considerations, future work will consist in optimising the RTD epitaxial structure design in order to improve the associated RF power performance in the low-THz band ( $\sim 100-300$  GHz).

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