

# GaInNAs quantum-well vertical-cavity surface-emitting lasers emitting at 2.33 $\mu\text{m}$

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**Abstract.** In the present paper, the comprehensive fully self-consistent optical-electrical-thermal-recombination model is used to determine the optimal structure of the possible GaInNAs quantum-well (QW) tunnel-junction (TJ) vertical-cavity surface-emitting lasers (VCSELs) with single-fundamental-mode operation at 2.33  $\mu\text{m}$  wavelength suited for carbon monoxide sensing applications. From among various considered structures, the diode laser with 4- $\mu\text{m}$  TJ and two 6-nm  $\text{Ga}_{0.15}\text{In}_{0.85}\text{N}_{0.015}\text{As}_{0.985}/\text{Ga}_{0.327}\text{In}_{0.673}\text{As}_{0.71}\text{P}_{0.29}$  QWs has the lowest threshold current and seems to be optimal for the above applications. Higher threshold currents are obtained for  $\text{Ga}_{0.15}\text{In}_{0.85}\text{N}_{0.015}\text{As}_{0.985}/\text{Al}_{0.138}\text{Ga}_{0.332}\text{In}_{0.530}\text{As}$  QW structures but the latter can be grown in reactors without P source which are used for fabrication of GaAs-based devices. Both the modelled VCSELs offer a very promising room temperature continuous wave performance and may represent an alternative choice to GaSb-based lasers.

**Key words:** simulation of a diode laser operation, QW VCSELs, mid-infrared radiation, dilute nitrides.

## 1. Introduction

There is now increasing interest in room temperature (RT) continuous wave (CW) regime of the mid-infrared semiconductor devices due to their possible applications such as distant air monitoring, medical diagnostics, wireless optical communication, thermovision measurements, and laser spectroscopy [1, 2]. Semiconductor lasers emitting radiation of wavelengths longer than 2  $\mu\text{m}$  are currently produced with the aid of the GaSb technology [3], however manufacturing of GaSb structures is relatively expensive and complex, thermal conductivities of GaSb-based semiconductors [4–7] are disappointingly low, carrier confinement in GaSb active regions [8, 9] is relatively low and GaSb substrates [10] are still expensive and of limiting sizes. The alternate substrate material is InP which is much cheaper than GaSb. Furthermore, InP-based devices can be manufactured using well known, much simpler and less expensive technology. Therefore, there is a wide interest to replace in the above applications the GaSb lasers with the InP-based ones produced using diluted nitrides as, for example, InNAs, GaInNAs, and GaInNAsSb.

Dilute nitride alloys have some unusual properties in comparison with most known semiconductors. An increase in their nitride contents leads to reductions of both the lattice constant and the energy gap. Therefore, choosing properly the mole fractions of indium and nitrogen, the strain within these nitride structures and their band gaps can be controlled as far as the layer thickness remains below a critical limit for creation of misfit dislocations. In the GaAs-based VCSELs, their application enables reaching both the 1.31- $\mu\text{m}$  and the 1.55- $\mu\text{m}$  emission bands [11] used in the fiber-optic communication. Advanced InP-based technology, on the other hand, is expected to reach even the 3.5- $\mu\text{m}$  emission.

In the present paper, the comprehensive fully self-consistent optical-electrical-thermal-recombination model is used to determine optimal structure of the possible GaInNAs quantum-well (QW) tunnel-junction (TJ) vertical-cavity surface-emitting lasers (VCSELs). The target wavelength equal to 2.33  $\mu\text{m}$  is selected in order to cover a strong absorption line of carbon monoxide (CO) [12] (Fig. 1).

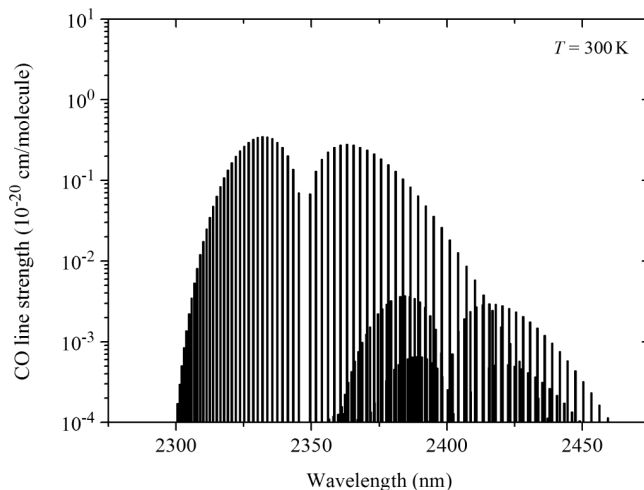


Fig. 1. Absorption lines of CO as a function of wavelength

## 2. The structure

A general concept of the modelled structure (Fig. 2) is similar to the currently most modern 2.33- $\mu\text{m}$  GaInAsSb/AlGaAsSb GaSb-based VCSEL proposed in [13–15]. Its intentionally undoped active region is assumed to be composed of 6-nm  $\text{Ga}_{0.15}\text{In}_{0.85}\text{N}_{0.015}\text{As}_{0.985}$  QWs separated by 10-nm  $\text{Ga}_{0.327}\text{In}_{0.673}\text{As}_{0.71}\text{P}_{0.29}$  (laser A) or  $\text{Al}_{0.138}\text{Ga}_{0.332}$

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In<sub>0.530</sub>As (laser B) internal barriers. External 30-nm barriers manufactured from the same material as the internal ones are assumed on both active-region sides. The active region is sandwiched by InP (laser A) or Ga<sub>0.47</sub>In<sub>0.53</sub>As (laser B) spacers, doped with silicon (5·10<sup>17</sup> cm<sup>-3</sup>) or zinc (5·10<sup>17</sup> cm<sup>-3</sup>) on the n and p sides, respectively. Above p-type spacer, the TJ composed of 15-nm p<sup>++</sup>-Al<sub>0.21</sub>Ga<sub>0.26</sub>In<sub>0.53</sub>As doped with carbon (2·10<sup>19</sup> cm<sup>-3</sup>) and 15-nm n<sup>++</sup>-Al<sub>0.21</sub>Ga<sub>0.26</sub>In<sub>0.53</sub>As doped with silicon (2·10<sup>19</sup> cm<sup>-3</sup>) is located. To minimise the absorption loss, the TJ is situated at the standing-wave node. Upper spacer is manufactured from InP (laser A) or Ga<sub>0.47</sub>In<sub>0.53</sub>As (laser B) doped with silicon up to 5·10<sup>17</sup> cm<sup>-3</sup>. The 3-λ cavity is terminated on both sides by distributed-Bragg-reflectors (DBRs): the 4-pair α-Si (162 nm)/SiO<sub>2</sub> (407 nm) top DBR and the fused 36.5-pair GaAs (175 nm)/Al<sub>0.90</sub>Ga<sub>0.10</sub>As (200 nm) bottom DBR. The bottom DBR is doped with silicon up to 2·10<sup>18</sup> cm<sup>-3</sup> (Al<sub>0.90</sub>Ga<sub>0.10</sub>As) and 5·10<sup>17</sup> cm<sup>-3</sup> (GaAs). Bottom DBR diameter is assumed to be equal to 60 μm, whereas the upper DBR diameter is larger by 6 μm than TJ diameter. The top contact is produced in a form of a ring of 10 μm width. It is separated from the top spacer with the 200-nm thick highly silicon-doped (5·10<sup>18</sup> cm<sup>-3</sup>) n<sup>+</sup>-Ga<sub>0.47</sub>In<sub>0.53</sub>As contact layer. The whole bottom 60 μm diameter surface of the 200-μm GaAs substrate doped with silicon up to 2·10<sup>18</sup> cm<sup>-3</sup> is covered by the bottom contact. The laser is attached to the cylindrical (height = diameter = 5 mm) copper heat sink with 3-μm indium solder.

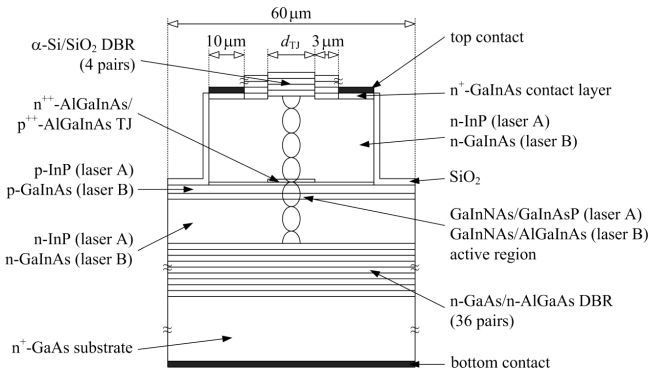


Fig. 2. The 2.33-μm QW TJ-VCSEL structure under consideration

### 3. The model

To simulate RT CW threshold operation of the GaInNAs QW TJ-VCSEL, we have adapted, our three-dimensional optical-electrical-thermal-recombination self-consistent model reported earlier by Sarzała and Nakwaski [16]. The model consists of four mutually interrelated parts:

a) The finite-element (FE) electrical model [17,18] characterizes both the current spreading including carrier drift and diffusion processes within the device volume between the top and the bottom contacts, the injection of both electrons and holes into the active region, and their radial diffusion within it before their monomolecular, bimolecular and Auger recombinations.

- b) The FE thermal model [17,19] gives details of a heat generation nonradiative recombination, reabsorption of radiation as well as the volume and the barrier Joule heating and its spreading from the heat sources toward the heat sink and within it.
- c) The optical model describes, for successive radiation modes, optical fields within the resonator. The model is based on the effective frequency method [20]. The lasing threshold is determined from the condition of the real propagation constant.
- d) The gain model, based on the Fermi's Golden Rule [17], gives information about the optical gain spectra. A brief description of the theoretical model for calculating the optical gain and electronic band structures of the strained QW active regions may be found in our previous publication [21].

The above well-conducted self-consistent approach allows us integration of various physical phenomena taking place within a VCSEL device.

### 4. The parameters

#### 4.1. Material parameters used in the electrical model.

Electrical conductivities of the n- and p-type semiconductor materials are calculated from Eqs. (1) and (2) given in [22]:

$$\sigma_n = en\mu_n, \quad (1)$$

$$\sigma_p = ep\mu_p, \quad (2)$$

where  $e$  is the electron charge,  $n$  and  $p$  are the free electron and hole concentrations,  $\mu_n$  and  $\mu_p$  are the electron and hole mobility.

Using the existing experimental data [23–31], we obtain the following expressions for the electron mobility in Si-doped GaAs and Al<sub>x</sub>Ga<sub>1-x</sub>As:

$$\mu_{n - \text{GaAs:Si}} = \frac{6600 \frac{\text{cm}^2}{\text{V} \cdot \text{s}}}{1 + \left( \frac{n}{5 \cdot 10^{17} \text{cm}^{-3}} \right)^{0.53}}, \quad (3)$$

$$\mu_{n - \text{AlGaAs:Si}} = \mu_{n - \text{GaAs:Si}} \cdot f(x), \quad (4)$$

$$f(x) = \begin{cases} \exp(-16x^2) & x \leq 0.5, \\ 0.054x - 0.009 & x > 0.5. \end{cases} \quad (5)$$

The free electron concentrations in Si-doped GaAs and Al<sub>x</sub>Ga<sub>1-x</sub>As for the donor concentration  $N_d$  are approximated using the data of [23–26]:

$$n_{\text{GaAs:Si}} = N_d, \quad (6)$$

$$n_{\text{AlGaAs:Si}} = n_{\text{GaAs:Si}} \cdot g(x), \quad (7)$$

$$g(x) = \begin{cases} 1 - 7.8x^2 & x \leq 0.35, \\ 1.14x - 0.36 & x > 0.35. \end{cases} \quad (8)$$

Using the data of [25, 32–39], we calculate electron mobility in Si- and Zn-doped InP from the following relations:

$$\mu_{n - \text{InP:Si}} = \frac{3900 \frac{\text{cm}^2}{\text{V} \cdot \text{s}}}{1 + \left( \frac{n}{10^{18} \text{cm}^{-3}} \right)^{0.51}}, \quad (9)$$

$$\mu_p - \text{InP:Zn} = \frac{120 \frac{\text{cm}^2}{\text{V} \cdot \text{s}}}{1 + \left( \frac{p}{2 \cdot 10^{18} \text{cm}^{-3}} \right)}. \quad (10)$$

On the basis of the experimental data of [25, 40], we assume zero activation energy in Si-doped InP:

$$n_{\text{InP:Si}} = N_d. \quad (11)$$

The relation between the free hole concentration in Zn-doped InP and the acceptor concentration  $N_a$  is taken from [39]:

$$p_{\text{InP:Zn}} = 0.75 N_a. \quad (12)$$

The electron mobility in Si- and Zn-doped  $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$  are approximated using the data of [41–46]:

$$\mu_n - \text{GaInAs:Si} = \frac{16700 \frac{\text{cm}^2}{\text{V} \cdot \text{s}}}{1 + \left( \frac{n}{6 \cdot 10^{16} \text{cm}^{-3}} \right)^{0.42}}, \quad (13)$$

$$\mu_p - \text{GaInAs:Zn} = \frac{250 \frac{\text{cm}^2}{\text{V} \cdot \text{s}}}{1 + \left( \frac{p}{6 \cdot 10^{17} \text{cm}^{-3}} \right)^{0.34}}. \quad (14)$$

Using the data of [40, 44, 47], we write the following relations between free carrier and dopant concentrations in Si- and Zn-doped  $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ :

$$n_{\text{GaInAs:Si}} = 0.55 N_d, \quad (15)$$

$$p_{\text{GaInAs:Zn}} = 0.90 N_a. \quad (16)$$

The rest of the electrical conductivities used in our model are equal to  $3 \cdot 10^{-3} \Omega^{-1} \text{m}^{-1}$  for the  $\alpha$ -Si [48], to  $1 \cdot 10^{-8} \Omega^{-1} \text{m}^{-1}$  for the  $\text{SiO}_2$  [49], to  $1.392 \cdot 10^7 \Omega^{-1} \text{m}^{-1}$  for the indium solder [50], to  $5.794 \cdot 10^7 \Omega^{-1} \text{m}^{-1}$  for the copper heat sink [51], and to  $5 \Omega^{-1} \text{m}^{-1}$  for the TJ [52]. We also assumed that contact resistances are equal to  $2.5 \cdot 10^{-6} \Omega \text{cm}^2$  [53].

The monomolecular  $A$ , the bimolecular  $B$ , the Auger  $C$ , and the ambipolar  $D$  recombination coefficients used in the simulation are taken from [54] and are equal to:  $1 \cdot 10^{-8} \text{s}^{-1}$ ,  $4 \cdot 10^{-10} \text{cm}^3 \text{s}^{-1}$ ,  $2.43 \cdot 10^{-28} \text{cm}^6 \text{s}^{-1}$ , and  $10 \text{cm}^2 \text{s}^{-1}$ , respectively.

In our calculations, for RT threshold VCSEL operation, we assumed that electrical parameters does not depend on the temperature. Their RT values are listed in Table 1.

**4.2. Material parameters used in the thermal model.** RT thermal conductivities for InP, AlGaAs, GaInAs, GaInAsP and AlGaInAs (Table 1) are calculated from thermal resistivities for binaries given in [55–59] using interpolation formulas found in [60] and bowing parameters taken from [61–66]. Their temperature dependences and analogous expressions for  $\alpha$ -Si,  $\text{SiO}_2$  and copper may be found in [67]. Because of extremely thin QW layers, the whole active region is assumed to exhibit the thermal conductivity of the barriers. For the indium solder we used the constant value equal to  $84 \text{Wm}^{-1} \text{K}^{-1}$  [68].

Table 1  
RT electrical  $\sigma$  and thermal  $k$  conductivities used in the simulation of the 2.33- $\mu\text{m}$  QW TJ-VCSELS

material	$\sigma$ ( $\Omega^{-1} \text{m}^{-1}$ )	$k$ ( $\text{Wm}^{-1} \text{K}^{-1}$ )
$\alpha$ -Si	$3 \cdot 10^{-3}$	0.98
$\text{SiO}_2$	$1 \cdot 10^{-8}$	1.44
$n^+$ - $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$	122933	4.41
n-InP (laser A)	18354	68.03
p-InP (laser A)	607	68.03
n- $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ (laser B)	25413	4.41
p- $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ (laser B)	945	4.41
tunnel junction	5	4.13
n-GaAs	26436	44.05
n- $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}$	2081	25.53
n-GaAs substrate	68555	44.05

**4.3. Material parameters used in the gain model.** RT values and temperature dependencies of the band parameters for binaries and the bowing coefficients used in the gain calculations are taken from [69–72]. Interpolation schemes for the ternary and quaternary alloys are given in [73] and [74]. The energy gap and the electron effective mass in GaInNAs have been calculated using formulas taken from [75] and [21], respectively. RT values of the most important parameters used in the gain calculations are listed in Table 2.

Table 2  
RT parameters used to determine gain spectra in the simulation of the 2.33- $\mu\text{m}$  QW TJ-VCSELS

parameter	unit	value (laser A)	value (laser B)
QW energy gap	eV	0.420	0.420
QW depth in conduction band	eV	0.346	0.413
QW depth in valance band	eV	0.188	0.121
waveguide depth in conduction band	eV	0.200	-0.137
waveguide depth in valance band	eV	0.199	-0.080
spin-orbit splitting	eV	0.360	0.360
Lorentz broadening	ps	0.1	0.1
QW refractive index	-	3.8	3.8
QW electron effective mass	$m_0$	0.074	0.074
QW heavy hole effective mass	$m_0$	0.284	0.284
QW light hole effective mass	$m_0$	0.038	0.038
barrier electron effective mass	$m_0$	0.052	0.050
barrier heavy hole effective mass	$m_0$	0.323	0.318
barrier light hole effective mass	$m_0$	0.076	0.069

**4.4. Material parameters used in the optical model.** The refractive indices for 2.33- $\mu\text{m}$  wavelength used in our model are equal to 3.328 for GaAs [76], to 2.911 for  $\text{Al}_{0.90}\text{Ga}_{0.10}\text{As}$  [77], to 3.120 for InP [78], to 3.2 for  $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$  [79], to 3.6 for  $\alpha$ -Si [80], to 1.433 for  $\text{SiO}_2$  [81], to 3.405 for Al-GaInAs TJ [82], to 3.440 for AlGaInAs barrier [82], to 3.36 for GaInAsP barrier [83], and to 3.8 for GaInNAs QW [84].

The absorption coefficient in n-GaAs is approximated using the data of [85]:

$$\alpha_n - \text{GaAs} = 5.1 \text{cm}^{-1} \left( \frac{n}{10^{18} \text{cm}^{-3}} \right)^{1.3}. \quad (17)$$

We assume that the absorption coefficient in n-AlGaAs can be obtained from linear interpolation of the absorption coefficients in GaAs and AlAs:

$$\alpha_n - \text{AlGaAs} = x\alpha_n - \text{AlAs} + (1 - x)\alpha_n - \text{GaAs}. \quad (18)$$

Using the data of [86] we also assume that:

$$\alpha_n - \text{AlAs} = 0.5\alpha_n - \text{GaAs}. \quad (19)$$

The absorption coefficients in n- and p-InP are approximated using the data taken from [87–89].

$$\alpha_n - \text{InP} = 2 \text{ cm}^{-1} \left( \frac{n}{10^{18} \text{ cm}^{-3}} \right), \quad (20)$$

$$\alpha_p - \text{InP} = 52 \text{ cm}^{-1} \left( \frac{p}{10^{18} \text{ cm}^{-3}} \right)^{1.2}. \quad (21)$$

The relations between the absorptions coefficients in n- and p-Ga<sub>0.47</sub>In<sub>0.53</sub>As and free carrier concentrations are taken from [90]:

$$\alpha_n - \text{GaInAs} = 4.48 \text{ cm}^{-1} \left( \frac{n}{10^{18} \text{ cm}^{-3}} \right), \quad (22)$$

$$\alpha_p - \text{GaInAs} = 7.97 \text{ cm}^{-1} \left( \frac{p}{10^{17} \text{ cm}^{-3}} \right). \quad (23)$$

Absorption coefficients for  $\alpha$ -Si and SiO<sub>2</sub> can be neglected [91,92]. For the p<sup>++</sup>-AlGaInAs/n<sup>++</sup>-AlGaInAs TJ the absorption coefficients are assumed to be equal to 1000 cm<sup>-1</sup> and 100 cm<sup>-1</sup>, respectively. The latter value is also assumed for the absorption coefficients of the AlGaInAs and GaInAsP barriers.

### 5. The results

For an application of the considered VCSELs as a sources of the carrier wave used in the gas-sensing applications, it is of primary importance to obtain the stable single-fundamental-mode LP<sub>01</sub> emission. Although in the TJ-VCSELs, contrary to oxide-confined devices, it may be achieved even for large diameters, we restrict our discussion to TJs with small diameters for which, as it will be shown later, threshold currents are relatively low. Wavelengths of the LP<sub>01</sub> modes as a function of the TJ diameters and number of QWs are plotted in Figs. 3 and 4. As one can see, although increases in the TJ size and in the number of QWs cause an increase in the emitted wavelength, for all calculated cases, both the simulated lasers show LP<sub>01</sub> operation with emission wavelength close to the 2.33  $\mu\text{m}$  emission and can cover strong absorption line of CO.

An increase in the emitted wavelength due to modifications of the TJ diameter or number of QWs is followed by reduction of the threshold gain (Figs. 5 and 6). The calculated threshold-gain values for both lasers are comparable, however for the laser with GaInAs spacers it was impossible to achieve threshold operation for TJ with diameter smaller than 4  $\mu\text{m}$  and for active region with single QW. The main reason for that result are higher temperatures (Figs. 7 and 8) obtained in the above laser caused by the low thermal conductivity (4.4 Wm<sup>-1</sup>K<sup>-1</sup>) of GaInAs spacers. In comparison, the thermal conductivity of InP is equal to 68 Wm<sup>-1</sup>K<sup>-1</sup>.

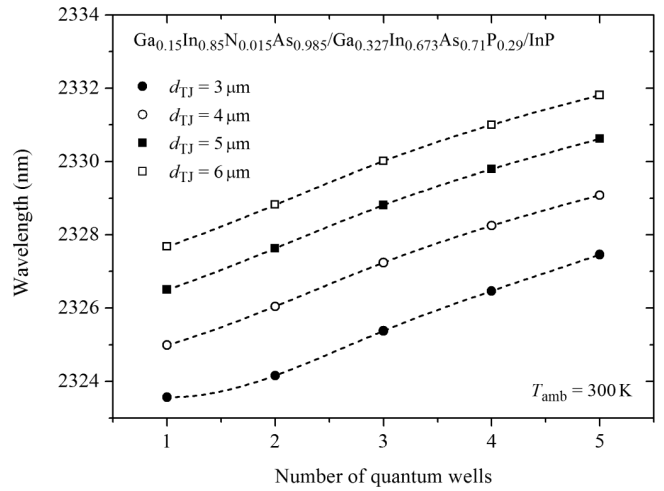


Fig. 3. RT dependence of the lasing wavelength as a function of the number of QWs determined for various TJ diameters of GaInAs/GaInAsP/InP QW 2.33- $\mu\text{m}$  VCSEL

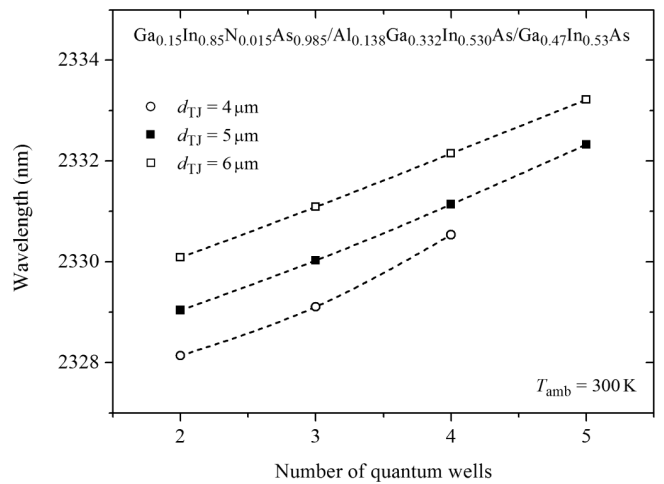


Fig. 4. RT dependence of the lasing wavelength as a function of the number of QWs determined for various TJ diameters of GaInAs/AlGaInAs/GaInAs QW 2.33- $\mu\text{m}$  VCSEL

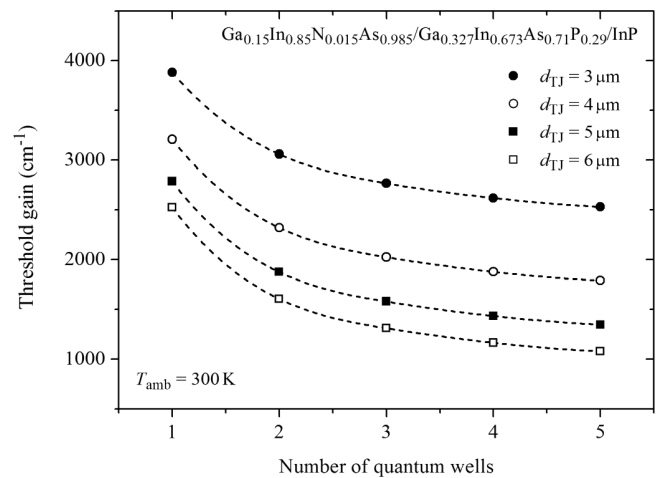


Fig. 5. RT dependence of the threshold gain as a function of the number of QWs determined for various TJ diameters of GaInAs/GaInAsP/InP QW 2.33- $\mu\text{m}$  VCSEL

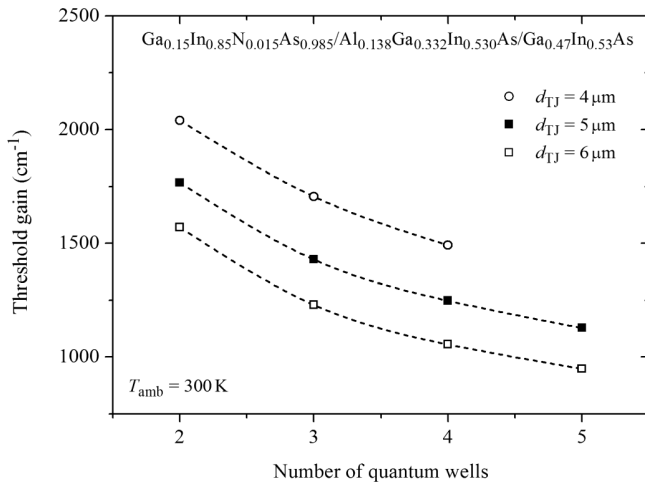


Fig. 6. RT dependence of the threshold gain as a function of the number of QWs determined for various TJ diameters of GaInNAs/AlGaInAs/GaInAs QW 2.33- $\mu\text{m}$  VCSEL

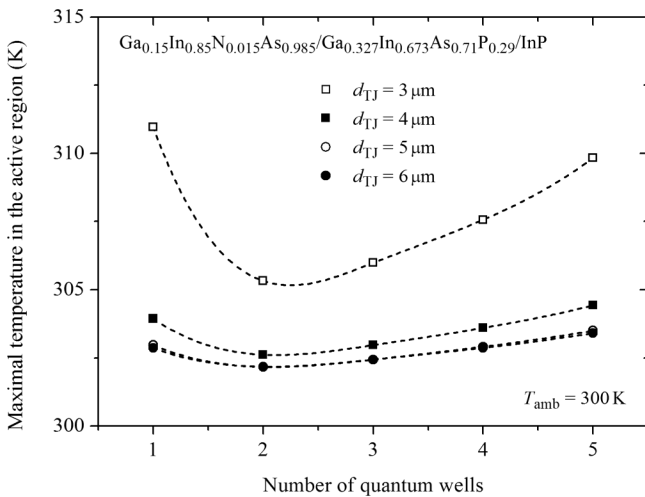


Fig. 7. Maximal temperature in the active region as a function of the number of QWs determined for various TJ diameters of GaInNAs/GaInAsP/InP QW 2.33- $\mu\text{m}$  VCSEL

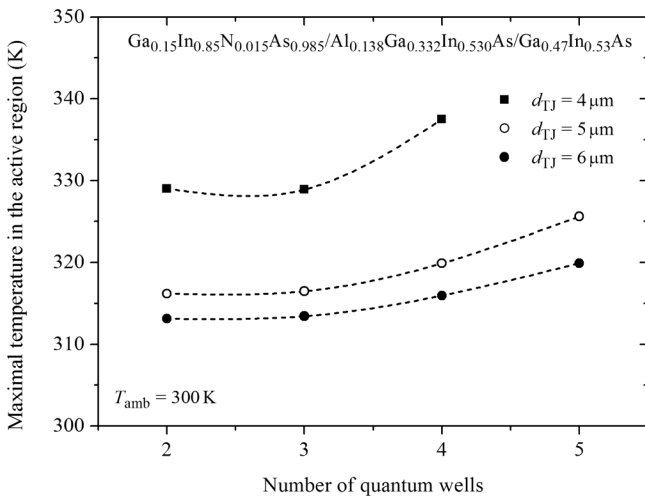


Fig. 8. Maximal temperature in the active region as a function of the number of QWs determined for various TJ diameters of GaInNAs/AlGaInAs/GaInAs QW 2.33- $\mu\text{m}$  VCSEL

To determine the optimal structures of the possible GaInNAs QW TJ-VCSELs, the threshold currents for various TJ diameters and numbers of QWs were calculated. As can be seen from Fig. 9, for the laser with InP spacers, the lowest thresholds were obtained for the TJ diameter equal to 4  $\mu\text{m}$ . In this case, for the active region with two QWs, the calculated threshold current was as low as 0.85 mA. Noticeably higher threshold currents were obtained for the laser with GaInAs spacers (Fig. 10). The optimal TJ diameter and number of QWs for this VCSEL were equal to 5  $\mu\text{m}$  and 2, respectively, and the lowest threshold current was close to 1.7 mA.

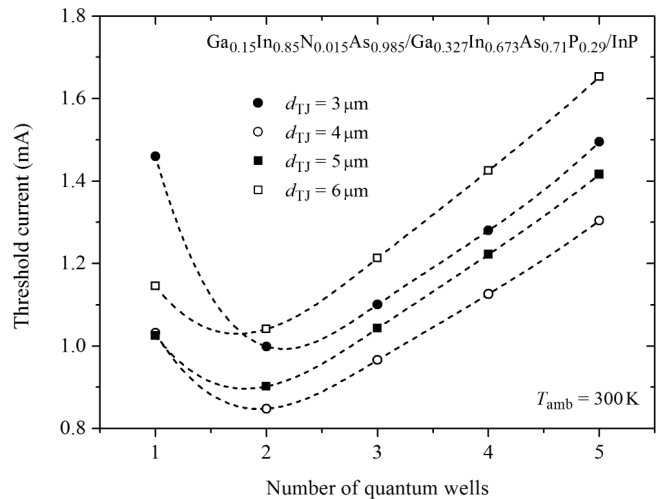


Fig. 9. RT dependence of the CW threshold current as a function of the number of QWs determined for various TJ diameters of GaInNAs/GaInAsP/InP QW 2.33- $\mu\text{m}$  VCSEL

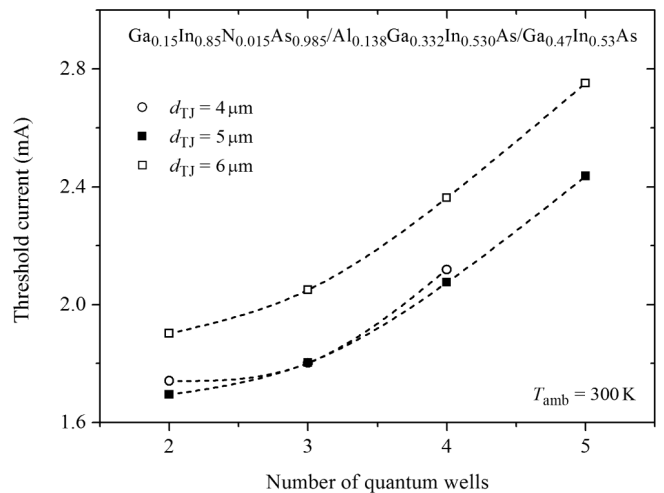


Fig. 10. RT dependence of the CW threshold current as a function of the number of QWs determined for various TJ diameters of GaInNAs/AlGaInAs/GaInAs QW 2.33- $\mu\text{m}$  VCSEL

## 6. Conclusions

We have used the comprehensive fully self-consistent optical-electrical-thermal-recombination model to determine the optimal structure of the possible GaInNAs QW TJ VCSELs with single-fundamental-mode operation at 2.33  $\mu\text{m}$  wavelength suited for CO detectors. We found that for GaInNAs/GaInAsP

QW TJ-VCSELs with InP spacers it is possible to obtain a RT CW lasing with the threshold current lower than 1 mA, which is similar to that of GaSb-based TJ-VCSELs. Higher threshold currents were obtained for laser with GaInNAs/AlGaInAs active region surrounded by the GaInAs spacers, but this structure can be grown in reactors without P source which are used for fabrication of GaAs-based devices. Both the simulated VCSELs are very promising RT CW laser sources of the 2.33- $\mu\text{m}$  carrier wave for the CO-sensing applications and can represent an alternative choice to GaSb-based lasers.

**Acknowledgements.** This work has been supported by the COST Action MP0805 and by the Polish Ministry of Science and Higher Education, grant No N N515 533338.

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