# THE LASING WAVELENGTH OF QW ACTIVE REGION OF AlGaAs SCH LASERS

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Computer simulations with Synopsys' Sentaurus TCAD are used to study the effect of the molar concentration of aluminum in the active and waveguide regions on the energy spectrum of carriers in Quantum Well (QW) and the optical spectral characteristics of radiation of semiconductor lasers with $Al_xGa_{1-x}As$ double heterostructures and separate confinement (SCH). Wavelength of single-mode lasers is shown to be almost independent of the concentration of aluminum in the waveguide itself, in a wide range of aluminum content, but to depend mainly on Al concentrations in QW region.

*Key words*: Semiconductor lasers, AlGaAs, TCAD, Synopsys, Computer modeling and simulation, separate confinement heterostructures.

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## 1. INTRODUCTION

Since around 1990, virtually all designs of semiconductor lasers are injection lasers with double heterostructure and separate confinement (SCH) [1], [2].

In SCH lasers electronic transitions and photons generation are localized in the most narrow-band part - a quantum well (QW), whose width can reach several tens of angstroms, and an optical waveguide is a region of width about 1 μm. This separate confinement of electronic and optical excitations can significantly lower the threshold current density of laser generation and increase the power of semiconductor lasers operating in at room temperature.

Due to the relative simplicity and perfection of technology, solid solutions of $Al_xGa_{1-x}As$ are used most commonly as wide-gap semiconductors in SCH lasers. Reaching the threshold current density of these lasers less than 1 kA/cm$^2$ at room temperature has opened up prospects for their practical application and served as a turning point in their production. However, further progress in this direction is associated with optimizing the design of laser diodes and, in particular, taking into account the role of QW width and the values of the molar concentration $x$ of aluminum in the QW and waveguide regions, possible effects of strains and heat released, optimizing doping concentrations, etc. Computer simulations taking into account the interplay between all these effects together are desirable.

In this paper, as our first description of a more complex problem, we show results of simulation of the influence of the molar concentration of aluminum in the QW and the waveguide region on the energy spectrum of charge carriers in the QW. It is useful to have these results as a reference in analysis of more complex modeling. In particular, we observe that not only energy levels in QW should be designed carefully (laser wavelength depends on them) but also the difference between QW energy levels and the QW depth itself is of importance on all opto-electrical laser characteristics as well [7].

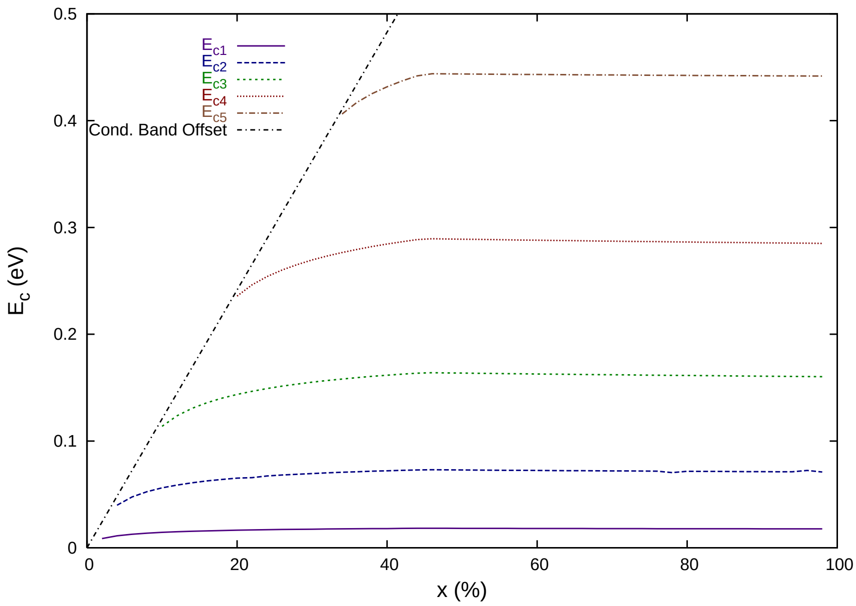


Fig. 1 – Conduction band energy levels for a 15 nm width of QW. It was assumed that Al concentration in QW is 0% and $x$ is Al concentration in waveguide.

We choose to conduct simulation in a commercial software package Sentaurus TCAD of Synopsys [4].

The structure of SCH lasers we are studying consists of $Al_xGa_{1-x}As$ layer as an $n$-type emitter of thickness 1.5 μm, with doping concentration of $10^{18}/cm^3$, waveguide of $Al_xGa_{1-x}As$ of thickness 0.12 μm with $n$-type doping concentration of $5 \cdot 10^{15}/cm^3$, an active laser region of $Al_xGa_{1-x}As$ of thickness 9, 12, 15 or 18 nm with $n$-type doping concentration of $10^{15}/cm^3$, again waveguide of $Al_xGa_{1-x}As$ of thickness 0.12 μm with $n$-type doping concentration of $5 \cdot 10^{15}/cm^3$, and a layer of $Al_xGa_{1-x}As$ as a $p$-type emitter of thickness 1.5 μm, with $p$-type doping concentration of $10^{18}/cm^3$.

An important aspect of using $Al_xGa_{1-x}As$ solid solutions is that this compound

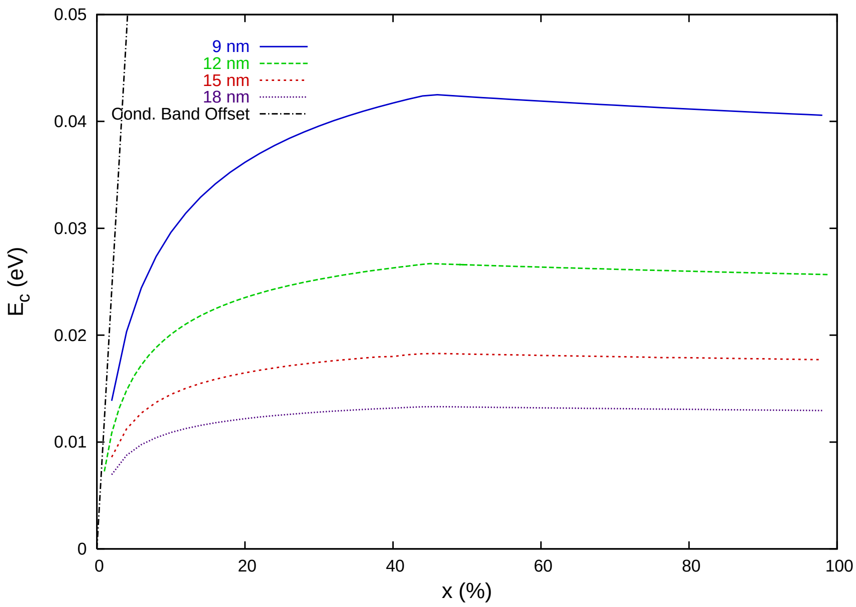


Fig. 2 – Comparison of the first energy level in QW for electrons for various QW widths, 9, 12, 15 and 18 nm. Al concentration in QW is 0% and $x$ is Al concentration in waveguide.

has two conduction-band minima. At $x < 0.45$, a direct transition between conduction and valance bands dominates, while for higher Al concentrations, an indirect transitions for $E_c(k)$, with electron wave-vector $k$ shifted in $X$ direction, $<100>$, are energetically favorable. An approximation that is used in Sentaurus TCAD for Al concentration dependence of energy gap $E_g$ at $T = 300$K has the form:

$$\begin{aligned} E_g(x) =& 1.42248 + 0.56267 \cdot x, \text{ for } x \leq 0.45, \\ E_g(x) =& 1.98515 + 0.14835 \cdot (x - 0.45) + 0.143 \cdot (x - 0.45)^2, \text{ for } x > 0.45. \end{aligned} \tag{1}$$

## 2. THE ENERGY SPECTRUM OF CARRIERS IN THE QW SCH LASERS

Emission of semiconductor SCH lasers is determined by interband transitions of electrons in the QW. Consequently, to determine the spectral characteristics of laser radiation it is important to know the energy spectrum of carriers in the QW.

Due to the specific structure of heterojunctions, this spectrum, as well as the wave functions describing the state of the carriers in the QW, can be found in the approximation of a rectangular potential well $V(y)$, on the basis of the stationary

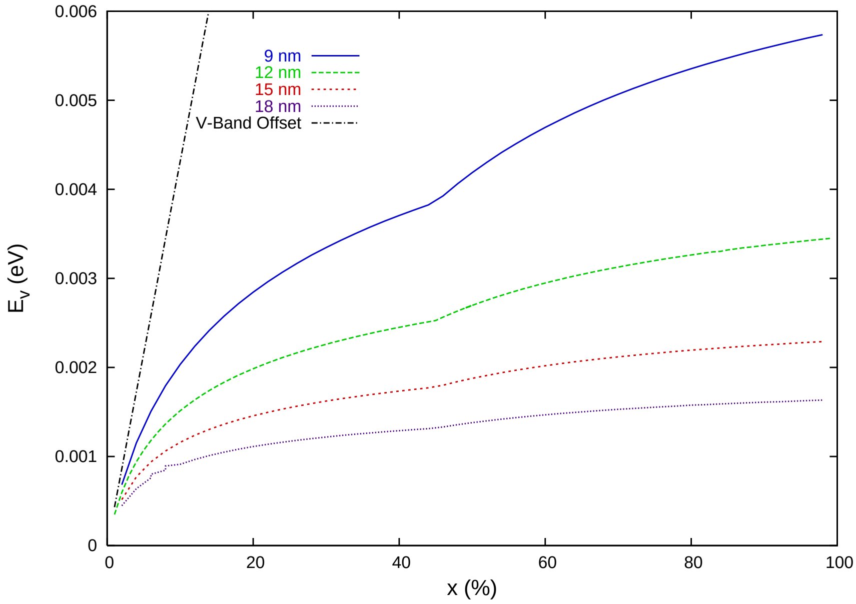


Fig. 3 – Comparison of the first energy level in QW for heavy holes for various QW widths, 9, 12, 15 and 18 nm. Al concentration in QW is 0% and $x$ is Al concentration in waveguide.

Schrödinger equation [3]:

$$\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial y}\left(\frac{1}{m(y)}\frac{\partial}{\partial y}+V(y)-E+\frac{\hbar^2 k^2}{2m(y)}\right)\right)\psi(y)=0, \tag{2}$$

where $k^2 = 2m(y)E/\hbar^2$, $\hbar$ is Planck's constant, $m(y)$ is effective mass (since the quantum well has different material properties than the waveguide, $m$ depends on the coordinate $y$, the axis assumed here to be directed perpendicular to the QW layer), and $E$ is energy of carriers relative to the bottom of quantum well.

Eigenstates of (2) could be found analytically [3]. They are in the form of symmetric and anti-symmetric stationary wave functions. The number of states in QW is limited and depends on QW width $L$ and its potential depth, which we will call conduction band and valance band offsets, for electrons and holes, respectively, as well it depends on effective masses of charge carriers.

Software package Synopsys Sentaurus TCAD solves Equation 2 numerically. There, energy of states in QW are found in Sentaurus's device log files, which are plain text files and can be easy parsed by using custom written Perl* scripts. The reason we use Perl is also that it integrates ergonomically with the entire Linux computational environment, which is our preferred, efficient operational system. We use

*PERL is "Practical Extraction and Report Language", `http://www.perl.org`

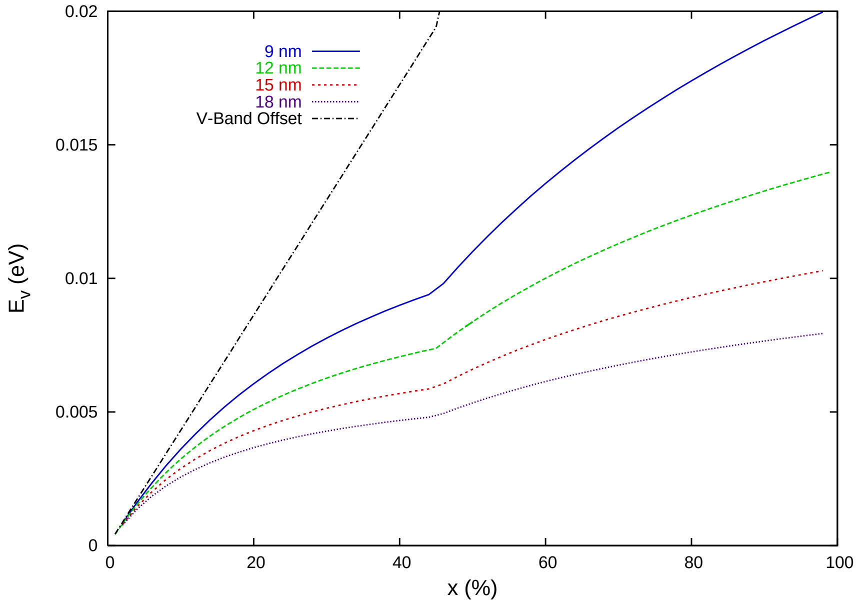


Fig. 4 – Comparison of the first energy level in QW for light holes for various QW widths, 9, 12, 15 and 18 nm. It was assumed that Al concentration in QW is 0% and $x$ is Al concentration in waveguide.

Perl scripting language for control of batch processing and changing parameters of calculations, as well for manipulation on resulting text data files. A more detailed description, with examples of scripts, is available on our laboratory web site†.

We simulated operation of lasers with quantum well width equal to 9, 12, 15, and 18 nm, and various contents $x$ of aluminum in the active region and in the waveguide. It was assumed that the effective masses of electrons $(m)$ and heavy $(m_h)$ and light $(m_l)$ holes, expressed in units of the rest mass of electron, varies linearly with molar concentration of alumina in $Al_xGa_{1-x}As$ [4], and the temperature is $T = 300$K. We have than, as a good approximation: $m(x) = 0.057 \cdot x + 0.067$, $m_h(x) = 0.139 \cdot x + 0.481$, and $m_l(x) = 0.186 \cdot x + 0.074$. Figure 1 presents typical results for conduction band energy levels for a 15 nm width of QW, as a function of Al concentration in waveguide, while Figure 2 compares dependencies of the first conduction band QW state energy $E_{c1}$ on Al concentration, for various QW widths, 9, 12, 15 and 18 nm.

Figure 3 compares dependencies of the first valance band QW energy state of heavy holes, $E_{hh1}$, on Al concentration, for various QW widths, 9, 12, 15 and 18 nm, while Figure 4 shows similar results for light holes.

We performed also calculations for dependence of QW energy levels on Al

†`http://www.ostu.ru/units/ltd/zbigniew/synopsys.php`

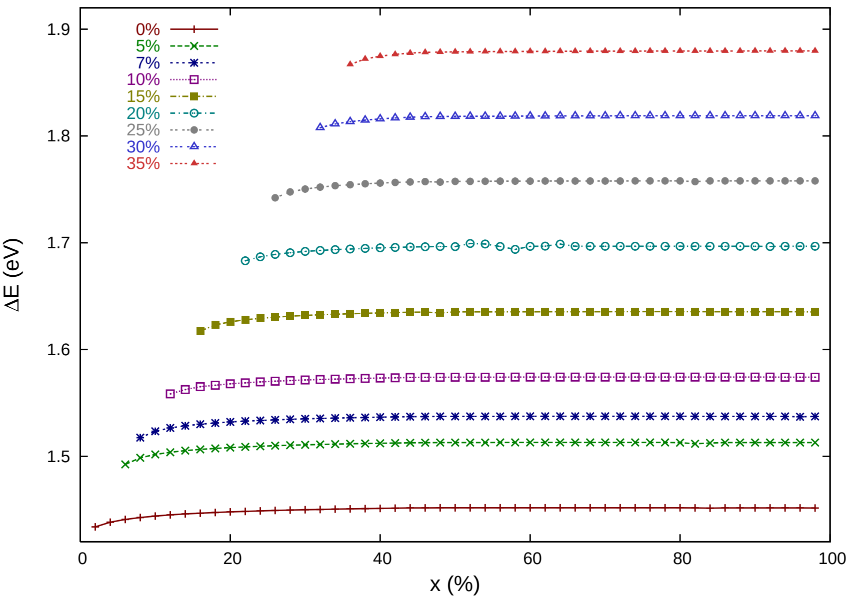


Fig. 5 – Transition energy between the first electron subband and the first heavy holes subband in QW, for 12 nm width of QW active region. $x$ is concentration of Al in waveguide, while every curve is computed for different values of Al concentration in active region of QW, as indicated in the figure.

concentration in waveguide, for a broad range of initial Al concentrations in QW, for all studied QW widths. A typical example data, for 12 nm width of QW, are shown in Figure 5.

A question arises, to what an extend the contribution of energy of QW states depends on the difference of Al concentrations between waveguide and the active region. To analyze that, we draw Figure 6. There, $E_{c1} + E_{hh1}$ is shown as a function of the difference between Al concentration in waveguide and in active region, $\Delta x$, for the case of 9 nm and 18 nm QW width, and different Al concentrations in the active region. The most interesting region, from the engineering point of view, is below $\Delta x$ of around $30\%$. We see that in that region, while at lower QW width of 9 nm differences between curves reach energies of around 10 meV, for QW width of 18 nm they become less than about 5 meV.

## 3. RADIATION CHARACTERISTICS OF AlGaAs-BASED SCH LASERS

Spectral characteristics of laser radiation are determined by the energy difference between the quantization levels of electrons and holes in the QW, as well as the characteristics of the resonator, which is used to enhance radiation. The maximum wavelength of the radiation produced in the active region of the laser diode may be

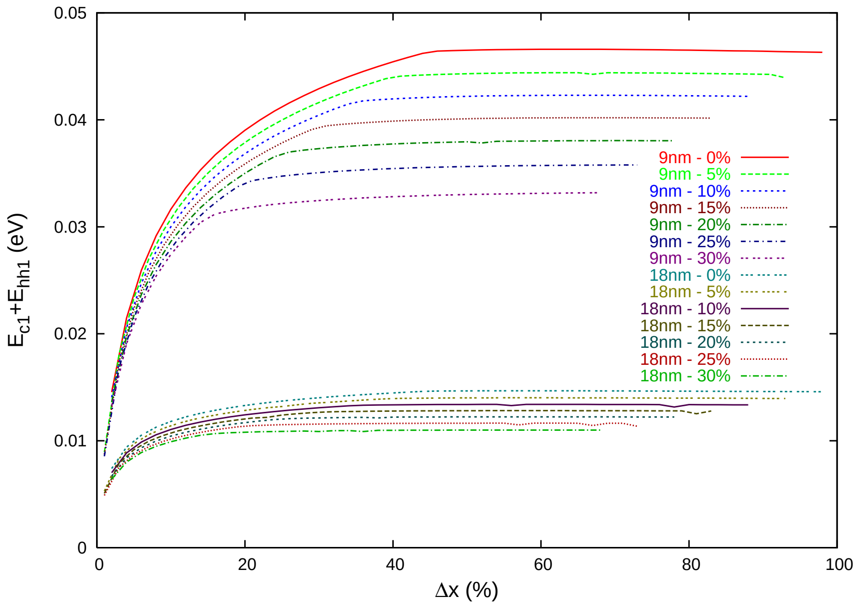


Fig. 6 – Comparison of QW states energy $E_{c1} + E_{hh1}$ as a function of the difference between Al concentration in waveguide and in the active region, $\Delta x$, for the case of 9 nm and 18 nm QW width, and different Al concentrations in the active regions, as indicated in the figure.

calculated by the formula:

$$\lambda = \frac{hc}{E_g + E_{c1} + E_{hh1}}, \tag{3}$$

where $h$ is Planck's constant and $c$ - the speed of light.

As shown by simulation results, the energy states of electrons, $E_{c1}$, and heavy holes, $E_{hh1}$, change very slowly with the changes in concentration difference of aluminum in the active region and waveguide.

Moreover, for a broad range of Al concentrations, the energy contribution from QW states does nearly not depend on the concentration of aluminum itself in the waveguide but is determined rather by Al concentration differences between the active region (QW) and waveguide.

The results of calculations of the wavelength $\lambda$, for SCH lasers with QW width equal to 9, 12, 15, and 18 nm, are presented in Figure 7. Markers in this figure correspond to wavelengths of high-power semiconductor lasers [5], and [6], produced in the Research Institute "Polyus" in Moscow. These lasers have active region (QW width) of 0.12 μm, with only background doping concentration. The lasing wavelength based on our calculations is shorter from the results observed experimentally, for about 10 nm.

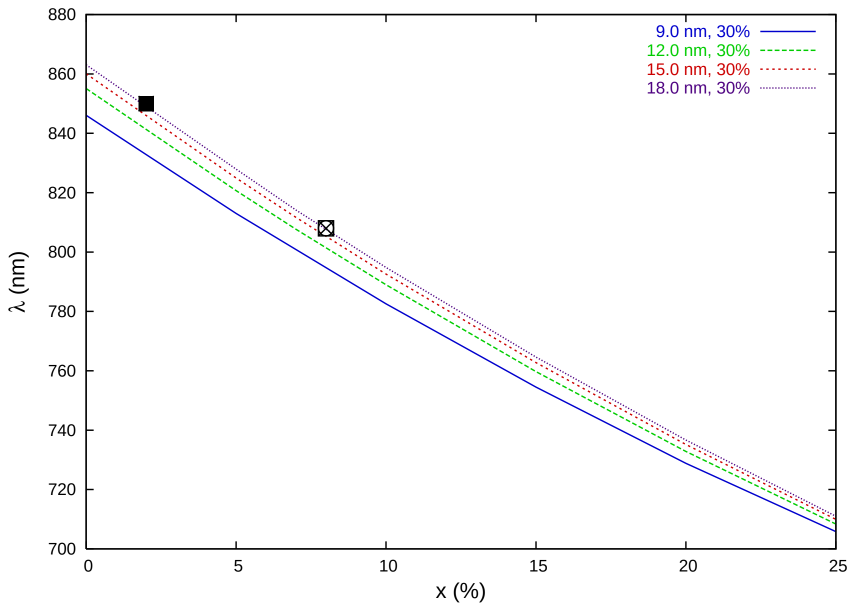


Fig. 7 – Lasing wavelength as a function of Al concentration in active region, when waveguide concentration is 30% of Al, for several values of QW width, as indicated in the figure. Markers correspond to wavelengths of high-power semiconductor SCH lasers produced at Research Institute ”Polyus” in Moscow.

We must point out however that Equation 3 does not take into account band gap renormalization due to finite carrier density. This correction depends on the carrier density at lasing threshold and it may be of the order of 10 meV, for carrier densities of the order of $10^{18}/\mathrm{cm}^3$. As other possible sources of contributions to lasing wavelength we consider thermal effects due to large energy released in active region and effects of strains. Our computer-modeling studies are continued in these directions.

We do not expect the existence of lasing action when Al concentration exceeds $45\%$, as electronic transitions would require then a change of wavevector $\Delta k > 0$, and these processes would require interaction with phonons. For that reason, however, studying physical processes around these Al concentrations is valuable.

## 4. CONCLUSIONS

In this single-mode lasers the main contribution to lasing wavelength $\lambda$ is determined by the semiconductor band gap in the QW, as well as the lowest energy states of electrons and holes in the QW.

At low Al concentrations in waveguide, energy levels in QW for both electrons and holes increases monotonically with concentration of aluminum, while at higher Al concentrations in waveguide, of around 50% and more, they become independent on concentration of aluminum.

With the increase of the concentration in active region, the lasing wavelength $\lambda$ decreases, in close agreement with results obtained at the Research Institute "Polyus" in Moscow. Research on the role of other possible contributions to lasing frequency is continued.

These results are important from the point of production of SCH lasers based on solid solutions of $Al_xGa_{1-x}As$ and can be used to optimize the design of these lasers. They are useful also as a reference in laser designing: not only energy levels in QW should be considered carefully (laser wavelength depends on them) but also the difference between uppermost QW energy levels and the QW depth itself is of importance on all opto-electrical laser characteristics as well [7].

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