

SQW PbSe/PbSrSe Emitted Wavelengths Calculations for Breath Analysis Applications

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Abstract

A theoretical model was developed to conduct the effects of non parabolicity and temperature on PbSe/Pb_{0.934}Sr_{0.066}Se nanostructure system. In this work we analyzed PbSe/Pb_{0.934}Sr_{0.066} SQW structure by calculating the quantized energy levels, confinement factor, modal gain and current density relationship taking into consideration the effects of non parabolic bands and operating temperatures. For the SQW system under investigation, it will be concluded that non parabolicity effects on emitted wavelengths are important to accurately determine the operable critical wavelength for detecting the biomarkers of interest in breath analysis applications. Moreover, the emitted wavelengths decreases with increasing temperature which makes this system suitable for absorption spectroscopy applications where a good tunable diode laser is needed at various temperatures.

Keywords: lead salt lasers, infrared, modal gain, confinement factor, non-parabolicity.

1. Introduction

Lead salts or IV-VI material systems are being desirable for several applications such as IR spectroscopy, low cost mid-IR sensors, mid-IR opto-electronic devices, and medical applications [1, 2]. Based on literature reports, health conditions such as Breast cancer and Lung Cancer have biomarker molecules in exhaled breath at wavelengths in the infra-red (IR) region. A new technique that may play a key role in detecting these biomarkers is Tunable Laser Spectroscopy (TLS) [1]. PbSe/Pb_{0.934}Sr_{0.066}Se quantum well laser structures, as part of TLS system, can be used to generate these critical wavelengths that can be absorbed by the various biomarkers molecules and hence detecting their presence in parts per million (ppm). Laser emission at these critical wavelengths is related to several system parameters [1, 2].

In this work, analysis and design are done on PbSe/Pb_{0.934}Sr_{0.066}Se single quantum well (SQW) laser structure. The effects of non parabolic band structure of this material system and temperature are included in a developed model and studied extensively. The developed model is being used to calculate energy levels, emitted wavelengths, and confinement factor data to determine the critical parameters of interest to accurately determine the operable critical wavelength and temperature for detecting the biomarker of interest.

2. Material and Methods

For a well material with parabolic bands in the growth direction (z-direction), the effective masses in the

Schrodinger-like equation are at the extrema of the bands and are independent of the energy. For a well material with non-parabolic bands, such as the system under investigation, two methods can be used to solve for the energy levels [3,4]. The first method uses the "effective mass" equation, also known as the Luttinger-Kohn (LK) equation and the second method is the "energy-dependent effective mass" (EDEM) method. The energy level shifts due to non-parabolicity effects differ depending on the method and system parameters used. Throughout this work, the effective mass of the barrier material is considered constant and independent of energy. Due to limitation in using the Luttinger-Kohn equation [3], the energy-dependent effective mass method was adopted in this work for all calculations and analysis.

The energy gap and effective masses of Pb_{1-x}Sr_xSe system dependence on temperature according to these relations:

$$E_g(x,T) = 0.150 + 3.608x - 1.31x^2 + (0.430 - 3.093x + 6.495x^2) \times 10^{-3} T \text{ (eV)}$$

(for $0 \leq x \leq 0.276, 0 < T \leq 350K$) (1)

and the empirical equation for the longitudinal mass [2]:

$$m_{||}^*/m_0 = 0.3013 \times E_g + 0.00407$$

(for $0.2 \leq E_g \leq 1.2 \text{ eV}$) (2)

where the barrier is Pb_{0.934}Sr_{0.066}Se with $E_g=0.46 \text{ eV}$ and effective mass= $0.142 m_0$, and the well is PbSe with its $E_g=0.28 \text{ eV}$ and effective mass= $0.08 m_0$ at 300K. In this study we ignored the non-parabolicity effects of the barrier material. The difference in the energy gaps between the well material and the barrier material is assumed to be equally divided between the conduction and valence bands. The offset energy or the barrier potential for this system is 0.09 eV. This assumption is made because measurements on the offset energy for this system have not been made. In this study, the conduction and valence-band mobility effective masses in the well are assumed equal and the effective masses of the carriers outside the well are assumed constant.

3. Results and Discussions

The conduction band energy levels calculation assuming parabolic and non-parabolic bands are shown in Fig. 1. As shown in the figure, the energy levels including the effects of non parabolicity are lower than those excluding the effects of non-parabolicity and this difference is higher for small well width values and decreases as the well width is increased. Moreover, this effect is higher for higher quantized energy levels. The emitted wavelength values at 300K for the system are show in Fig. 2 where the effects of band non parabolicity are included and compared to those excluding the effects of

band non parabolicity. One notice that the emitted wavelength values are higher including non-parabolicity and this difference is higher for smaller well widths and decreases as the well width increases. For applications that require critical wavelength calculation such as the breath analysis technique, it is important to include the effects of non-parabolicity to be able to obtain the desired accurate results for detecting the existence of volatile compounds at their corresponding wavelengths. Therefore, in what follows, the effects of non-parabolicity are included in all calculation of the system. Also, these calculations are done only on the first energy levels transitions between the conduction and valence bands.

The emitted wavelengths as a function of five temperatures: 77K, 200K, 150K, 250K, and 300K are shown in Fig. 3. For a fixed well width, the emitted wavelengths decreases with increasing temperature and increases with increasing well width at the same temperature. This graph is important for investigators who are using this material system in tunable diode laser absorption spectroscopy to measure certain markers in exhaled breath which are correlated with certain diseases [5]. Examples include the measurement of exhaled nitric oxide for Asthma at 5.2 μm [6,7], Acetone for Diabetes at 3.4 μm [8], Acetaldehyde for Lung Cancer at 5.7 μm [9]. By investigating Fig. 2, it will be obvious that at room temperature the system can't be used to detect Asthma or Lung Cancer and it can be used to detect Diabetes at around 4 nm well width. However, from Fig. 3, it can be shown that detecting Asthma and Lung Cancer biomarkers in the breath requires operating the system at 77K at well widths around 6 nm and 12 nm, respectfully.

Therefore it is important to include the effects of non-parabolicity to be able to calculate all the energy levels for the system. Similar results can be obtained for the valence band. The effects of temperature on the confinement factor are shown in Fig 4. The confinement factor increases with temperature at a fixed well width and this is due to the effects of temperature on the emitted wavelength as seen from Fig. 3. The confinement factor analysis are needed to determine the threshold current density needed for lasing to occur [10].

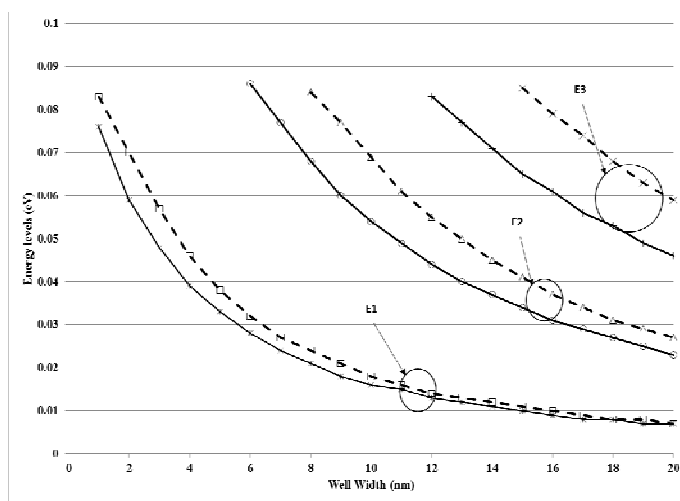


Fig. 1. The effects of non parabolicity (solid line) on the conduction band energy levels at 300K.

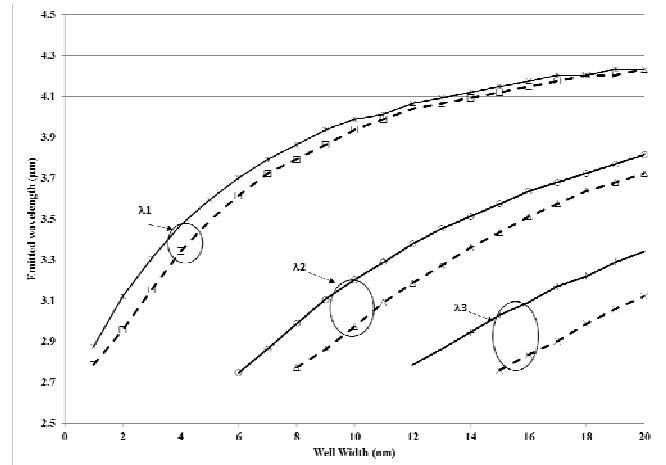


Fig.2. The effects of non parabolicity (solid line) on the emitted wavelengths at 300K.

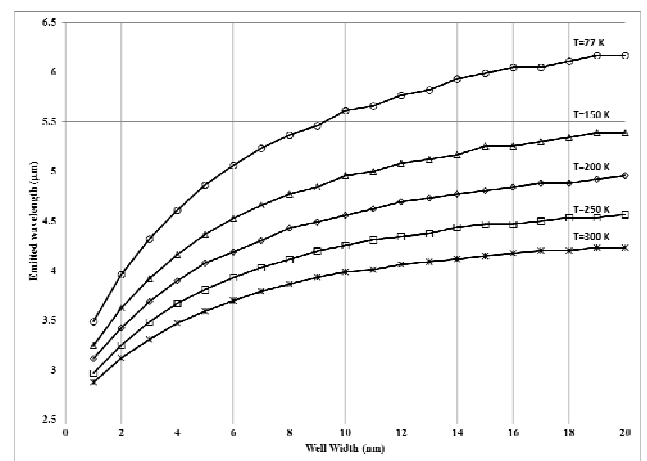


Fig.3. The effects of temperature on the emitted wavelengths. The effects of non-parabolicity are included in the calculations.

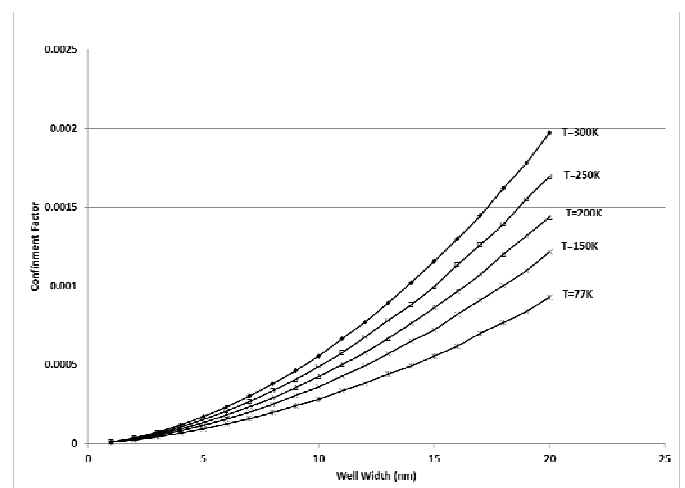


Fig. 4. The effects of temperature on the confinement factor as a function of well width. The effects of non-parabolicity are included in the calculations.

4. Conclusions

In this work we analyzed PbSe/Pb_{0.934}Sr_{0.066} SQW structure by calculating the quantized energy levels, emitted wavelengths, and confinement factor data. The effects of band non-parabolicity was studied and it was shown that non-parabolicity will have small but not negligible effect on emitted wavelengths. Some of the breath biomarkers can be detected with this system at room temperature, and others can be detected at different operating temperatures. To accurately detect a biomarker with this system, an accurate determination of the critical well width and operating temperature is a must.

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Fig. 1. The effects of non parabolicity (solid line) on the conduction band energy levels at 300K.

Fig.2. The effects of non parabolicity (solid line) on the emitted wavelengths at 300K.

Fig.3. The effects of temperature on the emitted wavelengths.The effects of non-parabolicity are included in the calculations.

Fig. 4. The effects of temperature on the confinement factor as a function of well width. The effects of non-parabolicity are included in the calculations.

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