An Analytical Model of SH-LED for Gas Sensor Instrumentation in Mid-infrared (2-5μm) Region

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ABSTRACT:  
In this paper, we present an analytical model of a P⁺-InAs₀.₃₆Sb₀.₂₀P₀.₄₄/ n⁰-InAs/n⁻-InAs single heterostructure light emitting diode (SH-LED) suitable for use as source in gas detection instrumentation system based on optical absorption gas spectroscopy in the mid-infrared spectral region at room temperature. The model takes into account all dominating radiative and non-radiative recombination processes, interfacial recombination and self-absorption in the active layer of the SH-LED structure. The effect of various radiative and non-radiative recombination mechanisms on the quantum efficiency and hence output power of the LED has been evaluated. The output power of the SH-LED has been computed as a function of bias current and compared/ contrasted with the reported experimental results.

Keywords— Gas instrumentation, Light emitting diode, Mid-infrared, Single heterostructure.

1. Introduction  
The mid-infrared (2-5μm) spectral region contains the strong fundamental absorption bands of a number of combustible and atmospheric pollutant gases like NH₃ (2.1 μm), HF (2.5μm), CH₄ (2.35 and 3.7 μm), N₂O (3.9 and 4.5 μm), SO₃ (4μm), CO₂ (4.27 μm) and CO (2.3 and 4.6 μm). Presently, the optical absorption based infrared gas detection techniques are becoming popular, as they are the only ones, which are truly gas specific and hence reliable for gas sensor instrumentation. The light sources for gas sensing must operate in a continuous wave regime, with optical power higher than 1 mW [1]. The ternary III-V semiconductor alloy InAs₁ₓSbx is a very promising material for the fabrication of mid-infrared light emitting diode as its energy gap covers the 3-5μm spectral range. But its room temperature continuous operation is limited by non-radiative recombination such as Shockley-Read-Hall (SRH) and Auger recombination process, which are the dominating recombination mechanisms for narrow bandgap semiconductor material system. Several double heterostructure junction [1]-[4], single heterostructure junction [5] and more recently, the homo-junction [6] mid-infrared light emitting diodes for various target wavelengths have been reported, but the systematic theoretical studies to characterize these light emitting diodes for their room temperature operation have received little attention. It is, therefore, necessary to develop an analytical model for the analysis of SH-LED operating in mid-infrared spectral region. As the technology of narrow bandgap semiconductors is not yet fully mature and the cost of experimental investigation is high, there is a need for further theoretical studies in the area to properly address the challenges ahead for the realization of room temperature SH-LED. The outcome of the theoretical studies will provide useful design guidelines for improving and optimizing the existing structures and development of new device prototype.

2. The Proposed SH-LED Structure  
The device under consideration is the single heterostructure based on P⁺-InAs₀.₃₆Sb₀.₂₀P₀.₄₄/ n⁰-InAs/ n⁻-InAs materials system. The schematic of the structure is shown in Fig. 1(a). It consists of a highly doped (P) layer of quaternary materials InAsSbP of larger bandgap over the undoped InAs layer (active layer) of smaller bandgap to form the heterojunction. This whole structure has been fabricated on N⁺-InAs substrate of the same conductivity as that of active region material. The energy band diagram of the heterojunction has been obtained by applying the Anderson’s model [7]. According to this model the proposed structure forms the staggered Type-IIb band alignment. The energy band diagram of the structure is shown in Fig. 1(b). The energy bandgaps of the two semiconductors, their valance and conduction bandage discontinuity and built-in-potential at n⁺-P⁺ interinterface after formation of heterojunction are related as
analytically using the boundary conditions. Equation (7) can be solved for the hole diffusion constant and diffusion length given by [8].

The one dimensional governing charge equation of the active region under forward bias is given by [8]:

\[ \nabla^2 (\Delta p(x)) = \frac{\Delta p(x)}{L_p^2} \]  \hspace{1cm} (7)

where \( \Delta p(x) \) is the injected hole density, \( L_p \) is the diffusion length given by \( L_p = \sqrt{D_p \tau} \), \( D_p \) is the hole diffusion constant and \( \tau \) is the minority carrier lifetime. Equation (7) can be solved analytically using the boundary conditions

\[ \frac{d\Delta p(x)}{dx} \bigg|_{x=0} = \frac{J}{qD_p} - \frac{s_p}{D_p} \Delta p(0) \]  \hspace{1cm} (8)

\[ \frac{d\Delta p(x)}{dx} \bigg|_{x=d} = 0 \]  \hspace{1cm} (9)

where \( J \) is the injected current density, \( q \) is the electronic charge, \( d \) is the thickness of active layer and \( s_p \) is the surface recombination velocity of holes at P-n heterointerface. The hole density in the active region is calculated using (7), (8) and (9) as

\[ \Delta p(x) = \frac{JL_p}{qD_p} \left[ \cosh \left( \frac{d-x}{L_p} \right) - \frac{L_p s_p}{D_p} \cosh \left( \frac{d}{L_p} \right) \right] \]  \hspace{1cm} (10)

The average hole density in the active region is given by

\[ \bar{\Delta p} = \frac{1}{d} \int_0^d \Delta p(x) \, dx = \frac{J}{q} \frac{\tau_e}{d} \]  \hspace{1cm} (11)

where \( \tau_e \) is the effective carrier lifetime when surface recombination is important and is given by

\[ \tau_e = \tau \frac{\sinh \left( \frac{d}{L_p} \right)}{\sinh \left( \frac{d}{L_p} \right) + \frac{L_p s_p}{D_p} \cosh \left( \frac{d}{L_p} \right)} \]  \hspace{1cm} (12)

For \( \frac{L_p s_p}{D_p} \ll 1 \) (12) reduces to

\[ \frac{1}{\tau_e} = \tau \frac{1}{\frac{1}{\tau} + \frac{s_p}{d}} \]  \hspace{1cm} (13)

where \( \tau \) is the net minority carrier lifetime given by
where \( \tau_{SRH} \) are the radiative, Auger and SRH recombination lifetimes of the minority carrier in the active region respectively and can be estimated using [9].

### 3.1 The Current-Voltage Characteristics of the Structure

The current through the forward bias DH-LED consists of two components

(i) Diffusion current arising from the minority carriers injected from neutral P⁺ and n⁰ regions. (ii) Drift current due to generation recombination in the depletion region at P⁺-n⁰ junction.

#### 3.1.1 The diffusion component

Due to the presence of discontinuities in the bandages at the heterointerface, the diffusion currents in heterostructure are different from that in homojunction. In the given structure, electrons having energy equal to \( V_d - \Delta E_c \) can reach the heterointerface of P⁺ region and similarly the holes from P⁺ region, having energy equal to the barrier \( V_d - \Delta E_v \) can reach to the interface at n⁰ region to constitute the total diffusion component of the current in the structure. The diffusion component of current is calculated by solving the standard one-dimensional diffusion equation (7) under forward bias using appropriate boundary conditions. The diffusion components of current due to injection of electrons and holes in P⁺ and n⁰ regions injected from n⁰ and P⁺ region respectively can be obtained as [10]

\[
I_{dn} = q \frac{AD_n}{L_p} n_{p0} \frac{L_n s_n}{D_n} \cos \left( \frac{d - x_p}{L_n} \right) + \sinh \left( \frac{d - x_p}{L_n} \right) \\
(15)
\]

\[
I_{sp} = q \frac{AD_p}{L_p} p_{n0} \frac{L_p s_p}{D_p} \cos \left( \frac{t - x_n}{L_p} \right) + \sinh \left( \frac{t - x_n}{L_p} \right) \\
(16)
\]

where \( n_{p0} \) and \( p_{n0} \) are the minority carrier concentration in P⁺ and n⁰ regions at equilibrium, \( L_n \) and \( L_p \) are the diffusion lengths for electrons and holes respectively, \( D_n \) and \( D_p \) are their respective diffusion coefficients, \( s_n \) and \( s_p \) are the surface recombination velocities for electron and holes at the interface. Here \( x_n \) and \( x_p \) are the width of the depletion region on the respective sides.

The total diffusion current component for the structure is given by

\[
I_d = (I_{sn} + I_{sp}) \exp \left[ \frac{qV}{kT} - 1 \right] \\
(17)
\]

#### 3.1.2 The generation-recombination component

The carriers generated in the depletion region are generally separated under the application of existing electric field. The transport of carriers across the heterojunction is strongly affected by the trap levels at the heterointerface inside the depletion region. The carrier generation-recombination in the active region is governed by the Shockley-Read-Hall equation. The electron and hole components of current arising from the generation recombination in the depletion region is given by

\[
I_{gr} = 2A \sqrt{3(kT)^3} \sigma N_f \left[ \frac{1}{m_{nn}^*} \frac{n_{p0} x_p}{V_{d1}} \frac{1}{m_{pp}^*} \frac{n_{n0} x_n}{V_{d2}} \right] \exp \left( \frac{qV}{2kT} \right) \]

(18)

where \( m_{nn}^* \) and \( m_{pp}^* \) are the effective masses of electron and holes in the n⁰ and P⁺ regions respectively, \( V \) is the applied voltage, \( W \) is the total depletion width, which is the function of applied voltage \( V \).

### 4. The Quantum Efficiency and Power Output of SH-LED

The radiative recombination lifetime \( \tau_R \) is given by

\[
\tau_R = \frac{1}{B_r p} \\
(19)
\]

Where \( B_r \) is the radiative recombination coefficient and \( p \) is the hole concentration.
The Auger recombination lifetime $\tau_A$ is given by

$$\tau_A = \frac{1}{A p^2} \quad (20)$$

Where $A$ is the Auger coefficient.

Using (19) and (20), the quantum efficiency, neglecting the SRH recombination is given by

$$\eta = \frac{B_r p}{B_r p + A p^2} \quad (21)$$

Also using charge neutrality condition the current density $J$ is given by

$$J = \frac{d q A p}{\tau} \quad (22)$$

Using (21) and (22), the output power $P$ of the SH-LED is given by

$$P = A_d \left(\frac{h v}{q}\right) B_r \left(n^4 q d \tau^2\right)^{\nu_3} J^\frac{3}{\nu_3} \quad (23)$$

From equation (23) the effect of various radiative and non-radiative recombination on the power output (or quantum efficiency) and output power with injection current density of the SH-LED can be evaluated.

4. Results and Discussions

Numerical computation has been done for $P^-$InAs$_{0.48}$Sb$_{0.22}$P$_{0.30}$/n$^0$-InAs/ n$^+$-InAs single heterostructure light emitting diode (SH-LED) at room temperature. The values of different parameters used in the model are summarized in the Table1. Some of the parameters of the quaternary materials (InAsSbP) have been computed from the parameters of the constituent binary/ternary materials using the linear interpolation formula.

Fig. 2 depicts the forward-bias current-voltage characteristics of the proposed structure. The graph shows the usual exponential rise in the current with the increase in the applied voltage. The cut-in voltage is approximately 0.27 V. Fig. 3 shows the effect of various recombination mechanisms on the quantum efficiency of the SH-LED. The study reveals that the quantum efficiency of the SH-LED is greatly affected by the non-radiative recombination mechanisms such as SRH and Auger recombination. It is seen that at room temperature operation the reduction in the overall efficiency is dominated by Auger recombination process.

Fig. 4 shows the variation of optical power output with the bias current. The experimental results reported by Krier et al. [5] for the same structure is shown by circles. It is found that theoretical results are in good agreement with the reported experimental results [5].

5. Conclusion

The study reveals that the quantum efficiency of the SH-LED source is significantly affected by non-radiative recombination process including surface recombination. The SRH recombination is dominating at low temperature while the Auger recombination is dominant at higher temperature. In order to improve the performance of room temperature mid-infrared LEDs based on narrow bandgap semiconductor it is necessary to suppress the SRH and Auger recombination. SRH recombination can be greatly reduced by improving the processing of the device whereas one has to modify the device structure suitably using the concept of bandgap engineering in order to reduce Auger recombination at room temperature. On the basis of the theoretical results, it is expected that this SH-LED can be used as a suitable source in gas instrumentation system. The model developed here would provide useful design guidelines for the experimentalists for developing device prototypes.

REFERENCES

[5] A. Krier and X.L. Huang, Design considerations for uncooled InAs mid-infrared light emitting diodes grown by liquid phase


IMPORTANT FIGURES AND GRAPHS

Fig. 1 (a) Schematic of the proposed SH-LED
(b) Energy band diagram

Fig. 2 Forward-bias current-voltage characteristics of the SH-LED

Fig. 3 The effect of various recombination mechanisms on the quantum efficiency of the SH-LED

Fig. 4 Variation of optical power output of the SH-LED with the drive current.