ELECTRON-PHONON INTERACTIONS IN INTERSUBBAND LASER HETEROSTRUCTURES

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We present a simple semianalytical model, which allows comprehensive analysis of the LO-phonon assisted electron relaxation in quantum well intersubband semiconductor lasers. Examples of scattering rate tailoring in type-I double quantum well heterostructures and analysis of the subband depopulation process in type-II heterostructures illustrate applicability of the model.

1. Introduction

Multiple quantum well (QW) heterostructures are used widely for novel intersubband semiconductor lasers operating in the technologically important mid-infrared and far-infrared spectral ranges. Essential to the laser heterostructure design is maintaining proper balance between the inter- and intrasubband electron scattering rates, which determine the electron density distribution in the laser active region. This balance influences not only the population inversion between the lasing states but also the threshold level for the electrical or optical pumping thus affecting the possibility of high-temperature continuous-wave laser operation. In polar semiconductors, electron relaxation is usually determined by polar excitations: LO-phonons and, at a higher level of electron concentration, plasmons. In this paper, we describe briefly a physical model of electron and polar phonon confinement, which allows tailoring of the scattering rates for the most important relaxation processes in intersubband laser heterostructures. A phenomenological approach based on the envelope function approximation will be employed consistently for the analysis of both the electron and phonon spectra. In part 2 we start with the dielectric continuum model, which provides a simple description of the polar mode confinement and allows also incorporation of the screening and plasmon effects. Several examples of electron-phonon scattering rate tailoring in type-I double quantum well heterostructures will illustrate the application of the model. To include into consideration narrow-gap type-I and, especially, broken-gap type-II laser heterostructures, where nonparabolicity and band-mixing effects in electron energy spectrum must be taken into account, we proceed in part 3 with multiband quantization scheme allowing simple semianalytical treatment of the electron confinement in such heterostructures. In part 4 we use this approach to evaluate and compare the rates of two competitive processes of the lower lasing state depopulation in type-II cascade laser heterostructures: direct interband tunneling through the heterostructure “leaky window” and interband electron transitions assisted by LO-phonon emission.
2. Dielectric Continuum Model for Polar Excitations in Layered Heterostructures

Energy spectrum of the polar excitations in a layered heterostructure can be characterized by a model Hamiltonian

\[ \hat{H}_{ph} = \frac{1}{8\pi} \sum_{m,n} \int d^3r \left\{ E_{mn}^2 \frac{\partial \omega_m(\omega)}{\partial \omega} \right\} = \frac{1}{2} \sum_{m,n} \left( \hat{a}_{mn}^* \hat{a}_{mn} + \hat{a}_{mn}^+ \hat{a}_{mn}^* \right) \hbar \omega_{mn}. \]  

(2.1)

Here, \( <...> \) denotes time-averaging, and a phenomenological dielectric function \( \epsilon(\omega) \) describes the frequency dispersion of the semiconductor susceptibility in each layer, ignoring spatial dispersion and mode damping. Real-valued potentials are assumed for quasi-2D polar modes \( \omega_{mn} \); all other notations are self-explanatory:

\[ E_{mn}(r,t) = -\nabla \Phi_{mn}(r,t), \quad \Phi_{mn}(z) = \hat{a}_{mn}(t)e^{iqz} + \hat{a}_{mn}(t)e^{-iqz}; \quad \hat{a}_{mn}(t) = e^{-i\omega_{mn}t} \hat{a}_{mn}. \]  

(2.2)

(2.3)

After the time averaging, Eq. (2.1) gives the expression for the amplitude of 2D polar mode

\[ \Phi_{mn}^2 = \frac{2\pi \hbar \omega_{mn} \varphi_{mn}^2}{L^2 \int dz (\varphi_{mn}^2 + q^2 \varphi_{mn}^2) \tilde{\omega}(\omega_{mn})}; \quad \tilde{\omega}(\omega) = \frac{1}{2} \frac{\partial \omega_m(\omega)}{\partial \omega}. \]  

(2.4)

The spatial distribution of the polar mode potential across the heterostructure is represented here by smooth envelope function \( \varphi_{mn}(z) \).

To simplify the calculation of the electron scattering rates in heterostructures it is often convenient to use bulk-like spectrum of polar excitations \( \omega_B \), that is assuming that the confined 2D electrons interact with dispersionless 3D bulk LO phonons.

\[ \Phi_B^2 = \frac{2\pi \hbar \omega_B \varphi_{mn}^2}{L^2 (q^2 + q_z^2) \epsilon_{eff}(\omega_{mn})}; \quad \epsilon_{eff}(\omega) = \tilde{\omega}(\omega_B). \]  

(2.5)

To facilitate comparison between the two models we write (2.4) in a similar manner

\[ \Phi_{mn}^2 = \frac{2\pi \hbar \omega_{mn} \varphi_{mn}^2}{L^2 q \epsilon_{eff}(m, q)}; \quad \epsilon_{eff}(m, q) = \int dz (\varphi_{mn}^2 + q^2 \varphi_{mn}^2) \tilde{\omega}(\omega_{mn}), \]  

(2.6)

thus introducing an effective dielectric constant for polar mode \( \omega_{mn} \)

\[ \epsilon_{eff}(m, q) = \frac{1}{2q} \int dz (\varphi_{mn}^2 + q^2 \varphi_{mn}^2) \tilde{\omega}(\omega_{mn}), \]  

(2.7)

and normalization condition for the envelope functions \( \varphi_{mn}(z) \)

\[ \frac{1}{2q} \int dz (\varphi_{mn}^2 + q^2 \varphi_{mn}^2) = 1. \]  

(2.8)
With this normalization, in a homogeneous material we would have \( \varepsilon_{\text{eff}}(m,q) = \varepsilon_{\text{eff}}^{(B)} \).

To characterize the coupling with polar modes, we consider the matrix element for the intersubband \( i-f \) electron transition induced by the mode potential (2.6):

\[
\left| M_{if}(m) \right|^2 = \frac{\pi e^2 \hbar \omega_{mq}}{L^2 q} \beta_{if}(m)(q). \tag{2.9}
\]

The quantity

\[
\beta_{if}^{(m)}(q) = \frac{I_{if}(m,q)}{\varepsilon_{\text{eff}}(m,q)}; \quad I_{if}(m,q) = \left| \int dz \Psi_i^*(z) \varphi_{mq}(z) \Psi_f(z) \right|^2. \tag{2.10}
\]

defines a dimensionless coupling parameter for a 2D polar mode \((m,q)\). Here, \( \Psi_i(z) \) and \( \Psi_f(z) \) are normalized envelope functions of the initial and final electron states in an intersubband transition, for certainty, in a scattering process \((i, K) \rightarrow (f, K-q)\) assisted by the emission of polar excitation quantum \( \hbar \omega_{mq} \). For bulk-like excitations with amplitudes (2.5), after integration over \( q_z \) the effective matrix element takes exactly the same form (2.9), with the coupling parameter

\[
\beta_{if}^{(B)}(q) = \frac{I_{if}^{(B)}(q)}{\varepsilon_{\text{eff}}^{(B)}}; \quad I_{if}^{(B)}(q) = \int dz' \Psi_i^*(z) \Psi_f(z') \int dz'' \Psi_i^*(z'') \Psi_f(z'') e^{-i[\hat{q} \cdot z]} \tag{2.11}
\]

So defined, this allows simple and illustrative comparison of the intersubband scattering rates, \( \Gamma_{if} \), calculated in these two models of excitation spectra:

\[
\Gamma_{if} = \frac{2\pi}{\hbar} \sum_{m,q} \left| M_{if}(m) \right|^2 \delta(E_i - E_f - \hbar \omega_{mq}) =
\]

\[
e^2 \int \frac{d^2 q}{2q} \sum_m \omega_{mq}(q) \beta_{if}^{(m)}(q) \delta(E_i - E_f - \hbar \omega_{mq}); \tag{2.12}
\]

\[
e^2 \omega_B \int \frac{d^2 q}{2q} \beta_{if}^{(B)}(q) \delta(E_i - E_f - \hbar \omega_B). \tag{2.13}
\]

If dispersion of the 2D polar spectrum is negligible, the sum rule would hold true

\[
\beta_{if}^{(B)}(q) = \sum_m \beta_{if}^{(m)}(q). \tag{2.14}
\]

However, as we shall demonstrate in the next section, the polar mode confinement effect in thin-layer QW heterostructures induces strong dispersion of the interface modes thus making the sum rule fail, so that instead of (2.14) we have the relationship

\[
\beta_{if}^{(w)}(q) < \sum_m \beta_{if}^{(m)}(q) < \beta_{if}^{(B)}(q). \tag{2.15}
\]
2.1. LO-phonon confinement in layered heterostructures

In low-doped binary materials, the polar LO-phonons dominate the electron relaxation. The model dielectric function can be chosen in the form

\[ \varepsilon(\omega) = \varepsilon_{\infty} \frac{\omega^2 - \omega_{LO}^2}{\omega^2 - \omega_{TO}^2}. \]  

(2.16)

Here, \( \omega_{LO} \) and \( \omega_{TO} \) are, correspondingly, the longitudinal and transverse bulk optical phonon frequencies. Bulk effective dielectric constant (2.5) becomes

\[ \varepsilon_{eff}^{(B)}(\omega_{LO}) = \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_0} \right)^{-1}, \quad \varepsilon_0 = \varepsilon_{\infty} \frac{\omega_{LO}^2}{\omega_{TO}^2}. \]  

(2.17)

In the dielectric continuum model, \(^6\) the polar mode potentials are found from the equation of electrostatics

\[ \nabla (\varepsilon \nabla \Phi_m) = 0. \]  

(2.18)

In conjunction with the model dielectric function (2.16), this gives two basic types of polar phonon modes in a layered heterostructure, which together form an orthogonal and complete set \(^7\):

- Dispersionless confined LO solutions with nodes at the layer boundaries \( z_l \)

\[ \varphi_{mq}^{(c)}(z) = \left[ \frac{4q/a_l}{q^2 + q_m^2} \right]^{1/2} \sin q_m(z - z_l); \]  

(2.19)

\[ a_l = z_{l+1} - z_l; \quad q_m = \frac{m\pi}{a_l}; \quad \omega_{mq}^{(c)} = \omega_{LO}. \]

- Dispersive interface solutions satisfying at the boundaries the electrostatic boundary conditions

\[ \varphi_{mq}^{(i)}(z) = \sum_{i=0}^{N} \left[ C_{i,1} e^{q(z_i-z)} + C_{i,2} e^{q(z-z_i)} \right]. \]  

(2.20)

\[ \varphi_i(z_l) = \varphi_{i-1}(z_l), \quad \varepsilon_i \frac{\partial}{\partial z} \varphi_i(z_l) = \varepsilon_{i-1} \frac{\partial}{\partial z} \varphi_{i-1}(z_l). \]  

(2.21)

The latter can be conveniently represented by a transfer matrix \(^8\)

\[ C(l) = Q(l)C(l-1); \quad Q(l) = \frac{1}{2\varepsilon_l} \begin{bmatrix} (\varepsilon_l + \varepsilon_{l-1}) e^{-q_{l-1}} & \varepsilon_l - \varepsilon_{l-1} \\ (\varepsilon_l - \varepsilon_{l-1}) e^{q_{l-1}} & (\varepsilon_l + \varepsilon_{l-1}) e^{q_{l-1}} \end{bmatrix}. \]  

(2.22)

Since \( C_1(0) = C_2(N) = 0 \), this requires

\[ [Q(1)Q(2)\ldots Q(N)]_{22} = 0. \]  

(2.23)
This relation, completed with phenomenological expressions for dielectric functions in each layer \( l \), determines the dispersion of the interface modes. As an example, we consider binary GaAs/AlAs system. For ternary alloys, the two-pole model should be used for the dielectric functions.\(^9\) This does not alter the potential distributions of the interface modes, though increases the number of modes and modifies also the mode coupling parameters. Parameters used in calculations are represented in Table 1.\(^{10}\) For a single-interface heterostructure, dispersion equation (2.23) takes the form

\[
\varepsilon_b(\omega) + \varepsilon_w(\omega) = 0 .
\]  

(2.24)

This gives two dispersionless single-interface modes \( \omega_{l,b(w)} \), barrier- or well-type according to the mode frequency range:

\[
\omega_{LO,b(w)} < \omega_{1,b(w)} < \omega_{TO,b(w)} .
\]  

(2.25)

These modes are characterized, correspondingly, by two different effective dielectric constants (2.7)

\[
E_{\text{eff},l,b(w)} = \frac{\varepsilon_b + \varepsilon_w}{2} \omega = \omega_{l,b(w)} .
\]  

(2.26)

In the case of a double-interface heterostructure, single-QW or single-barrier type, Eq.(2.18) has two solutions of different spatial symmetry, \( \omega_k \) and \( \omega_A \), corresponding to

![Fig. 1. Dispersion of the interface phonon energies (a) and inverse effective dielectric constants (b) for a single-barrier (labeled thick lines, barrier width 2 nm) and single-well (unlabeled thin lines, well width 4 nm) heterostructures. Solid lines represent symmetric (S) modes, dashed lines – antisymmetric (A) modes. For single-well modes, the dispersion is inverted comparing with the single-barrier modes. Dotted lines correspond to single-interface dispersionless modes.](image-url)
symmetric (S) or antisymmetric (A) combinations of single-interface modes of adjacent interfaces. Each solution can be also of \( b \)- or \( w \)-type. The effective dielectric constants for these four modes, for example in a single-QW heterostructure with layer sequence \( b-w-b \), are

\[
\varepsilon_{\text{eff},S}(A)_{b(w)} = \frac{\tilde{\varepsilon}_b + \tilde{\varepsilon}_w}{1 + \xi} e^{\mp qa_1 (b,w)} ; \quad \varepsilon_{bwb} = \frac{1 - s e^{-qa_1}}{1 + s e^{-qa_1}}.
\]  

Here, \( a_1 \) is the QW width, index \( s = +1 \) corresponds to the symmetric, and \( s = -1 \) corresponds to the antisymmetric solution. Both the mode energies and the effective dielectric constants demonstrate considerable dispersion at \( qa_1 < 1 \); see Figure 1. For \( qa_1 > 1 \), the overlap of different single-interface modes shrinks, so that, as a reasonable limit, we have \( \varepsilon_{\text{eff},S(A)} \rightarrow \varepsilon_{\text{eff},1} \). In the case of a single-barrier (\( w-b-w \)) heterostructure, we have to transpose indexes \( w \) and \( b \) and substitute \( 1/\xi \) for \( \xi \) in (2.27). This entails simple relationship \( \tilde{\xi}_{bwb}(s) = \xi_{wbw}(-s) \) and implies the opposite dispersion for interface modes of the same parity in single-barrier and single-well heterostructures. This important feature is illustrated in Figure 1, where we have chosen a smaller value for barrier layer width to resolve the curves. These two different types of interface mode behavior, single-well-like and single-barrier-like, can be also traced in more complex multiple-interface heterostructures.

Double quantum well (DQW) heterostructures are of the utmost importance for many different applications and very often are used as active region elements in intersubband lasers. For a DQW heterostructure with layer sequence \( a_1/a_2/a_3 \) it is convenient to adopt a classification scheme which divides all the interface modes into two groups: "outer" modes (O), localized in the limit \( a_1,a_3 > a_2 \) at the outer interfaces and "inner" modes (I), localized in the same limit at the inner interfaces. Both groups can be further subdivided into S-type and A-type modes. This classification complies with our previous scheme, since in the limit \( a_1,a_3 >> a_2 \) the outer modes behave like the interface modes of a single-well heterostructure formed by the outer interfaces. Inner modes, characteristic of barrier

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**Fig. 2.** Spatial distribution of the interface mode potentials in DQW heterostructures: (a) symmetric heterostructure, \( a_1/a_2/a_3 = 6/2/6 \) nm, (b) asymmetric heterostructure, \( a_1/a_2/a_3 = 2/2/6 \) nm. Thick lines represent inner (I), thin lines – outer (O) interface modes. Solid lines depict symmetric (S), dashed lines – antisymmetric (A) modes. Phonon wave vector is \( q = 0.5 \) nm\(^{-1} \). The heterointerfaces are shown by vertical dotted lines.
layer $a_2$, in the same limit behave like the interface modes of a single-barrier heterostructure. This classification represents to some extent the symmetry of the phonon envelope functions $\varphi_m(z)$. We shall use indexes S and A keeping in mind that an exact symmetry can be assigned to an envelope $\varphi_{m}(z)$ only if $a_1 = a_3$, see Figure 2a, though the main symmetry features of the potential distribution persist even in highly asymmetric DQW heterostructures; see Figure 2b. The classification scheme is not unique and should be chosen in accordance with the type of the heterostructure and the dominant electron transition. For example, if we consider the intrawell relaxation in a DQW heterostructure with wide inner barrier layer, we can adopt a classification scheme based on the eigenmodes of two isolated quantum wells. Indexes I/O should be then reassigned to the left and right QW. Finally, we use symbols b/w to denote barrier/well-type frequency range. It is important that for the inner antisymmetric (IA) mode the potentials from neighboring interfaces $l = 0,1$ and $l = 2,3$ combine constructively. This results in stronger overlap of the IA-phonon potentials with the initial and final electron states located in adjacent quantum wells. Moreover, the barrier-type mode IAb is characterized by the highest inverse dielectric function; see Figure 3b. We can expect, therefore, that IAb-phonons will dominate the interwell phonon-assisted electron transitions in DQW heterostructures with narrow barrier layers. It is worth noting also that the dispersion of both the phonon energies and effective dielectric constants is substantially more pronounced for the inner interface modes than for the outer modes, because the overlap of the potentials of the inner interfaces depends mostly on the narrow barrier width, $a_2$, while the dispersion of the outer modes depends on the total separation between the outer interfaces, $a_1+a_2+a_3$. We can readily discern this trend in Figure 3, which demonstrates all the qualitative features of a single-barrier-like and single-well-like mode behavior (compare with Figure 1) thus justifying our classification scheme. If any of the inner heterostructure layers, $a_1$, $a_2$, or $a_3$, is thick enough, the outer interface modes become dispersionless.$^{11}$

![Fig. 3. Dispersion of the interface phonon energies (a) and inverse effective dielectric constants (b) in an asymmetric DQW heterostructure, $a_1/a_2/a_3 = 2/2/6$ nm. Thick lines represent inner (I) interface modes and resemble the single-barrier modes of Fig. 1. Outer modes are shown by thin lines and are similar to single-well modes in Fig. 1. Solid lines represent symmetric (S), dashed lines – antisymmetric (A) modes.](image-url)
2.2. Examples of scattering rate tailoring

Several exemplary calculations of relaxation processes in QW heterostructures will illustrate our approach. Interwell phonon-assisted transitions in the DQW heterostructures are often used in intersubband laser design as an efficient depopulation process for the lower lasing states.\textsuperscript{12,13} Figure 4a shows the calculated rates of the 2-1 interwell electron transitions assisted by spontaneous emission of different interface phonons as a function of subband separation $E_{21}$. Initial kinetic energy of the electron is small ($\varepsilon_2 = 5$ meV) so that the emission threshold with a good accuracy represents the emitted phonon energy. In accordance with our qualitative considerations, inner antisymmetric barrier-type (IAb) mode dominates the interwell scattering process, though the total of all other mode rates is comparable. Note the remarkable difference between IAb and IAw-related rates, which is a direct consequence of the difference in effective dielectric constants for these modes; see Figure 3b. Outer symmetric (OS) modes do not participate noticeably in interwell scattering, because their envelopes are very smooth in the barrier region. The electron-phonon overlap is thus reduced to negligible overlap of the orthogonal initial and final electron states. Figure 4b shows the dependence of the interwell transition rate on the initial kinetic energy of the electron $\varepsilon_2$. The narrow QW width has been chosen $a_1= 7$ nm, so that $E_{21} = 39$ meV and the emission of confined well-type phonons is always possible (dashed-dotted line). Again, the IAb interface mode provides sharp increase of the transition rate at the electron kinetic energy $\varepsilon_2 \approx \hbar \omega_{LO,b} - E_{21} \approx 12$ meV. The first step-like increase of the scattering rate is due to the confined barrier-type phonons and is significantly smaller.

In Figure 5, we compare the total emission rate for all localized (interface and confined) modes with the results obtained by using the bulk-like approximation for phonon spectrum. In accordance with the sum rule for electron-phonon interaction,\textsuperscript{14} the total rate falls in the interval defined by the interaction with bulk-like phonons of well (w) or barrier (b) materials, except near the onset of resonant electron-phonon scattering.

![Fig. 4. Rate of the interwell 2-1 phonon-assisted electron transitions in an asymmetric DQW heterostructure; $a_1 = 10$ nm, $a_2 = 3$ nm: (a) Spontaneous emission of different interface phonons. The width of the narrow QW $a_1$ is changed from 5 nm to 8 nm to cover 2-1 subband separation shown in the figure. (b) Rate of spontaneous phonon emission as a function of electron initial kinetic energy ($a_1 = 7$ nm; subband separation $E_{21} = 39$ meV). Solid line shows the total rate, the contribution from all interface modes is shown by dashed line, and from all confined modes – by dashed-dotted line.](image-url)
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where the interwell transition rate is very sensitive to the phonon spectrum dispersion. Here, two sharply separated peaks are formed. Confined modes of the lowest energy are apparently dominant at the onset of the resonance, while the IAb-interface mode is primarily responsible for the next abrupt increase of the interwell transition rate. As one can see from Figure 4b, the IAb-interface mode dominates the transition process only near the resonance. Further off the resonance, the confined well-type modes become

Fig. 5. Rate of interwell transitions assisted by spontaneous phonon emission in a DQW heterostructure with layers $a_2 = 3$ nm, $a_3 = 10$ nm: (a) Individual contributions to the total rate (solid line) from all interface modes (dashed line), and from all confined LO-phonons (dashed-dotted line). (b) Comparison of the total transition rate (solid line) with the transition rates calculated using bulk-like phonon spectrum of barrier $(b)$ and well $(w)$ materials (dashed lines).

Fig. 6. Sum rule for electron-phonon interaction: (a) Comparison of the sum of the electron-phonon overlap integrals $I_{21}(q)$ for all confined and interface modes (solid line) with the overlap integral for bulk-like phonons (dashed line). Thin solid lines show separately the contributions from interface and confined modes. (b) Comparison of the sum of the effective coupling coefficients for all modes (solid line) with the coupling coefficients for bulk-like phonons in the barrier $(b)$ and well $(w)$ materials. DQW heterostructure with layer sequence $a_1/a_2/a_3 = 7/3/10$ nm.
more effective. As a result, in Figure 5b the curve representing the total rate of all localized modes is located closer to curve $w$, especially at large subband separation $E_{21}$.

The sum rule for electron-phonon interaction is illustrated also in Figure 6a. Here, we compare the sum of the electron-phonon overlap integrals (2.10) for confined and interface modes participating in 2-1 interwell electron transition with the overlap integral (2.11) for bulk-like phonons. Both curves practically coincide due to the completeness condition for phonon mode set used in our model. The corresponding interrelation between effective electron-phonon coupling constants (2.15) is shown in Figure 6b.

The interwell transition rate can be enhanced by increasing the electron-phonon overlap, for example, if the depopulated subband in the narrow QW anticrosses the second subband of the wider QW, while the energy separation from the first subband is tuned to the highest-energy LO-phonon mode. This resonant process is illustrated in Figure 7, which shows the rate of the interwell transition as a function of the narrow QW width $a_1$ instead of the subband separation used in Figure 5. The curves are labeled with the value of the wider QW width in nm. The curve labeled with $a_3 = 10$ nm corresponds to the solid curve in Figure 5 and also details individual contributions to the overall phonon-emission rate: dashed line – interface phonons, dashed-dotted line – confined phonons, which dominate the scattering process at this resonance. Peaks of the interwell transition rate are related to the resonant penetration of the initial electron state from the narrow QW into the adjacent wider QW due to 2-3 level anticrossing.

In dielectric continuum model, dielectric function $\varepsilon(\omega)$ can naturally incorporate plasmon-related effects either phenomenologically or through the dynamical Hartree corrections. This takes into account the collective response of the electronic subsystem to the laser radiation, which can significantly change the optical characteristics of the intersubband laser heterostructures under high level of electron injection. For example, in a QW with normal ordering of subband occupation, the intersubband resonant screening of the light-wave field usually narrows and blue-shifts the spectrum of the intersubband
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Figure 8 demonstrates significant anomalous red-shift and substantial narrowing of the optical gain spectra in an InGaAs QW with nonequilibrium inverted order of subband occupation. The curves are labeled with the value of the lower subband depopulation time $\tau_{\text{out}}$ in psec and illustrate the influence of the first subband bottom filling $n_1 \propto n_2 \tau_{\text{out}}/\tau_{21}$ on the optical spectra. Intersubband non-radiative relaxation time $\tau_{21}$ is determined primarily by electron-LO-phonon interaction and has been calculated here using the approach discussed above.

3. Multiband Description of Electron Confinement

In previous section, one-band effective mass approximation was used to describe the electron states involved in intersubband transitions. For narrow-gap type-I and staggered-gap type-II heterostructures used in novel intersubband lasers, the multiband treatment of the electron energy spectrum is a must. In multiband effective-mass theory, a mesoscopic electron state can be represented phenomenologically by a column of smoothly varying envelope functions. The number of these functions equals the number of energy bands explicitly considered in the model. In a homogeneous crystal, such a multicomponent wave function satisfies the Schrödinger equation with an effective matrix Hamiltonian $\hat{H}$. The general form of the effective Hamiltonian can be obtained by symmetry considerations, while the values of the phenomenological parameters used in the Hamiltonian are determined by fitting to experimental data. For most of the cubic $A_3B_5$ semiconductors the isotropic eight-band Kane model is rather good approximation. This model describes $kp$-mixing between two groups of orbital basis states, $\{S\}$ and $\{X, Y, Z\}$, characterized by opposite parities and coupled with spin states $\{\alpha, \beta\}$. The effective wave function of an arbitrary mesoscopic state is represented in this model by the column of smooth envelopes $\psi_n$, which consists of scalar ($n = 0$) and vector ($n = 1, 2, 3$) parts. With allowance for spin, these become, respectively, one even and three odd spinors.
\[ \Psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} ; \quad \psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} . \] (3.1)

The effective Hamiltonian of an isotropic 8-band model can be written in the matrix form
\[ \hat{H} = E_g \hat{e}_0 + \Delta \hat{e}_3 + \hat{p} \cdot \mathbf{p} + \gamma_0 p^2 \hat{e}_0 - \gamma_2 (\hat{J} \cdot \mathbf{p}) (\hat{J} + \hat{\sigma}) \cdot \mathbf{p}. \] (3.2)

Here, \( p = -i \nabla \) is the momentum operator, and we use the unit system with \( \hbar = 1 \). Symbols with hats represent square 8\( \times \)8 matrices in full basis set employed in the model. The matrices \( \hat{e}_0 \) and \( \hat{e}_3 \) are diagonal unit matrices with non-zero elements only in scalar \((\hat{e}_0; n = 0)\) or vector \((\hat{e}_3; n = 1, 2, 3)\) subspaces correspondingly. These matrices reveal the intraband nature of related operators, while nondiagonal operator \( \hat{P} \), describes the interband \( \psi_0 - \psi \) mixing. In an isotropic model the interband mixing is characterized by a single parameter - Kane's interband velocity: \( P = i < S | p_z | Z > / m_0 \).

The second term of the Hamiltonian describes the spin-orbit splitting of the zone-centered vector states by the amount \( \Delta \) due to coupling between the spin momentum \( \hat{\sigma} \) and the microscopic orbital momentum \( \hat{J} = 1 \) characteristic of three-fold degeneracy of the vector basis states \( \{X, Y, Z\} \). For matrix formulation of the model we shall use the basis given by four doublets of Kramers-conjugate \( (\nu = \pm 1) \) basis states
\[ \begin{pmatrix} - & - & - & - \\ - & + & - & + \\ - & - & + & + \\ - & + & + & - \end{pmatrix} \] (3.3)

In the vector subspace of basis (3.3) the matrix of spin-orbit coupling, \( \hat{\sigma} \cdot \hat{J} \), becomes diagonal
\[ \hat{\sigma} \cdot \hat{J} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \otimes \delta_{\nu \nu'} . \] (3.4)

As a result, the second term of the Hamiltonian (3.2) has nonzero matrix elements, \(-\Delta\), only for spin-orbit split-off states with \( n = 2 \), whereas the fourfold degenerate valence basis states with \( n = 1, 3 \) correspond to the energy zero.

Phenomenological coefficients \( \gamma_2 \) in the second-order terms of the Hamiltonian (3.2) can be obtained from the experimentally determined bulk effective masses of the charge carriers.\(^{21}\) The matrix structure of the term with \( \gamma_2 \) is closely related to the quasispin operator \( \hat{\Sigma} \), which is defined to satisfy the usual commutation rules and guarantee the conservation of the total angular momentum:
\[ \hat{\Sigma} = \hat{J} + \frac{1}{2} \hat{\sigma} , \quad \hat{\Sigma} \cdot \hat{\Sigma} = i \hat{\Sigma} , \quad [\hat{H}, (\hat{\Sigma} + r \times \mathbf{p})]_\nu = 0 . \] (3.5)

Operator \( \hat{\Sigma} \) determines also the matrix representation for the rotation of the coordinate system through the angle \( \varphi \) about a unit vector \( \hat{m} \):
\[ \hat{\varphi}_{\hat{m} \varphi} = e^{i (\hat{m} \cdot \hat{\Sigma}) \varphi} . \] (3.6)
Since the helicity of a free quasiparticle with momentum \( \mathbf{k} = \mathbf{k} m \), \( \hat{\mu} = (\hat{\Sigma} \cdot \mathbf{m}) \), is a good quantum number, the scalar invariant \( (\hat{\Sigma} \cdot \mathbf{p})^2 - \frac{\mathbf{p}^2}{4} = (\hat{\mathbf{J}} \cdot \mathbf{p} + \hat{\sigma} \cdot \mathbf{p}) \). This form is directly related to the projection operator onto the subspace of two-fold degenerate eigenstates characterized by the helicity \( \mu = \pm 3/2 \):

\[
\hat{\Lambda}_h = \frac{1}{2} \left( \hat{\mu}^2 - \frac{1}{4} \right) = \frac{1}{2} (\hat{\mathbf{J}} \cdot \mathbf{m}) \left( \hat{\mathbf{J}} + \hat{\sigma} \cdot \mathbf{m} \right) \; ; \; \hat{\Lambda}_h^2 = \hat{\Lambda}_h \; ; \; \text{Sp} \hat{\Lambda}_h = 2. \quad (3.7)
\]

The eigenstates with definite sign of the helicity can then be extracted with additional projector

\[
\hat{\Lambda}_\mu = \frac{1}{2} \left( 1 + \frac{\hat{\mu}}{\mu} \right). \quad (3.8)
\]

The matrix representation of corresponding operators in the basis of coupled momenta (3.3) is completely described by the matrix of helicity

\[
\hat{\mu} = \begin{bmatrix}
\frac{1}{2} \mathbf{m} \cdot \sigma & 0 & 0 & 0 \\
0 & \mathbf{m} \parallel \cdot \sigma + \frac{1}{2} m_z \sigma_z & 0 & -i\sqrt{3} \sigma_y (\mathbf{m} \parallel \cdot \sigma_y) \\
0 & 0 & \frac{1}{2} (m_z \sigma_z - \mathbf{m} \parallel \cdot \sigma_{\parallel}) & 0 \\
0 & i\sqrt{3} (\mathbf{m} \parallel \cdot \sigma_{\parallel}) \sigma_y & 0 & \frac{3}{2} m_z \sigma_z
\end{bmatrix}. \quad (3.9)
\]

This entails, for example, the matrix representation of the projector (3.7) in the vector subspace of (3.3):

\[
\Lambda_h = \frac{1}{2} \begin{bmatrix}
\frac{1}{2} m_{\parallel}^2 & 0 & -i\sqrt{3} (\mathbf{m} \cdot \sigma + m_z \sigma_z) \sigma_y (\mathbf{m} \parallel \cdot \sigma_{\parallel}) \\
0 & \frac{3}{2} m_{\parallel}^2 & 0 & 0 \\
i\sqrt{3} (\mathbf{m} \parallel \cdot \sigma_{\parallel}) \sigma_y (\mathbf{m} \cdot \sigma + m_z \sigma_z) & 0 & \frac{3}{2} m_{\parallel}^2 & 0
\end{bmatrix} \; . \quad (3.10)
\]

### 3.1. Analytical representation for the eigenstates

Classification of the eigenstates according to their helicity \( \mu \) facilitates obtaining an analytical representation for eigenstates. “Heavy” states (\( \mu = \pm 3/2 \)) can be obtained by using projection operator (3.7) and identity \( (\mathbf{m} \cdot \mathbf{J}) \psi = i \mathbf{m} \times \psi \):

\[
\psi_h = \begin{pmatrix}
0 \\
\psi_h
\end{pmatrix} U_h ; \quad \psi_h \propto \psi - (\mathbf{m} \cdot \mathbf{J}) \mathbf{m} + i(\mathbf{m} \cdot \sigma) (\mathbf{m} \times \psi) \; ; \quad (3.11)
\]

Corresponding matrix representation in the vector part of basis (3.3) is

\[
\psi_h \propto \Lambda_h \begin{pmatrix}
1 \\
0
\end{pmatrix} \propto \begin{pmatrix}
\frac{\sqrt{3} m_{\parallel}^2}{2} \\
0
\end{pmatrix} + i(\mathbf{m} \parallel \cdot \sigma_{\parallel}) \sigma_y (\mathbf{m} \cdot \sigma + m_z \sigma_z). \quad (3.12)
\]
“Light” states \( (\mu = \pm 1/2) \) are formed by \( \psi_0 \psi \) mixing, which is provided by interband velocity operator \( P \). Accordingly, the vector part of the light eigenfunction, \( \psi_l \), must transform like a dynamical polar vector. In our isotropic model, two operators, \( p \) and \( i\sigma \times p \), exhibit suitable transformation properties, therefore, \( \psi_l \) should be sought as a linear combination of the column \( k \) and the column \( q = (\sigma \cdot J)^k \):

\[
\psi_l = \begin{pmatrix} 1 \\ \psi_l \end{pmatrix} U_l; \quad \psi_l = iP(a + b(\sigma \cdot J))k . \tag{3.13}
\]

Substituting this representation into the Schrödinger equation, \( \hat{H}\psi_l = E\psi_l \), and taking into account that \( \hat{A}_h\psi_l = 0 \), we easily find the coefficients of the linear combination:

\[
a = \frac{\tilde{E} + \frac{1}{3}\Delta}{E(E + \Delta)}; \quad b = \frac{\frac{1}{3}\Delta}{E(E + \Delta)}; \quad \tilde{E} = E + \gamma_3 k^2 . \tag{3.14}
\]

Vector column \( \psi_l \) takes an especially simple form in the basis of coupled momenta (3.3) due to the diagonal representation of the spin-orbit coupling operator \( (3.4) \)

\[
\psi_l = iP \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{1}{E} \end{pmatrix} ; \quad k = \begin{pmatrix} (2k_z + q_z)/\sqrt{6} \\ (k_z - q_z)/\sqrt{3} \\ (i\sigma_z)/\sqrt{2} \end{pmatrix} . \tag{3.15}
\]

Normalizing spinor amplitudes \( U_h \) and \( U_l \) also include the spatial dependence of the envelopes \( U_{h,l} \propto \exp(ikr) \). We can use the projector (3.7) to obtain the quasiparticle dispersions. For heavy states

\[
E_h(k) = \frac{1}{2} \text{Sp}(\hat{A}_h\hat{H}) = -(\gamma_2 + \gamma_3)k^2 , \tag{3.16}
\]

while for the light bands the dispersion relations can be obtained from the equation

\[
\text{det} [(1 - \hat{A}_h) (\hat{H} - E)] = (E_g + \gamma_0 k^2 - E) + P^2 k^2 \frac{\tilde{E} + \frac{2}{3}\Delta}{E(E + \Delta)} = 0 . \tag{3.17}
\]

This equation is of third order in \( k^2 \) and results in three different types of light eigenstates, though only two solutions, \( \Psi_1 \) and \( \Psi_2 \), are physically relevant. They describe, respectively, the electron/light-hole and the spin-orbit split-off bands. The spurious solution \( \Psi_3 \) will be discussed in section 3.2 below.

In a heterostructure, spherical symmetry of the bulk energy spectrum is reduced to the axial symmetry group \( C_v \). We can significantly simplify the eigenvalue problem using the reflection symmetry \( \omega \) with respect to the plane formed by the heterostructure growth axis \( z \) and the electron in-plane momentum \( K \), chosen here along the \( x \)-axis, so that \( k = (K, 0, k_z) \). This transformation is equivalent to the product of the inversion, \( I \), and the
rotation by angle $\pi$ about the $y$-axis, $\omega_y$. In basis (3.3) corresponding matrix representation is

$$\hat{\omega}_y = i \hat{\omega}_y = (\hat{e}_0 - \hat{e}_3) \exp(i \pi \hat{\Sigma}_y) = (e_0 + e_3) \otimes i \sigma_y.$$  \hspace{1cm} (3.18)

We can choose the normalizing spinors $U_l$ and $U_h$ as eigenstates of the operator $\sigma_y$,

$$\sigma_y U_{i,h} = \eta U_{i,h}, \quad \eta = \pm 1,$$  \hspace{1cm} (3.19)

thus introducing in our model the eigenstate polarization $\eta$. From (3.18) it follows that this quantum number correlates with the eigenstate parity with respect to the $xz$-reflection. In basis (3.3), the matrix representations of the $xz$-reflection $\omega_{xz}$ and the time-reversal operation $\tau$ differ only by the complex conjugation operator $\Re$:

$$\hat{\tau} = \hat{\omega}_{xz} \Re.$$  \hspace{1cm} (3.20)

From (3.19) it thus follows that $\Re U_{i} = U_{-i}$, so that the time-reversal operation changes the sign of the eigenstate polarization $\eta$. The inversion operation $I$ does not change $\eta$, therefore, this quantum number can be used both in Kramers degeneracy condition

$$E(K, \eta) = E(-K, -\eta),$$  \hspace{1cm} (3.21)

and in the two-fold degeneracy condition

$$E(K, \eta) = E(K, -\eta),$$  \hspace{1cm} (3.22)

characteristic of the eigenstates in heterostructures with inversion symmetry. In asymmetrical heterostructures, such as InAs/GaSb DQW, this degeneracy is lifted and (3.22) fails. So defined, the state polarization significantly simplifies the matrix representation for $\Psi_h$ and $\Psi_l$, which is thus reduced to the four-component expressions:

$$\Psi_h = \begin{pmatrix} 0 \\ \Psi_h \end{pmatrix} U_h; \quad \Psi_h = \begin{pmatrix} \sqrt{3} K \\ 0 \\ -2k_z - i\eta K \end{pmatrix};$$  \hspace{1cm} (3.23)

$$\Psi_l = \begin{pmatrix} 1 \\ \Psi_l \end{pmatrix} U_l; \quad \Psi_l = iP \begin{pmatrix} (2k_z - i\eta K)^2 \sqrt{6}E \\ (k_z + i\eta K)^2 \sqrt{3} (E + \Delta) \\ K \sqrt{2} E \end{pmatrix}. \hspace{1cm} (3.24)$$

3.2. Phenomenological boundary conditions

At a heterointerface A-B, the phenomenological description of a mesoscopic state by an effective Hamiltonian (3.2) should be accomplished with appropriate boundary conditions (BC) for the A- and B-parts of the multicomponent wave function $\Psi$ (3.1). The most common approach to the matching procedure requires the component-by-component continuity of the envelopes $\psi_n$, thus assuming uniform microscopic structure of the contacting materials. At the A-B interface ($z = 0$) this approach entails the BC in the form\(^{22}\)

$$\Psi_A = \Psi_B; \quad \hat{j}_{zA} \Psi_A = \hat{j}_{zB} \Psi_B.$$  \hspace{1cm} (3.25)
The second condition provides for the current continuity across the interface. The flux operator matrix, $\mathbf{j}$, can be defined so that the current density $\mathbf{j} = \Psi^+ \hat{\mathbf{j}} \Psi$ satisfies the continuity equation

$$\text{div} \, \mathbf{j} = -\frac{\partial \Psi^+ \Psi}{\partial t} = i\Psi^+ \hat{H} \Psi - i(\hat{H} \Psi)^+ \Psi.$$  \hspace{1cm} (3.26)

BC (3.25) reveal significant drawback when degenerate spectrum of the constituent semiconductors is involved. In this situation, the transverse components of the momentum operator, $p_{x,y}$, directly enter the current operator. This makes BC (3.25) dependent on the mesoscopic structure of the electron state, in this case – on the in-plane electron wave-vector $K$. Microscopic uniformity also implies the identity of the A-B basis states, which is inconsistent with the actual diversity of the effective Hamiltonian parameters in constituent semiconductors. Finally, the most important disadvantage of the conventional BC (3.25) is the lack of the adjustable parameters required in any kind of the phenomenological models to allow fitting in experimental data. Several authors have already suggested more general phenomenological BC, which reject the unjustified assumption of the component-by-component continuity of the envelopes and make no specific assumptions about the basis functions on each side of the heterointerface. Here, we shall restrict our analysis with the simplest diagonal form of the boundary conditions

$$\psi_{nA} = F_n \psi_{nB}^*; \quad \psi'_{nA} = G_n \psi'_{nB}. \hspace{1cm} (3.27)$$

Each envelope $\psi_n$ is a spinor in basis (3.3), so that BC parameters $F_n$ and $G_n$ should be considered as $2 \times 2$ matrices. The internal structure of these blocks, however, is severely restricted by axial symmetry assumed for the heterostructure energy spectrum. Invariance under rotations about $z$-axis leads to the diagonal structure of each $2 \times 2$ block, since the matrix of the rotation operator $\omega_\varphi$ is diagonal, see (3.6) and (3.9). The symmetry under $xz$-reflection $\omega_{xz}$ (3.18) makes diagonal elements equal, while the time-reversal symmetry $\tau$ (3.20) imposes the real values for these matrix elements. So, finally, each $2 \times 2$ block in BC is represented by a real number, $F_n$ or $G_n$, multiplied by $2 \times 2$ unity matrix of the Kramer’s subspace, $\delta_{\nu \nu'}$. It is important that BC with such a matrix structure do not mix electron states with different polarizations $\eta$. This significantly simplifies the eigenvalue problem: 4-component analytical solutions (3.23-3.24) can be used together with phenomenological BC (3.27) in reduced $4 \times 4$ matrix representation.

Phenomenological matching parameters, $F_n$ and $G_n$, are independent on the mesoscopic characteristics of the electron state, though they are interrelated due to the current continuity condition at the A-B interface

$$j_{zA} = j_{zB}. \hspace{1cm} (3.28)$$

In model (3.2) the continuity equation (3.26) is satisfied by the expression

$$\mathbf{j} = \Psi^+ \hat{\mathbf{P}} \Psi + (\gamma_0 \hat{e}_0 - \gamma_3 \hat{e}_3 )(\Psi^+ \mathbf{P} \Psi + \text{h.a.}) - \frac{1}{2} \gamma_2 \left[ \Psi^+ \left( \hat{j}(\mathbf{p} \cdot \hat{\mathbf{j}}) + \hat{\mathbf{j}}(\mathbf{p} \cdot \hat{\mathbf{\sigma}}) \right) + \text{h.a.} \right], \hspace{1cm} (3.29)$$

where h.a. stands for Hermitian adjoint. The z-component of the flux $\mathbf{j}$ is represented in basis (3.3) as
\[ j_z = -iP \left[ \psi_0^* \frac{\sqrt{3} \psi_1^* + \psi_2}{\sqrt{3}} - c.c. \right] - i\gamma_0 (\psi_0^* \psi_0^* - c.c.) + i\gamma_3 (\psi_1^* \psi_1^* + \psi_2^* \psi_2^* - c.c.) \]
\[ + i(\gamma_2 + \gamma_3) (\psi_1^* \psi_1^* - c.c.) - \frac{\sqrt{3}}{2} \gamma_2 \left[ \psi_3^* (p_x - i \sigma_y p_y) \psi_1 + c.c. \right]. \]  

(3.30)

Here, c.c. stands for complex conjugate. An arbitrary mesoscopic state expansion includes 4 independent partial solutions, one heavy and three light,
\[ \Psi = \Psi_h + \Psi_{B1} + \Psi_{B2} + \Psi_{B3}, \]  

(3.31)

therefore, each wave-function component in (3.30) can be varied independently. The current continuity (3.28) then imply the following relationships between BC parameters and parameters of the constituent Hamiltonians
\[ F_0 F_1 = F_0 F_2 = \frac{P_B}{P_A}; \quad F_1 F_3 = \frac{\gamma_{2B}}{\gamma_{2A}}; \]
\[ F_0 G_0 = \frac{\gamma_{0B}}{\gamma_{0A} }; \quad F_1 G_1 = F_2 G_2 = \frac{\gamma_{3B}}{\gamma_{3A}}; \quad F_3 G_3 = \frac{(\gamma_2 + \gamma_3)_B}{(\gamma_2 + \gamma_3)_A}. \]  

(3.32)

One matching parameter, for instance \( F_0 \), can be conveniently treated as a phenomenological parameter of the BC.

It should be noted that BC in general form (3.27) can be used only if all partial solutions have been included in the expansion (3.31). However, the third \( k^2 \) root of the dispersion equation (3.17), \( k_{13}^2 \propto -P^2/\gamma_0 \gamma_3 >> k_{11}^2, k_{12}^2 \), gives spurious solution with a matrix structure following from (3.24):
\[ \Psi_{13} \propto \left[ \begin{array}{c} \pm \frac{1}{\sqrt{3}} \\ \sqrt{2} \\ 1 \\ 0 \end{array} \right] U_{13}(z). \]  

(3.33)

This solution appears due to the influence of remote bands treated perturbatively and is beyond the applicability of the Kane model. Therefore, when considering the mesoscopic electron states, we have to truncate both the expansion (3.31) and the BC set (3.27) providing them only for smooth envelopes. Assuming \( U_{15} << U_{11}, U_{12} \), we can neglect spurious amplitudes in expansion (3.31) and omit them in the matching condition for envelopes (3.27). First three matching conditions for envelope derivatives with \( n = 0,1,2 \) contain large terms \( k_{13} U_{15} \). These terms are cancelled out from the linear combination of the boundary conditions with \( n = 1,2 \) since, according to (3.32), we have \( F_1 = F_2 \), and consequently \( G_1 = G_2 \). Remaining boundary condition with \( n = 0 \) determines unphysical amplitude \( U_{13} \), which we do not consider explicitly, and thus may be skipped. As a result, we arrive at the following truncated BC set for smooth envelopes only
\[ \Psi_{A,B} \approx (\Psi_h + \Psi_{B1} + \Psi_{B2})_{A,B}; \]  
\[ \psi_{A} = F_0 \psi_{B}; \]  
\[ (\psi_1' - \sqrt{2} \psi_2')_A = G_1 (\psi_1' - \sqrt{2} \psi_2')_B; \]  
\[ \psi_{3B} = G_3 \psi_{3B}. \]  

(3.34)  
(3.35)  
(3.36)  
(3.37)
Similar truncation procedure should be used any time we encounter strongly evanescent solutions, which is the case, for example, for spin-split or heavy-hole bands in type-II heterostructures, which will be considered in the next section.

3.3. Electron energy spectrum of basic heterostructures

Analytical representation of the Kane model eigenstates completed with phenomenological BC provides the tool for a semianalytical treatment of the electron confinement in the most basic intersubband laser heterostructures. Narrow-gap semiconductor materials used in the mid-infrared lasers are characterized by large spin-orbit splitting of the valence band $\Delta$. In the limit $\Delta \gg E$, small envelopes with $n = 2$ can be omitted in (3.24). Split-off light solution $\Psi_l^2$ becomes spurious, therefore, an arbitrary mesoscopic state should be represented by a superposition of smooth wave packets of only two partial solutions - one light and one heavy, $\Psi \approx \Psi_l + \Psi_h$. Correspondingly, the matching condition (3.36), which determines the spurious amplitudes, should be skipped.

Large values of the valence band offsets simplify the boundary conditions even more. Let us assume that the mesoscopic state $\Psi$ is mostly localized in layer B and the energy of the state is far off the valence band top in the A-material. The heavy solution can then be treated as a spurious one in the layer A. Proceeding with our truncation scheme, small amplitude $U_{hA}$ can be neglected and BC (3.37) skipped, so that the A- and B-parts of the mesoscopic state $\Psi$ are matched at the interface by BC (3.35) only.

As a first example, we consider the energy spectrum of an asymmetric narrow-gap type-I single-QW heterostructure with layer sequence A1-B-A2; see Figure 9a, inset. We do not consider strain-induced and space-charge effects here. In the flat-band

![Diagram](image_url)

Fig. 9. Band diagram of an asymmetric type-II InAs/GaSb DQW heterostructure. Asymmetric type-I QW heterostructure is shown schematically in the inset. (a) “Leaky” DQW heterostructure modeling a single stage of an intersubband cascade laser. Direct interband tunneling depopulation of the lower lasing subband through the heterostructure leaky window $\delta$ is shown by a bold arrow ($\Gamma$). (b) Isolated type-II DQW heterostructure with first electron-like and first light-hole-like subbands anticrossed. Interband LO-phonon assisted depopulation process ($\Gamma_{ph}$) is shown by an arrow.
approximation, the wave function of a confined state is represented in the QW layer B as a superposition of light and heavy solutions with opposite $k$

$$\Psi_B = \sum_{l,h,\pm} \Psi_{l,h}(\pm k_{l,h}), \quad (3.38)$$

while in the barrier regions A1 and A2 we consider only smooth evanescent light solutions with $k_{A1} = -i\lambda_{A1}$ and $k_{A2} = i\lambda_{A2}$. Matching $\Psi_{A1}$, $\Psi_B$, and $\Psi_{A2}$ by BC (3.35) with $n = 0, 1, 3$, we easily obtain the dispersion equation in the form

$$D(E) = \tilde{\lambda}_{1,2}^2 + (\tilde{\lambda}_1 + \tilde{\lambda}_2)k_j \cot \beta_l - k_j^2$$

$$+ (\zeta_1 \tilde{\lambda}_1 + \zeta_2 \tilde{\lambda}_2)k_h \cot \beta_h - \zeta_1 \zeta_2 k_h^2 - (\zeta_1 + \zeta_2)k_l k_h \frac{1 - \cos \beta_l \cos \beta_h}{\sin \beta_l \sin \beta_h} = 0. \quad (3.39)$$

Here, $\beta_{l(h)} = k_{l(h)} a_B$, \( \tilde{\lambda} = \xi \lambda \), \( \tilde{\lambda}_x = \tilde{\lambda} \pm \eta K \), \( \eta = \frac{1}{2} \eta (1 - \xi + \zeta) \), and

$$\xi = \frac{1}{E_B^2} \frac{E_B}{E_A}; \quad \zeta = \frac{3K^2}{4k_h^2 + K^2} \left( 1 - \frac{E_B^2}{E_A(E_{A}(B) - E_{G(4)A})} \right).$$

Indexes 1 and 2 in Eq. (3.39) refer, respectively, to interfaces A1-B and B-A2. The energy $E$ in each layer is referenced to the top of the valence band, and, according to the dispersion equations (3.16) and (3.17), with a good approximation we have

$$k_{h}^2 + K^2 \approx -2m_h E_B; \quad k_{l(4)}^2 + K^2 \approx 2m_{l(4)}(E_{A(4)} - E_{G(4)A})/E_{G(4)A}. \quad (3.40)$$

In an asymmetrical QW, linear terms $\sim \eta K$ determine subband “spin” splitting, which is more pronounced in valence band, where $\xi < 0$. In the case of a symmetrical QW, the terms with $\eta K$ are cancelled out so that the double degeneracy of the energy spectrum is restored. For conduction-band states, the electron confinement is described by a simplified dispersion equation obtained in the limit $m_l \gg m$. This is exactly the first line of Eq. (3.39).

It is important that the dispersion equation (3.39) holds the same general form even for more complex heterostructures and, therefore, can be conveniently used in a great variety of situations. In this work, as an example, we shall study asymmetric InAs/GaSb DQW heterostructure shown in Figure 9a. This structure models a single stage of a cascaded active region of a type-II intersubband laser. The energy $E$, each layer is referenced to the top of the valence band, and, according to the dispersion equations (3.16) and (3.17), with a good approximation we have

$$k_{h}^2 + K^2 \approx -2m_h E_B; \quad k_{l(4)}^2 + K^2 \approx 2m_{l(4)}(E_{A(4)} - E_{G(4)A})/E_{G(4)A}. \quad (3.40)$$

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substantially different from type-I single-QW heterostructure shown schematically in the inset, nevertheless the matching of the wave function components at the interfaces still leads to the dispersion equation in the same general form (3.39), with only changes for $\lambda_1$ and $\lambda_2$:

$$D(E) = 0 ; \quad \lambda_1 = k_{lA} \cot k_{lA}a_{A1} ; \quad \lambda_2 = -ik_{lA}.$$  (3.41)

For InAs/GaSb/InAs triple QW heterostructure with an additional InAs QW layer, which models the so-called W active region of type-II lasers, the dispersion equation can be obtained in the same fashion

$$D(E) = 0 ; \quad \lambda_1 = k_{lA} \cot k_{lA}a_{A1} ; \quad \lambda_2 = k_{lA2} \cot k_{lA2}a_{A2}.$$  (3.42)

In the limit $\zeta \to 0$ this equation describes also asymmetric type-I DQW heterostructure. Finally, in the limit $\lambda_2 \to \infty$ we obtain simple dispersion equation for an asymmetric two-layer InAs/GaSb DQW heterostructure isolated on both sides by AlSb barrier layers (Figure 9b):

$$\zeta \left( k_{lA} \cot \beta_{lA} + \frac{\eta K}{2} \right) \left( k_{lB} \cot \beta_{lB} - \frac{\eta K}{2} \right) +$$

$$\zeta \left( k_{hB} \cot \beta_{hB} - \frac{\eta K}{2} \right) = 0 . \quad (3.43)$$

Using the above dispersion equations makes the analysis of the subband structure very illustrative. Since at $K = 0$ the light- and heavy-particle subbands are decoupled, it is convenient to consider them first separately. This separation can be accomplished formally in the limit $m_h \to \infty$, which eliminates the terms with $\zeta$ from the dispersion equation. Figure 10 shows exemplary calculation of the subband structure in the leaky window of an isolated
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InAs/GaSb DQW heterostructure schematically represented in Figure 9b. Parameters used in calculations are represented in Table 2.10 Solid and dashed lines represent subbands with opposite polarizations $\eta$, which are split due to the lack of inversion symmetry in this heterostructure. Note, that this splitting is much more pronounced for B-type (light-hole) states. Strong anticrossing between the light subbands is readily seen in Figure 10a and can be easily traced in the complete picture of the electron energy spectrum shown in Figure 10b. In this heterostructure, the top of the first light-hole subband LB1 is above the bottom of the first InAs-related electron-like subband LA1, so that the subbands anticrossing occurs at a final value of the in-plane wave vector $K$. In intersubband laser design, the lower lasing states (subband LA1) should be located in the upper part of the leaky window. Figure 11 shows on the enlarged scale the subband alignment for a smaller value of the InAs QW width. With $d_A$ decreasing, the electron-like subband moves toward the upper edge of the leaky window so that the anticrossing finally occurs at $K \approx 0$. Here, we cannot assign any definite type (electron- or hole-like) to the states of the subband extremities $L1^\pm$, and linear terms dominate the subband dispersion. Note, that at the anticrossing this linear subband splitting is equally distributed between the $L1^\pm$ subbands. It is important that the anticrossing gap is smaller than LO-phonon energy in constituent semiconductors, $\hbar \omega_{LO} \approx 30$ meV, so that the tunneling depopulation of the lower lasing state can be favorably complemented with phonon-assisted transitions, which will be considered in the next section.

4. Subband Depopulation in Type-II Laser Heterostructures

In this section, we use the results of the previous parts to analyze the lower lasing state depopulation in type-II cascade laser heterostructures. InAs/GaSb/AlSb material system is very promising for implementation of high-temperature mid-infrared intersubband lasers covering the 3-5 $\mu$m atmospheric window. Comparing with type-I QCL,12 higher conduction band offset at InAs/AlSb interface allows extension of the laser operation at
shorter wavelength, simultaneously reducing the leakage current. Cross-gap alignment between InAs and GaSb allows also better blocking of the injected electrons in the upper lasing states, while the lower lasing state depopulation can be favorably accomplished by two efficient processes: direct interband tunneling through the InAs/GaSb “leaky window” and LO-phonon assisted interband electron transition. In type-II lasers, the direct interband tunneling has always been considered as a basic depopulation mechanism whereas the interband LO-phonon assisted tunneling is habitually treated as an inefficient one due to a symmetry difference between the initial and final electron states involved in the transition. Here, we make a comparative study of these two processes and show that symmetry constraint for LO-phonon emission can be essentially removed in coupled InAs/GaSb quantum wells by significant nonparabolicity and band-mixing effects inside the heterostructure leaky window.

4.1. Interband tunneling in InAs/GaSb “leaky” heterostructure

One of the attractive features of type-II “broken gap” heterostructures for the intersubband cascade laser design is the opportunity of direct interband tunneling depopulation of the lower lasing states located in the heterostructure leaky window. The rate of this process can be easily evaluated using the dispersion equation (3.41). Imaginary term $\lambda_j$ corresponding to the outgoing electron wave in the collector region makes the energy eigenvalues in the leaky window complex with imaginary part $-i\hbar\Gamma/2$. The quantity $\Gamma$ represents the interband tunneling depopulation rate, which is proportional to the inverse lifetime of the quasibound electron state. Figure 12 shows two upper light-type energy levels ($K = 0$) in the leaky window $\delta$ of the InAs/GaSb DQW heterostructure depicted in Figure 9a. The level positions $\varepsilon$ are counted from the InAs conduction band minimum. Levels LA1 and LB1 demonstrate typical anticrossing behavior, changing the type of the state localization (A- or B-layer) beyond the anticrossing point; see also Figure 13. At the anticrossing point, the electron density spreads equally over both coupled quantum wells, so that the interband tunneling rates (or the energy level widths) are equal for the upper (L$-$) and lower (L$+$) anticrossing levels; see Figure 12b. Before the anticrossing, the quasibound A-type states are substantially

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**Fig. 12.** Anticrossing between two upper light-type energy levels in the leaky window. Position of the energy levels $\varepsilon$ in the leaky window (a) and the energy level width $\hbar\Gamma$ (b) as a function of the InAs QW width $a_A$ at two values of GaSb QW width, $a_B = 16$ nm (solid lines) and $a_B = 10$ nm (dashed lines).
narrower than the B-type states, since the tunneling from the A-levels, localized mostly in InAs layer, requires two interfaces to penetrate.

All these features of the quasibound states in the leaky window $\delta$ can be easily inferred and analyzed from the phase of the electron reflection coefficient.\textsuperscript{31,32} Restoring the amplitude of the incoming wave, $U^-$, in the right half-space InAs-layer, the reflection coefficient can be expressed through the function $D(\varepsilon)$ from Eq. (3.41)

$$ R(\varepsilon) = \left( \frac{U^+_\varepsilon}{U^-_{\varepsilon}} \right) = \frac{D^*(\varepsilon)}{D(\varepsilon)}. \quad (4.1) $$

Since there is no propagating wave in the left barrier region, the latter relation readily follows also from the time-reversal symmetry of the reflection process. In the vicinity of a resonant state, the phase of the reflection coefficient undergoes $\pi$ phase shift and the peak of the phase derivative with respect to energy has Lorentzian shape. The value of the full peak width at half maximum represents the inverse lifetime $\Gamma$ of the quasibound state. Figure 14 illustrates the evolution of the light-type quasibound levels ($K = 0$) in the heterostructure leaky window, $0 < \varepsilon < \delta$, as the GaSb quantum well width $a_B$ increases. The InAs quantum well width is constant, $a_A=12$ nm, thus keeping the bottom of the subband LA1 in the middle of the leaky window. In subplot (a) the narrow peak LA1 corresponds to the lowest electron-like level localized mostly in InAs quantum well A. Much wider peak LB1 corresponds to the highest light-hole subband in the GaSb quantum well B. When the A- and B-type levels anticross (b), the decay rates of the light quasibound states become comparable. This situation, when occurs in the middle of the leaky window, reveals the highest rate of the interband tunneling process. The broadened
peaks $L^{+}$ and $L^{-}$ represent symmetrical and antisymmetrical combinations of A- and B-type levels under the anticrossing condition. After the anticrossing, the LA1 level width shrinks, see subplot (c). The anticrossing broadening can be readily traced also in the case of anticrossing between LA1 and the next light-hole-like level, LB2; shown in subplot (d), peaks $L^{2\pm}$. This subplot demonstrates also significant narrowing of the B-type levels when they are verging the leaky window edges.

The decrease in InAs QW width $a_A$ pushes the lower lasing level LA1 upwards, simultaneously decreasing the level width associated with the interband tunneling. Since the uppermost position of the LA1 subband reduces the thermal backfilling of the lower lasing states, it would be beneficial to keep LA1 as high as possible in the leaky window. However, it is readily seen from Figure 12 that in the most important range, $8\text{nm}<a_A<9\text{nm}$, the direct tunneling rate $\Gamma$ practically vanishes and cannot be adjusted by changing GaSb QW width $a_B$. On the other hand, the interband tunneling from the lower lying light-type subband LB1 is still efficient. The energy separation between these two subbands can be adjusted by proper design of the GaSb QW width $a_B$, therefore, for the depopulation of the lower lasing states in subband LA1 we may employ a competitive depopulating transitions LA1→LB1 assisted by LO-phonon emission.$^{32,33}$

Fig. 14. Light quasibound states in the leaky window $\delta = 150 \text{ meV}$. All curves are normalized to the highest peak value and labeled with the full peak width at half maximum. Each subplot is labeled with the GaSb QW width $a_B$. The width of the InAs QW is $a_A = 12\text{nm}$.
4.2. Phonon enhancement of the depopulation process

To demonstrate the possibility of the electron-LO-phonon resonance in interband transitions, we consider an isolated InAs/GaSb DQW heterostructure shown schematically in Figure 9b. This model structure explicitly reveals some important features of the depopulation process determined by the heterostructure asymmetry. Strain and space-charge related effects are not included in these exemplary calculations. To optimize the depopulation of the lowest electron-like subband, LA1, we need to provide for anticrossing with the highest light-hole-like subband, LB1, which also enhances the electron-phonon wave function overlap in the phonon emission process. This subband anticrossing can be arranged in the upper part of the leaky window if InAs QW width is about $a_\lambda \sim 9$ nm. We shall calculate and compare the LO-phonon emission rate for two different values of the InAs QW width, $a_\lambda=9$ nm and $a_\lambda=8.5$ nm, the later allowing for the higher position of the subband LA1; see Figure 12.

![Graph](image_url)  

Fig. 15. Electron-phonon resonance in InAs/GaSb DQW heterostructure. Upper subplot shows LO-phonon emission rate $\Gamma_{ph}$ calculated for two values of InAs QW width $a_\lambda=9$ nm (curve set a) and $a_\lambda=8.5$ nm (curve set b). Smaller width of the InAs QW provides for the higher position of the lower lasing states in the leaky window. Three regions of the phonon emission rate, R1-R3, correspond to three different type of resonant transition in Brillouin zone. Lower subplot shows the total effective density of the final electron states $D(\varepsilon)$ for the phonon emission transitions. Level broadening $\Gamma$ is taken 0.1 meV (thick solid lines), 1 meV , and 5 meV (thin lines in each curve set).
The upper limit for the phonon-assisted depopulation rate, $\Gamma_{\text{ph}}$, can be obtained assuming the final states for electron transitions to be unoccupied. Since the LO-phonon energies are very close in both constituent materials (see Table 2), we neglect polar mode confinement and calculate the phonon emission rate using model bulk-like phonon spectrum and Eq. (2.13). The coupling constant can be simply averaged with respect to the layer widths:

$$\beta_{\text{eff}} = (\beta_{\text{A}} a_{\text{A}} + \beta_{\text{B}} a_{\text{B}})/(a_{\text{A}} + a_{\text{B}}).$$  \hspace{1cm} (4.2)

Index $f$ in Eq. (2.13) counts nondegenerate spin-split subbands. Since the spin is entangled in the multiband electron state envelopes $\Psi_i$ and $\Psi_f$, the electron-phonon interaction couples the initial electron state with the final states in either spin-split subbands. The integration over the $q$ – directions in Eq. (2.13) returns factor $\pi$ for each subband, which would recover usual factor $2\pi$ in case of non-split subbands. The width of the quasibound electron states in leaky window is determined by interband tunneling and in the upper part of the window is about 1 meV; see Figure 12. This small level broadening can be included in the $\Gamma_{\text{ph}}$ rate calculations by using Lorentzian lineshape function with half-width $\Gamma$ instead of the $\delta$-function. With electron-phonon coupling constant $\beta = 1$, the last integral in (2.13) characterizes the effective density of the final states $D_f$ available in the subband $E_f$ for electron transitions assisted by LO-phonon emission.

Figure 15 shows the depopulation rate $\Gamma_{\text{ph}}$ calculated as a function of the GaSb QW width $a_{\text{B}}$ for two different values of the InAs QW width. For a narrower InAs QW, the lower lasing subband LA1 has moved higher in the leaky window, and, as a result, all the resonances occur at larger values of the GaSb QW width, $a_{\text{B}}$. The increase of $a_{\text{B}}$ in the range from 5 nm to 10 nm, while keeping the energy position of the initial electron-like subband LA1 practically unchanged, makes it possible to scan the final states in the hole-like subbands $E_f$, here - the light subband LB1 and the heavy subband H2, which thus move toward the upper part of the heterostructure leaky window. Figure 15 clearly

![Fig. 16. Electron energy spectrum of an InAs/GaSb DQW with layer widths $a_{\text{A}} = 8.5$ nm and $a_{\text{B}} = 9$ nm. (a) subband diagram in the upper part of the leaky window illustrating three basic interband transitions assisted by the LO-phonon emission. The most important resonant transition, R1, is indirect in Brillouin zone. (b) Effective density of states for electron subbands participating in the phonon-emission transitions. Level broadening parameter is $\Gamma = 0.1$ meV (solid lines), 1 meV (dashed lines), and 5 meV (dashed-dotted lines).]
demonstrates three distinctive regions in the LO-phonon emission rate, R1-R3, which are related to three consecutive resonances. The first, most remarkable resonance, R1, corresponds to the onset of the LA1→LB1 phonon-assisted transition, as illustrated in Figure 16a. For brevity, the initial electron state in the LA1 subband is taken with zero in-plane momentum, so that the electron wave vector in the final state is equal to the emitted phonon wave vector, $K_f = q$. The anticrossing between LA1 and LB1 subbands results in resonant penetration of the LA1 subband states into the adjacent GaSb QW B and ensures sufficient electron-phonon overlap for this indirect interwell A→B transition. R1-related transitions are indirect also in the $K$-space, since the top of the upper light-hole-like subband LB1 is displaced to the final value of $K$ due to the subband spin splitting inherent to asymmetric heterostructures.\textsuperscript{34,35} This splitting is especially strong in heterostructures based on the narrow-gap semiconductor materials.\textsuperscript{36} In Figure 16a, for convenience, we show the split subbands with only one sign of the spin polarization. The Kramers degeneracy condition (3.21), imposed on any system by time-reversal symmetry, should be used here to restore the complete subband structure. Note, that the final momentum transfer is important for the high phonon emission rate in R1 resonance, because the optimum value of the electron-phonon overlap $I(q)$ can be engineered close to the peak of the effective density of the final electron states at the top of LB1 subband; see Figure 16b and corresponding peaks 1a and 1b in the lower subplot of Figure 15.

With $a_0$ increasing, phonon-assisted LA1→LB1 transitions become less efficient, firstly, because of corresponding decrease of the effective final density of states away of the top of the LB1 subband, and secondly, due to the suppression of the electron-phonon overlap $I(q)$ both at small and at the large momentum transfers. This can be readily seen from Figure 17, showing the electron-phonon overlap integrals for interband transitions.

**Fig. 17.** Electron-phonon overlap integral $I(q)$ for LA1→LB1 (solid line) and LA1→H2 (dashed line) transitions in an InAs/GaSb DQW with layer widths $a_A = 9$ nm and $a_B = 8$ nm.
as a function of the transferred (phonon) wave vector $q = K_f$. For a “vertical” transition with zero momentum transfer ($q = 0$), the electron-phonon overlap integral $I(q)$ is reduced simply to the overlap between orthogonal initial and final electron states, and thus vanishes. This explains the pronounced minimum in the phonon emission rate between the peaks R1 and R2. The final electron states for the latter resonance belong to the ring of the LB1 subband saddle points, which are again characterized by a high efficient density of states; see Figure 16b and peaks 2a and 2b in the lower subplot of Figure 15. For $a_L = 9$ nm, the peak of the effective density of states is more pronounced and is also favorably located at small negative values of $K_f$, where the electron-phonon overlap for LA1(0)→LB1($K_f$) electron transition is again significant; see Figure 17. For $a_L = 8.5$ nm, both the density peak 2b and electron-phonon overlap are less pronounced and, correspondingly, the peak rate value R2 is relatively small. Finally, the increase of the phonon emission rate in the region R3 corresponds to the onset of electron transitions into the H2 subband. The overall rate of the phonon emission is significantly depressed here because the most important transitions to the subband top, characterized by the highest effective density of states (peaks P3a and P3b in the lower subplot of Figure 15) correspond to inefficient vertical transitions with nearly zero electron/heavy-hole overlap integral $I(q)$. Most of the R3 rate is actually determined by the transitions to the H2-subband states with $K_f < -0.1$ nm$^{-1}$, where the LA1-H2 overlap significantly increases due to the light-heavy state mixing effect in the H2 subband, see Figure 17.

Finally, we compare the LO-phonon emission rates calculated for two different values of the InAs QW width; see the upper plot in Figure 15. For a narrower InAs QW, represented by curve set (b), the lower lasing subband LA1 has been relocated to the extreme upper part of the leaky window. Still, the overall magnitude of the main peak R1 remains practically unchanged. This means that phonon-assisted depopulation can be conveniently employed even when the lower lasing level is designed near the upper edge of the heterostructure leaky window, where direct interband tunneling depopulation becomes inefficient. This design is beneficial for the laser performance providing for the highest value of the matrix element for intrawell optical lasing transition and simultaneously preventing thermal backfilling of the lower lasing states.

5. Conclusions

LO-phonon assisted scattering determines intersubband electron relaxation in novel quantum well semiconductor lasers. We describe a simple phenomenological model, which allows comprehensive analysis of the LO-phonon mediated processes in intersubband laser heterostructures. As an application of our approach, we consider the process of the lower lasing level depopulation in type-II InAs/GaSb intersubband laser active region. We show that LO-phonon assisted transitions can significantly enhance the depopulation process comparing with direct interband tunneling through the heterostructure leaky window, traditionally considered as the main depopulation mechanism in type-II lasers. Inclusion of the phonon-assisted depopulation into the laser design scheme allows relocation of the lower lasing level into the upper part of the leaky window thus ensuring higher oscillator strength for the lasing transition and simultaneously preventing thermal backfilling of the lower lasing states.
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References