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Spontaneous radiative recombination and nonradiative Auger recombination in quantum-confined heterostructures

L.V. Asryan

Abstract. **General approach is described to the rates, fluxes and current densities associated with spontaneous radiative and nonradiative Auger recombinations in heterostructure lasers with different types of a quantum-confined active region (quantum wells, quantum wires, and quantum dots). The proper way of defining the spontaneous radiative and Auger recombination coefficients and their dimensionality are discussed. It is shown that only in a quantum dot, true time constants can be introduced for spontaneous radiative and nonradiative Auger recombinations, which are independent of the injection level. Closed-form elegant expressions are presented for the radiative recombination coefficient as an explicit function of temperature and parameters in bulk and quantum-confined structures. These expressions clearly demonstrate inappropriateness of the common practice of deriving the recombination coefficients in low-dimensional heterostructures from the bulk values.**

Keywords: *spontaneous radiative recombination, nonradiative Auger recombination, semiconductor lasers, heterojunctions, quantum wells, quantum wires, quantum dots.*

1. Introduction

Quantum wells (QWs) are extensively used as the active region in the basic optoelectronic device – the diode laser [1 – 4]. It was predicted [5, 6] and then successfully demonstrated (see, e.g. [7 – 9]) that the use of even lower-dimensional hetero-structures, such as quantum wires (QWRs) [10] and especially quantum dots (QDs) (see [11] for review), can significantly improve performance characteristics of semiconductor lasers.

Operation of a semiconductor laser is strongly affected by recombination processes in the structure. The intensity of each recombination process is characterised by its rate. Here, the spontaneous radiative recombination and the nonradiative Auger recombination are discussed.

Important parameters describing the rates of the recombination processes are the spontaneous radiative recombination coefficient or, simply, the radiative constant B, and the nonradiative Auger recombination coefficient or, simply, the Auger constant C. Despite the fact that considerable study is being given to low-dimensional laser structures, it became a common practice to use the bulk coefficients B_{3D} and C_{3D} and the size of the quantum-confined region to obtain the corresponding coefficients in the latter. Such an approach assumes (often implicitly) that the latter coefficients scale with the size of the quantum-confined region (see below). The shortcomings of this approach were systematically reviewed in [12] for the first time, where a physically appropriate way of presenting the recombination rates in a QW was set out explicitly from derivations within a common framework.

Here, to develop the entire picture, the expressions will be presented for the rates, fluxes and current densities associated with spontaneous radiative recombination and nonradiative Auger recombination in all types of low-dimensional heterostructures (QWs, QWRs, and QDs) used as the active region in injection lasers. For comparison, the corresponding expressions for a bulk active region will also be presented.

L.V. Asryan Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, USA; e-mail: asryan@mse.vt.edu; web-site: http://www.mse.vt.edu/people/faculty/asryan.html

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2. Basic equations

2.1 Bulk active region

In a three-dimensional (3D) region, the appropriate quantities are the rates per unit time per unit volume, which are given as follows:

$$R_{\rm spon}^{\rm 3D} = B_{\rm 3D} n_{\rm 3D} p_{\rm 3D}, \tag{1}$$

$$R_{\rm Auger}^{\rm 3D} = C_{\rm 3D} n_{\rm 3D}^2 p_{\rm 3D} \tag{2}$$

(measured in $[L]^{-3}[T]^{-1}$).

In Eqn (1), the product of the electron and hole 3D-densities, n_{3D} and p_{3D} (each measured in $\rm cm^{-3}$), reflects the fact that the spontaneous radiative recombination is a bimolecular process, i.e., each single act of recombination involves two carriers, an electron and a hole.

The product of $n_{3D}^2 p_{3D}$ in Eqn (2) reflects the fact that the Auger recombination is a trimolecular process, i.e., each single act of recombination involves three carriers, two electrons and a hole in the particular case of the CHCC process [13] discussed here for definiteness ('C' stands for the conduction band and 'H' stands for the heavy-hole valence band). There can be other Auger processes, such as the CHHS process ('S' stands for the spin-split-off valence

band), for which the recombination rate is proportional to $n_{3D}p_{3D}^2$ (since this process involves an electron and two holes in each single act).

In order that R_{spon}^{3D} and R_{Auger}^{3D} be measured in cm^{-3} s^{-1}, B_{3D} and C_{3D} have dimensionality cm^3 s^{-1} and cm^6 s^{-1}, respectively.

Together with the injection current itself, a useful and meaningful quantity in diode lasers is the current density per unit of an area perpendicular to the injection direction. The injection current density is measured in A cm^{-2} and is the product of the electron charge and the injection flux.

Both the spontaneous radiative and Auger recombinations consume injected carriers in diode lasers. Hence some portion of the total injection flux goes into the fluxes of these recombinations. These latter fluxes are obtained as the products of the linear size (thickness) b of the bulk recombination region along the direction of the current injection and the rates per unit time per unit volume [given by Eqns (1) and (2)]:

$$bR_{spon}^{3D} = bB_{3D}n_{3D}p_{3D}, \tag{3}$$

$$bR_{Auger}^{3D} = bC_{3D}n_{3D}^2p_{3D} \tag{4}$$

(measured in $[L]^{-2}[T]^{-1}$). The spontaneous radiative and Auger recombination current densities are

$$j_{spon}^{3D} = ebR_{spon}^{3D} = ebB_{3D}n_{3D}p_{3D}, \tag{5}$$

$$j_{Auger}^{3D} = ebR_{Auger}^{3D} = ebC_{3D}n_{3D}^2p_{3D}. \tag{6}$$

The expression for B_{3D} in a nondegenerate bulk material is presented in Table 1.

2.2 Quantum well

In a two-dimensional (2D) heterostructure (QW), it is appropriate to define the rates per unit time per unit area of a QW plane. These rates are given as follows:

$$R_{spon}^{2D} = B_{2D}n_{2D}p_{2D}, \tag{7}$$

$$R_{Auger}^{2D} = C_{2D}n_{2D}^2p_{2D} \tag{8}$$

(measured in $[L]^{-2}[T]^{-1}$), where n_{2D} and p_{2D} are the 2D-carrier densities measured in cm^{-2}. Since R_{spon}^{2D} and R_{Auger}^{2D} are measured in cm^{-2} s^{-1}, B_{2D} and C_{2D} have dimensionality cm^2 s^{-1} and cm^4 s^{-1}, respectively.

The expression for B_{2D} in a nondegenerate 2D-material is presented in Table 1. It was derived using the matrix element of interband optical transitions within the framework of $\boldsymbol{k}\cdot\boldsymbol{p}$ theory.

The same Eqns (7) and (8) present the recombination fluxes in a single QW.

The current densities associated with recombinations in a structure with multiple QWs are

$$j_{spon}^{2D} = eN_{QW}B_{2D}n_{2D}p_{2D}, \tag{9}$$

$$j_{Auger}^{2D} = eN_{QW}C_{2D}n_{2D}^2p_{2D}, \tag{10}$$

where N_{QW} is the number of QWs.

2.3 Quantum wire

In a one-dimensional (1D) heterostructure (QWR), it is appropriate to define the rates per unit time per unit length of a QWR. These rates are given as follows:

$$R_{spon}^{1D} = B_{1D}n_{1D}p_{1D}, \tag{11}$$

$$R_{Auger}^{1D} = C_{1D}n_{1D}^2p_{1D} \tag{12}$$

(measured in $[L]^{-1}[T]^{-1}$), where n_{1D} and p_{1D} are the 1D-carrier densities measured in cm^{-1}. Since R_{spon}^{1D} and R_{Auger}^{1D}

Table 1.

Structure	Spontaneous radiative recombination coefficient*,**	Unit	Reference
Bulk	$B_{3D} = \frac{4}{3}\sqrt{2}\pi^{3/2}\alpha\sqrt{\varepsilon}\frac{\hbar^2}{[(m_c+m_{hh})k_BT]^{3/2}}E_g\left(\frac{P}{\hbar c}\right)^2$	$[L]^3[T]^{-1}$	[14]***
QW****	$B_{2D} = \frac{4}{3}\pi\alpha\sqrt{\varepsilon}\frac{\hbar}{(m_c+m_{hh})k_BT}E_0\left(\frac{P}{\hbar c}\right)^2$	$[L]^2[T]^{-1}$	Derived here (see also [12], [15], [16])
QWR****	$B_{1D} = \frac{2}{3}\sqrt{2\pi}\alpha\sqrt{\varepsilon}\frac{1}{[(m_c+m_{hh})k_BT]^{1/2}}E_0\left(\frac{P}{\hbar c}\right)^2$	$[L][T]^{-1}$	Derived here
QD****	$B_{0D} = \frac{1}{\tau_{QD}^{spon}} = \frac{8}{3}\alpha\sqrt{\varepsilon}\frac{E_0}{\hbar}\left(\frac{P}{\hbar c}\right)^2$	$[T]^{-1}$	[14]

Parameters: $\alpha = e^2/\hbar c$ is the fine structure constant; e is the electron charge; $\hbar$ is the Planck's constant; c is the velocity of light in vacuum; ε is the dielectric constant; m_c and m_{hh} are the electron and heavy-hole effective masses; k_B is the Boltzmann constant; T is the temperature; E_g is the bandgap of the bulk material; $E_0 = E_g + \varepsilon_n + \varepsilon_p$ is the optical transition energy; ε_n and ε_p are the lowest quantised energy levels (subband edges) of an electron and a hole in the conduction and valence bands respectively, measured from the corresponding band edges; Kane's parameter P is given as follows

$$P^2 = \frac{\hbar^2}{2}\left(\frac{1}{m_c} - \frac{1}{m_0}\right)\frac{E_g(E_g+\Delta_0)}{E_g+2\Delta_0/3};$$

m_0 is the free-electron mass; Δ_0 is the energy of the spin-orbit splitting (the use of parameter P is convenient in view of its slight dependence on the material type [18]).

*Both in the conduction and valence bands, a single subband and parabolic dispersion are assumed in the directions of free motion. **The ratio $P/\hbar c$ is dimensionless. ***To compare the expression for B_{3D} with those in low-dimensional structures, Eqn (10) of [14] is simplified assuming only heavy-holes are involved. ****The energy E_0 of the optical transition between the lowest subband edges (lowest levels) in the conduction and valence bands enters into the expressions for B in quantum-confined structures instead of the bandgap E_g in the expression for B_{3D}.

are measured in cm^{-1} s^{-1}, B_{1D} and C_{1D} have dimensionality cm s^{-1} and cm^2 s^{-1}, respectively.

The expression for B_{1D} in a nondegenerate 1D-material is presented in Table 1. Like the expressions for the radiative constant in bulk-, QW-, and QD-structures, the expression for B_{1D} was derived within the framework of $\boldsymbol{k}\cdot\boldsymbol{p}$ theory.

The recombination fluxes in a single layer of QWRs are

$$N_{lin}B_{1D}n_{1D}p_{1D}, \tag{13}$$

$$N_{lin}C_{1D}n_{1D}^2p_{1D}, \tag{14}$$

where N_{lin} is the linear density of QWRs (measured in cm^{-1}) in the layer (see [17]); the dimensionality of fluxes is $[L]^{-2}[T]^{-1}$.

The current densities associated with recombinations in a structure with multiple layers of QWRs are

$$j_{spon}^{1D} = eN_{QWR-layer}N_{lin}B_{1D}n_{1D}p_{1D}, \tag{15}$$

$$j_{Auger}^{1D} = eN_{QWR-layer}N_{lin}C_{1D}n_{1D}^2p_{1D}, \tag{16}$$

where $N_{QWR-layer}$ is the number of layers with QWRs.

2.4 Quantum dot

In a zero-dimensional (0D) heterostructure (QD), it is appropriate to define the rates per unit time per a single QD. In view of the quantum-size effect in all the three directions in a QD, there is no volume, area or length, with respect to which the transition rates should be counted. In [14], the following equation was derived for the spontaneous radiative recombination rate in a QD:

$$R_{spon}^{0D} = B_{0D}f_nf_p = \frac{f_nf_p}{\tau_{QD}^{spon}}, \tag{17}$$

where f_n and f_p are the electron and hole level occupancies (probabilities of occupation of the levels) in a QD, which are the analogues of the carrier densities in a bulk region, QW, and QWR; R_{spon}^{0D} is measured in $[T]^{-1}$.

The Auger recombination rate in a QD can be written as follows:

$$R_{Auger}^{0D} = C_{0D}f_n^2f_p = \frac{f_n^2f_p}{\tau_{QD}^{Auger}} \tag{18}$$

(measured in $[T]^{-1}$). Since R_{spon}^{0D} and R_{Auger}^{0D} are measured in s^{-1}, and f_n and f_p are dimensionless, then B_{0D} and C_{0D} have dimension of s^{-1}. Hence B_{0D} и C_{0D} can be viewed as the reciprocals of the spontaneous-radiative (τ_{QD}^{spon}) and Auger recombination times (τ_{QD}^{Auger}), respectively:

$$B_{0D} = \frac{1}{\tau_{QD}^{spon}}, \tag{19}$$

$$C_{0D} = \frac{1}{\tau_{QD}^{Auger}}. \tag{20}$$

The expression for $B_{0D} = 1/\tau_{QD}^{spon}$ is presented in Table 1.

The recombination fluxes in a single layer of QDs are

$$N_sB_{0D}f_nf_p = N_s\frac{f_nf_p}{\tau_{QD}^{spon}}, \tag{21}$$

$$N_sC_{0D}f_n^2f_p = N_s\frac{f_n^2f_p}{\tau_{QD}^{Auger}}; \tag{22}$$

(the dimensionality of fluxes is $[L]^{-2}[T]^{-1}$), where N_s is the surface density of QDs (measured in cm^{-2}) in the layer.

The current densities associated with recombinations in a structure with multiple layers of QDs are

$$j_{spon}^{0D} = eN_{QD-layer}N_sB_{0D}f_nf_p = eN_{QD-layer}N_s\frac{f_nf_p}{\tau_{QD}^{spon}}, \tag{23}$$

$$j_{Auger}^{0D} = eN_{QD-layer}N_sC_{0D}f_n^2f_p = eN_{QD-layer}N_s\frac{f_n^2f_p}{\tau_{QD}^{Auger}}, \tag{24}$$

where $N_{QD-layer}$ is the number of layers with QDs.

3. Discussion

(1) One can see from Table 1 that, in the general case, the spontaneous radiative recombination coefficient is an inverse power function of $\sqrt{T}$

$$B_{rD} \propto \frac{1}{T^{r/2}}, \tag{25}$$

where r is the dimensionality of the structure: $r = 3$, 2, 1, and 0 in bulk, QW, QWR, and QD, respectively. Such a T-dependence is simply a consequence of the T-dependence of the effective densities of states in the conduction and valence bands, which in the general case are

$$N_{c,v}^{rD} \propto T^{r/2}. \tag{26}$$

(2) A comparison of the above equations for different low-dimensional structures shows that, only in a QD, true time constants can be introduced for the spontaneous radiative and Auger recombinations, τ_{QD}^{spon} and τ_{QD}^{Auger}, which are independent of the level occupancies f_n and f_p, i.e., of the injection (pump) current, and hence are true recombination lifetimes.

Nevertheless, it became a common practice to exploit the spontaneous radiative and Auger recombination times also in bulk, QW, and QWR structures. Defining

$$\frac{1}{\tau^{spon}} = Bn, \tag{27}$$

$$\frac{1}{\tau^{Auger}} = Cn^2, \tag{28}$$

the recombination rates become

$$R_{spon} = \frac{p}{\tau^{spon}}, \tag{29}$$

$$R_{Auger} = \frac{p}{\tau^{Auger}}. \tag{30}$$

As seen from Eqns (27) and (28), τ^{spon} and τ^{Auger} depend on the carrier density (electron density here, for definiteness), i.e., on the pump current, and hence are not true time constants. The appropriate quantities in bulk, QW, and QWR structures are the corresponding recombination coefficients, B and C. In contrast, τ_{QD}^{spon} and τ_{QD}^{Auger} are true time constants in a QD. Using the recombination coefficients in a QD, B_{0D} and C_{0D}, is equivalent to using the time constants.

(3) Only in the bulk region, the current densities scale with the thickness b of the region [Eqns (5) and (6)]. In the cases of QWs [Eqns (9) and (10)], QWRs [Eqns (15) and (16)], and QDs [Eqns (23) and (24)], j_{spon} and j_{Auger} do not scale with the linear size (thickness of the QW, thickness of the layer with QWRs or QDs). This is natural, since in all these low-dimensional structures the size is so small that the quantum-size effect is manifested. A QW, a layer with QWRs, and a layer with QDs act as a 2D-layer, i.e., a layer with no linear size in the transverse direction, which is why they are considered quantum-confined. The size of the structure does affect the quantised energy levels and hence the optical transition energy E_0, thus affecting B [see Table 1] and C, but this kind of size-dependence is never scaling.

(4) A common practice of deriving the recombination coefficients in low-dimensional structures from the bulk values leads to the strong (scaling) dependence on the recombination region size a^*. This is demonstrated in Table 2.

Just as the carrier density in a quantum-confined heterostructure can not be obtained from the bulk value (which is nevertheless often done) and should be derived independently using the corresponding density of states, so can not be obtained and so should be derived the spontaneous radiative and Auger recombination coefficients. Presented in Table 1 are the appropriate expressions for the spontaneous radiative recombination coefficient B as a function of temperature and parameters in bulk and quantum-confined structures. These expressions reveal the absence of any scaling dependence on the size and show clearly that a simplified bulk-value approach illustrated in Table 2 is completely inappropriate in quantum-confined structures. There is indeed a size-dependence of B, which comes from such a dependence of the transition energy E_0 in low-dimensional structures; as mentioned above, this dependence is not scaling.

Table 2. Recombination coefficients in low-dimensional structures obtained using bulk values B_{3D} and C_{3D}.

Quantum-confined structure	QW	QWR	QD
Spontaneous radiative recombination coefficient	$\frac{B_{3D}}{a}$	$\frac{B_{3D}}{a^2}$	$\frac{B_{3D}}{a^3}$
Nonradiative Auger recombination coefficient	$\frac{C_{3D}}{a^2}$	$\frac{C_{3D}}{a^4}$	$\frac{C_{3D}}{a^6}$

The same conclusion is true for the Auger recombination coefficient C in quantum-confined structures. Calculation of the Auger constant is more complicated than that of the radiative constant and usually requires numerical methods. In contrast to B, there are no closed-form expressions, which would give reasonable estimates for C. In addition, extracting C from experiments is a difficult task. As a consequence, there is a wide scatter in reported values for C even in a bulk material [13].

*Another shortcoming of the common procedure is that the recombination region size, i.e. the size of the region of actual localization of a carrier, is larger (often considerably) than the geometrical size of a quantum-confined region defined by its heteroboundaries with the surrounding material.

4. Conclusions

General approach has been described to the rates, fluxes and current densities associated with spontaneous radiative and nonradiative Auger recombinations in heterostructure lasers with a quantum-confined active region (quantum wells, quantum wires, and quantum dots). The proper way of defining and the dimensionality of the spontaneous radiative and Auger recombination coefficients have been discussed. Only in a QD, true time constants can be introduced for spontaneous radiative and Auger recombinations, which are independent of the injection level. Closed-form elegant expressions have been presented for the radiative recombination coefficient as an explicit function of temperature and parameters in bulk and quantum-confined structures. These expressions clearly demonstrate inappropriateness of the common practice of deriving the recombination coefficients in low-dimensional heterostructures from the bulk values.

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