# Population inversion study of GaAs／AlGaAs three－quantum－well quantum cascade structures 

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#### Abstract

A population inversion study of $\mathrm{GaAs} / \mathrm{Al}_{\mathrm{x}} \mathrm{Ga}_{1-\mathrm{x}} \mathrm{As}$ three－quantum－well quantum cascade structures is presented．We derive the population inversion condition（PIC）of the active region（AR）and discuss the PICs on different structures by changing structural parameters such as the widths of quantum wells or barriers in the AR．For some instances，the PIC can be simplified and is proportional to the spontaneous emission lifetime between the second and the first excited states，whereas some other instances imply that the PIC is proportional to the state lifetime of the second excited state．


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The quantum cascade laser（QCL）has become an im－ portant source of coherent radiation in the mid－infrared region，and its frequency range has been extended to the terahertz region ${ }^{[1]}$ ．The QCL currently exhibits excel－ lent performance ${ }^{[2-7]}$ ．Theoretical research is an effective tool to facilitate laser fabrication ${ }^{[8]}$ ．In this letter，we study the mechanisms by which the widths of quantum wells（QWs）and barriers in the active region（AR）can affect the population inversion of QCL．

The time－independent Schrodinger equation of an elec－ tron with mass $m$ in one－dimensional potential $V(x)$ is

$$
\begin{equation*}
\widehat{H}(x) \phi(x)=-\frac{\hbar^{2}}{2} \frac{\mathrm{~d}}{\mathrm{~d} x}\left(\frac{1}{m} \frac{\mathrm{~d} \phi}{\mathrm{~d} x}\right)+V(x) \phi(x)=E \phi(x) \tag{1}
\end{equation*}
$$

where $V(x)$ includes $-e F x$ ，the potential caused by the applied electric field $F$ ，and $e$ is the electron charge．To solve Eq．（1），the wave function and potential are dis－ cretized．$N+1$ points are selected to equally divide the AR ，and the position coordinate of the electron can be expressed as $x_{j}=j \times h_{0}$ ，where $h_{0}$ is the step length，$j$ $=0,1,2, \cdots, N$ ，and $x_{j+1}=x_{j}+h_{0}$ ．The total length of the AR of the QCL is $L_{\mathrm{a}}=N h_{0}$ ．At each selected point，the wave function and potential are $\phi_{j}=\phi\left(x_{j}\right)$ and $V_{j}=V\left(x_{j}\right)$ ，respectively．The first－order deriva－ tive of the discrete wave function at two adjacent points can be expressed in the finite difference approximation as $\frac{1}{m} \frac{\mathrm{~d} \phi\left(x_{j}\right)}{\mathrm{d} x}=\frac{\phi\left(x_{j}\right)-\phi\left(x_{j-1}\right)}{m_{j} h_{0}}$ ．To obtain the second－order derivative of the discrete wave function，three adjacent points must be considered，resulting in the following ex－
pression：

$$
\begin{align*}
\frac{\mathrm{d}}{\mathrm{~d} x}\left(\frac{1}{m} \frac{\mathrm{~d} \phi\left(x_{j}\right)}{d x}\right) & =\frac{1}{m_{j+1} h_{0}^{2}}\left[\phi\left(x_{j+1}\right)-\phi\left(x_{j}\right)\right] \\
& -\frac{1}{m_{j} h_{0}^{2}}\left[\phi\left(x_{j}\right)-\phi\left(x_{j-1}\right)\right] \tag{2}
\end{align*}
$$

After taking Eq．（2）into Eq．（1），we obtain the matrix equations of the AR：

$$
\begin{array}{r}
(\mathbf{H}-E \mathbf{1}) \phi(x)=\sum_{j=\mathbf{0}}^{N}\left[-\mathbf{u}_{j} \phi\left(\mathbf{x}_{j-\mathbf{1}}\right)\right. \\
\left.+\left(d_{j}-E\right) \phi\left(x_{j}\right)-u_{j+1} \phi\left(x_{j+1}\right)\right]=0 \tag{3}
\end{array}
$$

in which the Hamiltonian is a symmetric diagonal ma－ trix，wherein 1 is the unit matrix，the diagonal matrix element is $d_{j}=\frac{\hbar^{2}}{2 h_{0}^{2}}\left(\frac{1}{m_{j+1}}+\frac{1}{m_{j}}\right)+V_{j}$ ，and the adjacent non－diagonal matrix element is $u_{j}=\frac{\hbar^{2}}{2 m_{j} h_{0}^{2}}$ ．Setting $x_{0}$ and $x_{N}$ as the boundary coordinates of AR，the boundary conditions of the region are

$$
\begin{align*}
\phi\left(x_{0}\right) & =\phi\left(x_{N}\right)  \tag{4}\\
\left.\frac{1}{m_{0}} \frac{\mathrm{~d} \phi}{\mathrm{~d} x}\right|_{x=x_{0}} & =\left.\frac{1}{m_{N}} \frac{\mathrm{~d} \phi}{\mathrm{~d} x}\right|_{x=x_{N}} \tag{5}
\end{align*}
$$

We also obtain the matrix equation of the AR：

$$
(\mathbf{H}-E \mathbf{1}) \phi=\left(\begin{array}{cccccc}
\left(d_{1}-E\right) & -u_{2} & 0 & \cdot & \cdot & -u_{1}  \tag{6}\\
-u_{2} & \left(d_{2}-E\right) & -u_{3} & \cdot & \cdot & \cdot \\
0 & -u_{3} & \left(d_{3}-E\right) & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & -u_{N-1} & \left(d_{N-1}-E\right) & -u_{N} \\
-u_{1} & \cdot & \cdot & \cdot & -u_{N} & \left(d_{N}-E\right)
\end{array}\right)\left(\begin{array}{c}
\phi\left(x_{1}\right) \\
\phi\left(x_{2}\right) \\
\phi\left(x_{3}\right) \\
\cdot \\
\phi\left(x_{N-1}\right) \\
\phi\left(x_{N}\right)
\end{array}\right)=\mathbf{0} .
$$

The solutions of the matrix equation yield the eigen energies and wave functions of the AR. In our calculations the electron density of the AR is sufficiently small that we can neglect Poisson's equation ${ }^{[9]}$.

Research results show a high probability of rapid subband thermalization through electron-electron scattering processes ${ }^{[10]}$. For thermalized subbands, the emission process in the AR dominates the tunneling output, which is extremely fast that the density of electrons in the first subband shown in Fig. 1 is nearly zero. The rate equations for the AR are

$$
\begin{align*}
& \frac{\mathrm{d} N_{3}}{\mathrm{~d} t}=\frac{J}{e L_{\mathrm{a}}}-\frac{N_{3}}{\tau_{3}},  \tag{7}\\
& \frac{\mathrm{~d} N_{2}}{\mathrm{~d} t}=\frac{N_{3}}{\tau_{32}}-\frac{N_{2}}{\tau_{2}} \tag{8}
\end{align*}
$$

where $N_{i}\left(N_{i}=2,3\right)$ is the electron concentration in the $i$ th subband and $J$ is the electrical current density. $1 / \tau_{3}=$ $1 / \tau_{32}+1 / \tau_{31}$, where $\tau_{3}$ is the state lifetime (SL) or relaxation time (RT) of the third subband, and $\tau_{32}$ and $\tau_{31}$ are the reciprocals of the spontaneous emission rate (SER) between the third subband and two other subbands in Fig. 1, respectively. The SL or RT of the second subband $\tau_{2}$ satisfies $1 / \tau_{2}=1 / \tau_{21}+1 / \tau_{\mathrm{op}}$, where $\tau_{21}$ is the reciprocal of the SER between the second subband and the first subband, $\tau_{\text {op }}$ is the reciprocal of the intersubband polar-optical-phonon (POP) scattering rate between the second and the first subbands. In other words, $\tau_{32}, \tau_{31}$, and $\tau_{21}$ are the RTs of spontaneous emissions and can be expressed as ${ }^{[11]}$

$$
\begin{equation*}
\frac{1}{\tau_{\mathrm{if}}}=\gamma_{0}^{3 \mathrm{D}} \times\left|F_{\mathrm{i} \rightarrow \mathrm{f}}\right| \tag{9}
\end{equation*}
$$

where $\gamma_{0}^{3 \mathrm{D}}=\frac{e^{2} n w_{0}^{2}}{6 \pi \varepsilon_{0} m^{*} c^{3}}$ and

$$
\begin{equation*}
F_{\mathrm{i} \rightarrow \mathrm{f}}=\frac{2 m^{*}\left(E_{\mathrm{f}}-E_{\mathrm{i}}\right)}{\hbar^{2}}\left|Z_{\mathrm{i} \rightarrow \mathrm{f}}\right|^{2} \tag{10}
\end{equation*}
$$

where $n$ is the refractive index, $m^{*}$ is the electron effective mass, $\omega_{0}=\left(E_{\mathrm{i}}-E_{\mathrm{f}}\right) / \hbar$, where $E_{\mathrm{i}}$ and $E_{\mathrm{f}}$ are the eigen energies of the initial and final states of spontaneous emission, respectively, $\varepsilon_{0}$ is the vacuum permittivity, $c$ is the light velocity, and $\left|Z_{\mathrm{i} \rightarrow \mathrm{f}}\right|$ is the dipole matrix element. $\tau_{\text {op }}$ is the intersubband POP scattering relaxation time (SRT) between the second and the first subbands. Based on D. Ahn and S. L. Chuang's work ${ }^{[12]}$, $\tau_{\text {op }}$ can be expressed as

$$
\begin{align*}
\frac{1}{\tau_{\mathrm{op}}} & =E_{\mathrm{q}} \frac{2 e^{2}}{8 \sqrt{2} \pi \hbar^{2}} \sqrt{\frac{m^{*}}{E_{\mathrm{t}}}}\left[\frac{1}{\varepsilon_{0}}\left(\frac{1}{\varepsilon_{\infty}}-\frac{1}{\varepsilon_{\mathrm{s}}}\right)\right]\left(n_{\mathrm{q}}+1\right) \\
& \times\left.\int_{0}^{\pi} \frac{1}{|\cos \phi|} \mathrm{d} \phi\right|_{\phi \neq \frac{\pi}{2}} ^{x_{x_{0}}} \phi_{1}(z) \phi_{2}(z) \mathrm{d} z \int_{x_{0}}^{x_{N}} \phi_{1}\left(z^{\prime}\right) \\
& \times \phi_{2}\left(z^{\prime}\right) \mathrm{d} z^{\prime}\left(e^{-\frac{\sqrt{8 m^{*} E_{t}}}{\hbar}} \cos \phi\left|z-z^{\prime}\right|+1\right) \tag{11}
\end{align*}
$$

where $E_{\mathrm{q}}$ is the energy of POP, $E_{\mathrm{t}}=\hbar^{2} k_{\mathrm{t}}^{2} / 2 m^{*}, k_{\mathrm{t}}$ is the wave vector of the electron in the plane parallel to
the QWs, and $\varepsilon_{\infty}$ and $\varepsilon_{\mathrm{s}}$ are the optical and static dielectric constants, respectively. The phonon occupation number $n_{\mathrm{q}}$ is given by the Bose-Einstein distribution $n_{\mathrm{q}}=\left\{\exp \left[\left(\hbar \omega_{\mathrm{q}}\right) / k_{\mathrm{B}} T\right]-1\right\}^{-1}$, where $k_{\mathrm{B}}$ is the Boltzmann constant.

Supposing that the electric current $J$ injects into the third subband without loss, then it can be obtained from Eqs. (7) and (8),

$$
\begin{equation*}
N_{3}-N_{2}=\frac{J}{e L_{\mathrm{a}}} \tau_{3}\left(1-\frac{\tau_{2}}{\tau_{32}}\right), \tag{12}
\end{equation*}
$$

which is the population inversion condition (PIC) of QCL.

As shown in Fig. 2, the widths of the four barriers are denoted as $W_{\mathrm{B} 1}, W_{\mathrm{B} 2}, W_{\mathrm{B} 3}$, and $W_{\mathrm{B} 4}$, and the widths of the three QWs are denoted as $W_{\mathrm{W} 1}, W_{\mathrm{W} 2}$, and $W_{\mathrm{W} 3}$. For component $x$, the electron effective masses of $\mathrm{Al}_{x} \mathrm{Ga}_{1-x}$ As and GaAs are $m_{\text {GaAs }}^{*}=(0.063+0.087 x) m_{0}$ and $m_{\text {AlGaAs }}^{*}=0.063 m_{0}$, respectively, where $m_{0}$ is the free-electron mass. The conduction band discontinuity at $\mathrm{Al}_{x} \mathrm{Ga}_{1-x} \mathrm{As} / \mathrm{GaAs}$ heterointerface is $\Delta E_{c}=0.79 x$ eV , and the applied electric field is $F=10 \mathrm{kV} / \mathrm{cm}$. If $W_{\mathrm{B} 1}=4 \mathrm{~nm}, W_{\mathrm{W} 1}=0.5 \mathrm{~nm}, W_{\mathrm{B} 2}=1 \mathrm{~nm}, W_{\mathrm{W} 2}=15.5$ $\mathrm{nm}, W_{\mathrm{B} 3}=2 \mathrm{~nm}, W_{\mathrm{W} 3}=3 \mathrm{~nm}$, and $W_{\mathrm{B} 4}=6.5 \mathrm{~nm}$, then three subbands contribute to the performance of the AR. The three subbands are denoted as subband1, subband2, and subband3, and the corresponding eigen energies are marked as $E_{1}, E_{2}$, and $E_{3}$. The energy difference $E_{2}-E_{1} \approx 35.4-(-0.39)=35.79 \mathrm{meV}$ is very close to the POP energy of the AR: $E_{\mathrm{op}}=$ $E_{\mathrm{op}-\mathrm{AlGaAs}} \frac{L_{\mathrm{AlGaAs}}}{L_{\mathrm{a}}}+E_{\mathrm{op}-\mathrm{GaAs}}\left(1-\frac{L_{\mathrm{AlGaAs}}}{L_{\mathrm{a}}}\right) \approx 35.79 \mathrm{meV}$, where $E_{\text {op-AlGaAs }}$ and $E_{\text {op-GaAs }}$ are the POP energies of $\mathrm{Al}_{x} \mathrm{Ga}_{1-x} \mathrm{As}$ and GaAs , respectively, and $L_{\mathrm{op}-\mathrm{AlGaAs}}$ and $L_{\mathrm{op}-\mathrm{GaAs}}$ are total thicknesses of $\mathrm{Al}_{x} \mathrm{Ga}_{1-x} \mathrm{As}$


Fig. 1. Three-level diagram of the AR.


Fig. 2. Three-quantum-well AR, $W_{\mathrm{B} 1}=4 \mathrm{~nm}, W_{\mathrm{W} 1}=0.5$ $\mathrm{nm}, W_{\mathrm{B} 2}=1 \mathrm{~nm}, W_{\mathrm{W} 2}=15.5 \mathrm{~nm}, W_{\mathrm{B} 3}=2 \mathrm{~nm}, W_{\mathrm{W} 3}=3$ $\mathrm{nm}, W_{\mathrm{B} 4}=6.5 \mathrm{~nm}$, and applied electric field $F=10 \mathrm{kV} / \mathrm{cm}$.
and GaAs in the AR, respectively. The POP energy is $E_{\text {op-AlGaAs }}=36.25+1.83 x+17.12 x^{2}-5.11 x^{3} \mathrm{meV}$, and $E_{\mathrm{op}-\mathrm{GaAs}}=35 \mathrm{meV}$. The energy difference $E_{3}-E_{2}=$ $64.9-35.4=29.5 \mathrm{meV}$ shows that the lasing wavelength (LW) is approximately $42.03 \mu \mathrm{~m}$.

We set $E_{\mathrm{t}}=E_{\mathrm{op}}$ in calculating intersubband POP SRT. Setting $W_{\mathrm{B} 1}=4 \mathrm{~nm}, W_{\mathrm{B} 2}=1 \mathrm{~nm}, W_{\mathrm{B} 3}=2 \mathrm{~nm}$, and $W_{\mathrm{B} 4}=6.5 \mathrm{~nm}$, the spontaneous emission lifetimes (SELs) $\tau_{32}, \tau_{31}$, and $\tau_{21}$, together with the POP SRT between subband2 and subband $1 \tau_{\mathrm{op}}$, and the LW of the QCL as functions of $W_{\mathrm{W} 1}, W_{\mathrm{W} 2}$, and $W_{\mathrm{W} 3}$ were calculated. The calculation results are shown in Fig. 3. Setting $W_{\mathrm{W} 1}$ as the linear variable, $W_{\mathrm{W} 2}$ is changed correspondingly, and $W_{\mathrm{W} 3}$ is changed slightly to make sure that $E_{2}{ }^{-}$ $E_{1} \approx E_{\mathrm{op}}$. The calculated values of $W_{\mathrm{W} 1}, W_{\mathrm{W} 2}$, and $W_{\text {W3 }}$ are listed in Table 1. Among the three SELs, $\tau_{31}$ has the longest time (Fig. 3(a)). When $\tau_{31} \approx 17.66 \mu$ s and $\tau_{32} \approx 0.69 \mu \mathrm{~s}$, the ratio $\tau_{32} / \tau_{31}$ has the maximum value 0.039 , then $\tau_{3}=\frac{\tau_{32} \times \tau_{31}}{\tau_{31}+\tau_{32}}=\tau_{32} \frac{1}{1+\frac{\tau_{32}}{\tau_{31}}} \approx \tau_{32} \frac{1}{1+0.039} \approx \tau_{32}$. A comparison between Figs. 3(a) and (b) shows that the ratio $\tau_{\mathrm{op}} / \tau_{21}$ has the maximum value $1.57 \times 10^{-4}$, then $\tau_{2}=\frac{\tau_{\mathrm{op}} \times \tau_{21}}{\tau_{21}+\tau_{\mathrm{op}}}=\tau_{\mathrm{op}} \frac{1}{1+\frac{\tau_{\mathrm{op}}}{\tau_{21}}} \approx \tau_{\mathrm{op}} \frac{1}{1+1.57 \times 10^{-4}} \approx \tau_{\mathrm{op}}$. Under these considerations, the PIC of the QCL is $N_{3}-N_{2} \approx$ $\frac{J}{e L_{\mathrm{a}}} \tau_{32}\left(1-\frac{\tau_{\mathrm{op}}}{\tau_{32}}\right)$, and the ratio $\tau_{\mathrm{op}} / \tau_{32}$ has the maximum value $1.5 \times 10^{-4}$ (Fig. 3). Then, we obtain

$$
\begin{equation*}
N_{3}-N_{2} \approx \frac{J}{e L_{\mathrm{a}}} \tau_{32} \tag{13}
\end{equation*}
$$

Thus, PIC can be simplified to Eq. (13). Assigning $W_{\mathrm{W} 1}=3 \mathrm{~nm}, W_{\mathrm{W} 2}=14.15 \mathrm{~nm}$, and $W_{\mathrm{W} 3}=3 \mathrm{~nm}, \tau_{32}$ has the maximum value, and the AR has the maximum population inversion (MPI). The corresponding LW is 46.44 $\mu \mathrm{m}$, which is also the longest wavelength in Fig. 3(b), and the shortest one is $41.33 \mu \mathrm{~m}$ at $W_{\mathrm{W} 1}=1 \mathrm{~nm}, W_{\mathrm{W} 2}$ $=15.25 \mathrm{~nm}$, and $W_{\mathrm{W} 3}=2.95 \mathrm{~nm}$.

Figures $4(\mathrm{a})$ and $4(\mathrm{~b})$ show the results when $W_{\mathrm{W} 1}$ is set as the linear variable, $W_{\mathrm{W} 3}$ is changed correspondingly, and $W_{\mathrm{B} 4}$ is changed slightly by setting $W_{\mathrm{B} 1}=4$ $\mathrm{nm}, W_{\mathrm{B} 2}=1 \mathrm{~nm}, W_{\mathrm{W} 2}=15.5 \mathrm{~nm}$, and $W_{\mathrm{B} 3}=2 \mathrm{~nm}$. The calculated values of $W_{\mathrm{W} 1}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$ are listed in Table 2. Similar to Fig. 3, $\tau_{31}$ has the longest time among the three SELs, and $\tau_{31}$ changes from approximately $7.93 \mu$ s to 2.20 ms . As shown in Fig. 4, $\tau_{32} / \tau_{31}<0.045$, $\tau_{\mathrm{op}} / \tau_{21}<0.94 \times 10^{-4}$, and $\tau_{\mathrm{op}} / \tau_{32}<0.98 \times 10^{-4}$. Hence, PIC can be also simplified to Eq. (13). The LW corresponding to the PIC is approximately $42.03 \mu \mathrm{~m}$, which is


Fig. 3. (a) SELs $\tau_{32}, \tau_{31}$, and $\tau_{21}$ as functions of $W_{\mathrm{W} 1}, W_{\mathrm{W} 2}$, and $W_{\mathrm{W} 3}$. (b) POP SRT between subband2 and subband1 $\tau_{\mathrm{op}}$ and LW of QCL as functions of $W_{\mathrm{W} 1}, W_{\mathrm{W} 2}$, and $W_{\mathrm{W} 3}$. $W_{\mathrm{W} 1}$ is set as the linear variable shown in the horizontal coordinate, $W_{\mathrm{W} 2}$ is changed correspondingly, and $W_{\mathrm{W} 3}$ is changed slightly to make sure that $E_{2}-E_{1} \approx E_{\text {op }}$.

Table 1. Calculated Values of $W_{\mathrm{W} 1}, W_{\mathrm{W} 2}$, and $W_{\mathrm{W} 3}$ Corresponding to Fig. 3.

| Variable | $W_{\mathrm{W} 1}$ | $W_{\mathrm{W} 2}$ | $W_{\mathrm{W} 3}$ |
| :---: | :---: | :---: | :---: |
|  | 0.50 | 15.50 | 3.00 |
|  | 0.75 | 15.45 | 3.00 |
| Value (nm) | 1.00 | 15.25 | 2.95 |
|  | 1.25 | 15.00 | 3.05 |
|  | 1.75 | 14.90 | 2.95 |
|  | 2.00 | 14.70 | 3.00 |
|  | 2.25 | 14.55 | 3.00 |
|  | 2.50 | 14.45 | 3.00 |
|  | 2.75 | 14.30 | 3.00 |
|  | 3.00 | 14.15 | 3.00 |



Fig. 4. (a) $\tau_{32}, \tau_{31}$, and $\tau_{21}$ as functions of $W_{\mathrm{W} 1}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$. (b) $\tau_{\mathrm{op}}$ and LW of QCL as functions of $W_{\mathrm{W} 1}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$. $W_{\mathrm{W} 1}$ is set as the linear variable shown in the horizontal coordinate, $W_{\mathrm{W} 3}$ is changed correspondingly, and $W_{\mathrm{B} 4}$ is changed slightly to make sure that $E_{2}-E_{1} \approx E_{\text {op }}$.
also the longest wavelength in Fig. 4 (b), and the shortest wavelength is $31.88 \mu \mathrm{~m}$ when $W_{\mathrm{W} 1}=3 \mathrm{~nm}, W_{\mathrm{W} 3}=$ 0.85 nm , and $W_{\mathrm{B} 4}=6.55 \mathrm{~nm}$.

Setting $W_{\mathrm{W} 2}$ as the linear variable, $W_{\mathrm{W} 3}$ is changed correspondingly, and $W_{\mathrm{B} 4}$ is changed slightly when $W_{\mathrm{B} 1}$ $=4 \mathrm{~nm}, W_{\mathrm{W} 1}=0.5 \mathrm{~nm}, W_{\mathrm{B} 2}=1 \mathrm{~nm}$, and $W_{\mathrm{B} 3}=2 \mathrm{~nm}$. We obtain $\tau_{32}, \tau_{31}, \tau_{21}$, and $\tau_{\text {op }}$, and the LW is shown in Fig. 5. The calculated values of $W_{\mathrm{W} 2}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$ are listed in Table 3. For all the calculated AR structures, despite the longest $\tau_{\mathrm{op}} \approx 1.78 \mathrm{~ns}, \tau_{\mathrm{op}} / \tau_{21}<0.28 \times 10^{-2}$ and $\tau_{\mathrm{op}} / \tau_{32}<0.24 \times 10^{-2}$. Meanwhile, the ratio $\tau_{32} / \tau_{31}$ changes as the structure of AR changes. For example, $\tau_{32} / \tau_{31} \approx 0.64$ at $W_{\mathrm{W} 2}=12 \mathrm{~nm}, W_{\mathrm{W} 3}=4 \mathrm{~nm}$, and $W_{\mathrm{B} 4}=6.4 \mathrm{~nm}$, and $\tau_{32} / \tau_{31} \approx 1.88 \times 10^{-4}$ at $W_{\mathrm{W} 2}=16$ $\mathrm{nm}, W_{\mathrm{W} 3}=2.4 \mathrm{~nm}$, and $W_{\mathrm{B} 4}=6.5 \mathrm{~nm}$. Thus, $\tau_{3}$ cannot be simply replaced by $\tau_{32}$, and the PIC of the QCL becomes

$$
\begin{equation*}
N_{3}-N_{2} \approx \frac{J}{e L_{\mathrm{a}}} \tau_{3} \tag{14}
\end{equation*}
$$

By calculating $\tau_{3}$, we find that the MPI about the structures of the AR in Fig. 5 is the structure when $W_{\mathrm{W} 2}=$ $15 \mathrm{~nm}, W_{\mathrm{W} 3}=3.3 \mathrm{~nm}$, and $W_{\mathrm{B} 4}=6.5 \mathrm{~nm}$, and that the corresponding LW is $44.93 \mu \mathrm{~m}$, where the longest and shortest wavelengths are 46.27 and $25.89 \mu \mathrm{~m}$, respectively.

The results in Fig. 6 are $\tau_{32}, \tau_{31}$, and $\tau_{21}$, together with $\tau_{\mathrm{op}}$ and LW as functions of $W_{\mathrm{B} 3}, W_{\mathrm{W} 3}$, and $W_{\mathrm{W} 2}$. Setting $W_{\mathrm{B} 3}$ as the linear variable, $W_{\mathrm{W} 3}$ is changed


Fig. 5. (a) $\tau_{32}, \tau_{31}$, and $\tau_{21}$ as functions of $W_{\mathrm{W} 2}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$. (b) $\tau_{\mathrm{op}}$ and LW of QCL as functions of $\mathrm{W}_{W 2}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4} . W_{\mathrm{W} 3}$ is set as the linear variable shown in the horizontal coordinate, $W_{\mathrm{W} 3}$ is changed correspondingly, and $W_{\mathrm{B} 4}$ is changed slightly to make sure that $E_{2}-E_{1} \approx E_{\mathrm{op}}$.

Table 2. Calculated Values of $W_{\mathrm{W} 1}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$ Corresponding to Fig. 4.

| Variable | $W_{\mathrm{W} 1}$ | $W_{\mathrm{W} 3}$ | $W_{\mathrm{B} 4}$ |
| :---: | :---: | :---: | :---: |
|  | 0.50 | 3.00 | 6.50 |
|  | 0.75 | 2.90 | 6.45 |
| Value (nm) | 1.00 | 2.80 | 6.55 |
|  | 1.25 | 2.75 | 6.50 |
|  | 1.50 | 2.45 | 6.50 |
|  | 1.75 | 2.30 | 6.55 |
|  | 2.00 | 2.20 | 6.55 |
|  | 2.25 | 1.90 | 6.55 |
|  | 2.50 | 1.65 | 6.55 |
| 2.75 | 1.40 | 6.50 |  |
|  | 3.00 | 0.85 | 6.55 |

correspondingly, and $W_{\mathrm{W} 2}$ is changed slightly at $W_{\mathrm{B} 1}$ $=4 \mathrm{~nm}, W_{\mathrm{W} 1}=0.5 \mathrm{~nm}, W_{\mathrm{B} 2}=1 \mathrm{~nm}$, and $W_{\mathrm{B} 4}=$ 6.5 nm . The calculated values of $W_{\mathrm{B} 3}, W_{\mathrm{W} 3}$, and $W_{\mathrm{W} 2}$ are listed in Table 4. As shown in Fig. 6, for the calculated structures of $\mathrm{AR}, \tau_{\text {op }} / \tau_{21}<0.82 \times 10^{-2}$ and $\tau_{\text {op }} / \tau_{32}<2.05 \times 10^{-3} . \tau_{32}$ may be longer than $\tau_{31}$ and reach $47.12 \mu \mathrm{~s}$. The ratio $\tau_{32} / \tau_{31}$ prominently changes so that the PIC of the QCL is also expressed as Eq. (14). The LW corresponding to the PIC is approximately 80 $\mu \mathrm{m}$, and the longest and shortest wavelengths are 187.88 and $30.54 \mu \mathrm{~m}$, respectively.
In Fig. 7, $\tau_{32}, \tau_{31}, \tau_{21}, \tau_{\text {op }}$, and LW of the QCL as functions of $W_{\mathrm{B} 2}$ and $W_{\mathrm{B} 4}$ were calculated by setting $W_{\mathrm{B} 2}$ as the linear variable. Hence, $W_{\mathrm{B} 4}$ is changed correspondingly at $W_{\mathrm{B} 1}=4 \mathrm{~nm}, W_{\mathrm{W} 1}=0.5 \mathrm{~nm}, W_{\mathrm{W} 2}=$ $15.5 \mathrm{~nm}, W_{\mathrm{B} 3}=2 \mathrm{~nm}$, and $W_{\mathrm{W} 3}=3 \mathrm{~nm}$. The calculated values of $W_{\mathrm{B} 2}$ and $W_{\mathrm{B} 4}$ are listed in Table 5. As shown in Fig. $7, \tau_{\text {op }} / \tau_{21}<0.75 \times 10^{-2}, \tau_{\text {op }} / \tau_{32}<0.78 \times 10^{-3}$, and $\tau_{32} / \tau_{31}<0.058$. Thus, the PIC of the QCL can be expressed as Eq. (13), and the MPI can be obtained when $W_{\mathrm{B} 2}=4 \mathrm{~nm}$ and $W_{\mathrm{B} 4}=6.55 \mathrm{~nm}$, where the corresponding LW is $40.79 \mu \mathrm{~m}$, and the longest and shortest wavelengths in Fig. 7(b) are 42.03 and $40.13 \mu \mathrm{~m}$, respectively.
In conclusion, we analyze the QCL structures of $\mathrm{GaAs} / \mathrm{Al}_{0.15} \mathrm{Ga}_{0.85} \mathrm{As}$ and consider the ARs of the different widths of wells and barriers. We also discuss the PIC of the QCL. For some special cases, the PIC can be simplified and is proportional to the SEL between


Fig. 6. (a) $\tau_{32}, \tau_{31}$, and $\tau_{21}$ as functions of $W_{\mathrm{B} 3}, W_{\mathrm{W} 3}$, and $W_{\mathrm{W} 2}$. (b) $\tau_{\mathrm{op}}$ and LW of QCL as functions of $W_{\mathrm{B} 3}, W_{\mathrm{W} 3}$, and $W_{\mathrm{W} 2} . W_{\mathrm{B} 3}$ is set as the linear variable shown in the horizontal coordinate, $W_{\mathrm{W} 3}$ is changed correspondingly, and $W_{\mathrm{W} 2}$ is changed slightly to make sure that $E_{2}-E_{1} \approx E_{\mathrm{op}}$.


Fig. 7. (a) $\tau_{32}, \tau_{31}$, and $\tau_{21}$ as functions of $W_{\mathrm{B} 2}$ and $W_{\mathrm{B} 4}$. (b) $\tau_{\mathrm{op}}$ and LW of QCL as functions of $W_{\mathrm{B} 2}$ and $W_{\mathrm{B} 4} . W_{\mathrm{B} 2}$ is set as the linear variable shown in the horizontal coordinate, and $W_{B 4}$ is changed correspondingly to make sure that $E_{2}-E_{1} \approx E_{\mathrm{op}}$.

Table 3. Calculated Values of $W_{\mathrm{W} 2}, W_{\mathrm{W} 3}$, and $W_{\mathrm{B} 4}$ Corresponding to Fig. 5.

| Variable | $W_{\mathrm{W} 2}$ | $W_{\mathrm{W} 3}$ | $W_{\mathrm{B} 4}$ |
| :---: | :---: | :---: | :---: |
|  | 12.0 | 4.00 | 6.4 |
|  | 12.5 | 3.90 | 6.5 |
|  | 13.0 | 3.90 | 6.5 |
|  | 13.5 | 3.80 | 6.5 |
| Value (nm) | 14.0 | 3.70 | 6.5 |
|  | 14.5 | 3.70 | 6.5 |
|  | 15.0 | 3.30 | 6.5 |
|  | 15.5 | 3.00 | 6.5 |
|  | 16.0 | 2.40 | 6.5 |
|  | 16.5 | 1.50 | 6.5 |
|  | 17.0 | 0.45 | 6.5 |

Table 4. Calculated Values of $W_{\mathrm{B} 3}, W_{\mathrm{W} 3}$, and $W_{\mathrm{W} 2}$ Corresponding to Fig. 6.

| Variable | $W_{\mathrm{B} 3}$ | $W_{\mathrm{W} 3}$ | $W_{\mathrm{W} 2}$ |
| :---: | :---: | :---: | :---: |
|  | 1.0 | 2.35 | 15.45 |
|  | 1.5 | 2.75 | 15.40 |
|  | 2.0 | 3.00 | 15.50 |
|  | 2.5 | 3.25 | 15.50 |
| Value (nm) | 3.0 | 3.55 | 15.45 |
|  | 3.5 | 3.75 | 15.45 |
|  | 4.0 | 3.90 | 15.50 |
|  | 4.5 | 4.00 | 15.50 |
|  | 5.0 | 4.00 | 15.50 |
|  | 5.5 | 4.05 | 15.40 |
|  | 6.0 | 4.15 | 15.50 |

Table 5. Calculated Values of $W_{\mathrm{B} 2}$ and $W_{\mathrm{B} 4}$ Corresponding to Fig. 7.

| Variable | $W_{\mathrm{B} 2}$ | $W_{\mathrm{B} 4}$ |
| :---: | :---: | :---: |
|  | 0.50 | 6.65 |
|  | 1.0 | 6.50 |
|  | 1.5 | 6.50 |
| Value (nm) | 2.0 | 6.50 |
|  | 2.5 | 6.60 |
|  | 3.0 | 6.40 |
|  | 3.5 | 6.50 |
|  | 4.0 | 6.55 |

the second and the first excited states only, whereas some other cases imply that the PIC is proportional to the SL of the second excited states. Our results show the SELs between the states and the intersubband POP SRT between the second and the first subbands depend on the widths of the wells and barriers. Some optimal results are discussed in detail. The expressions of $\tau_{32}$, $\tau_{31}, \tau_{21}, \tau_{3}, \tau_{2}, \tau_{\mathrm{op}}$, and PIC show the mechanism behind the obtained results. The changes in the widths of the QWs and barriers in AR lead to changes in the wave functions of the electron at different eigen states, which consequently cause changes in $\tau_{32}, \tau_{31}, \tau_{21}, \tau_{3}, \tau_{2}$, and $\tau_{\text {op }}$. Different PICs are obtained when different ARs are adopted.

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