

Mode Selection and Tuning Mechanisms in Coupled-Cavity Terahertz Quantum Cascade Lasers

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Abstract—We present a model for longitudinal mode competition in coupled-cavity (CC) terahertz (THz) quantum cascade lasers (QCLs) by using a scattering matrix method and multi-mode reduced rate equations (RREs). The dependence of the mode selection and tuning characteristics on various device parameters is systematically investigated, including the net waveguide loss, the optical length of the passive cavity, and the heat-sink temperature for different relationship between the active and passive cavity lengths. The changes in eigenmode frequencies due to variations of device parameter are calculated before solving the RREs. The mode selection and tuning results obtained from solving the non-linear RREs could be well explained by the linear scattering matrix analysis. The mode tuning process simulated by the proposed model is compared with experimentally measured data, yielding good agreement. Comprehensive study of the influence of the key device parameters on the performance of CC THz QCLs provides potential design rules for single-mode operation with either wide frequency tunability or high stability.

Index Terms—Coupled-cavity, mode tuning, quantum cascade lasers (QCL), terahertz (THz).

I. INTRODUCTION

THE terahertz (THz) region of the electromagnetic spectrum (frequency: 0.5–10 THz, wavelength: 600–30 μm ,

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photon energy: 2–40 meV) has attracted considerable attention recently for its potential applications in chemical sensing, non-invasive imaging and spectroscopy [1]–[3]. THz quantum cascade lasers (QCLs) were first successfully demonstrated in 2002 [3]. Over the last decade, THz QCL technology has witnessed rapid development, and THz QCLs can now emit output powers >1 W [4], within the 1.2–5.4 THz range [5]–[7], and operate at temperatures of up to ~ 200 K in pulsed mode [8]. Single-mode operation THz QCLs with wide frequency tuning range are particularly required for sensing, spectroscopic, and imaging applications [9], [10]. However, the intrinsic frequency tuning range of single cavity QCLs by adjustment of the injection current and temperature are limited to approximately 0.05 cm^{-1} and 0.1 cm^{-1} , respectively [11], [12]. A variety of tuning techniques for THz QCLs have been reported. Large tuning range (>20 GHz) THz emission have been achieved by applying external grating, MEMS, or heterogeneous active region in QCLs [13]–[15], but suffer from slow tuning, operation difficulties or device complexity.

Coupled-cavity (CC) THz QCLs offer fast frequency tuning as a function of localized electrical heating of an optically coupled passive cavity [16]–[18]. The spectral function of coupled-cavity GaAs/AlGaAs THz QCLs has been calculated using transfer (T)-matrix method [16]. However, the mode modulation depth predicted by T-matrix approach (12%) is much smaller than the measured (62%) due to the absence of influence of laser action in active cavity. It was also concluded that the interplay between the photon density and electron population of the intersubband laser levels has to be included to accurately describe the experimentally observed switching of the mode structure. In addition, single-mode operation with excellent side mode suppression ratio (SMSR) above 34 dB was obtained in [17], where the T-matrix approach accurately predicted the eigenmode frequencies. However, the most important property of the CC QCLs, namely, mode selection and frequency tunability and their dependence on the key device parameters have not been systematically investigated. Discrete Vernier frequency tuning of CC THz QCLs was analyzed in [18], where the gain spectrum of the QCL was not taken into account in the mode hopping simulations. All reported theoretical analyses of CC THz QCLs have used only the transfer matrix method, which can only predict mode-selective filtering characteristics

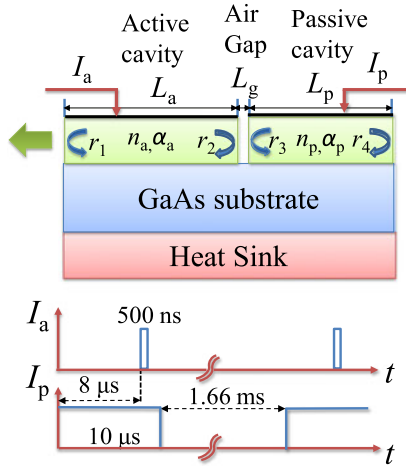


Fig. 1. Schematic diagram of the coupled-cavity multimode quantum cascade laser configuration.

below threshold. In this work, we combined the scattering matrix method and multi-mode reduced rate equations (RREs) analysis coupled with the full RE Schrödinger-Poisson (S-P) energy balance electron scattering transport calculations [19], to accurately model the mode selection and tuning characteristics in CC THz QCLs. The scattering matrix method is used to calculate the eigenmode frequencies and threshold gain, while the multi-mode RREs coupled with S-P simulation describe the laser behavior above the threshold, especially the influence of the gain spectrum. Systematical investigation of the dependences of the mode selection and frequency tunability on key device parameters in CC THz QCLs were conducted for different relationships between the active cavity length (L_a) and the passive cavity length (L_p), see Fig. 1, i.e. $L_a > L_p$, $L_a \sim L_p$ and $L_a < L_p$. An analog approach was applied to analyze and design CC diode lasers by Coldren *et al.* [20]–[22]. In spite of the recognized importance of the mode selection and frequency tuning in CC THz QCLs, no related theoretical investigation has yet been reported.

The purpose of this paper is threefold. Firstly, to generalize the RRE model from single-mode THz QCLs [19] to multi-mode THz QCLs, so that the interplay between the multi-mode photon densities and the electron densities of the intersubband laser levels could be accurately described. Secondly, to evolve the model for CC QCLs based on the scattering matrix method and integrate it with the multi-mode RREs. This allows us to formulate design rules for CC THz QCLs based on our observations of how mode selection and tuning characteristics depend on the key device parameters. The spectral power density (SPD) distribution of the eigenmodes and their dependence on the net waveguide loss and the effective refractive index of the passive cavity, and the heat sink temperature of the CC device are investigated. Finally, the proposed model contains eigenmode calculations for CC THz QCLs, on which the multi-mode RREs are based, so that the continuous frequency tuning of the dominant mode could also be modelled.

Fundamentally, the CC structure leads to a frequency-dependent threshold gain. The net waveguide loss and effective refractive index of the passive cavity determine the modulation

depth and phase of the threshold gain, respectively, which combines with the gain spectrum determines the dominant mode and the SMSR. Furthermore, it was found that eigenmode distributions on the threshold gain spectrum play an important role in mode tunability of CC THz QCLs especially when $L_p \geq L_a$. Various locations of eigenmodes (at peaks, rising and falling edges) can enhance the mode tunability. Technically, by varying the passive cavity refractive index over a wide range and observing the effect this has on mode and frequency tunability, we are able to choose a passive cavity length or drive current that provides a suitable mode tunability. Likewise, by exploring the heatsink temperature over a wide range, we are able to choose a temperature that provides the desired combination of mode and continuous frequency tunability. The proposed modelling approach has been validated by experimentally observed mode tuning as a function of heating power applied to the passive cavity.

The article is organized as follows. Section II describes the scattering matrix based linear coupled-resonator analysis used to calculate the threshold gain and eigenmode frequencies. This is followed by multi-mode RRE analysis for mode selection characteristics, in Section III. The results and discussion of the effects of device parameters on mode selection and frequency tuning are given in Section IV. Section V compares the simulation results with experimental data. Finally, Section VI presents our conclusion.

II. LINEAR COUPLED-RESONATOR ANALYSIS

The exemplar device selected for modelling is a 150- μm -wide and 11.6- μm -thick THz CC QCL with a bound-to-continuum active region based on GaAs/Al_{0.15}Ga_{0.85}As material system, as described in [23]. The key parameters in this two-section CC THz QCL are shown in Fig. 1, where the active cavity of length L_a and the passive cavity of length L_p are separated by a narrow air gap with length of L_g . We focus on a device with an active cavity length $L_a = 1.5$ mm and an air gap length $L_g = 13$ μm , which are the dimensions of a fabricated device we used to experimentally verify our theoretical model. To simulate three different geometries of the device ($L_a > L_p$, $L_a \sim L_p$, and $L_a < L_p$), passive cavity lengths L_p of 0.25 mm, 1.4 mm, and 3.4 mm were used. The operational condition of the CC THz QCL device simulated in this article is the same as described in [18] where the active cavity is driven by 500 ns-long pulses, which is triggered by a 600 Hz reference frequency and the passive cavity is heated using a train of 10- μs -long current pulses at a repetition rate of 8.21 kHz, gated by the same 600 Hz reference, as shown in Fig. 1. In this scheme, the amplitude of the active cavity current pulses is fixed at 0.75 mA (above the lasing threshold) and the amplitude of the passive cavity pulses vary below its threshold to control the dominant longitudinal mode of the device. We can neglect thermal crosstalk between the active and passive cavities due to the narrow pulses applied on both cavities.

When the passive cavity is operated below threshold or well above optical power rollover point, it can be assumed to behave as a linear equivalent mirror [20]. Based on complex scattering transmission matrix theory [22], the air gap and passive cavity can be described by an effective complex mirror. This way

the CC QCL can be described as a single cavity (SC) with an effective complex mirror.

The net transfer function of the CC QCLs can be described by [20]:

$$H(\nu) = \frac{t_a t_p S_{s21} \sqrt{(1-r_4^2)(1-r_1^2)}}{1 - (S_{s12}^2 - S_{s11}^2) r_1 r_4 t_a^2 t_p^2 - S_{s11} r_4 t_p^2 - S_{s22} r_1 t_a^2} \quad (1)$$

The parameters in (1) are defined in Table I. The eigenmode frequencies of the CC QCL, ν_m , are determined by the frequencies where the transfer function has local maxima or zeros of the denominator of $H(\nu)$ [20]. The linear coupled-resonator analysis of the coupled cavity above is essential for accurate frequency tuning analysis in CC QCLs. Firstly, the CC eigenmode calculation and updating with the varying device parameters (the net waveguide loss, the optical cavity lengths and heat sink temperatures) are necessary for frequency tunability study. Secondly, the threshold gain experienced by the CC eigenmodes can be selectively lowered by an appropriate selection of the device parameters. The threshold gains at the eigenmodes combine with the gain spectrum to predict the potential dominant mode, which is nearest to the net gain maximum above threshold.

III. MODE COMPETITION ANALYSIS THROUGH REDUCED RATE EQUATION AND THERMAL EQUATION

Mode competitions in CC THz QCLs can be described by multi-mode reduced rate equations for each longitudinal eigenmode frequency, calculated from the linear coupled resonator analysis. The multi-mode rate equations are a modification of those for single-mode QCLs [19] based on the classical QCL model as shown below:

$$\frac{dN_3(t)}{dt} = \frac{\eta_3 I_a(t)}{q} - (N_3(t) - N_2(t)) \sum_{m=1}^N G_m S_m(t) - \frac{N_3(t)}{\tau_3} \quad (2)$$

$$\frac{dN_2(t)}{dt} = \frac{\eta_2 I_a(t)}{q} + (N_3(t) - N_2(t)) \sum_{m=1}^N G_m S_m(t) + \frac{N_3(t)}{\tau_{32}} + \frac{N_3(t)}{\tau_{sp}} - \frac{N_2(t)}{\tau_2} \quad (3)$$

$$\frac{dS_m(t)}{dt} = M (N_3(t) - N_2(t)) G_m S_m(t) - \frac{S_m(t)}{\tau_{pm}} + \frac{M \beta_{sp} N_3(t)}{\tau_{sp}} \quad (4)$$

$$\frac{dT_p(t)}{dt} = \frac{1}{m_p c_p} \left[I_p(t) V_p(t) - \frac{T_p(t) - T_0}{R_{th}} \right] \quad (5)$$

where $N_3(t)$ and $N_2(t)$ are the carrier populations in the upper and lower laser levels (ULL/LLL), respectively, and $S_m(t)$ represents the photon population in mode m . Equation (4) contains N photon population equations for the longitudinal eigenmodes. The parameters (η_3 , η_2 , G_p , M , β_{sp} , τ_3 , τ_{32} , τ_2 ,

TABLE I
DEVICE PARAMETERS USED IN NUMERICAL SIMULATIONS
(UNLESS STATED OTHERWISE)

Symbol	Description	Value / Definitions
r_{eff}	Reflection coefficient of the effective mirror	$r_{eff} = S_{S11} [1 + \sigma \bar{R} / (1 - \bar{R})]$
σ	Gap factor	$\sigma = S_{s21} S_{s12} / S_{s11} S_{s22}$
\bar{R}	Resonance of r_{eff}	$\bar{R} = S_{s22} r_3 \exp(-2j\beta_p L_p)$.
$S_{s11}, S_{s12}, S_{s21}, S_{s22}$	Scattering coefficients [22]	Varies
$t_{a,g,p}$	Single pass transmission factor of the air gap, active and passive cavity	$t_{a,g,p} = \exp(-j\beta_{a,g,p} L_{a,g,p})$
$\tilde{\beta}_{a,g,p}$	Propagation constant of the air gap, active and passive cavity	$\tilde{\beta}_{a,g,p} = \beta_{a,g,p} - j\alpha_{a,g,p}/2$
$L_{a,g}$	Active cavity and air gap length	1.5 mm and 13 μ m
L_p	Passive cavity length	0.25 mm, 1.4 mm, and 3.4 mm
$\beta_{a,g,p}$	Real part of the propagation constant	$\beta_{a,g,p} = 2\pi n_{a,g,p} \nu_m / c$
$\alpha_{a,g,p}$	Net waveguide loss of the air gap, active and passive cavity	9 cm^{-1} , 0 cm^{-1} , and 9 cm^{-1}
$n_{a,g,p}$	Effective refractive index of the active and passive cavity	3.61, 1.0, 3.61
$\varphi_{r_{eff}}$	Phase angle of r_{eff}	Varies
ν_m	Eigenmode frequency for mode m	Varies
α_m	Effective mirror loss	$\alpha_m = (1/L_a) \ln[1/(r_1 r_{eff})]$
Γg_{th}	Threshold modal gain	$\Gamma g_{th} = \alpha_a + \alpha_m$
τ_{pm}	Photon lifetime for mode m	$\tau_{pm} = 1/[v_{gm} (\alpha_a + \alpha_m)]$
v_{gm}	Group velocity of mode m	Varies
η_3	Injection efficiency into ULL	54.41%
η_2	Injection efficiency into LLL	1.65%
η_m	Power output coupling coefficient for mode m	Varies
I_a	Active cavity current	0.75 A
I_p	Passive cavity current	Varies
G_m	Gain factor of mode m	$G_m = G_p / [1 + ((\nu_p - \nu_m) / (\Delta\nu/2))^2]$
G_p	Peak gain factor of the Lorentzian gain spectrum	$5.3 \times 10^4 \text{ s}^{-1}$
ν_p	Peak gain frequency	2.795 THz
$\Delta\nu$	FWHM of gain spectrum	500 GHz
M	Number of periods in active cavity	90
β_{sp}	Spontaneous emission factor	1.627×10^{-4}
τ_3	Total carrier lifetime in ULL	$5 \times 10^{-12} \text{ s}$
τ_{32}	Non-radiative relaxation time from ULL to LLL	$1.76 \times 10^{-10} \text{ s}$
τ_2	Total carrier lifetime in LLL	$2.1 \times 10^{-11} \text{ s}$
τ_{sp}	Spontaneous emission lifetime	$5 \times 10^{-10} \text{ s}$
R_{th}	Thermal resistance	9.92 K/W
q	Electronic charge	$1.6 \times 10^{-19} \text{ C}$
\hbar	Reduced Planck constant	$6.58 \times 10^{-16} \text{ eVs}$

and τ_{sp}) used in the equations are summarized in Table I. The electron transport parameters are obtained from the full self-consistent energy-balance Schrödinger-Poisson scattering transport calculation for the given lasing cavity current I_a described in [24], [25]. The dependence of RRE parameters on the temperature and terminal voltage should be considered if I_a varies. However, I_a is fixed at 0.75 mA in this work. Therefore the parameters mentioned above are all constant as shown in Table I. Once solved, the emission output power can be obtained

by $P_m(t) = \eta_m h \nu_m S_m(t) / \tau_{pm}$. We focus on the steady-state solutions of the multi-mode RRE in order to investigate mode selection and frequency tunability in CC THz QCL.

Equation (5) is the thermal model which describes the lattice temperature in the passive cavity $T_p(t)$ as functions of the chip mass m_p , the effective specific heat capacity c_p and the cold finger temperature T_0 . Here we only show the thermal model for the passive cavity, but that for the active cavity should be included if I_a varies. By setting (5) to zero, the steady state solution is given by $\Delta T_p = I_p V_p R_{th}$, where R_{th} is the thermal resistance, and I_p and V_p are the current amplitude and voltage applied to the passive cavity, respectively [26]. Therefore, any tuning of the current at the passive cavity changes its lattice temperature, which in turn perturbs the refractive index of the passive cavity. This changes the reflectivity of the effective mirror, and can result in a mode hop of the dominant CC mode to a mode with the maximum net gain.

IV. RESULTS AND DISCUSSIONS

The dominant mode and the corresponding SMSR in a CC THz QCL are determined by both the device parameters in (1) and the RRE parameters of the RRE model (2)–(5). Using the scattering matrix method and the multi-mode RRE model, we have investigated the influence of the key parameters on mode selection in CC THz QCLs, including the net waveguide loss, effective refractive index of the passive cavity, and the heat sink temperature of the CC device. The Lorentzian gain spectrum with peak gain factor G_p at 2.795 THz and full-width-half-maximum (FWHM) of 500 GHz [27] is applied in our simulation. Laser emission between 2.7 THz and 2.85 THz is our mode tuning range of interest. In reality, tuning one parameter will induce several parameters change simultaneously. In this section we change one parameter at a time, to gauge the individual effects of the various parameters over which we might hope to have some control. The usefulness of this method lies in the observation that the individual effects can be superimposed [21]. Via numerical simulation we can decouple these effects and understand how each parameter influences mode selection characteristics in CC THz QCL. The default device parameters, if not otherwise specified, are given in Table I. The effective refractive index of the waveguide active cavity is 3.61 at 2.7 THz with the index dispersion $dn/d\nu = 5.66 \times 10^{-14} (\text{Hz})^{-1}$, calculated using COMSOL Multiphysics. The net waveguide losses in the active and passive cavity are assumed to be invariant for the different eigenmodes, for simplicity.

A. Comparison Between Single- and Coupled-Cavity QCLs

We start our analysis with a comparison between the mode competition characteristics in a SC and CC THz QCL. The net transfer function and the threshold gain of a 1.5 mm-long SC and a CC QCL with $L_a = 1.5$ mm, $L_g = 13 \mu\text{m}$ and $L_p = 0.25$ mm are shown in Fig. 2(a) and (b), respectively. The eigenmode frequencies for the SC QCL (black circles) start from 2.712 THz with the mode spacing of 27.7 GHz, which is free spectral range (FSR) of the single cavity. The eigenmode frequencies of the CC QCL (red circles) are at 2.714, 2.74,

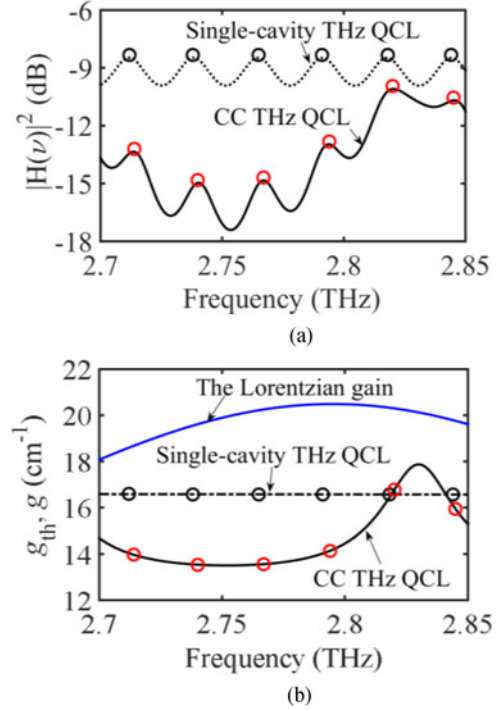


Fig. 2. Comparison of the (a) net transfer function and (b) the threshold gain between a 1.5-mm-long SC (in dotted lines) and a CC THz QCL ($L_a = 1.5$ mm, $L_g = 13 \mu\text{m}$ and $L_p = 0.25$ mm) (in solid lines). The black and red circles indicate the eigenmodes for the SC and CC THz QCL, respectively. The Lorentzian gain is shown in solid blue in plot (b).

2.767, 2.794, 2.82, 2.845, and 2.872 THz with the mode spacing predominantly determined by the FSR of the lasing cavity. The eigenmodes for a THz QCL are labelled from mode 1 to 6 with increasing frequency in the following discussions. The threshold gain (the total loss) are identical for the eigenmodes in the SC QCL if neglecting the net waveguide loss dispersion, as shown in Fig. 2(b). The CC structure leads to a frequency-dependent threshold gain, which exhibits a modulation with a period determined by the FSR of the passive cavity (166.2 GHz). It is observed from Fig. 2(b) that the maxima of the net gain, $g_n(\nu) = g(\nu) - g_{th}(\nu)$ are at mode 4 (2.791 THz) for the SC and at mode 3 (2.757 THz) for the CC case.

In order to verify the dominant mode predicted from the linear cavity resonator analysis above, the emission spectrum with $I_a = 0.75$ A for the SC and CC QCL are obtained by solving the multi-mode RRE and shown in Fig. 3(a) and (b), respectively. The dominant mode results are consistent with the prediction above. In addition, SMSR of 27.73 dB and 32.18 dB are obtained for the SC and CC THz QCL, respectively, as shown in Fig. 3.

B. Mode Competition Dependences on the Key Device Parameters in CC THz QCLs

1) *The Influence of Passive Cavity Net Waveguide Loss α_p* : Net waveguide loss in the passive cavity α_p is defined as $\langle \alpha_{ip} \rangle - \langle g_p \rangle$, where $\langle \alpha_{ip} \rangle$ and $\langle g_p \rangle$ are the average internal waveguide loss and modal gain in the passive cavity,

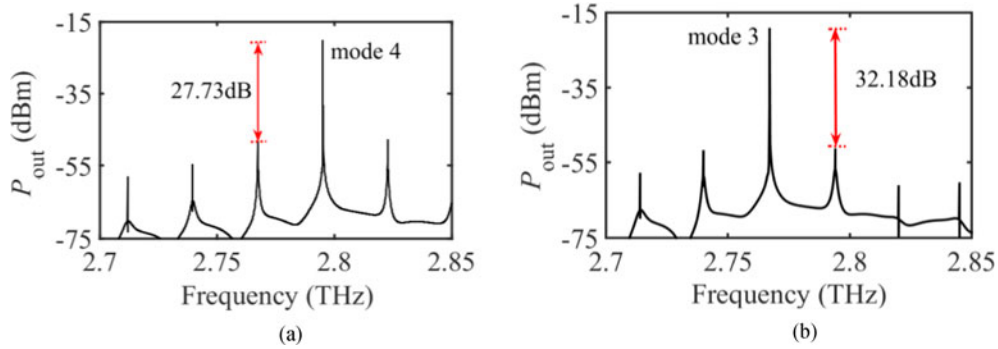


Fig. 3. The emission spectrum with $I_a = 0.75$ A for (a) the 1.5-mm-long SC and (b) the CC THz QCL ($L_a = 1.5$ mm, $L_g = 13$ μ m and $L_p = 0.25$ mm).

respectively. Therefore, positive and negative α_p indicate that modal gain is smaller and larger than the internal waveguide loss in the passive cavity, respectively. The passive cavity starts lasing when its modal gain overcomes the total loss of the passive cavity (the internal waveguide loss plus the mirror loss of the passive cavity α_{mp}), namely $\alpha_p = -\alpha_{mp}$. Our model is valid when the active cavity is lasing and passive cavity is not [21], so in the following discussions we limited $\alpha_p \geq -\alpha_{mp}$. α_{mp} is 23, 4, and 1.7 cm^{-1} when L_p is 0.25 mm, 1.4 mm and 3.4 mm, respectively. The net waveguide loss α_p has a significant influence on the modulation depth of the frequency-dependent threshold gain g_{th} in a CC THz QCL. Varying modulation depth of g_{th} induces the net gain relationship among the eigenmodes change, which in turn alters the dominant mode and its SMSR.

Fig. 4 summarizes the dependence of mode selection characteristics on α_p for different passive cavity lengths L_p . When $L_p = 0.25$ mm, the threshold gain spectra g_{th} with α_p of -23 , -12 and 9 cm^{-1} are shown in Fig. 4(a1), where the eigenmodes are marked by circles. When α_p is -12 cm^{-1} , g_{th} exhibits a sharp increase at the eigenmode frequency of 2.831 THz. The sharp peak decreases close to the baseline of 12.5 cm^{-1} when α_p is -23 cm^{-1} (reaching the lasing threshold of the passive cavity) and is very similar to the case of a single cavity. The peak value of g_{th} with α_p of 9 cm^{-1} is intermediate. In order to show how the g_{th} profile varies with α_p , the peak value of g_{th} as a function of α_p at 2.831 THz is shown in Fig. 4(a2). There is a maximum when α_p is -12 cm^{-1} , determined by (1). Increasing the peak value of g_{th} results in maximum net gain transfers from mode 5 to mode 3, which is verified by the emission spectra shown in Fig. 4(a3). It is noted that there is no emission at mode 5 of 2.831 THz when α_p is -12 cm^{-1} [red dotted curve in Fig. 4(a3)] due to its gain (20.1 cm^{-1}) being below threshold. Furthermore, it can be predicted that at 2.831 THz, lasing is not possible when α_p is between -17 and 1 cm^{-1} , as indicated by the dotted line in Fig. 4(a2). We can conduct the same analysis for other modes to determine the potential tuning range of α_p that supports lasing.

When L_p and L_a are comparable as in the case of Fig. 4(b), the eigenmodes are spaced by about the same amount with the modulation period of g_{th} . When α_p is -4 and 9 cm^{-1} , the g_{th} differences between eigenmodes are small so that the dominant mode is mainly determined by the gain spectrum peak at 2.795

THz. In addition, the SMSR in both cases are smaller compared with the results of $L_p < L_a$ shown in Fig. 4(a3). The gain at each eigenmode is below its threshold when α_p is -2 cm^{-1} so that the emission power are all less than -55 dBm in Fig. 4(b3) (red dotted curve). Also, we found that mode 5 at 2.814 THz is not able to lase when α_p is between -3 to -0.2 cm^{-1} .

In the third case with $L_p > L_a$ as in Fig. 4(c), α_p with the local maxima of the peak value of g_{th} increased to -0.9 cm^{-1} (c2) where THz emission at mode 3 is observed while other modes are suppressed (c1 and c3). However, with the decreased peak amplitude of g_{th} when α_p is -1.7 and 9 cm^{-1} (blue dash and dotted and red dotted lines in c1), the dominant mode changes to near gain spectrum peak at 2.793 THz and 2.82 THz, respectively (c3). It is obtained from c2 that mode 11 at 2.828 THz is not able to lase when α_p is between -1.2 to -0.1 cm^{-1} .

Comprehensive simulation reveals that the main eigenmode frequencies are 2.714, 2.74, 2.767, 2.794, 2.821, 2.845 and 2.872 THz for L_p are values of 0.25 mm, 1.4 mm and 3.4 mm. However, they vary when α_p is in the rising regions in Fig. 4(a2), (b2) and (c2). When $L_p = 0.25$ mm, the two eigenmodes of 2.821 THz and 2.845 THz merge into one mode at 2.83 THz when α_p is between $-23 \sim -10$ cm^{-1} . When $L_p = 1.4$ mm with α_p of $-4 \sim 10$ cm^{-1} , all eigen modes decrease about 10 GHz. When $L_p = 3.4$ mm with α_p of $-1.7 \sim 7$ cm^{-1} , the eigenmode spacing decreases to around 12 GHz, which is close to the FSR of the passive cavity. By using this model, one can obtain the net waveguide loss values that allow each eigenmode lases. In addition, by controlling the modulation depth of threshold gain spectrum through net waveguide loss, one can design the CC QCL device to lase at a desired eigenmode with good SMSR above 30 dB, also achieve mode tuning by control of the passive current amplitude to tune the net waveguide loss of the passive cavity. When tuning α_p , it is observed that $L_a \sim L_p$ is more stable with less tunability and $L_a < L_p$ has better mode tunability but with reduced SMSR. The mode tunability of $L_a > L_p$ is intermediate, with good SMSR above 30 dB.

2) *The Influence of Passive Cavity Optical Length $n_p L_p$:* Optical length of the passive cavity $n_p L_p$ determines phase of the g_{th} spectrum through the effective mirror reflection coefficient r_{eff} . Therefore, perturbation of the effective refractive index of the passive cavity induces a phase shift of the g_{th} spec-

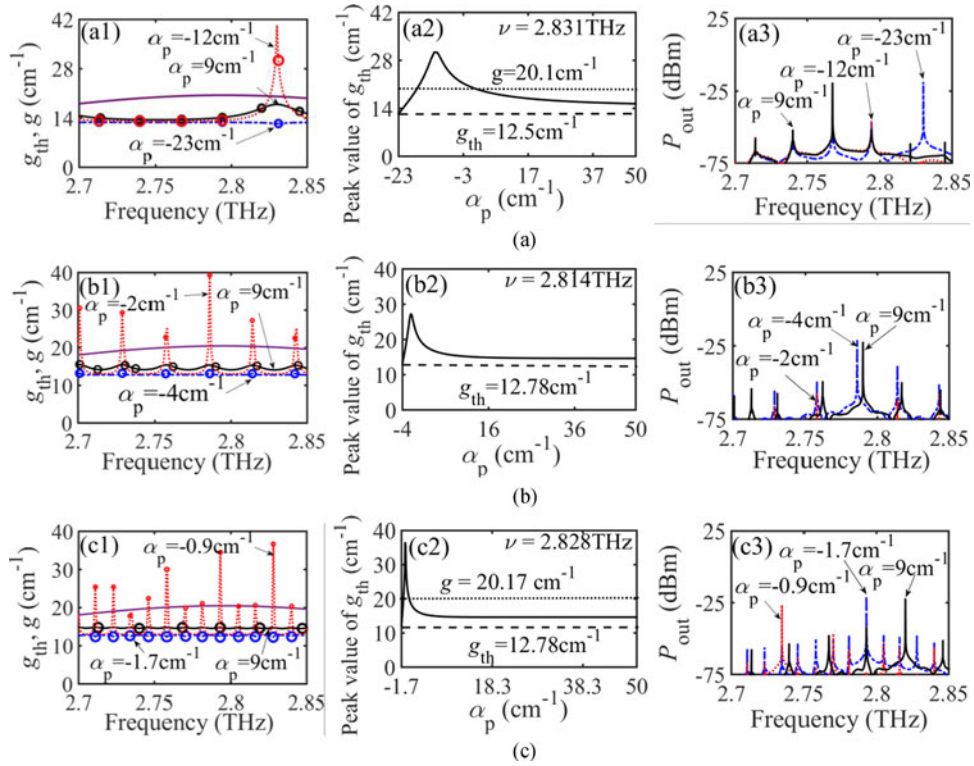


Fig. 4. The dependence of mode selection on the passive cavity net waveguide loss α_p for the long, medium and short passive cavities: (a) $L_p = 0.25$ mm (b) $L_p = 1.4$ mm and (c) $L_p = 3.4$ mm, where (a1), (b1) and (c1) show the threshold gains at various α_p with the Lorentzian gain indicated by purple solid lines, the eigenmodes are marked by circles; (a2), (b2) and (c2) plot the peak value of g_{th} as a function of α_p , where the dashed lines indicate the active cavity g_{th} when the total loss of passive cavity is exactly overcome by the modal gain of the passive cavity, and the dotted line indicate the active cavity gain at the eigenmode frequency showed in the plot; the emission spectra at various α_p are shown in (a3), (b3) and (c3), respectively.

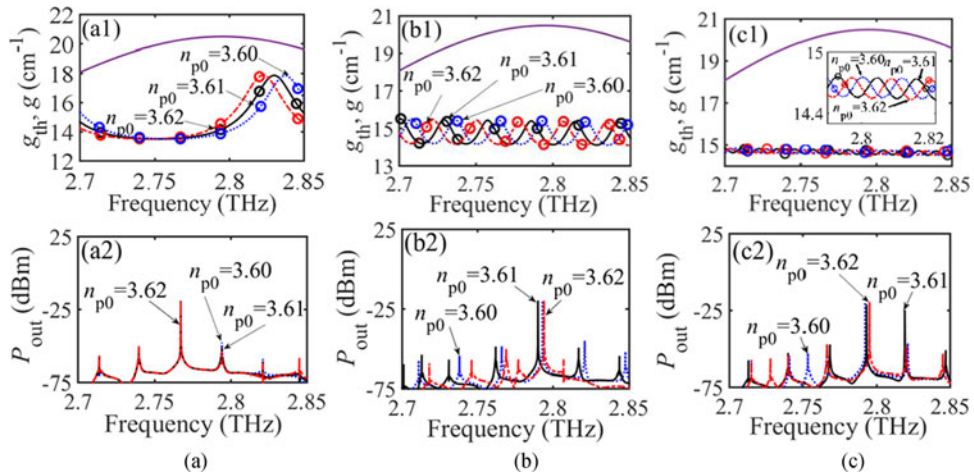


Fig. 5. The dependence of mode selection characteristics on the passive cavity effective refractive index (represented by the effective refractive index at 2.7 THz n_{p0}) for the long, medium and short passive cavities: (a) $L_p = 0.25$ mm (b) $L_p = 1.4$ mm and (c) $L_p = 3.4$ mm, where the Lorentzian gain spectra are indicated by purple solid lines, the threshold gains with n_{p0} of 3.60, 3.61 and 3.62 are given in red dash and dotted, black solid and blue dotted lines, respectively in (a1), (b1) and (c1) with the eigenmodes marked by circles; the emission spectrum with n_{p0} of 3.60, 3.61 and 3.62 are shown in red dash and dotted, black solid and blue dotted lines, respectively in (a2), (b2) and (c2), respectively.

trum. Depending on the phase angle of r_{eff} , red shift coefficient of g_{th} spectrum varies with L_p . Tuning adjustments of 0.01 in the effective refractive index of the passive cavity about the reference value of 2.7 THz, n_{p0} , were found to cause red shifts of 7 GHz in g_{th} for $L_p = 0.25$ mm and 1.4 mm [Shown in Fig.

5(a1) and (b1)]. While the red shift coefficient when $L_p = 3.4$ mm is about 4 GHz / 0.01, as a function of n_{p0} , as shown in Fig. 5(c1). The eigenmode frequencies are invariant when n_{p0} varies by ± 0.01 and $L_p = 0.25$ mm, but have a slight shift when $L_p = 1.4$ mm and 3.4 mm, as indicated in Fig. 5(b1) and

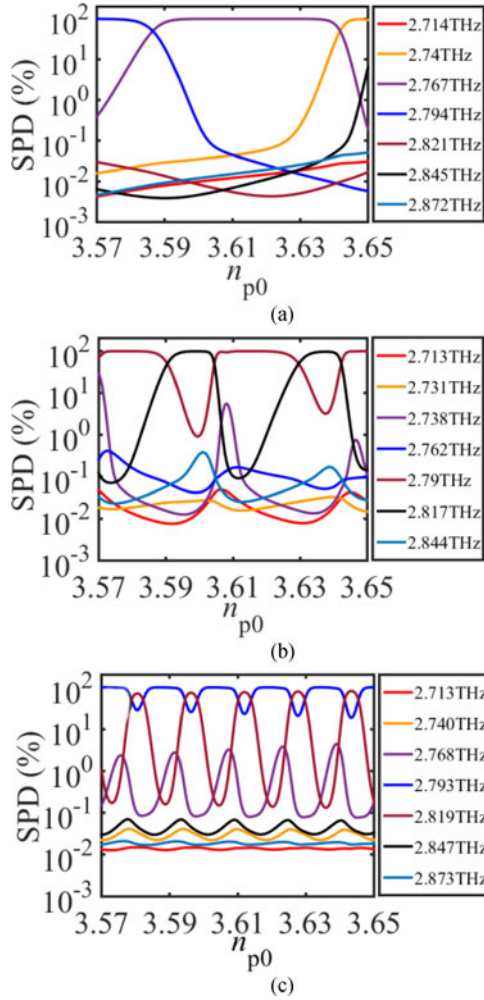


Fig. 6. The steady state SPD as a function of n_{p0} for the long, medium and short passive cavities: (a) $L_p = 0.25$ mm; (b) $L_p = 1.4$ mm and (c) $L_p = 3.4$ mm.

(c1). If we neglect small changes in the eigenmode frequencies, it is observed that there is no mode hopping for all these three passive cavity lengths, as shown in Fig. 5(a2), (b2) and (c2). This could be explained by the net gain at these frequencies having no significant change as a function of n_p as shown in (a1), (a2) and (a3), respectively.

Change in n_{p0} reflects the influence of varying driving current applied to the passive cavity due to the injection heating effect, commonly used mechanism for frequency tuning in coupled-cavity semiconductor lasers. The passive cavity current induced perturbation of the refractive index results in a change of the dominant mode and SMSR. We vary n_{p0} over a wide range of ± 0.04 to fully explore mode tunability via control of the passive cavity current. The result is the number of mode switching amongst different mode frequencies attainable for a given tuning range. On the other hand, the passive cavity length may be adjusted to provide the desired mode tunability. The steady state SPDs as a function of n_{p0} (varying by ± 0.04) for $L_p = 0.25$ mm, 1.4 mm and 3.4 mm are calculated and shown in Fig. 6(a), (b) and (c) respectively. Mode hopping amongst modes 4, 3 and 2 at 2.794, 2.767, 2.74 THz, respectively, with excellent SMSR is observed with n_{p0} varying from 3.57 to 3.65 in Fig. 6(a)

when $L_a > L_p$. With the same variation of n_{p0} , periodical mode hopping between only two modes is observed for the cases $L_a \sim L_p$ and $L_a < L_p$. As shown in Fig. 6(b), when $L_p = 1.4$ mm, mode 5 at 2.79 THz and mode 6 at 2.817 THz alternately and gradually swap their power when n_{p0} varies every 0.038, whereas in Fig. 6(c) with $L_p = 3.4$ mm, mode 4 at 2.793 THz and mode 5 at 2.819 THz transfer their dominant roles more frequently variations of just 0.016 in n_{p0} . However, good SMSR is not obtained when mode 5 is dominant in this case. Again, the mode tuning results obtained from solving the nonlinear RREs could be well explained by the net gain relationship amongst the eigenmodes obtained from linear resonator analysis. As shown in Fig. 5(a1), the net gain differences between the eigenmodes when $L_p < L_a$ are much greater than those when $L_p \sim L_a$ and $L_p > L_a$ due to the longer modulation period of g_{th} . We predict that mode tuning amongst more eigenmodes would occur when $L_a > L_p$ with greater variation in n_{p0} . However, due to the typical peak gain generally being much higher than g_{th} when $L_a \sim L_p$ and $L_a < L_p$ in CC THz QCLs, as shown in Fig. 5(b1) and (c1), the maximum net gain is always around the peak gain at 2.795 THz. For this reason the dominant modes for $L_p = 1.4$ mm and 3.4 mm are always between 2.79 THz and 2.82 THz in Fig. 6(b) and (c).

Furthermore, the eigenmode distribution in the g_{th} spectrum determines the mode tunability as well. Suppose for instance that, one of the two dominant modes lies at rising edge and the other at falling edge of g_{th} so that a red phase shift results in net gain of the mode at rising edge decreasing, while that of the mode at falling edge increases simultaneously. This scenario is illustrated by the two eigenmodes at 2.793 and 2.819 THz when $n_{p0} = 3.60$, as shown in the inset of Fig. 5(c1) with blue circles. This process gives rise to mode swapping only between these two modes when n_{p0} varies from 3.57 to 3.65 where g_{th} has a red shift of two full cycles. Therefore, no matter how wide the tuning range of n_{p0} , mode switching is only possible between two modes close to the gain spectrum peak in Fig. 6(b) and (c). In addition, if both of the eigenmodes lie at rising or falling edge of g_{th} profile, tuning n_{p0} might not change the dominant mode since their net gain relationship would not change. Based on the mode selection characteristic analysis in CC THz QCLs above, we found that in order to enhance mode tunability to obtain mode switching among more modes when $L_a \sim L_p$ and $L_a < L_p$, we can either decrease the gain spectrum peak or increase the threshold gain so as to increase the net gain differences among the eigenmodes. Alternatively, we can increase the modulation depth of the threshold gain to enhance the net gain differences by controlling the net waveguide loss as discussed in Section IV-B1. Furthermore, with a certain gain spectrum, the desired eigenmodes should distributed at different edges of the g_{th} profile so that their net gain changes with n_{p0} asynchronously. Last but not least, given a limited passive current tuning range, adjusting the effective refractive index could be replaced by altering cavity length at the design stage as a much easier way to enhance the mode tuning capability. For instance, for a CC THz QCL with $n_{p0} = 3.61$ and $L_p = 0.25$ mm, if the passive cavity current applied to the passive cavity is varied from 0–2 A, which induced lattice temperature in the passive cavity varies from 0–195 K. This in turn results in n_{p0}

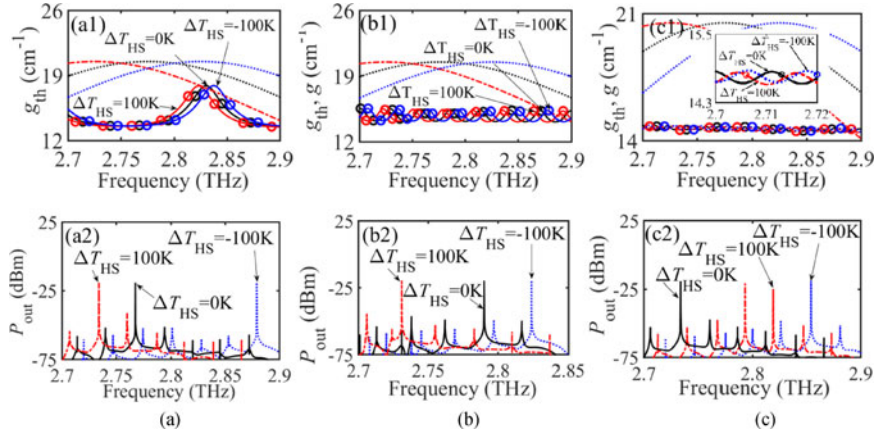


Fig. 7. Threshold gains and the emission spectra for heat sink temperature variation of ± 100 K in CC THz QCLs for the long, medium and short passive cavities: (a) $L_p = 0.25$ mm; (b) $L_p = 1.4$ mm; (c) $L_p = 3.4$ mm.

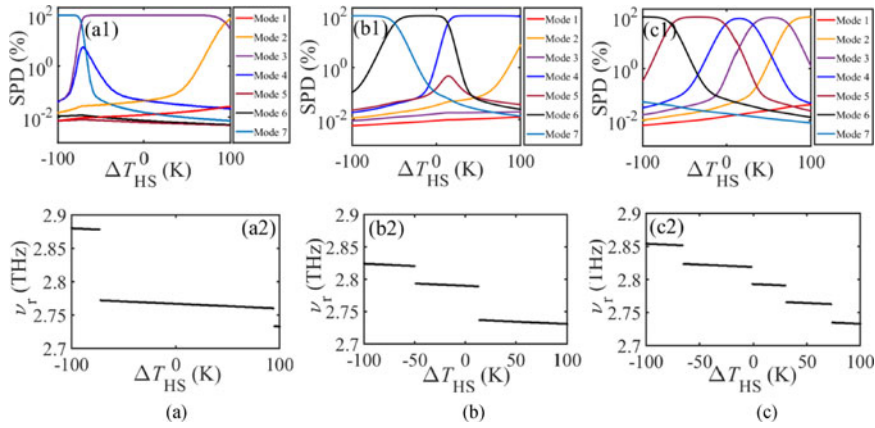


Fig. 8. The steady state SPD and the dominant mode frequency ν_r as a function of the heat sink temperature variation for the long, medium and short passive cavities: (a) $L_p = 0.25$ mm; (b) $L_p = 1.4$ mm; (c) $L_p = 3.4$ mm.

changes from 3.61 to 3.63 where no mode tuning occurs as shown in Fig. 6(a). However, if we increase L_p to around 0.252 mm (corresponding to tuning n_{p0} to 3.642 in Fig. 6(a), where mode hopping occurs), tuning between modes 3 and 2 can be obtained with a lesser tuning range for n_{p0} . Therefore, we can choose an appropriate passive cavity length to suit a limited current tuning range in order to obtain mode tuning.

3) *The Dependence on the Heat Sink Temperature T_{HS} :* When the heat sink temperature varies, on one hand, the refractive index of both the active cavity and the passive cavity, n_{a0} and n_{p0} , varies with temperature coefficient $dn/dT_{HS} = 9.5 \times 10^{-5}$ [18]. Simultaneously, the gain spectrum peak has a red shift with the coefficient of around 500 MHz/K on average [28]. Consequently, the eigenmode frequencies red shift with a temperature coefficient of 60–80 MHz/K due to variance in n_{a0} , which is consistent with the 63–90 MHz/K reported in [18], whilst the threshold gain has a red shift coefficient of 70 MHz/K on average as predicted from our simulation. Therefore the eigenmode frequencies, threshold gain and gain peak shift at different rates with temperature, which leads to mode tuning.

In order to show the mode tuning process induced by control of the heat sink temperature, the threshold gain and emis-

sion spectra with a heat sink temperature variation ΔT_{HS} of ± 100 K, and with $L_p = 0.25$ mm, 1.4 mm, and 3.4 mm are depicted in Fig. 7(a), (b) and (c), respectively. The net gain maximum has red shifts from mode 7 at 2.879 THz to mode 3 at 2.767 THz, then to mode 2 at 2.733 THz when ΔT_{HS} is -100 K, 0 K and 100 K, respectively, as shown in Fig. 7(a1). The results are consistent with the emission spectra shown in Fig. 7(a2). With ΔT_{HS} values of -100 K, 0 K and 100 K corresponding to n_{p0} of 3.60, 3.61 and 3.62, respectively, no mode hopping is observed from the emission spectrum shown in Fig. 5(a2). Similar comparisons with each pair of passive cavity lengths give the same result. Mode hopping among more modes could be obtained by control of the heat sink temperature compared with only tuning the passive cavity current. The red shift of both gain spectrum peak and eigenmode frequencies play an important role in mode switching. And the eigenmode shifting leads to continuous frequency tuning of the dominant mode as well. The updated net gains among the altered eigenmodes determine the next dominant mode and the corresponding SMSR.

Even though THz QCLs with the operation temperatures varying from 8 K to 200 K is now available [8], the output powers at higher temperature would be very low. However, by

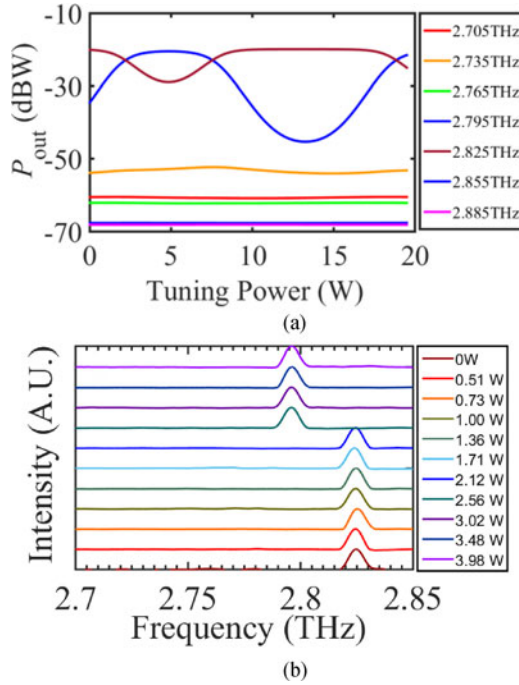


Fig. 9. Comparison of the mode tuning by passive cavity current between (a) the numerical simulation result and (b) the experimental data.

varying the heat sink temperature ΔT_{HS} at a wide tuning range from -100 K to 100 K, allows us to fully explore the effect on frequency tuning ability (amongst how many different modes) and thus to make a choice of heat sink temperature or peak gain frequency that provide a suitable combination of mode switches and continuous frequency tuning. For real CC THz devices, the active and passive cavity temperatures can also be manipulated by careful selection of excitation pulse duration and magnitude, as well as the thermal resistance of chip to submount interface, which has a marked impact on overall temperature change.

Fig. 8(a), (b) and (c) depict the steady state SPD as a function of ΔT_{HS} for $L_p = 0.25$ mm, 1.4 mm and 3.4 mm, respectively. The change of the dominant mode frequencies ν_r as a function of ΔT_{HS} are plotted as well, to illustrate the continuous frequency tuning of the dominant modes. We find that more mode hopping occurs when varying ΔT_{HS} from -100 K to 100 K in shown in Fig. 8(a), (b) and (c), than when n_{p0} varies from 3.60 to 3.62 , as shown in Fig. 6(a), (b) and (c), respectively. In addition, during each dominant mode period the dominant mode frequencies continuously red shift with increasing heat sink temperature. Mode hopping amongst 3 modes 7, 3 and 2, and a continuous frequency tuning of 11 GHz in mode 3 is achieved in Fig. 8(a2). Mode hopping amongst 3 modes with continuous frequency tuning of 4 GHz, 4 GHz and 6 GHz in each mode are realized when $L_p = 1.4$ mm, as shown in Fig. 8(b1) and (b2). When $L_p = 3.4$ mm, successive mode hopping from 6 to 2 with continuous frequency tuning from 2 – 5 GHz are observed in Fig. 8(c1) and (c2). Therefore, in these cases with the same ΔT_{HS} , mode tunability is improved with $L_a < L_p$ in this case compared with $L_a \sim L_p$ but with reduced SMSR.

From the analysis above, we demonstrate the sensitivity of the dominant mode, SMSR, as well as the emission frequency

to the key device parameters in a CC THz QCL for different ratios of active cavity and passive cavity. Due to the longer active cavity length, the mirror loss is greatly reduced in the CC THz QCLs compared with that in diode lasers. This results in a gain spectrum high above the threshold gain spectrum while they are comparable in diode lasers as demonstrated in [20]. Therefore, multiple modes have net gain above zero in CC THz QCLs, which makes the mode tuning characteristics more complicated. The mode competition and selection mechanism depend on the ratio of the lasing and passive cavity length and the eigenmode locations in the threshold gain spectrum as well. Frequency tuning in a CC THz QCL is normally realized by control the passive cavity current I_p for discrete mode hopping or the heat sink temperature T_{HS} for both mode hopping and continuous frequency tuning. It is observed that $L_a > L_p$ is more stable without mode hopping than $L_a \sim L_p$ and $L_a < L_p$ when tuning I_p or T_{HS} , which is consistent with the case in CC diode lasers [20]. However, when tuning I_p over a wider range, depending on L_p , $L_a > L_p$ exhibits mode tuning amongst more modes compared to the cases $L_a \sim L_p$ and $L_a < L_p$ when the eigenmodes near the gain peak are located at similar edges of the g_{th} profile. Mode tuning among more modes could be realized when $L_a \sim L_p$ and $L_a < L_p$ if eigenmodes located at different edges or locations of g_{th} spectrum so that their net gain changes with I_p asynchronously. When tuning the heat sink temperature, continuous frequency tuning is observed for three different ratios of L_a and L_p . However, a wider continuous frequency tuning range with a less discrete mode tuning could be obtained for the same variation of T_{HS} when $L_a > L_p$ compared with $L_a \sim L_p$ and $L_a < L_p$. Furthermore, frequency tunability could be enhanced with a proper combination of drive currents in both cavities and the heat sink temperature. There are a variety of sensing, spectroscopy, and imaging applications that require tunable THz laser sources [29]–[31]. By using the CC THz QCLs, we can control the convenient parameters (such as the cavity lengths, the injection currents, and the heat sink temperature) to achieve desired frequency tuning range. For example, discrete (continuous) tuning of 100 GHz (10 GHz) has recently been achieved experimentally from CC QCLs through appropriate cavity length optimization [32].

V. COMPARISON BETWEEN SIMULATION RESULT AND EXPERIMENTAL RESULT: MODEL VERIFICATION

The theoretical model described above is verified by experimental data for mode tuning by controlling the tuning power applied on the passive cavity current (the product of I_p and terminal voltage V_p). The comparison is carried for the fabricated CC QCL with $L_a = 1.5$ mm, $L_g = 13$ μ m and $L_p = 3.4$ mm described in [18]. As shown in Fig. 9(a), mode switching between Mode 5 at 2.825 THz and Mode 4 at 2.795 THz is anticipated from the numerical simulation when the tuning power in the passive cavity varies from 0 to 3.8 W, which agrees very well with the experimental data shown in Fig. 9(b), [18]. By using multi-mode RRE modelling, which involves the influence of the gain spectrum, more accurate results can be obtained than the simplified numerical approach described in [18], which

is based on the scattering matrix method only. In addition, the simulation results predict that mode tuning is only available between the two modes even with wider tuning power above 3.8 W. By developing a scattering matrix method in conjunction with multi-mode RREs, complete modelling of multi-mode competition in CC QCLs is predicted and analysed.

VI. CONCLUSION

Multi-mode reduced rate equations for THz QCLs were developed and the complete model for a coupled cavity THz QCL is established in this work. The accuracy of the proposed modelling approach has been validated with experimental data. Mode selection and frequency tuning capability of CC THz QCLs are investigated for different ratios of the lasing and passive cavity lengths. The net waveguide loss and the refractive index of the passive cavity determined the modulation depth and the phase of the threshold gain, respectively. Increase in heat sink temperature leads to red shifting of eigenmode frequencies, the threshold gain spectrum and the gain spectrum at different rates. The dominant mode and the SMSR are determined by the updated net gain relationship among the modes. The longer cavity lengths of THz QCLs result in a gain spectrum peak high above the threshold gain, which makes mode competition more complicated than in diode lasers. For discrete mode tuning capability, $L_a > L_p$ is more stable than $L_a \sim L_p$ and $L_a < L_p$, where the eigenmode distributions in the threshold gain spectrum influences mode competition as well. $L_a < L_p$ is more mode tunable than $L_a \sim L_p$ but with reduced SMSR. For continuous frequency tunability, wider continuous frequency tuning range could be obtained when $L_a > L_p$ compared with $L_a \sim L_p$ and $L_a < L_p$. The modelling approach demonstrated in this work provides a tool for numerical analysis for laser dynamic in multi-mode and multi-cavity QCLs.

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