The origin of self-focusing effect in terahertz quantum cascade lasers

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Abstract. The terahertz quantum cascade lasers (THz-QCLs) are the compact and coherent terahertz light sources based on the inter-subband transition and resonant tunneling of carriers in semiconductor superlattice. In recent studies on tapered THz-QCLs, it was found that the self-focusing effect in the active region of the devices may cause the abnormal increase of the far-field divergence of the laser beam. By simulating the propagation of optical mode in QCL waveguide and considering both the nonlinearity effect and thermal accumulation in the active region, we propose that the refractive index change caused by the third-order nonlinearity of multi-quantum-wells in active region may be the key reason for the self-focusing in THz-QCLs. This result indicates that the nonlinear effect may have great impact on the beam quality of QCLs which must be carefully considered in applications of THz-QCLs, such as the THz imaging systems.

1. Introduction

Quantum cascade lasers (QCLs), whose emission wavelengths can cover the frequency range from mid-infrared to terahertz (THz) regions[1, 2], are light sources based on the inter-subband transitions and resonant tunnelings of carriers in multiple quantum wells. The THz-QCLs have great applications in the fields of security check, free space optical communication, spectroscopy and imaging. However, the small output power and large divergence of the laser beam still limit the applications of THz-QCLs. To improve the output power maintaining the single-mode operation, the tapered gain region had been widely used in near-infrared diode and mid-infrared QCLs[3, 4, 5].

Recently, we developed the THz-QCLs with tapered gain region and demonstrated the power amplification effect[6]. The SEM imaging of the devices is shown in Fig.1a. The devices are composed of a ridged region of 0.5 mm×103 μm (length×width) and a tapered region of 2 mm length and with 0°, 3°, 5°, and 8° tapered angles, respectively. In the experiment, we observed an abnormal increase of far-field divergence of the tapered THz-QCLs. More specifically, the horizontal divergence of a far field laser beam decreases with increasing the tapered angle only when the angle is smaller than 5°, and then it increases with further increasing the angle. Generally speaking, the increase of the aperture of the output facet will decrease the divergence...
Figure 1. (a) SEM image of the tapered THz QCLs. (b) Conduction band energy diagram for two periods of multi-quantum-wells in the THz-QCL studied in Ref.[6]. The thicknesses of the GaAs quantum wells and Al$_{0.15}$Ga$_{0.85}$As barriers of one period are, from left to right, 12.6/4.4/9.3/0.6/16.9/0.9/16.6/1.0/14.3/1.2/ 12.5/1.5/11.4/2.5/11.4/3.3 nm. The barriers are in bold font and the underlined layer are doped with Si to 3×10$^{16}$ cm$^{-3}$. The designed bias is 2.55 kV/cm. The red subbands are upper and lower laser levels, and the subbands labeled with numbers 1∼4 are levels involved in the third order nonlinearity of the medium.

of laser beam, and the abnormal increase of the divergence may be due to the emergence of high-order transverse modes in the waveguide[7]. However, in our experiment, there are absorption stripes on the two sides of the ridges of the device which strongly suppress the high-order transverse modes. Then the observation suggests that there is self-focusing effect in the large tapered angle and high power THz-QCLs. The self-focusing can be caused by either the Kerr nonlinearity of the medium (Kerr lensing effect) or the thermal accumulation (thermal lensing effect). For the former case, if the laser medium possesses large third order susceptibility $\chi^{(3)}$, the refractive index $n$ for a high intensity light beam itself is modified by $\Delta n_{th} = n_2 I$, where $I$ is the optical intensity. For the latter case, the temperature gradient within the medium causes a refractive index change according to the local temperature as $\Delta n_{th} = \alpha_T T$, where $\alpha_T$ is the thermal coefficient and $T$ is the local temperature. Then we want to answer whether the optical nonlinearity or the thermal accumulation accounts for the self-focusing in tapered THz-QCLs.

2. Simulation of nonlinearity and thermal accumulation in THz-QCL
To specify the origin of the self-focusing in THz-QCL, we need to include the index changes caused by the Kerr lensing and the thermal lensing into the simulation of the optical mode propagation. For the Kerr lensing, we first calculate the third order susceptibility of the active region superlattice. The conduction band diagram of the THz-QCLs studied in Ref.[6] is calculated and is shown in Fig.1b. The calculated energy separation between the two laser levels (red lines) is 11.3 meV (~2.75 THz), the observed laser wavelength is 103 $\mu$m (~2.9 THz). The subbands labeled with 1∼4 are levels give birth to the third order optical nonlinearity. The density matrix equations can be employed to calculate the third order nonlinear susceptibility,

$$\frac{dp_{mn}}{dt} + (\gamma_{mn} + i\omega_{0}^{mn})\rho_{mn} = \frac{ie}{\hbar} \sum_{q} (z_{mq}\rho_{qn} - z_{qn}\rho_{mq})$$

$$\frac{dp_{mn}}{dt} + \hat{R}_{m} = \frac{ie}{\hbar} \sum_{q} z_{mq}\rho_{qm} - z_{qm}\rho_{mq},$$

(1)
where $m, n, q$ run over $1 \sim 4$, $\gamma_{mn}$ is the relaxation rate of the off-diagonal element of the density matrix, $\omega_{0mn}$ is the transition frequency, $z_{mn}$ is the optical dipole between the subbands $m$ and $n$, and $\tilde{R}_m$ represents all relaxation and pumping terms for the subband $m$ in the absence of the radiation fields. $\epsilon$ is the electron charge and $\hbar$ is the reduced Plank constant. The radiation field is considered as a sum of components with slowly varying amplitudes $F_{mn}$ and corresponding frequencies $\omega_{mn}$ near to the transition frequencies $\omega_{0mn}$. Solving the steady-state solution of Eq.(1), we can calculate the polarization of the system to arbitrary order of the nonlinearity and arbitrary field intensity. Since we are only concerned about the third order term which cause the index change, we expand the polarization in powers of the field amplitudes assuming weak enough field to get a analytical expression for the third order nonlinear susceptibility as

$$
\chi^{(3)} \approx \frac{ie\epsilon z_{12} z_{23} z_{34} z_{14} N_e}{\hbar \Gamma_{41}} \left[ \frac{1}{\Gamma_{31}} \left( \frac{n_2 - n_3}{\Gamma_{32}} + \frac{n_2 - n_1}{\Gamma_{21}} \right) - \frac{1}{\Gamma_{42}} \left( \frac{n_3 - n_4}{\Gamma_{43}} - \frac{n_2 - n_3}{\Gamma_{32}} \right) \right],
$$

where $\Gamma_{mn} = \gamma_{mn} + i(\omega_{0mn} - \omega_{mn})$, $N_e$ is the density of electrons in the active region, $n_m = \rho_{mn}$ is the subband population. Then the second order nonlinear refractive index is given by $n_2 = \chi^{(3)}/2n_0$, where $n_0$ is the linear refractive index.

For the energy diagram shown in Fig.1b, the calculated energy separations $\Delta E_{12}$, $\Delta E_{23}$, and $\Delta E_{34}$ are 11.3, 11.1, and 10.5 meV, respectively. The corresponding dipole matrix elements are $z_{12} = 6.46$ nm, $z_{23} = 7.08$ nm, $z_{34} = 15.94$ nm, and $z_{14} = 3.13$ nm. Using $N_e = 5 \times 10^{15}$ cm$^{-3}$, assuming that all the population is in the upper laser level 2, and all $\gamma_{mn} = 10$ meV except $\gamma_{41} = 20$ meV, and neglecting all detunings, we can get a $\chi^{(3)} \sim 2.2 \times 10^{-5}$ esu and corresponding nonlinear refractive index $n_2 \sim 5.17 \times 10^{-8}$ cm$^2$/W. Such a large nonlinearity is attributed to the large dipole moments. Of course, this value is an estimated upper limit of the nonlinear refractive index. The real value depends on the subband lifetimes, populations and even the temperature. So we use a smaller value $n_2 \sim 5 \times 10^{-9}$ cm$^2$/W in our simulation.

To study thermal lensing effect in THz-QCLs, we need simulate the temperature distribution in QCLs. The thermal model of QCLs has been widely studied. Here we just give a brief note on it, the details can be found in Ref.[8, 9] and the references therein. The heat diffusion in QCLs is described by the heat equation $\nabla \cdot [\kappa \nabla T] + Q = 0$, where $\kappa$ is the thermal conductivity tensor, $T$ is the temperature, and $Q$ is the heat generated per unit volume. The equation can be solved by standard finite-difference approach. Since the active region of the QCLs consist of near one thousand layers of quantum wells, the thermal conductivity is highly anisotropic. In the simulation, the thermal conductivity in the growth direction is significantly lower (typically one order lower) than thermal conductivity parallel to the layers. The detailed parameters of thermal conductivity of QCLs’ active region, the waveguide layers, the substrate as well as the heat sink can be also found in Ref.[9].

In Fig.2, we present the simulated temperature distributions of $0^\circ$- and $8^\circ$-tapered THz-QCLs. It can be seen that the temperature in the center of $8^\circ$-device is higher than that of $0^\circ$-device due to the larger width. For both devices, the temperature gradient is mainly along the growth direction. In the direction parallel to the layer, the temperature gradient is much smaller. This is because the conduction with the heat sink is the main way of the heat abstraction in QCLs. After the simulation of temperature distribution, the local temperature and the thermal coefficient $\alpha_T = 3.3 \times 10^{-4}$K$^{-1}$ are employed to study the thermal lensing effect in QCLs.

3. The origin of the self-focusing in tapered THz-QCLs
The optical mode within the waveguide of tapered THz-QCLs is described by the standard Helmholtz equation with the index changes due to the Kerr lensing and thermal lensing effects, and is solved with Beam propagation method[10]. Then the far-field distribution of the laser beam can be obtained from the optical mode distribution at the output facet according to the Rayleigh-Sommerfeld diffraction integral theory[11].
Figure 2. The simulated temperature distribution on the front facet of (a) 0°- and (b) 8°-tapered THz-QCLs. The temperatures of the environment and the heat sink are set to 10 K.

Figure 3. The experimental and simulated angles of full width at half maximum (FWHM) of the horizontal far field laser beam of the tapered THz-QCLs.

In Fig.3, we show the experimental and simulated results of horizontal full width at half maximum (FWHM) of the far field laser beam of the tapered THz-QCLs. As shown by the experimental data, the far-field divergence of tapered THz-QCLs decreases with increasing the tapered angle only when the angle is smaller than 5°. The divergence increase with further increasing the angle, see the experimental FWHM of 8° device. In the simulation side, the calculated divergence always decreases with increasing the angle if non of the lensing effects is considered (see the dashed line in Fig.3). Considering the thermal effect is also helpless. As shown in Fig.2, since the temperature gradient in the direction parallel to the quantum well layers is very small, the thermal lensing effect only slightly increases the far-field divergence of tapered THz-QCLs (the solid line in Fig.3). Even if we use a larger thermal coefficient $\alpha_T$, the simulated result cannot recover the experimental result. However, if the Kerr lensing effect is considered, the simulated result (data points •) can accurately recover the experimental result (data points ○). These comparisons suggest that the refractive index change caused by Kerr lensing, i.e. the third order optical nonlinearity of the active region may be the main reason for the abnormal increase of the divergence of tapered THz-QCLs.

4. Conclusions
In summary, we have presented the simulation of the mode propagation and the far-field distribution of THz-QCLs. By including the self-focusing effect caused by the third-order optical
nonlinearity of the superlattice in the active region, the simulation can recover the abnormal increase of the far-field divergence of the laser beam. This result suggests that the optical nonlinearity may have a great influence on the far-field beam quality of THz-QCLs, which should be carefully considered in future imaging application based on the THz-QCLs.

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References
[1] J. Faist, F. Capasso, Sivco, D. L. Sivco, C. Sirtori, A. L. Hutchinson, and A. Y. Cho 1994 *Science* **264** 553
[2] B. S. Williams 2007 *Nat. Photonics* **1** 517
[3] D. Vijayakumar, O. B. Jensen, and R. Ostendorf, T. Westphalen, and B. Thestrup 2010 *Opt. Express* **18** 893
[4] S. Menzel, L. Diehl, C. Pfugl, A. Goyal, C. Wang, A. Sanchez, G. Turner, and F. Capasso 2011 *Opt. Express* **19** 16229
[5] A. Lyakh, R. Maulini, A. Tsekoun, R. Go, C. Kumar, and N. Patel 2012 *Opt. Express* **20** 4382
[6] Y. F. Li, J. Wang, Ning Yang, J. Q. Liu, T. Wang, F. Q. Liu, Z. G. Wang, W. D. Chu, and S. Q. Duan 2013 *Opt. Express* **21** 15998
[7] L. Nähle, J. Semmel, W. Kaiser, S. Höfling, and A. Forchel 2007 *Appl. Phys. Lett.* **91** 181122
[8] C. A. Evans, D. Indjin, Z. Ikonic, P. Harrison, M. S. Vitiello, V. Spagnolo, and G. Scamarcio 2008 *IEEE J. Quan. Electron.* **44** 680
[9] K. Pierscinski, O. Pierscinska, M. Iwinska, K. Kosiel, A. Szerling, P. Karbownik, and M. Buga 2012 *J. Appl. Phys.* **112** 043112
[10] C. C. Wang 1996 *Phys. Rev. Lett.* **16** 344C346
[11] J. Wang, W. D. Wu, X. L. Zhang, and S. Q. Duan 2011 *Information and Electronic Engineering* **9** 365