Development of Intersubband Terahertz Lasers Using Multiple Quantum Well Structures

by

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Abstract

This thesis describes an experimental and theoretical effort in developing intersubband THz lasers using multiple-quantum-well structures. Scarcity of compact solid state sources in this frequency range, and to demonstrate a novel unipolar laser technology, motivated this research. Transport studies for realizing THz intersubband population inversion, new methods for long-wavelength mode confinement, and far-infrared spectral measurement techniques are critical steps in achieving this goal.

Conduction-band three-level subband systems in triple-quantum-well structures using GaAs/Al\textsubscript{0.3}Ga\textsubscript{0.7}As heterostructures were proposed, designed, and simulated by a numerical method. The numerical simulation is a self-consistent solution among the Schrödinger equation, Poisson equation, and rate equations. Electrons are injected by resonant tunneling to populate the upper subband; the lower subband is depopulated by fast longitudinal optical (LO) phonon scattering. THz emission devices consist of many modules of such triple-quantum-structures with the three-level systems cascade connected to each other. Dynamic charge of electron is provided by the $\delta$-doping per module. Temperature-dependent intersubband scattering plays a key role in transport modeling and therefore the degree of population inversion. Systematic calculations were performed to address issues of hot electron effect, lattice heating, and non-equilibrium optical phonons. Guidelines for device design and optimization were provided. The measured dc I-V at cryogenic temperature confirmed the design expectations.

Plasma confinement is used for making THz laser cavities. The minimum cavity loss can only be achieved by using metallic waveguides. The first metallic waveguide, which incorporates non-alloyed ohmic contact, was successfully fabricated by combining wafer bonding and selective etching techniques. Schemes for THz emission couplings were investigated by quantifying coupling loss, including surface coupling by gratings and edging coupling by facets.

The first free-space THz spectral measurement system was developed using a Fourier Transform Infrared (FTIR) spectrometer. This experimental set-up was successfully demonstrated in resolving THz emission by using step-scan and lock-in tech-
niques, and a fast Ge:Ga photon detector. Spontaneous intersubband THz emission was observed with linewidth narrower than 0.65 THz, and center frequency at the designed value of 3.8 THz. Different triple-quantum-well structures were designed, grown, and tested. The measured emission power levels were one order of magnitude lower than calculated values, and possible extra cavity loss mechanisms were discussed. To verify the triple-quantum-well structure design, a mid-infrared absorption measurement was performed on a sample grown on semi-insulating substrate. Information such as subband energy separations, dipole moments, and linewidth broadening, was extracted from the absorption spectrum and gave a good confirmation on numerical simulations and MBE growth quality of the MQW structures.

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Chapter 1

Introduction

1.1 Intersubband transitions for infrared generations

Since the invention of ultra-thin semiconductor layer growth techniques, such as molecular beam epitaxy, band-gap engineering has become a powerful tool to create new semiconductor structures that possess novel physical properties and device applications [1, 2]. Electronic states, wavefunctions, and carrier density can be tailored in semiconductor heterostructures. Intersubband transitions in these structures are especially attractive for optical applications, due to their large dipole moments as revealed by effective mass theory [3]. This figure of merit benefits both detector and laser developments. Stimulated by the concept of resonant tunneling proposed by Esaki and Tsu [4], Kazarinov and Suris discussed the possibility of light amplification in an electrically-pumped superlattice structure in 1971 [5]. A large dipole moment of intersubband transition was first observed on experiment in 1985 [6, 7] by an absorption measurement. The first intersubband emission was observed by Helm et al. in the far-infrared frequency range in a voltage-biased superlattice structure under resonant tunneling conditions [8, 9]. In the past decade, quantum well infrared
detection based on intersubband absorption has been well developed, and state-of-the-art quantum well photodetector (QWIP) chips have been fabricated working at wavelengths of 4 μm and 10 μm [10, 11]. However, the development of intersubband emitters and lasers have stagnated. This is largely due to the fact that for detection, most of the carriers are on the ground state, which is the case corresponding to thermal equilibrium; while for emission, an appropriate transport scheme has to be designed to realize population inversion between the two subbands for radiative transitions.

Depending on the dimensions of the quantum wells or superlattices, intersubband emission can be designed in frequency range from mid-infrared to far-infrared and terahertz (THz) using III-V semiconductor heterostructures [12, 13]. In the last ten years, a number of detailed feasibility studies have been proposed on electrically pumped intersubband lasers working in mid-infrared [14, 15, 16] and far-infrared frequencies [17, 18, 19, 20]. A detailed analysis of these proposals was given by Smet (Ref. [13]). Most of these papers presented quantitative numbers for the optical part, i.e., lasing frequency, gain, cavity loss. However, appropriate transport design to realize population inversion was still the major obstacle. The invention of a mid-infrared quantum cascade laser by Faist et al. at Bell Labs in 1994 [21] brought into the first successful intersubband laser in history. This type of laser and the subsequent superlattice laser demonstrated by the same group will be reviewed.

1.1.1 Mid-infrared quantum cascade lasers

The basic structure of a quantum cascade laser consists of an active section and a digitally graded gap injector. The active section usually has three subband levels $E_3$, $E_2$, and $E_1$ in a double or triple quantum wells. The lasing transition is between $E_3$ and $E_2$. For mid-infrared wavelength at 4 μm for example, $E_3 - E_2 \sim 300$ meV. $E_1$ level is designed to be about one longitudinal optical (LO) phonon energy below $E_2$, so that $E_2$ level can be emptied by rapid LO-phonon scattering. Since the
intersubband LO-phonon scattering from $E_3$ to $E_2$ is slowed down due to the large in-plane momentum transfer, global subband population inversion can be realized between $E_3$ and $E_2$. Under designed bias, the miniband formed by the superlattice in the digitally graded gap is aligned with the upper level $E_3$ to inject electrons. This graded gap region is important for the transport design of a quantum cascade laser and serves for a two-fold purpose. Firstly, the bias voltage drop $(eV \sim E_3 - E_1)$ between two adjacent cascade active sections needs to be spread along a wider region to avoid high electrical field across the structure. The digitally graded gap is also a better option than an alloy graded gap in terms of material growth [22]. Secondly, the hot electrons from the active region can relax their extra energy by intrasubband and intersubband LO-phonon emissions, and get thermalized within the digitally graded gap region before entering the next stage.

The operation of quantum cascade unipolar lasers are less temperature dependent, compared with the interband diode lasers working at the same frequency by using narrow band gap semiconductor materials. This is due to the intersubband nature of optical transitions, LO-phonon governed carrier transport ($\hbar \omega_{LO}/k \sim 400$ K), and negligible intersubband Auger scattering [23, 24]. The performance of quantum cascade lasers has significantly improved in the past four years since its invention. By using vertical (intrawell) transitions and Bragg reflection by the minigap formed in the superlattice injector to block upper level leakage, the lasing threshold current density was greatly reduced from $\sim 10$ KA/cm$^2$ to $\sim 1$ KA/cm$^2$ [25, 26, 27]. Continuous-wave operation has been achieved at 110 K, and Watt-level peak power of pulsed operation has been obtained at 20 K at $\lambda \sim 5$ μm wavelength [28]. By using a plasmon-enhanced waveguide to improve longer-wavelength mode confinement, continuous-wave operation of quantum cascade lasers above 8 μm were also demonstrated [29, 30, 31, 32]. It is believed that the present quantum cascade laser technology can cover 3 μm - 11 μm mid-infrared wavelength, in pulsed mode operation at room temperature or continuous-wave operation at liquid nitrogen temperature, and single
So far, all the demonstrated quantum cascade lasers were made of GaInAs/AlInAs quaternary system grown on lattice-matched InP substrate. The device design benefited from smaller electron effective mass and larger barrier heights compared to GaAs/AlGaAs material system. The contrast of the refractive indices within the quaternary systems makes dielectric cladding layer for mid-infrared waveguide available by MBE growth [21]. The non-alloyed ohmic contact to these material systems also simplifies the fabrication and avoids detrimental plasma loss at the metal/semiconductor junction regions. The development of GaAs/AlGaAs based quantum cascade lasers is presently under the way by several groups [35, 36, 37]. Once successful, it offers an alternative to the GaInAs/AlInAs based quantum cascade lasers.

An interesting observation for the quantum cascade laser is that, although the structure is designed with the expectation of global subband population inversion, due to the band nonparabolicity, the optical gain of a quantum cascade laser only depends on the local \( k \)-space population inversion around \( k_{||} = 0 \) (\( k_{||} \) is the in-plane wavevector). The degree of actual population inversion is thus significantly enhanced, since most of the electrons on subband \( E_2 \) do not cancel the population on \( E_3 \) in counting the inverted population. Faist \textit{et al.} demonstrated a quantum cascade laser without global subband population inversion [38], in which case the active section is a two-level system and the lifetime of electrons on lower subband was intentionally designed to be longer than that of the intersubband scattering time from upper subband to lower subband. This laser, with more electrons on lower level than the upper level, achieved lasing action with threshold current density only twice greater than a similar structure designed into three-level system with global subband population inversion [38]. Most of the quantum cascade lasers adopted three-level system design, because it helps to reduce the number of electrons on the bottom of the lower subband, thus increases the local \( k \)-space population inversion. Figure 1-1 described this situation schematically for both the two-level and three-level cases.
Figure 1-1: (a) Two-level mid-infrared quantum cascade laser based on local k-space population inversion. Electrons leak out $E_2$ subband at a slower rate than the inter-subband scattering rate from $E_3$ to $E_2$ by LO-phonon scattering, resulting in more electrons on $E_2$ subband than $E_3$ subband. Optical gain only depends on local k-space population inversion in the vicinity of $k_{||} = 0$, due to band nonparabolicity, as indicated by the dashed circle region. Electrons scattered to $E_2$ subband from $E_3$ subband loss energy by sequential intrasubband LO-phonon scattering. The graded shadow indicates electron occupation in $k_{||}$ space. (b) Three-level quantum cascade laser with global subband population inversion. Optical gain depends on the local k-space population inversion as the case in (a), but the degree of population inversion is enhanced by reducing the total population on $E_2$ level.
1.1.2 Mid-infrared superlattice lasers

As just pointed out, if the optical gain of intersubband transition only depends on the local k-space population inversion, the global subband population inversion, a more stringent condition, is not required. Thus, an intersubband laser will be easier to realize in terms of the transport design. The criterion to satisfy this condition is that the dispersion relations of the two subbands differ from each other. The study of the energy minibands in semiconductor superlattice was pioneered by Esaki and Tsu [4] in 1969. The miniband formation in superlattice structure was later investigated and demonstrated in experiment by Dingle and coworkers in 1975 [39]. A theoretical proposal of using a band-aligned superlattice to realize an infrared intersubband laser was put forward as early as 1987 by Yuh et al. [14]. Until very recently, the first intersubband superlattice lasers working at mid-infrared wavelength were demonstrated by Scamarcio et al. at Bell Labs [40, 41]. The active section of such a laser structure is simply made of two minibands formed by the superlattice. The miniband separation corresponds to the mid-infrared radiation. A digitally graded gap is used to bridge the lower miniband of a previous stage to the higher miniband of the next stage for electron injections. Population inversion in local k-space is automatically achieved by the dispersion relations of the two minibands.

By using a one-dimensional tight-binding approximation, the miniband dispersion relations in the reduced Brillouin zone are plotted schematically in Figure 1-2 [42]. In each miniband, electrons tend to occupy the lower states because of fast intraminiband scattering [40]. In quasi-thermal-equilibrium condition, the upper states of each miniband are empty, and the lower states are occupied, as indicated by the Fermi level on each miniband. Lasing transition therefore occurs at the Brillouin zone edge, where the energy separation is the smallest, and population inversion is readily achieved. This situation is completely analogous to the interband diode lasers, if the lower miniband is considered as the “hole” band. For interband diode lasers, population inversion can always be achieved under injection condition in the
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Figure 1-2: (a) Valence band and conduction band dispersion relations for a direct band gap semiconductor material in the first Brillouin zone. Under injection condition, $E_{fe}$ is the electron quasi Fermi level in conduction band and $E_{fh}$ is the hole quasi Fermi level in valence band. Lasing transition occurs at the Brillouin zone center. (b) Dispersion relations of the first and second minibands of a mid-infrared superlattice laser, $E_1 = E_1(k_z, k_{\parallel})$ and $E_2 = E_2(k_z, k_{\parallel})$, in the first Brillouin zone. The lasing transition occurs at the Brillouin zone edge, where energy separation is minimum. Quasi Fermi level is assumed for each miniband.
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p-n junction region, with electrons on the bottom of the conduction band, and holes on the top of the valence band as indicated in Figure 1-2. The only difference is that the local k space is at zone center \( \Gamma \)-point, between fourth (valence) and the fifth (conduction) energy bands in semiconductor crystals, instead of the Brillouin zone edge for superlattices which have only first and second minibands. One should therefore think that the semiconductor superlattices are one-dimensional "artificial crystals", with the semiconductor bulk replaced by the MBE-grown heterostructure.

Both the quantum cascade lasers and superlattice lasers rely on local k-space population inversion, due to specific dispersion relations. However, in terms of the transport design and under what condition the population inversion can be realized, these two types of lasers have a fundamental difference. The quantum cascade lasers rely only on nonparabolic dispersion relation for local k-space population inversion. Because both the upper subband and lower subband are bent in the same direction shown in Figure 1-1, to maximize population inversion at \( k_{\parallel} \sim 0 \), the electrons on the upper subband are encouraged to occupy the low \( k_{\parallel} \) states, whereas the electrons on the lower subband are encouraged to reside on the high \( k_{\parallel} \) states (subband bottom). Fortunately, due to the nature of phonon scattering and large subband separation corresponding to mid-infrared frequency range, the constant injection of high-energy electrons from upper subband upsets the thermal-equilibrium distribution of electrons on the lower subband. Thus, as long as this highly non-equilibrium distribution is maintained on lower subband, without a third subband to quickly remove electrons from the lower subband, population inversion can still be realized with a two-level design ([38]). However, if the lower subband could not maintain highly non-equilibrium distribution, such as the case in which the energy separation between upper and lower subbands is brought down to \( \sim 1-2 \) LO-phonon energy, quantum cascade laser has to be implemented by a three-level design with global population inversion. The interminiband superlattice lasers, on the other hand, are only two-level systems. Thus there is no global population inversion. Shown in Figure 1-2, the dispersion relations
of the two minibands in $k_z$ space are bent in opposite directions. The near-thermal-equilibrium distributions of electrons on both the upper and the lower minibands are desirable to maximize the population inversion. This is a less stringent requirement for transport design, provided that the electrons become thermalized on each miniband. For a superlattice laser, the electron distribution in $k_{\parallel}$ space does not play a role in determining the population inversion. Thus, the energy separation between the two minibands can be reduced, and much longer-wavelength superlattice lasers can be realized with the present simple two level design. It is worth mentioning that, nonparabolicity is a material's property, which may vary from one material system to another. This local k-space population inversion may not be a full advantage that a quantum cascade laser can take if its host material system is changed into one with smaller nonparabolicity. For superlattice lasers, however, the local k-space population inversion is due to the miniband dispersion relations, which is resulted solely from the superlattice structure engineering and is regardless of the host material system.

Compared with quantum cascade lasers, the electrically pumped superlattice lasers are simpler in transport design, and have impressive high output power and high temperature performance [43]. Besides the fact that population inversion is easier to achieve for superlattice lasers under injection, the wide-spread wavefunctions of the miniband states make the dipole moment of intersubband transition extremely large. The corresponding oscillator strength between miniband states with the same $k_z$ index is around 10 at the Brillouin zone edge [40, 43], compared to the oscillator strength of 1 for interwell or intrawell transitions in quantum cascade lasers [28, 32]. The sub-threshold spontaneous emission spectra of superlattice lasers are usually broader than the quantum cascade laser working at the same frequency [41, 40, 43]. This is caused by the miniband energy dispersion along $k_z$ direction, especially when its slope is comparable to the in-plane $k_{\parallel}$ dispersion relation. Injected electrons, when hot from the previously stage, start to populate high $k_{\parallel}$ and $k_z$ states. The in-plane states do not contribute to emission broadening significantly due to the intersubband
transition nature (there is still some broadening due to band nonparabolicity). The $k_z$ states, however, will contribute to emission broadening directly, in a way similar to the interband radiative transitions between the conduction band and the valence band. In designing a superlattice laser, the slope of the miniband dispersion should be engineered as steep as possible. It will benefit both local $k$-space population inversion and emission linewidth.

1.1.3 Other methods for infrared generations based on intersubband transitions

Mid-infrared optically pumped intersubband lasers

Optical pumping provides an alternative approach to electrical pumping for making intersubband lasers. It selectively sends carriers to the desired subband level without biasing the multiple quantum well structures. Since it doesn’t involve carrier transport in the vertical direction (growth direction), possible inhomogeneity in electrically pumped multiple quantum well structures due to high field domain formation is avoided. Optically pumped intersubband lasers were first proposed as early as 1993 [44, 45]. Practical development of optically pumped mid-infrared intersubband lasers has been carried out by Julien’s group via intraband and interband pumping schemes in recent several years [46, 47, 48]. An CO$_2$ laser pumped mid-infrared intersubband laser working at 15.5 $\mu$m was recently demonstrated by this group [49]. The lasing threshold was about 0.5 MW/cm$^2$. Watt-level output power was achieved at cryogenic temperature, and lasing action persisted to 110 K. This first optically-pumped intersubband laser, using GaAs/AlGaAs material system, bears complete similarity to the mid-infrared quantum cascade lasers in terms of the active region design and schemes for realizing population inversion. Global subband population inversion is designed by using a three level system analogous to the quantum cascade lasers, i.e., the lower subband of the radiative transition was emptied through fast LO-phonon
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scattering to the ground level which is one LO-phonon energy below. Electrons on the ground level of the multiple quantum wells are pumped to the upper level by the CO2 laser. The intersubband scattering time for electrons from upper level to lower level by LO-phonon emission, due to a large momentum transfer, is longer than the intersubband scattering time between the lower level and the ground level. The optical gain also depends on local k-space population inversion through band nonparabolicity, although this effect may not be as prominent as in quantum cascade lasers, due to smaller subband energy separation and smaller nonparabolicity parameter in GaAs/AlGaAs material system. The mode confinement was achieved by a MBE-grown 5 μm thick AlAs cladding layer from the bottom side and air from the top side. Since there is no need to provide electrical contacts, free carrier loss in laser cavity is minimized.

It is necessary to point out a powerful experimental characterization method that benefited the development of the first optically pumped intersubband laser: two-color free electron laser pump-probe measurements. The optically-pumped nature of emission experiments makes pump-probe measurement very suitable and ready to perform for the emission devices. The two output wavelengths of the two-color free electron laser are continuously tunable from THz frequency range to mid-infrared. The pulse width can be made as short as a few hundred femtoseconds. Key parameters, such as electron lifetime on excited states, optical gain at the emission frequency, and cavity loss were obtained [47, 50]. Device parameters can thus be tuned to finally reach the lasing threshold.

Infrared generations by nonlinear optics of intersubband transitions

Due to large dipole moment of intersubband transitions, quantum wells possess large nonlinear susceptibilities such as $\chi^{(2)}$ and $\chi^{(3)}$ [10, 51]. In asymmetrical quantum wells, step quantum wells, or quantum wells in strong electric field, $\chi^{(2)}$ can be designed very large (in $10^{-7}$ m/V range) by optimizing dipole moments at double
resonance. Especially at low temperatures the linewidth shrinks and thus further enhances the susceptibility at resonance. A number of experiments have demonstrated the giant $\chi^{(2)}$ by second harmonic generations [52, 53, 54, 55, 56]. To generate infrared radiation by frequency down conversion, difference frequency mixing and parametric oscillator can be used. Sirtori et al. demonstrated the first far-infrared generation at about 5 THz by difference frequency mixing, using large $\chi^{(2)}$ at double resonance in a coupled double quantum well structure [57]. A nano Watt power level was achieved with two CO$_2$ lasers as the pump. The interaction length in this experiment was shorter than the coherent length, thus phase matching condition is generally not required. For both difference frequency mixing and parametric oscillator, phase matching condition needs to be satisfied to achieve large output power. To meet this requirement, quasi-phase matching was proposed by introducing periodically modulated $\chi^{(2)}$, where the periodicity compensates for the k-vector difference between the pump and the signal [58]. This idea is similar to the quasi-phase matching used for bulk nonlinear optical materials [59, 60]. For quantum wells, the large Stark shift can be used to tune $\chi^{(2)}$ off resonance with metallic grating deposited on the surface of the quantum well wafers. Another solution for phase matching is to use Stark shift to tune the first order susceptibility of the intersubband transitions in quantum wells, thus the refractive index of medium [61, 62] is tuned to the phase-matching condition. So far there have been no experimental demonstrations of the above voltage-tuned quasi-phase matching or phase matching in multiple quantum wells. Recently, a concept of optical parametric oscillators without phase matching was proposed [63]. When the loss of the idler or signal is large enough to be comparable to the mismatched wavevector, i.e., wave attenuates too quickly within one wavelength, the momentum conservation restriction is relaxed. The localization of waves in real space leads to wavevector spreading in the momentum space, and hence phase matching is not a required condition.

Compared to an optical parametric oscillator, difference frequency mixing is less
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preferable for device applications, because it needs two “pumping” sources with slightly different frequency. In a way similar to a laser, an optical parametric oscillator needs a pumping source and threshold gain to operate. An optically-pumped laser utilizes the first order susceptibility of intersubband transitions in quantum wells but needs to design a population inversion scheme, whereas optical parametric oscillator utilizes second order susceptibility without a requirement for population inversion. For optical parametric oscillators, the threshold pumping might be much higher, and the phase matching and pumping coupling issues need to be accomplished. The advantage of parametric oscillators is that they may offer much larger tunability compared with optically pumped lasers, which is a very desirable feature for spectroscopic applications [64].

Lasers without population inversion using multiple quantum well structures

Lasers without population inversion were first proposed by Harris [65, 66] in 1989. This concept is based on Fano-type quantum interference in absorption and emission processes. When two upper states are coupled to each other, i.e., their lifetime broadening is comparable to the coupling, both the absorption from a lower state to the upper state and the emission from the upper state to the lower state will have two paths. At certain frequencies, the amplitudes of these two paths interfere destructively for absorption process, and constructively for emission process, causing vanished absorption and enhanced emission. Optical gain is thus possible even there is no population inversion between the lower state and the upper state. Experimentally, this coupling-induced transparency by quantum interference was first observed in Sr vapor [67], then in coupled double quantum well structures with resonant tunneling and broadened upper states by leakage [68, 69]. The later achievements are inspiring, since multiple quantum well structures are “artificial atoms” and their subband levels, coupling strength, and linewidth broadening can be designed and tailored in
certain range to meet the specific requirements for this Fano-type interference. The idea of building semiconductor lasers without population inversion based on inter-subband transitions was first proposed by Imamoglu and coworkers in 1994, with a design example at mid-infrared frequency using coupled double quantum wells [70]. This opens a new possibility to generate coherent infrared radiation based on inter-subband transitions. However, the realization of such a bold idea depends on many critical numbers. Especially, the electron dephasing time due to electron-electron scattering can be very short compared to that in an atomic system. Also, pushing such a laser to operate at longer wavelength into THz range seems very difficult. The smaller energy separation corresponding to THz frequency makes it improbable to selectively broaden upper levels without affecting the lower level's lifetime.

1.2 Existing coherent terahertz sources and applications

Terahertz frequency (1-10 THz, or 30-300 μm wavelength) is beyond the operation capability of electronic devices such as transistors, which utilize classic diffusive transport. Even today's start-of-the-art heterojunction bipolar transistor (HBT) can only reach 100 ~ 200 GHz frequency range, limited by the transient time and device parasitic RC time constant. On the other hand, photonic devices such as interband laser diodes can only be operated at frequencies above the material's band gap, which is greater than 10 THz (40 meV) even for narrow-gap lead salt semiconductors. Terahertz frequency is thus among the most underdeveloped electromagnetic spectral region, because of the lack of compact, coherent solid-state sources.

Molecular gas lasers are capable of generating terahertz radiations from 0.1 THz to 8 THz range. Population inversion is achieved between vibrational or rotational energy levels of the molecules by selective optical pumping such as using a CO₂ laser [71]. Molecular gas lasers can be continuous-wave operated at room temperature due
to the extremely sharp linewidth. However, they are usually bulky and consume a lot of power. Solid state diode lasers, using narrow band gap semiconductor materials such as lead salt and BiSb, can be operated down to $\sim 10$ THz frequency at cryogenic temperatures [24]. Free electron lasers are high-power lasers that can generate high quality laser radiation. The operating frequency can be tuned in a broad range covering the terahertz (1-10 THz) frequency [72]. Unfortunately, free electron lasers are too expensive and corpulent to be used for practical applications. The only solid state lasers available today that work in THz frequency range are p-type Ge lasers [73]. Crossed magnetic (0.3-3 Tesla) and pumping electric fields ($0.5-2$ kV/cm) need to be applied to the laser crystal. Differences between the scattering rates of light holes and heavy holes by LO phonons, with appropriate $B/E$ ratio, gives hole state population inversion and thus optical gain. The p-Ge lasers have the advantage of great field-dependent tunability, but they need to be operated at cryogenic temperatures with typically $<1\%$ duty cycle and $\sim 1 \mu$sec maximum pulse duration. The requirement of a strong magnetic field makes device less compact for practical usage.

The applications of coherent THz solid state sources lie in three major categories: (1) high-resolution THz spectroscopy for chemical and biological applications, including gas analysis, atmospheric pollution monitoring, and chemical agent detections. These types of applications are based on absorption measurements and require the tunability of the lasers [74]. (2) Non-invasive semiconductor wafer characterizations. The free carriers in doped semiconductor wafers typically have plasma frequencies in THz frequency range. The doping density profile and carrier mobility variations on wafer level can be characterized by time-domain or frequency-domain THz reflection or transmission measurements with spatial resolution comparable to the THz wavelength [75, 76]. This technique is especially desirable for III-V semiconductor wafer characterizations, because an ohmic contact is not readily available without annealing. (3) Local oscillators used in THz heterodyne detections of atomic and molecular species in interstellar space [77].
1.3 Electrically-pumped intersubband THz lasers

The quest of developing an electrically pumped intersubband THz laser has a two-fold impetus: (1) to demonstrate a novel intersubband-transition-based laser technology in THz frequency range; (2) to provide a compact coherent solid-state THz source for practical applications.

Although mid-infrared electrically pumped quantum cascade lasers and superlattice lasers were invented several years ago, major obstacles remain for the development of THz intersubband lasers. The narrow subband separation corresponding to THz frequencies (4-40 meV) makes selective population of subbands difficult. As we will see, local k-space population inversion, which is the situation for mid-infrared quantum cascade lasers, intersubband superlattice lasers, and other semiconductor lasers, can not be effectively utilized in THz intersubband laser design. For mode confinement, in addition, the long wavelength requires new methods to make a laser cavity. Presently, the research project in which the author is engaged at MIT has been the only one in this field.

A critical step in developing a THz intersubband laser is the transport design to realize population inversion. As analyzed in subsections 1.1.1 and 1.1.2, the successful development of electrically pumped mid-infrared intersubband lasers by Bell Labs reveals that population inversion can be realized through two approaches: (1) global subband population inversion by engineering intersubband scattering rates, and (2) local k-space population inversion by designing the subband dispersion relations. Based on this fact, the author believes there are two options to choose to realize population inversion in an electrically pumped THz intersubband laser. Since band nonparabolicity is negligible for subband separation corresponding to THz frequencies, the optical gain will not depend on local k-space population inversion such as the case in mid-infrared quantum cascade lasers, but instead will depend on the global subband population inversion. Therefore a THz intersubband laser using multiple quantum well structure has to be designed to guarantee overall subband population
inversion. THz lasers depending on local \textbf{k}-space population inversion are possible by borrowing the idea of mid-infrared superlattice lasers in a parallel way. The question is, with the band widths comparable to the small energy separation between minibands for THz frequency generation, it might be impractical to implement such a superlattice structure. A THz laser based on local \textbf{k}-space population inversion is possible, however, in $k_{\parallel}$ space in valence band, which is pointed out by a recent work.

The above three possibilities are illustrated in Figure 1-3 with both the multiple quantum well (superlattice) structures and subband dispersion relations described schematically.

Scheme-1 is a three-level system using coupled triple quantum well structures, designed to realize global intersubband population inversion. At designed bias, the energy separation between $E_3$ and $E_2$ corresponds to THz frequency (typically $10 \sim 20$ meV), and the energy separation between $E_2$ and $E_1$ is greater or comparable to the LO-phonon energy. Also, $E_1$ subband is aligned to $E_3'$ of the next identical triple quantum well module at this bias, so that electrons can undergo resonant tunneling to populate the upper subband of the next module. Since the intersubband scattering rate between $E_2$ and $E_1$ by LO phonons is much faster than that between $E_3$ and $E_2$ for which LO-phonon scattering is not available, the intersubband population inversion between $E_3$ and $E_2$ can be achieved.

Scheme-2 is a superlattice design borrowed from the mid-infrared superlattice lasers for local \textbf{k}-space population inversion. Two minibands are formed in $k_z$ space by the superlattice structure. The energy separation between the bottom of the lower miniband and the bottom of the upper miniband is about one LO-phonon energy, to guarantee that an electron can be scattered by at least one LO phonon within each stage. The lasing transition occurs at the Brillouin zone edge with energy separation corresponding to THz frequency. As mentioned above, since the miniband energy width is comparable to the interminiband separation, selective injection of electrons from the first miniband of the previous stage to the second miniband of the next stage
Figure 1-3: Design options for THz intersubband lasers. (a) Scheme-1, three-level system designed for global intersubband population inversion. (b) Scheme-2, local $k_z$-space population inversion with a superlattice structure. (c) Scheme-3, local $k_{||}$-space population inversion in valence band, due to non-monotonic light hole subband dispersion relation.
is difficult, and band alignment is critical in designing such a functioning superlattice structure.

Scheme-3 is proposed by a recent publication [20] for local $k$-space population inversion. In that, lasing depends on the local in-plane $k_{||}$ space in valence band. This proposal takes the advantage of more complicated valence band structure. In a simple single quantum well structure cascade connected in valence band, light hole subband is coupled with heavy hole subband of the next quantum well which corresponds to resonant tunneling by energy level alignment. The inverted light-hole effective mass leads to non-monotonic dispersion relation in the in-plane $k_{||}$-space. Thus the lasing transition occurs at the minimum of light hole dispersion relation. Provided intrasubband scattering process is fast enough, it can be assumed that holes have near-thermal-equilibrium distribution on each subband. As indicated by the Fermi levels on the heavy hole subband and the light hole subband, local $k_{||}$-space population inversion can be automatically achieved at the minimum energy separation.

1.4 Thesis outline

The research in this Thesis focuses on the three-level design in Scheme-1, with expectation to achieve global subband population inversion and realize a conduction band intersubband THz laser. Chapter 2 presents the numerical simulation method, a multiple quantum well design of the three-level system, and basic transport modeling based on rate equations. The THz spontaneous emission power and optical gain are given in Chapter 3, with discussions on THz emission coupling, mode confinement, plasma loss, and metallic waveguide, based on numerical results. Chapter 4 gives more detailed treatments of transport modeling with the presence of hot electron effect, hot LO-phonon effect, and lattice heating. It is shown that non-equilibrium LO phonons have a significant effect in degrading subband population inversion. A more complete temperature-dependent transport modeling is proposed for calculating
subband population inversion. Chapter 5 presents the experimental set-up for THz emission measurements, device processing, especially the metallic waveguide fabrication technique developed in this research project. THz emission spectra were resolved using Fourier Transform Infrared (FTIR) spectrometer. Several triple-quantum-well structures with different design parameters have been designed, fabricated, and measured. These results are presented in Chapter 6, followed by conclusions in Chapter 7.
Chapter 2

Multiple Quantum Well Structure Design

2.1 Introduction

Design of multiple quantum well structure (MQW) involves engineering subband levels corresponding to THz frequency generation, and ensuring the presence of population inversion when the structure is under an appropriate bias. For a given semiconductor heterostructure, the subband levels are obtained by solving the Schrödinger equation in the presence of electrostatic potential. The electrostatic potential is given by the Poisson equation for a certain charge distribution in the quantum wells. For unipolar devices with only conduction band involved, the charge is due to electrons and the ionized donors. To obtain a self-consistent solution between the Schrödinger equation and Poisson equation, it is therefore necessary to know how the electrons distribute in a MQW structure, given subband energy levels and wavefunctions. This transport modeling in such a quantum mechanical system lies in the central role in device modeling of the THz emitters. Literature in this field is lacking, even though the transport studies of quantum-effect semiconductor devices dated back 20 years ago. Most quantum-effect semiconductor devices, based on perpendicular transport
(carriers transport along heterostructure growth direction), deal with tunneling behaviors through double barrier, double quantum wells, or a superlattice structure, with the quantum region sandwiched by two heavily doped electron or hole reservoirs which are treated as semi-classical regions [1, 2, 78]. The device modeling and simulation techniques for such tunneling diodes, mostly for microelectronic applications, are well developed [79, 80, 81, 82, 83, 84, 85]. In addition, since the quantum region of these devices is relatively short, typically several hundred angstroms (Å) which is comparable to the coherent length, carriers are assumed to be ballistic [81, 82]. Electron or hole concentration in the quantum region depends on the contact’s Fermi levels. Complicated MQW structures incorporating multiple stages of quantum well modules, however, are generally proposed for optical applications such as electrically pumped intersubband lasers. The transport study and experimental realization of such structures only began with the invention of quantum cascade lasers. There are two basic distinctions in transport modeling between these types of MQW structures and the extensively studied resonant tunneling devices: (1) since the structure are usually much longer than the coherent length, intersubband scattering is an important transport mechanism; (2) carriers in the MQWs are provided by the internal doping, not from the contacts. These assumptions provide the basis for the modeling and design of THz emission MQW structures.

2.2 Numerical simulation

2.2.1 Device modeling

To design an intersubband MQW structure for THz generation, a reasonable device model needs to be established for numerical simulations. It should include the Schrödinger equation, Poisson equation, and intersubband transport mechanisms such as phonon-assisted tunneling. Such a numerical simulation should give subband energy levels, wavefunctions, and carrier population on each subband.
Firstly, electrostatic potential needs to be obtained by the Poisson equation for a given charge distribution:

$$\frac{d}{dz}[\varepsilon_r(z)\varepsilon_0 \frac{d}{dz} V(z)] = -e[N_D^+(z) - n(z)]$$  \hspace{1cm} (2.1)$$

where $\varepsilon_r(z)$ is the relative dielectric constant of the semiconductor heterostructure. $N_D^+$ is the ionized donor distribution, and $n(z)$ is the electron concentration. $e$ is one electron charge. Holes are absent for conduction band MQWs doped only with donors. $z$ is the coordinate along MQW growth direction. The electron concentration is expressed as

$$n(z) = \sum_i n_i \psi_i(z)$$  \hspace{1cm} (2.2)$$

where $\psi_i(z)$ is the envelope wavefunction of the $i$-th subband and $n_i$ is the two-dimensional (2D) electron population on that subband. Assuming the material-determined conduction band profile is $E^0_C(z)$, the bent conduction band profile, with the presence of electrostatic potential $V(z)$, is $E_C(z) = E^0_C(z) - qV(z)$. By solving the one-dimensional Schrödinger equation:

$$\frac{\partial}{\partial z} \left[ \frac{1}{m^*(z)} \frac{\partial}{\partial z} \psi(z) \right] + \frac{2}{\hbar^2} [E - E_C(z)] \psi(z) = 0$$  \hspace{1cm} (2.3)$$

where $m^*(z)$ is the effective mass of electron in the heterostructure. $E = E_i$ and $\psi(z) = \psi_i(z)$ give the energy level and subband wavefunction of the $i$-th subband.

To obtain a self-consistent solution between the Schrödinger equation and the Poisson equation, the electron population on each subband needs to be obtained. Here lies the basic distinction in transport modeling between the MQW structure used in this research and the device modeling on tunneling diodes, which rely on electron reservoirs at the contacts. Since we are dealing with the discrete energy levels, electron transport in the MQW structure is governed by rate equations. Electron population on each subband is determined by intersubband scattering and resonant tunneling.
Another important assumption is that, for sufficiently long MQW structures, carriers are provided by the internal doping. Unlike tunneling diodes, contacts do not affect the transport behavior in MQW region, except for providing the electrical connection. This assumption has been demonstrated experimentally by comparing I-V curves of a n⁺-i-n⁺ structure with an n⁺-n-n⁺ structure, in which case n⁺-i-n⁺ behaves as an insulator (n⁺ is the doped contact, i is a MQW region without doping, and n is the same MQW region with doping) [86]. Under this global charge neutrality condition and from rate equations corresponding to static state, electron population on each subband can be obtained through:

\[ \sum_i n_i = \int N^+ D_i(z)dz \]  \hspace{1cm} (2.4)

and

\[ \frac{dn_i}{dt} = \sum_{j \neq i} \frac{n_j}{\tau_{ji}} - \sum_{k \neq i} \frac{n_k}{\tau_{ik}} = 0 \]  \hspace{1cm} (2.5)

In above, the total number of electrons equals to the total ionized donors in one module. \( \tau_{ji} \) is the intersubband scattering time for electrons from \( j \)-th subband to \( i \)-th subband, and \( \tau_{ik} \) is the intersubband scattering time from \( i \)-th subband to \( k \)-th subband. Intersubband scattering times are determined by the subband wavefunctions, energy levels, and electron subsystem and phonon subsystem temperatures. Detailed quantification and discussion of temperature-dependent intersubband scattering will be given in Chapter 4.

Figure 2-1 illustrates the flow chart of device modeling for numerical simulation of MQW structures. The solution should be self-consistent among Poisson equation 2.1, Schrödinger equation 2.3, and rate equations 2.5.
2.2.2 Simulation code

The numerical simulation of the MQW structures has been implemented by a modified "Semiconductor Electrostatics by QUantum AnaLysis" code. The original code, called SEQUAL in abbreviation, was written by McLennan and Datta at Purdue University [87] to simulate tunneling-diode types of quantum effect devices. It is a self-consistent numerical solution between Schrödinger equation and Poisson equation. The quantum region, such as semiconductor quantum wells or heterostructures, is sandwiched by two contacts. Electrons are assumed coming from the contacts which are in local thermodynamic equilibrium with defined Fermi levels, and injected into the quantum region by ballistic transport. Depending on the boundary conditions, the subband energy levels in the quantum region are quasi-bound states or real bound states, which can be obtained respectively by propagating state calculation or eigenstate calculation. Generally, this code does not fit the simulation model for the MQW structures used in this research, which is proposed in Figure 2-1. In this numerical code, since electrons in the quantum region are supplied by the contacts,
the band bending due to electrostatic potential will not be correct, and therefore the calculated subband energy levels would deviate. To incorporate rate equations into the numerical simulation to give the correct electron distribution within the quantum region, the original SEQUAL code was modified to fit this purpose [88]. In the modified version, the electron population on each subband is assigned using rate equations based on intersubband scattering times, then enters the code for further iterations. Charge neutrality is guaranteed in the quantum region. This modified SEQUAL code has been extensively used for the simulation and design of the THz emission MQW structures.

2.3 Triple-quantum-well design: M10

Structure parameters

A three-level system with the intention to achieve global subband population inversion, which is implemented by a triple-quantum-well structure proposed in Figure 1-3(a), is adopted in designing the intersubband THz lasers. It has the advantages of simplicity, easy to design with a reasonable scheme for realizing population inversion, and reduced free carrier loss by eliminating heavily doped classic buffer regions for inter-module connections. To increase the optical gain and confinement factor, the emission MQW device consists of many modules of such triple-quantum-wells, which are cascade connected when applied with appropriate bias [89]. At this designed bias, the voltage drop across the structure should be uniformly distributed among the modules, due to global charge neutrality indicated by Equation 2.4. In this case each triple-quantum-well module will emit at the same frequency with the same inverted population as other modules. Net negative charge in the active region due to electron diffusion from the contacts is ignored, provided that the contact/MQW junction width is much smaller than the total length of the MQW region. There are seven parameters for this triple-quantum-well structure, which will be used to tune
Figure 2-2: Design parameters of a triple-quantum-well structure and their primary functionality.

The optical performance for a THz intersubband laser, including emission frequency, inverted population, and gain. The primary functionalities of these parameters are illustrated in Figure 2-2.

Adjusting the widths of the quantum wells, $W_3$, $W_2$, and $W_1$ will primarily determine the subband levels $E_3$, $E_2$, and $E_1$, so that $\Delta E_{32}$ corresponds to THz emission, and $\Delta E_{21}$ allows for fast intersubband LO-phonon scattering at designed bias. The middle barrier $B_2$, controlling the coupling between subbands $E_3$ and $E_2$, is an important parameter. It determines dipole moment $z_{32}$, the key parameter for intersubband optical transition, and intersubband scattering time $\tau_{32}$. The $\delta$-doping per module provides dynamic charge to populate subbands. In the case of $\tau_{32} > \tau_{21}$, it will lead to inverted population between $E_3$ and $E_2$ subbands. A design of such a triple-quantum-well structure, named M10, is specified in Table 2.1. The barrier is made of Al$_{0.3}$Ga$_{0.7}$As and the well is GaAs. The device consists of totally 10 modules of such triple-quantum-well structure. The length of active region is $313.6 \, \text{Å} \times 10 = 0.3136 \, \mu\text{m}$.
CHAPTER 2. MULTIPLE QUANTUM WELL STRUCTURE DESIGN

Table 2.1: M10 triple-quantum-well structure parameters

<table>
<thead>
<tr>
<th>$W_3$</th>
<th>$W_2$</th>
<th>$W_1$</th>
<th>$B_3$</th>
<th>$B_2$</th>
<th>$B_1$</th>
<th>$N_D$ (in buffer well)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24 ML</td>
<td>23 ML</td>
<td>31 ML</td>
<td>17 ML</td>
<td>9 ML</td>
<td>7 ML</td>
<td>$0.9 \times 10^{11}/\text{cm}^2$</td>
</tr>
</tbody>
</table>

(1 ML = 2.825 Å).

Quasi-bound states vs. real-bound states

Figure 2-3 shows, for a single triple-quantum-well module of M10 structure at zero bias, the subband energy levels calculated from quasi-bound state simulation. The energy levels are obtained by checking the transmission coefficient. $E_1$, $E_2$, and $E_3$ are ground states located in the buffer well, emitter well, collector well respectively, and $E_4$, $E_5$, and $E_6$ are first excited states in the buffer well, emitter well, and collector well. Strictly speaking, due to boundary conditions, the electrons in the MQW structure are in propagating states, and have a finite time to escape a quantum well [84]. Quasi-bound state calculation can give this escape time by measuring the associate subband’s broadening from the transmission coefficient. From the blow-up of a resonance peak corresponding to $E_1$ level, for example, the subband energy broadening is only $\Delta E_1 \sim 0.1$ meV. Correspondingly, the escape time of electrons is on the order of $\tau_{esc} \sim h/\Delta E_1 \sim 10$ ps. This is a relatively longer process compared with intersubband scattering time. Thus the level broadening due to finite lifetime of subbands can be ignored. In this case, real-bound state calculations do not differ significantly from the quasi-bound state calculations, and give similar results. For comparison, Table 2.2 gives the subband levels obtained by both the quasi-bound state calculation and real-bound state calculation for the same single triple-quantum-well module of M10 structure at zero bias. It suggests the validity of using real-bound state calculations in designing and simulating THz emission MQW structures. Compared with the quasi-bound state calculation, real-bound state calculation is an eigenvalue solver, and thus saves significant simulation time and gives orthogonal
Table 2.2: Quasi-bound state vs. real-bound state calculations

<table>
<thead>
<tr>
<th>subband level (meV)</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
<th>$E_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>quasi-bound state calculation</td>
<td>35.4</td>
<td>50.4</td>
<td>62.3</td>
<td>144.4</td>
<td>193.8</td>
<td>239.1</td>
</tr>
<tr>
<td>real-bound state calculation</td>
<td>35.5</td>
<td>49.7</td>
<td>62.1</td>
<td>144.5</td>
<td>192.8</td>
<td>238.8</td>
</tr>
</tbody>
</table>

subband wavefunctions. In following simulations, real-bound state calculations are employed using the modified SEQUAL code.

Structure simulation

The numerically simulated subband levels as functions of bias per module for M10 structure are plotted in Figure 2-4. A positive bias means the conduction band on emitter well side is raised against collect well side. Due to Stark shift, $E_3$ rises above $E_2$ and $E_2$ rises above $E_1$ level with the increasing bias. In simulations, it is assumed that all the electrons per module are located in the buffer well on $E_1$ level, the ground state of the triple-quantum-well. The designed operation bias is $V_o = 49$ meV/module, where $E'_1$ level in the preceding module is aligned with $E_3$, the upper level of the following module through the 17 ML thick injector barrier. Thus $E_3$ level can be populated by electrons from $E'_1$ through resonant tunneling. At this bias, $E_3 - E_2 = 15.3$ meV, which corresponds to 3.8 THz intersubband radiation. Also, the energy separation between $E_2$ and $E_1$ is about 34 meV. Considering the electrons are generally energetic due to non-zero in-plane momentum $k_{||}$, this energy separation is sufficient to open up fast polar longitudinal optical phonon (LO-phonon) scattering in GaAs ($\hbar \omega_{LO} = 36$ meV). $E_2$ level is therefore depopulated. In the ideal case, i.e., the intersubband scattering time between $E_2$ and $E_1$, $\tau_{21}$, is much shorter than that between $E_3$ and $E_2$, $\tau_{32}$, electrons from ionized dopants will occupy only $E'_1 - E_3$ states and the $E_2$ level will be empty, $n_{1'-3} \sim N_D$, $n_2 \sim 0$. A self-consistent simulation corresponding to this case is plotted in Figure 2-5, which gives the conduction band profile, magnitude-square wavefunctions, and the electron distribution based
Figure 2-3: Transmission coefficient of a single triple-quantum-well module of M10 structure at zero bias.
on the above extreme-case intersubband scattering rates. At resonant tunneling, the wavefunctions of $E_1'$ and $E_3$ are delocalized, i.e., both of them are evenly distributed in the buffer well of the preceding module and emitter well of the following module. The anti-crossing gap is $\Delta_o = 1.9$ meV, as indicated by the narrowest energy separation between $E_1'$ and $E_3$ in Figure 2-5. The anti-crossing gap will cause additional emission linewidth broadening for $E_3 \rightarrow E_2$ radiative transition.

In describing the resonant tunneling behavior, the term **coherent tunneling time** has been proposed [13, 90], which is estimated from the Rabi oscillation frequency. An electron wavepacket can be decomposed into the superposition of the two delocalized states at resonant tunneling condition. The wavepacket oscillates between these two states with a period inversely proportional to their energy splitting. In this case, the **coherent tunneling time** can be estimated by $\tau_{coh} = h/2\Delta_o \sim 1 \text{ ps} [90]$. However, it is believed that this term should be carefully examined and the author recommends not to use it in describing the intersubband transport process. Since $E_1'$
Figure 2-5: (a) Self-consistent simulation of M10 structure at required bias, where $E_1'$ is aligned with $E_3$. (b) The corresponding charge distribution in the self-consistent solution. The positive charge is due to the sheet donors by $\delta$-doping in the buffer wells.
and $E_3$ subbands are obtained as the eigenstates of the MQW structure, the effect of injector barrier thickness $B_3$ is already taken into consideration. Provided that in intersubband scattering calculations, these two states are used as the initial or final states, there is then no independent "tunneling" process through the injector barrier. The thickness of the injector barrier influences the transport behavior by affecting the coupling between the wavefunctions of $E_1'$ state and $E_3$ state, which eventually affects the intersubband scattering times from $E_1'$, or $E_3$, to other subband levels in the MQW structure. Electron transport is greatly facilitated at resonant tunneling, in that subband wavefunctions are delocalized to maximize the coupling with other subbands. The intersubband transport processes are thus enhanced through, for example, phonon scattering.

In Figure 2-6, the delocalization of the $E_1'$ and $E_3$ states at resonant tunneling is illustrated as a parameter of the energy separation between $E_1'$ and $E_3$ levels at anti-crossing. The delocalization occurs within approximately $|E_1' - E_3| \leq 1.5\Delta_o$. The thinner the injector barrier is, the stronger $E_1'$ and $E_3$ will be coupled to each other, and thus the larger the anti-crossing gap $\Delta_o$ will be. $B_3 = 17$ ML is chosen for the M10 structure design as a trade-off between the resonant tunneling and other considerations. At anti-crossing gap, both $E_1'$ and $E_3$ will be occupied by electrons and thus give intersubband emission with additional linewidth broadening of $\Delta_o$. This broadening should be reduced by using a relatively thicker injector barrier. Also, a thick injector barriers tends to isolate two neighboring triple-quantum-well modules, so that electrons will be more confined within a module, and undesirable inter-module intersubband scattering which do not favor designed population inversion, such as $E_2' \rightarrow E_2$ and $E_3' \rightarrow E_2$ by LO-phonon scattering, can be totally blocked. The ideal design is the case where resonant tunneling is the only process by which modules communicate with each other, to favor carrier injection and population inversion.

The intersubband scattering time $\tau_{32}$ is an uncertainty, since the LO-phonon scattering window may be opened due to the hot electron effect, even though nominally
the subband separation between $E_3$ and $E_2$ is designed below one LO-phonon energy. The thickness of middle barrier, $B_2 = 9$ ML is a trade-off between optimizing the dipole moment $z_{32}$ for intersubband optical transition, and reducing the $E_3 \to E_2$ scattering rate. The anticrossing gap between $E_3$ and $E_2$ through this middle barrier is simulated to be $\Delta_m = 11.2$ meV. At designed bias, $E_3 - E_2 \sim 1.4\Delta_m$, resulting in dipole moments $z_{32} = 25$ Å and $z_{12} = 22$ Å for THz emission. The collector barrier is chosen to be relatively thin, $B_1 = 7$ ML, to facilitate fast LO-phonon intersubband scattering $\tau_{21}$ between $E_2$ and $E_1$. With the presence of both middle barrier and collector barrier, the direct LO-phonon scattering for electrons from $E_3$ level to $E_1$, $\tau_{31}$, is a much slower process. This intersubband scattering process does not affect population inversion, but increases the current density that running through the device, which is not desirable. This current can be reduced by increasing the collector barrier thickness $B_1$.

At operating bias, $E'_1$ is aligned with $E_3$, and their combined electron population is assumed to be $n_3$. The electron population on $E_2$ is $n_2$. Assuming full ionization of the $\delta$-doping, then Equations 2.4 and 2.5 can give subband populations and population
CHAPTER 2. MULTIPLE QUANTUM WELL STRUCTURE DESIGN

inversion:

\[
\begin{align*}
    n_3 &= \frac{\tau_{32}}{\tau_{32} + \tau_{21}} N_D, \\
    n_2 &= \frac{\tau_{21}}{\tau_{32} + \tau_{21}} N_D, \\
    \Delta n_{32} &= \frac{\tau_{32} - \tau_{21}}{\tau_{32} + \tau_{21}} N_D.
\end{align*}
\]

The current density of the device at operating bias is

\[J_o = e^{n_3} \frac{n_3}{\tau_{32}} + e^{n_3} \frac{n_3}{\tau_{31}} = e^{\frac{\tau_{32} + \tau_{31}}{(\tau_{32} + \tau_{21})\tau_{31}} N_D}.
\]

In the above expressions, the intersubband scattering time is the same for \(\tau_{32}\) and \(\tau_{1'2}\) for simplicity. Since \(E_1'\) and \(E_3\) are separated with a small energy, Maxwell distribution can be used to determine electron occupations on these two levels: \(n_3(1')/n_3(3) = e^{-\Delta_o/kT_{3e}}\), where \(T_{3e}\) is the electron temperature of \(E_3\) subband. Then there are

\[
\begin{align*}
    n_3(1') &= \frac{e^{-\Delta_o/kT_{3e}}}{1 + e^{-\Delta_o/kT_{3e}}} n_3, \\
    n_3(3) &= \frac{1}{1 + e^{-\Delta_o/kT_{3e}}} n_3.
\end{align*}
\]

For low electron temperature \(kT_{3e} \ll \Delta_o\), \(n_3(3) \sim n_3\), and \(n_3(1') \sim 0\). For high electron temperature \(kT_{3e} \gg \Delta_o\), \(n_3(3) \sim n_3(1') \sim \frac{1}{2} n_3\).

The sheet doping per module for M10 structure, provided by the \(\delta\)-doping \(N_D = 0.9 \times 10^{11}/cm^2\), is a reasonably number. As a result, electrons on each subband are kept sufficiently low. The nonlinear conduction band bending due to the presence of dynamic charge is small, and subband levels are relatively insensitive to the electron distribution in the quantum wells. This is highly desirable in designing a robust THz emission MQW structure, especially considering that the small subband energy
Figure 2-7: Subband level separations of M10 structure using self-consistent simulation, as functions of intersubband scattering time ratio, \( \tau_{21}/\tau_{32} \).

Separations are in the 10 meV range for THz emissions. The electron-electron intersubband scattering rate on \( E_3 \) level, which scales with electron density, will not contribute significantly to the intersubband scattering time \( \tau_{32} \) [13].

Figure 2-7 shows the self-consistent simulation of M10 structure as functions of different intersubband scattering time ratio \( \tau_{32}/\tau_{21} \). This ratio determines electron distribution in quantum wells by Equation 2.8. Uncertainties of the intersubband scattering rates will not affect the triple-quantum-well design significantly. The low level doping per module used in M10 structure causes subband energy levels to vary within only 1 \( \sim \) 2 meV between extreme cases of the intersubband scattering times, from ideal population inversion \( (\tau_{21}/\tau_{32} \rightarrow 0) \) to reversed population inversion \( (\tau_{21}/\tau_{32} > 1) \).
2.4 High-field domain

THz emission structures consist of multiple triple-quantum-well modules. These modules are cascade connected through resonant tunneling at designed bias. When the applied voltage deviates from this designed bias, resonant tunneling condition cannot be satisfied for all the modules. As a result, voltage across the device will not be uniformly distributed and the so-called high-field domain will develop. High-field domain development has been well studied and understood in superlattices \cite{91,92,93,94,95}. This concept can be extended to the multiple-module MQW structures, with subband levels of a single quantum well in superlattices replaced by the subbands within a MQW module, as shown in Figure 2-8.

Case-(a) corresponds to the multiple modules of triple-quantum-well structure at zero bias. With bias slightly above zero, \(0 \leq V \leq N_m(\Delta_o + \Delta E_1)\) \cite{93}, electrons transport through the MQWs by ground state to ground state resonant tunnelings, indicated in case-(b). \(\Delta_o\) is the anticrossing gap of \(E_1\) subbands between adjacent modules, \(\Delta E_1\) is the energy broadening of \(E_1\) level, due to scattering, and \(N_m\) is the total number of modules in the device. At bias higher than \(N_m(\Delta_o + \Delta E_1)\), ground state energy alignment is impossible for all the modules. If the voltage drop is uniformly distributed as illustrated in case-(c'), then each module is off the resonant tunneling condition, and current will be blocked. Thus case-(c') possesses negative differential resistance (NDR), which is not a stable condition. A stable scheme, at the same bias, is illustrated by case-(c), in which the voltage drop breaks into two domains, a low-field region, with a small voltage drop corresponding to \(E'_1 \rightarrow E_1\) tunneling, and a high-field region with \(E'_1 \rightarrow E_3\) resonant tunneling. In this case, charge transport is facilitated.

The necessary voltage increment to place one more additional module into high field domain is \cite{95},

\[
e\Delta V = E_3 - E_1
\] (2.12)
Figure 2-8: High-field domain development in multiple-module MQW structures used for THz emissions.
Considering the gradual change of the bias, the development of one more module into high-field domain may place other modules into off-resonance condition, and the current will drop inevitably. This is especially true for large subband energy separation $E_3 - E_1$, or the total number of modules within the device is small. A necessary condition for the multiple-module quantum well structure to tolerate this high-field domain development without decreasing the current significantly is:

$$N_m(\Delta_o + \Delta E_1) \geq E_3 - E_1$$

(2.13)

Effectively, using larger number of modules will smear out the current dip when one more high-field domain is developed. On the other hand, this current dip, which occurs periodically with increasing the biasing voltage, gives direct information on intersubband energy separation, via Equation 2.12. Using small number of modules can exhibit this feature, so that the I-V curve can be used directly to measure subband separations.

For THz emission devices made of multiple modules of triple-quantum-wells, it is expected that device will start to emit even at very low bias, due to the sequential high-field domain development. This high-field domain, corresponding to $E'_1 \rightarrow E_3$ resonant tunneling, propagates and expands from one end of the device to the other end until the bias reaches the designed value.

### 2.5 I-V curves of M10 at 4.2 K

The THz emission MQW structures used in this research are grown by our collaborator of this research project, Prof. Michael Melloch at Purdue University. His MBE machine is dedicated for GaAs/AlGaAs growth. High mobility 2DEGs in the range of $\sim 10^7$ cm$^2$/V-s can be routinely obtained from his machine.

Table 2.3 lists the MBE growth sequence of M10 device. The 10 modules of triple-quantum-well structure is sandwiched by two graded doped contact layers, grown on
Table 2.3: M10 device MBE growth sequence

<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Doping Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2 µm GaAs, Si doped with 2 × 10^{18}/cm³</td>
<td></td>
</tr>
<tr>
<td>0.1 µm GaAs, Si doped with 1 × 10^{18}/cm³</td>
<td></td>
</tr>
<tr>
<td>0.1 µm GaAs, Si doped with 8 × 10^{17}/cm³</td>
<td></td>
</tr>
<tr>
<td>0.32 µm GaAs/Al_xGa_{1-x}As, 10 triple-quantum-well modules</td>
<td></td>
</tr>
<tr>
<td>0.1 µm GaAs, Si doped with 2 × 10^{17}/cm³</td>
<td></td>
</tr>
<tr>
<td>0.1 µm GaAs, Si doped with 4 × 10^{17}/cm³</td>
<td></td>
</tr>
<tr>
<td>0.2 µm GaAs, Si doped with 2 × 10^{18}/cm³</td>
<td></td>
</tr>
</tbody>
</table>

[1 0 0] n⁺ GaAs substrate

lattice matched n⁺ GaAs substrate. The contact layers are to provide electrical connection to the MQW active region.

The equivalent bulk doping of the active region is the δ-doping per module divided by the length of one module, \( N_D/l_m \sim 3 \times 10^{16}/\text{cm}^3 \). Thus the contact and active region form an n⁺-n junction, and electrons from the contacts will diffuse into the MQW region. To examine the charge neutrality assumption in MQW modules, the electron concentration in the contact/MQWs junction region is simulated by a classic Poisson solver [96] with two different doping densities in the contacts. The dopant is assumed to be fully ionized. The device simulation temperature is 40 K. It is seen that the diffusion length is about several hundred Angstroms, and only the module closest to the contact has electrons exceeding the internal doping. Depending on the contact doping level, the diffusion electron concentration drops to about one order of magnitude below the equivalent bulk doping level of MQWs in the second module. Charge neutrality is thus considered as a valid assumption for most of the modules in M10 device.

The M10's I-V curve was measured at 4.2 K with the device directly submerged in liquid helium. The size of the device is typically 100 µm × 100 µm mesa etched. Figure
Figure 2-9: Electron concentration (per cm$^3$) at the contact/MQWs junction for M10 device, simulated by a classic Poisson solver at temperature of T=40 K. Two doping levels are used in the contact, $2 \times 10^{17}$/cm$^3$ and $8 \times 10^{17}$/cm$^3$.

2-10(a) shows the positive biased dc I-V curve with loop sweep voltage between 0 V and 2.7 V. The current increases until it is clamped around $V = 1$ V, where negative differential resistance appears. The current oscillates as a function of the bias from 1 V to 2.4 V. Beyond 2.5 V, the current increases exponentially. When voltage sweeps back, current also traces back except in the negative differential region.

According to the numerical simulation, $E_4$ subband, which is the first excited state in the buffer well, is 110 meV above $E_1$ subband, as revealed by the simulation results in Figure 2-5(a) at designed bias and Figure 2-10(b) at bias of 110 meV/module. Since $E_4$ and $E_1$ are located in the same quantum well, this intrawell intersubband energy separation is essentially insensitive to the bias voltage across the module, i.e., there is little Stark shift. At $V = 1$ V, each module in M10 device shares about 100 mV voltage drop, corresponding to $E'_1 \rightarrow E_4$ energy alignment. Current therefore reaches its maximum. At voltages higher than this value, the energy misalignment between $E'_1$
Figure 2-10: (a) Measured M10 device dc I-V curve at 4.2 K, with loop sweep voltage between 0 V and 2.7 V. The current density at designed operation bias $V_o = 0.49$ V is $J_o = 0.39$ KA/cm$^2$. (b) Simulated M10 subband levels at bias of 110 mV/module.
and $E_4$ causes the decrease of current and thus negative differential resistance appears. The period of the current oscillation, in region of $1 < V < 2.4$ V, is approximately $\Delta V = 0.15$ V, and this corresponds to explicit high-field domain formation in each module of the M10 device. As the simulation result in Figure 2-10(b) shows, 150 mV increase will make $E'_1$ level surpass the middle barrier and the other barriers behind it, letting electrons on $E'_1$ subband shoot directly to the continuum state above the middle barrier. This above-barrier state can be considered as a virtual state corresponding to the first excited state in the emitter well or the collector barrier. It takes 0.15 V extra voltage to form the high-field domain corresponding to $E'_1 \rightarrow \text{continuum state}$ alignment for each module, which coincides well with the current oscillation $\Delta V = 0.15$ V shown in the I-V curve. Ten modules take totally 1.5 V, making the negative differential resistance region extended from 1 V to 2.4 V. The amplitude of the current oscillation keeps increasing at higher bias voltage. This is understandable, since with more modules aligned with $E'_1 \rightarrow \text{continuum state}$ configuration, resonant tunneling will permit higher current, compared with the $E'_1 \rightarrow E_4$ resonant tunneling.

The hysteresis in the looped I-V curve, at the voltages corresponding to one high-field domain formation, is associated with the charge storage in the quantum wells. On one side, subband level depends on band bending, which can be caused by the the charge storage in the quantum well; one the other side, the charge storage in a quantum well also depends on the subband levels, i.e., the charge can be released during resonant tunneling when subband levels are aligned. This mutual dependence between subband levels and the stored charge thus gives bistable behavior when the voltage is swept to high and low when crossing the resonant tunneling. It should be noted that due to charge neutrality assumption, band bending is limited by the doping level in the modules, i.e., the total electrons that can be provided in each module. In M10 structure, the doping per module is low. The maximum band bending can be estimated by $\frac{1}{2} m_e N_D / \varepsilon_0 \epsilon_r \sim 20$ mV. Apparently, this small band bending can
Figure 2-11: Measured pulsed I-V curves of M10 device with different pulse widths. The pulse frequency is the same for the three curves.

only cause small hysteresis, as shown in Figure 2-10(a). The large hysteresis around $V = 2.5 \, \text{V}$, corresponding to high-field domain formation for the last module, is obviously due to the contact effect. As discussed before, the large amount of charge in this module is provided by electron diffusion from the heavily doped contact, instead of from the module’s internal $\delta$-doping.

For bias above $2.5 \, \text{V}$, the current increases exponentially, due to the single-barrier tunneling for electrons on $E'_1$ subband through the 17 ML thick injector barrier. This situation is similar to the Fowler-Nordheim tunneling [84], and the current vs. voltage relation can be described by the WKB approximation:

$$I \sim \exp[-2 \int k(z)dz], \quad (2.14)$$

where $k(z) = \sqrt{\frac{2m^*}{\hbar^2}} |V(z) - E|$. 
CHAPTER 2. MULTIPLE QUANTUM WELL STRUCTURE DESIGN

The high-field domain formation due to expected energy alignment $E'_1 \rightarrow E_3$ at designed operation bias $V = 0.49$ V, however, is not seen in the dc I-V curve in Figure 2-10(a). Figure 2-11 shows the measured pulsed I-V curves for M10 device with different pulse width but with the same pulse frequency. The ac current was measured using a calibrated lock-in amplifier or a box car. For pulse width longer than 1 ms (10% duty cycle), the I-V has similar behavior to the dc I-V curve measured in Figure 2-10(a). Dramatic change is seen for pulse width as short as 0.1 ms (1% duty cycle), where the current is clamped and stops to increase at the designed bias $V_o = 0.49$ V. For a pulse width in-between, current hops to the value corresponding to dc case at a bias beyond $V_o$, as is shown in an example for the curve with 0.3 ms pulse width. This pulsed I-V measurement is a clear verification of energy alignment at the designed bias. It remains to be answered why the I-V relation depends on the measurement conditions such as the pulse width. The current hopping phenomenon in time scale of $\sim 0.1$ msec can be due to device heating. The temperature-dependent transport behavior will be addressed in Chapter 4.

Besides M10, a device named M100 was also grown and tested. This device is identical to M10 but has 100 modules of triple-quantum-well structure with the same $\delta$-doping per module. Its dc I-V was measured at 4.2 K and is shown in Figure 2-12. Clearly, at the designed bias of $V_o = 4.9$ V, current reaches its maximum and then is followed by a negative differential resistance region. Also, a current bump around $V = 2.5$ V is observable, which corresponds to the $E'_1 \rightarrow E_2$ alignment according to the simulation in Figure 2-4. At the designed bias, all the modules are aligned corresponding to $E'_1 \rightarrow E_3$ resonant tunneling. At higher bias, high-field domains will develop and propagate throughout the structure. Unlike the M10 device, current oscillations associated with high-field domain development are not observed for the M100 device. This smoothly-changing current in the whole bias region reveals that the condition in Equation 2.13 is satisfied for the M100 device. The high-field domain developments, corresponding to the switching of resonant tunneling from $E'_1 \rightarrow E_3$
Figure 2-12: Measured dc I-V curve of M100 device. The current density at designed bias $V_o = 4.9$ V is $J_o = 0.68$ KA/cm$^2$. 
Figure 2-13: Measured dc I-V curves of M10p and M10pp devices. The current densities at designed bias of $V_o = 0.49\,\text{V}$ is $J_o = 1.3\,\text{KA/cm}^2$ for M10p and $J_o = 3.6\,\text{KA/cm}^2$ for M10pp.

to $E'_1 \rightarrow E_4$, and from $E'_1 \rightarrow E_4$ to $E'_1 \rightarrow \text{continuum state}$, needs to share additional voltage $\Delta V = \frac{1}{e}(E_4 - E_3) = 0.06\,\text{V}$ and $\Delta V = \frac{1}{e}(E_{\text{con}} - E_4) = 0.15\,\text{V}$ respectively. Considering the 1-2 meV anticrossing gap and another 1-2 meV subband linewidth broadening, Equation 2.13 can be satisfied easily for $N_m = 100$ modules.

Two other devices, named M10p and M10pp, were also grown with their I-V curves measured. These two devices have the same 10 modules of triple-quantum-well structure as M10 device, except the $\delta$-doping in the buffer well is $1.5 \times 10^{11}/\text{cm}^2$ for M10p device and $3.0 \times 10^{11}/\text{cm}^2$ for M10pp device respectively. Their dc I-V curves are shown in Figure 2-13.

The dc I-V relations of M10p and M10pp devices are similar to M10 device, except with much larger current densities at designed bias. Using Equation 2.9, combined with the information of $\delta$-doping per module in the buffer well and the measured
Table 2.4: Effective scattering time $\tau_{\text{eff}}$

<table>
<thead>
<tr>
<th>Device</th>
<th>M10</th>
<th>M100</th>
<th>M10p</th>
<th>M10pp</th>
</tr>
</thead>
<tbody>
<tr>
<td>modules</td>
<td>10</td>
<td>100</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>$N_D$</td>
<td>$0.9 \times 10^{11}/\text{cm}^2$</td>
<td>$0.9 \times 10^{11}/\text{cm}^2$</td>
<td>$1.5 \times 10^{11}/\text{cm}^2$</td>
<td>$3.0 \times 10^{11}/\text{cm}^2$</td>
</tr>
<tr>
<td>measured $J_o$</td>
<td>0.39 KA/cm²</td>
<td>0.68 KA/cm²</td>
<td>1.3 KA/cm²</td>
<td>3.6 KA/cm²</td>
</tr>
<tr>
<td>$\tau_{\text{eff}} = eN_D/J_o$</td>
<td>37 ps</td>
<td>21 ps</td>
<td>18 ps</td>
<td>13 ps</td>
</tr>
</tbody>
</table>

current densities at the designed bias, the effective scattering time $\tau_{\text{eff}}$ for the four devices are summarized in Table 2.4. From Equation 2.9, the current density is expressed as $J_o = eN_D/\tau_{\text{eff}}$, and the effective scattering time is defined as

$$\tau_{\text{eff}} = \frac{(\tau_{32} + \tau_{21})\tau_{31}}{\tau_{32} + \tau_{31}}. \quad (2.15)$$

Even though all of these four devices have the same triple-quantum-well structure, their intersubband scattering times are different. Compared with M10 device, M100 device has the same $\delta$-doping per module but much larger current density. Considering 100 modules dissipate more $P = IV$ electric power and therefore more device heating, the shortened effective scattering time for M100 can be explained by the temperature-dependent intersubband scattering rate. The same understanding holds for M10p and M10pp devices. This issue will be addressed in details in Chapter 4. It should also be noted that in the above effective scattering time calculations, full-ionization of the $\delta$-dopant is assumed. This sets the upper limit for $\tau_{\text{eff}}$.

As another check of the M10 structure’s design, the device dc I-V was measured with reverse bias at 4.2 K. Figure 2-14(a) shows dc current vs. reverse bias voltage. The current is turned on around $V = -1.5$ V. Figure 2-14(b) shows the simulated subband levels under this reverse bias. Clearly, the current turn-on at this bias corresponds to the case where $E'_3$ subband, now the lowest level of a module, is aligned with $E_4$ subband of the next module. Electrons are injected to the $E_4$ level by resonant tunneling and intersubband radiative transitions at $\hbar \omega = E_4 - E_3 \sim 140$
Figure 2-14: (a) Simulated subband levels under reverse bias of $V = -0.15$ V/module. (b) Measured reverse biased dc I-V curve of M10 device.
meV should occur, corresponding to $\lambda \sim 9 \, \mu$m mid-infrared radiation.

### 2.6 Summary

A device model has been established for the design and simulation of the THz emission MQWs. A triple-quantum-well structure, M10, was designed by numerical simulations. Subband levels, population inversion, and current density are properly quantified based on electron transport modeling proposed in this chapter. The triple-quantum-well structure design was verified by the I-V measurements at 4.2 K on M10 device and its variants. Practical considerations, including high-field domain formation and contact effect, are discussed in detail for a thorough understanding of the device’s behaviors. The author believes the optical performance of a THz emission MQW structure relies on a good understanding and control of its transport modeling. This chapter is a basic step toward this goal.
Chapter 3

THz Emission, Coupling, and Loss

3.1 Introduction

To achieve THz lasing, it requires the optical gain generated by the intersubband transition must exceed the cavity loss. An initial step in developing a THz laser using MQW structures is to be able to observe the intersubband spontaneous emission and resolve the emission spectrum. Since the wavelength of intersubband radiative transition is determined by the MQW design and can be tailored arbitrarily, frequency-dependent parameters, such as spontaneous emission power, optical gain, and cavity loss, need to be obtained for feasible device design. Long wavelength of THz radiation imposes difficulty in realizing optical confinement. A plasma waveguide made with heavily doped contact layers offers an alternative but possesses large cavity loss. A metallic waveguide is promising and will be shown to be necessary for making a low-loss THz laser cavity. In this chapter, THz radiative transition and optical gain, grating coupling for spontaneous emission, and plasma cavity loss will be analyzed. Detailed numerical results are given for the emission device design.
3.2 Spontaneous emission and gain

The deviations of THz radiative transition rates and optical gain follow Yariv's treatment [97] with a little modification using envelope wavefunction approximation for intersubband cases [13, 98]. Using the dipole interaction approximation, the interaction Hamiltonian of an electron with electromagnetic field is

\[ H' = -eE(r, t) \cdot r. \]  

(3.1)

By quantizing electromagnetic field \( E(r, t) \) in a plane wave form with wavevector \( k \) and polarization \( \sigma = 1, 2 \), the interaction Hamiltonian in volume \( V \) with dielectric constant \( \epsilon = \epsilon_r \epsilon_0 \) can be written as

\[ H' = i\epsilon \sqrt{\frac{\hbar \omega_k}{2\epsilon}} [a^\dagger_{k,\sigma} e^{-ik \cdot r} - a_{k,\sigma} e^{ik \cdot r}] \hat{e}_{k,\sigma} \cdot r. \]  

(3.2)

Using Fermi's Golden Rule, and executing the annihilation and creation operators, the transition rate from initial state \( |i, n_{k,\sigma} > \) to final state \( |f, n_{k,\sigma} + 1 > \) is

\[ W_{i \rightarrow f}^{k,\sigma} = \frac{2\pi}{\hbar} |H'|^2 \delta(E_i - E_f - \hbar \omega_k) \]  

(3.3)

\[ = \frac{\pi \epsilon^2 \omega_k}{V \epsilon} |< \hat{e}_{k,\sigma} \cdot r | i > |^2 (n_{k,\sigma} + 1) \delta(E_i - E_f - \hbar \omega_k), \]  

(3.4)

where \( n_{k,\sigma} \) is the number of photons in mode \((k, \sigma)\). In obtaining the above expression, \( e^{ik \cdot r} \sim 1 \) since the optical wavelength is much greater than the size of MQWs where the radiative transition occurs. The spontaneous emission rate, and stimulated emission rate of generating a photon into mode \((k, \sigma)\) are then

\[ W_{i \rightarrow f, sp}^{k,\sigma} = \frac{\pi \epsilon^2 \omega_k}{V \epsilon} |\hat{e}_{k,\sigma} \cdot r_{if}|^2 \delta(E_i - E_f - \hbar \omega_k), \]  

(3.5)
CHAPTER 3. THZ EMISSION, COUPLING, AND LOSS

\[ W_{i \rightarrow f, st}^{\mathbf{k}, \sigma} = \frac{\pi e^2 \omega_k}{V \epsilon} |\hat{\mathbf{e}}_{k, \sigma} \cdot \mathbf{r}_{if}|^2 \delta(E_i - E_f - \hbar \omega_k) n_i^{\mathbf{k}, \sigma}, \]

(3.6)

where \( \mathbf{r}_{if} \equiv \langle f | \mathbf{r} | i \rangle \) is the dipole moment between initial and final states.

For subbands, the initial and final states can be expressed as

\[ |i \rangle = \frac{1}{\sqrt{S_{xy}}} e^{i \mathbf{k}_\| \cdot \mathbf{r}_i} \psi_i(z) U_0(\mathbf{r}), \]

\[ |f \rangle = \frac{1}{\sqrt{S_{xy}}} e^{i \mathbf{k}_\| \cdot \mathbf{r}_f} \psi_f(z) U_0(\mathbf{r}), \]

(3.7)

where \( \psi_i(z) \) and \( \psi_f(z) \) are subband wavefunctions obtained from effective mass Schrödinger Equation 2.3. \( U_0(\mathbf{r}) \) is the periodic Bloch wave function of the host crystal. \( S_{xy} \) is the in-plane area. \( \mathbf{k}_\| \) is the in-plane wavevector of the subband’s envelope wavefunction. The dipole moment is

\[ \mathbf{r}_{ij} = \frac{1}{S_{xy}} \int d\mathbf{r}_i d\mathbf{z} e^{i (\mathbf{k}_f - \mathbf{k}_i) \cdot \mathbf{r}_i} \langle \mathbf{r}_i \psi_f^*(z) \psi_i(z) U_0^*(\mathbf{r}) U_0(\mathbf{r}) \rangle \]

\[ = \delta_{\mathbf{k}_f \parallel - \mathbf{k}_i \parallel} \hat{z} \int dz \psi_f^*(z) z \psi_i(z). \]

(3.8)

The above expression is obtained by approximating \( \psi_i(z) \) and \( \psi_f(z) \) as slowly varying envelope wavefunctions compared with \( U_0(\mathbf{r}) \). The integration can thus be performed over each lattice cell with \( \psi(z) \) treated as constants, then summed over all the lattice cells. Due to the periodicity of \( U_0(\mathbf{r}) \) and the fact that the integration \( \int_{W_S} d\mathbf{r} U_0^*(\mathbf{r}) U_0(\mathbf{r}) = 0 \) over one Wigner-Seitz cell due to the odd parity argument, \( U_0^*(\mathbf{r}) U_0(\mathbf{r}) \) in the above integration can be removed.

Equation 3.8 imposes in-plane momentum conservation for intersubband optical transitions. By defining intersubband dipole moment as \( z_{if} \equiv \int dz \psi_f^*(z) z \psi_i(z) \), with in-plane momentum conservation satisfied, the spontaneous emission rate and stimu-
lated emission rate of intersubband radiative transition into a specific mode is:

\[ W_{i \rightarrow f, sp}^{k, \sigma} = \frac{\pi e^2 \omega_k}{V \epsilon} |\hat{e}_{k, \sigma} \cdot \hat{z}|^2 z_{if}^2 \delta(E_i - E_f - \hbar \omega_k), \]  

(3.9)

\[ W_{i \rightarrow f, st}^{k, \sigma} = \frac{\pi e^2 \omega_k}{V \epsilon} |\hat{e}_{k, \sigma} \cdot \hat{z}|^2 z_{if}^2 \delta(E_i - E_f - \hbar \omega_k)n_{k, \sigma}. \]  

(3.10)

The spontaneous emission rate is then obtained by summing over all the optical modes. In 3D case, the optical mode density is \( \frac{V}{(2\pi)^3} \) in k-space. Thus

\[
W_{i \rightarrow f, sp}^{3D} = \sum_{k} \sum_{\sigma} W_{i \rightarrow f, sp}^{k, \sigma}
= \int d\mathbf{k} \frac{V}{(2\pi)^3} \frac{\pi e^2 \omega_k}{V \epsilon} z_{if}^2 \delta(E_i - E_f - \hbar \omega_k)
= \int_0^\infty k^2 dk \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\varphi \frac{1}{(2\pi)^3} \frac{\pi e^2 c_0 k}{\epsilon n} z_{if}^2 \delta(\hbar \omega - \hbar c_0 k/n)
= \frac{e^2 n \omega^3 z_{if}^2}{3\pi \epsilon_0 \hbar c_0^3}.
\]  

(3.11)

When summing over the polarization (\( \sigma = 1, 2 \)), the one-dimensional nature of subband wavefunctions requires that E field only be polarized along the z-direction, which is the MQW growth direction, and this is the so-called dipole selection rule. \( \hbar \omega = E_i - E_f \) is the photon energy. Photon dispersion relation is used in the above equation, \( \omega_k = c_0 k/n \), where \( c_0 \) is the speed of light in vacuum and \( n = \sqrt{\epsilon_r} \) is the medium's refractive index.

An important parameter in measuring intersubband radiative transitions is the dimensionless oscillator strength, defined as \( f_{if} = \frac{2m^* \omega z_{if}^2}{\hbar} \). The expression of oscillator strength can be obtained by ratioing the radiative lifetime with the decay time of a classic Hertzian dipole. An alternative expression for the spontaneous emission rate using oscillator strength is
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\[ W_{i\rightarrow f,sp}^{3D} = \frac{e^2}{6\pi \epsilon_0 m^* c_0^2} \omega_{if}^3. \]  \hspace{1cm} (3.12)

The above expressions for the spontaneous emission rate is calculated for the free-space case where there is no confinement for photons. This is not true for laser devices which have optical cavities. For THz lasers, the ideal confinement is realized by using a metallic waveguide. It is therefore necessary to obtain the spontaneous emission rate in 2D case. Since the metallic waveguide sandwiching the MQW region is typically several microns in thickness, only the basic TEM mode exists in such a cavity. With the absence of high order transverse modes, the mode density is then \( \frac{S_{xy}}{(2\pi)^2} \) in \( k_{\parallel} \)-space. The 2D spontaneous emission rate can then be obtained

\[
W_{i\rightarrow f,sp}^{2D} = \int dk_{\parallel} \frac{S_{xy}}{(2\pi)^2} \pi e^2 \omega_{k} z_{if}^2 \delta(E_i - E_f - \hbar \omega_k) \\
= \int_0^\infty kdk \int_0^{2\pi} \theta d\theta \frac{S_{xy}}{(2\pi)^2} \pi e^2 c_0 k \frac{\omega_{k}}{V\epsilon n} z_{if}^2 \delta(\hbar \omega - \hbar c_0 k/n) \\
= \frac{e^2}{2t_c \epsilon_0 \hbar c_0^2} \omega_{if}^3. \hspace{1cm} (3.13)
\]

where \( t_c \) is the thickness of the confined MQW region in metallic waveguide. By using oscillator strength, the 2D spontaneous emission rate can also be expressed as

\[ W_{i\rightarrow f,sp}^{2D} = \frac{\epsilon^2}{4t_c \epsilon_0 m^* c_0^2} \omega_{if}^3. \hspace{1cm} (3.14)\]

It is necessary to compare the 2D spontaneous emission rate with the 3D. From expressions 3.12 and 3.14, we obtain

\[
\frac{W_{sp}^{2D}}{W_{sp}^{3D}} = \frac{3}{4} \frac{\lambda_s}{t_c}, \hspace{1cm} (3.15)
\]

where \( \lambda_s = 2\pi c_0/n\omega \) is the emission wavelength in semiconductor.

Since for THz frequency, the emission wavelength in semiconductor is typically
several tens of microns, about one order of magnitude greater than the active region thickness, the 2D spontaneous emission rate is then much greater than the 3D spontaneous emission rate. This behavior is similar to microcavity effect [99]. The emission efficiency is enhanced due to electronic radiative transitions being coupled into fewer optical modes with fastest rates.

The intersubband spontaneous radiative transition time, $\tau_{sp} = 1/W_{sp}$, is plotted in Figure 3-1 for 3D and 2D cases as functions of the emission frequency in THz range, using typical values of dipole moments in intersubband transitions. For M10 design as an example, the calculated dipole moment and intersubband energy separation in Chapter 2, result in $\tau_{sp}^{3D} \sim 28 \mu$s. Considering the effective intersubband scattering time, revealed by the I-V measurement, is on the order of 10 ps due to nonradiative intersubband transitions, the quantum efficiency of THz spontaneous emission is very low, $\eta_{sp} \sim \tau_{sp}/\tau_{eff} \sim 10^{-6}$. For an emission device which draws milli-Watt electric power for example, the generated intersubband optical power will be in nano-Watt range. Compared with mid-infrared intersubband emitters, the quantum efficiency is three orders of magnitude lower due to $\omega^3$-dependent spontaneous emission rate in Equation 3.11.

From Equation 3.6, the stimulated emission rate for a specific mode is proportional to the number of photons on that mode. Considering linewidth broadening, photon distribution can be described by a lineshape function,

$$n^{k,\sigma} = n_i g(f),$$

(3.16)

where $n_i$ is the total number of photons in the mode and $g(f)$ is the normalized lineshape function $\int_{-\infty}^{\infty} g(f) df = 1$. For homogeneous broadening of Lorentzian type with $\Delta f$ as the full width at half maximum (FWHM), $g(f)$ is

$$g(f) = \frac{\Delta f/2\pi}{(\Delta f/2)^2 + (f - f_0)^2}.$$  

(3.17)
Figure 3-1: Calculated intersubband spontaneous emission times in 3D case (a) and 2D case (b) as functions of the emission frequency, with different dipole moment (Å).
As opposed to the spontaneous emission rate calculations, the calculation of stimulated emission rate does not integrate over the optical modes, and thus it does not depend on 2D or 3D case. By plugging in Equation 3.16 into Equation 3.6 and performing the integration of all the photons on that mode, the stimulated emission rate is expressed as

\[ W_{st} = \frac{\pi e^2 \omega}{\hbar V \varepsilon} z_i^2 N_1 g(f). \]  

(3.18)

It should be noted that the stimulated absorption rate is the same as the stimulated emission rate \( W_{ab} = W_{st} \) because the identical calculation. In order to obtain the expression for optical gain, wave intensity \( I = \frac{\hbar \omega c^2}{n} \) is plugged into Equation 3.18 and results in

\[ W_{st} = \frac{\hbar \omega c^2}{4 \hbar \varepsilon_0 m^* \omega} f_{i f} I g(f). \]  

(3.19)

In the presence of population inversion, the wave intensity increases when propagating in the medium, and the optical gain is defined as \( dI/dx = G(f) I_i \). By subtracting the photons generated by stimulated emission with the photons absorbed by stimulated absorption, we obtain \( dI/dx = \hbar \omega (N_i W_{st} - N_f W_{ab}) \). The gain expression is then expressed as

\[ G(f) = \frac{\Delta N e^2 \omega z_i^2 g(f)}{2 n \varepsilon_0 c_0 \hbar} = \frac{\Delta N e^2 f_{i f} g(f)}{4 n \varepsilon_0 c_0 m^*}, \]  

(3.20)

\[ G_0 = \frac{\Delta N e^2 \omega z_i^2}{\pi n \varepsilon_0 c_0 \hbar \Delta f} = \frac{\Delta N e^2 f_{i f}}{2 \pi n \varepsilon_0 c_0 m^* \Delta f}, \]  

(3.21)

where \( \Delta N = N_i - N_f = (n_i - n_f)/l_m \) is the bulk subband population inversion, and \( G_0 \) is the peak gain at \( f = f_0 \).

Figure 3-2 gives the calculated peak gain as a function of frequency with different dipole moments. The linewidth is assumed to be 0.5 THz. It is noted that the peak
Figure 3-2: Calculated peak gain as a function of emission frequency with different dipole moment (Å). The intersubband population inversion is $3 \times 10^{10}/\text{cm}^2$ and the length of one module is $l_m = 300$ Å.
gain is inversely proportional to the linewidth, and for a fixed dipole moment, it is linearly proportional to the emission frequency. In M10 design as an example, for an intersubband population inversion of $3 \times 10^{10}/\text{cm}^2$, the peak gain is $G_0 \sim 340 \text{ cm}^{-1}$ at designed operating bias. The gain of THz lasers is comparable to mid-infrared quantum cascade lasers due to an expected factor of 10 narrower emission linewidth [9] but also a factor of 10 lower emission frequency.

When the lasing threshold is reached, the output power is limited by the saturated wave intensity within the laser cavity [100]. For the M10 design with three-level system, from the expression of subband population inversion derived by rate equations in Section 2.3, the stimulated emission lifetime is limited by $\tau_{st}^{\text{sat}} \equiv 1/W_{st}^{\text{sat}} \sim \tau_{21}$ to maintain subband population inversion between $E_3$ and $E_2$ levels. The corresponding saturation wave intensity $I_{l}^{\text{sat}}$, from Equation 3.18, is

$$I_{st}^{\text{sat}} = \frac{\Delta f \hbar \epsilon_0 n c_0}{2 \tau_{st}^{\text{sat}} z_3 c^2},$$

(3.22)

The laser output power per facet can be estimated by

$$P \sim r S f I_{l}^{\text{sat}},$$

(3.23)

where $r$ is the light reflection coefficient at the semiconductor/air interface. From above expressions, the lasing output power is independent of the frequency. It is proportional to the linewidth broadening $\Delta f$ and inversely proportional to the dipole moment square. Large dipole moment and narrow linewidth increase peak gain, but decrease the lasing output power. To get some estimation for a THz laser, considering in M10 design $\tau_{21}$ is about 1 ps due to intersubband LO-phonon scattering, the saturation emission lifetime $\tau_{st}^{\text{sat}}$ is taken for 2 ps. The saturation wave intensity $I_{l}^{\text{sat}}$ and the corresponding emission power, for single mode output case, is plotted in Figure 3-3 as functions of dipole moment with different linewidth broadening. Typically, the output power is several tens of mW due to the narrow THz emission.
Figure 3-3: Wave intensity (Mega-Watt per centimeter square) in cavity and THz laser power output as functions of dipole moment with different linewidth. Saturation stimulated emission lifetime is taken as $\tau_{sat} = 2$ ps. The edge emitting facet area is assumed to be $S_f = 20 \ \mu m \times 3 \ \mu m$, and air/semiconductor interface reflection coefficient is $r = 0.55$. 
linewidth. Quantum cascade lasers and superlattices lasers have \( \sim \) Watt level output power [28, 40] due to much broader linewidth for mid-infrared intersubband emission and much shorter \( \tau_{21} (\sim 0.1 \text{ ps}) \) intersubband scattering time, which result in a greater wave intensity that can be sustained within the laser cavity.

### 3.3 Photon rate equation and sub-threshold spectrum

Sub-threshold emission is a combination of spontaneous emission and stimulated emission. It is an important emission region which, in addition to emission linewidth, yields the information on optical gain and cavity loss. The photon rate equation can not only be used to derive the emission spectrum in sub-threshold region, but also treat emission coupling, output power, gain and loss on a unified basis. Understanding this prospect is necessary and helpful for THz emission measurements and device design.

Figure 3-4 is a schematic showing the rate equation for THz photon's creation and annihilation in an optical cavity. \( E_3 \) and \( E_2 \) are subbands with electron population \( N_3 = n_3/l_m \) and \( N_2 = n_2/l_m \) respectively. The THz photon generation rate by spontaneous emission, considering the linewidth broadening, is \( N_3 g(f)/\tau_{sp} \) per frequency per volume; photon annihilation rate by cavity loss is \( \gamma N_i \), where \( N_i \) is the THz photon density per frequency per volume and \( \gamma = \alpha c_0/n \) is the photon loss rate. \( \alpha \) is the total cavity loss, including cavity dissipation loss and photon emission loss by coupling, \( \alpha = \alpha_{dis} + \alpha_{coup} \). With the presence of inverted population and therefore optical gain \( G(f) \), the cavity loss is reduced to \( \alpha - G(f) \) (or increased if for negative gain without population inversion between \( E_3 \) and \( E_2 \)). In steady state, the photon creation rate and annihilation rate are equal to each other,
Figure 3-4: A schematic showing in optical cavity, photon created by spontaneous emission and stimulated emission, and annihilated by stimulated absorption and cavity loss including emission escape.

\[ \frac{N_3}{\tau_{sp}} g(f) = \gamma N_1(f) = (\alpha - G(f)) \frac{c_0}{n} N_1(f). \]  
\hspace{1cm} (3.24)

Therefore the THz photon density in the cavity per volume per frequency is

\[ N_1(f) = \frac{N_3}{\tau_{sp}} g(f) \frac{1}{(\alpha - G(f)) c_0 / n}. \]  
\hspace{1cm} (3.25)

The rate at which THz photons are emitted out of the device is determined by the emission coupling rate \( \gamma_{coup} = \alpha_{coup} c_0 / n \),

\[ N_{em}(f) = \gamma_{coup} N_1(f) \]
\[ = \frac{N_3}{\tau_{sp}} g(f) \frac{\alpha_{coup}}{\alpha - G(f)}. \]  
\hspace{1cm} (3.26)

The device emission power spectrum can then be obtained:

\[ P_{em}(f) = \hbar \omega V \dot{N}_{em}(f) \]
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\[ P_0 g(f) \frac{\alpha_{\text{coup}}}{\alpha - G(f)} \]

where \( P_0 \) denotes the spontaneous radiation power by intersubband optical transition and expressed as

\[ P_0 = \hbar \omega V \frac{N_3}{\tau_{sp}} = \Delta E_{32} N_m A \frac{n_3}{\tau_{sp}}, \]

where \( A \) is the device area and \( N_m \) is the number of MQW modules in device.

If there is no gain present in the device, the emission is purely spontaneous. The emission spectrum is \( P_{em}(f) = P_0 g(f) \alpha_{\text{coup}} / \alpha \) and the total emission power is \( P^t_{em} = P_0 \alpha_{\text{coup}} / \alpha \). The presence of gain enhances the emission power by stimulated emission. By integrating Equation 3.27 and using the expressions in Equations 3.20 and 3.17 for gain and lineshape function, the total emission power is

\[ P^t_{em} = P_0 \frac{\alpha_{\text{coup}}}{\alpha} \sqrt{\frac{\alpha}{\alpha - G_0}}, \]

where \( G_0 \) is the peak gain expressed in Equation 3.21. The power enhancement factor due to stimulated emission is then

\[ f_P = \sqrt{\frac{\alpha}{\alpha - G_0}}. \]

Figure 3-5(a) plots the device emission power as a function of the peak gain with different cavity loss. When the gain approaches cavity loss, emission power increases dramatically and the sub-threshold region is dominated by stimulated emission.

For Lorentzian-type lineshape, the emission power spectrum is also a Lorentzian, but its linewidth is changed due to the presence of gain (or absorption). By rewriting Equation 3.27, the emission power spectrum can be expressed as

\[ P_{em}(f) = P^t_{em} g'(f), \]
Figure 3-5: (a) Ratio of device emission power to the spontaneous emission power, as a function of peak gain with different cavity loss. (b) Emission spectrum showing emission linewidth with different peak gain. The arrow indicates the original linewidth corresponding to zero peak gain.
where \( g'(f) \) is the normalized Lorentzian line shape function with a linewidth:

\[
\Delta f' = \Delta f \sqrt{\frac{\alpha - G_0}{\alpha}} = \Delta f / f_p.
\] (3.32)

The emission linewidth is reduced by the same enhancement factor \( f_p \) if optical gain is present in the medium. As indicated in Figure 3-5(b), the measured linewidth from spontaneous emission spectrum is different from the linewidth used in calculating the optical gain. If population is not inverted between the two subbands, which corresponds to the case of intersubband absorption \( (G_0 < 0) \), the measured emission linewidth is broader than the true gain linewidth.

### 3.4 Grating coupling for intersubband emission

For intersubband transitions in conduction band multiple quantum wells (MQWs), the dipole-interaction selection rule allows only the electric field to be polarized perpendicular to the plane of quantum wells [101]. Consequently, for unpatterned MQWs, edge-coupling is used for intersubband emission and detection. [21, 49, 11]. For edge emissions, the cavity loss due to facet coupling is:

\[
\alpha_{fac} = \frac{1}{2L} \ln(R_1 R_2),
\] (3.33)

where \( R_1 \) and \( R_2 \) are the facet reflectivities at the two ends, and \( L \) is the cavity length. For GaAs/air interface, \( R_1 = R_2 = 0.3 \), which gives facet coupling loss of \( \alpha_{fac} = 12 \text{ cm}^{-1} \) for a 1 mm long sample. For large cavity dissipation loss \( \alpha_{dis} > 100 \text{ cm}^{-1} \), only a small portion of the THz photons generated by intersubband transitions will be coupled out of the device, according to Equation 3.29. Considering the weak intersubband radiation power \( P_0 \), a better coupling scheme which offers larger coupling loss is needed to couple more THz photons out of the device for emission measurements. Besides, for device applications at longer wavelength in
THz range, it is desirable to couple the radiation through the surface to yield a better mode pattern. Metallic grating coupling has been one of the preferred techniques for intersubband emission measurements [9, 89]. Theoretical studies of grating coupling have been carried out for the detection scheme in which case the light is coupled into the device [102, 103, 104, 105]. Grating coupling for emission is an important issue for the design of surface-emitting intersubband THz emitting diodes (LEDs) and lasers. However, it has not been analyzed quantitatively. In this section, a general numerical method is presented for the analysis of grating coupling. Major results were published in Ref. [106]. They show that the grating coupling can result in a large cavity loss $\alpha_g$, which is desirable for coupling out the intersubband spontaneous radiation power, but it should be kept low in laser designs to lower the lasing threshold. This numerical method can also be applied to the detection scheme, in which it can be extended to a broader frequency range that cannot be tackled by the previous analytical method [102, 103, 104, 105]. The result of grating coupling for detection is attached in Appendix A.

A diffractive grating coupler functions by introducing parallel wavevectors along the semiconductor surface, and therefore it changes the direction of light propagation.
as well as the polarization. The emitted light due to intersubband transitions in MQWs can then be converted to the surface-emitting direction. In the coordinate system chosen in Figure 3-6, the emission $E$ field from intersubband transitions is polarized along the $z$ direction, and it propagates in parallel with the surface. The $H$ field is assumed to be along the $x$ direction, which is the wave that can be diffracted by the grating. For emission devices, the emitted photons are usually confined in a two-dimensional (2D) layer of MQWs. This can either be accomplished by dielectric cladding waveguide for short wavelengths [21], or by plasma confinement for longer wavelengths at THz frequencies [18, 89, 107]. The well-developed selective etching and lift-off techniques [108], which will be described in detail in Chapter 5, can be used to form a metallic confinement layer on the opposite side of the grating. Therefore, it is assumed that the waves diffracted by the grating toward the $-z$ direction form standing waves in the 2D active layer. The total field in the presence of a grating can then be written as

$$H_x = \sum_{n=\pm 1} B_n e^{i(k_n z + \kappa_n z)}, \quad z > 0,$$

$$H_x = e^{ik_0 y} + \sum_{n=\pm 1} [A_n \sin (k'_n z) + A'_n \cos (k'_n z)] e^{i k_n z}, \quad z < 0. \quad (3.34)$$

Here, $e^{ik_0 y}$ is the TEM traveling wave excited by the intersubband transitions with a normalized amplitude. $k_0 = n_0 \omega / c$ and $k'_0 = n'_0 \omega / c$, where $n_0$ and $n'_0$ are the refractive indices of the air and the semiconductor MQW respectively, assuming isotropic dielectric constant in the semiconductor. $k_n$ and $k'_n$ are the wavevectors for the $n$-th diffracted waves toward the $+z$ and $-z$ directions, respectively. Since the grating introduces parallel wavevectors along the propagation direction of the TEM wave, the dispersion relations for the diffracted wavevectors are:

$$k_{ny}^2 + k_{nz}^2 = k_0^2, \quad (3.35)$$

$$k_{ny}^2 + k'_{nz}^2 = k'_0^2. \quad (3.36)$$
Equation 3.37 can be understood with the aid of Figure 3-6, where ST and ST' are optical paths of the diffracted waves toward +z and −z directions, respectively. The phase delay from S to T and from S to T' should differ from the phase delay from S to S' (a grating period) by 2πn. That is, \( k_0'p - k_0p \cos(\angle TSS') = 2\pi n \) and \( k_0'p - k_0p \cos(\angle T'SS') = 2\pi n \), which leads to Equation 3.37. The E field is given by

\[
E_y = -\frac{1}{i\omega \varepsilon} \frac{\partial H_z}{\partial z}, \quad \text{(3.38)}
\]

\[
E_z = \frac{1}{i\omega \varepsilon} \frac{\partial H_z}{\partial y}. \quad \text{(3.39)}
\]

The amplitudes \( A_n, A'_n, \) and \( B_n \) of the diffracted waves are determined by the two boundary conditions at \( z = -t \), which is the bottom of the confined MQWs active region, and \( z = 0 \), which is the interface between the semiconductor and the air. The former, assuming a perfectly conducting metallic layer at \( z = -t \) to simplify calculations, gives \( A'_n = -A_n \cot(k'_{nz}t) \) by requiring a vanished \( E_y \) component. The later requires \( E_y \) to be zero at metallic regions of the grating, and both \( E_y \) and \( H_x \) to be continuous at aperture regions of the grating. Thus at \( z = 0 \), we can equate \( E_y \) on both sides, and relate \( A_n \) with \( B_n \): \( k'_{nz}A_n/n_0^2 = ik_{nz}B_n/n_0^2 \). The diffraction coefficients \( B_n \) are then determined by the following set of linear equations,

\[
\sum_{n=\pm 1}^{\pm \infty} n_0^2 k_{nz} B_n e^{ik_{ny}} = 0, \quad -a + mp < y \leq a + mp,
\]

\[
\sum_{n=\pm 1}^{\pm \infty} \left[ 1 + \frac{in_0^2 k_{nz}}{n_0^2 k'_{nz}} \cot(k'_{nz}t) \right] B_n e^{ik_{ny}} = e^{ik'_{ny}}, \quad a + mp < y \leq -a + (1 + m)p, \quad \text{(3.40)}
\]

where \( m \) is an integer.

Numerically, the above boundary conditions can be mapped onto a grid in the
Figure 3-7: Emission coupling efficiency and cavity loss of the grating coupling, including all orders of the diffracted waves, with three different filling factors. \( n_0 = 1 \) for air and \( \eta'_0 = 3.4 \) for semiconductor (GaAs). The frequency of the light is 5 THz, and \( t = 3 \) μm. The second y axis shows the grating coupling loss, \( \alpha_g = \eta/t \).
y direction. The coefficients $B_n$ are then simultaneously solved from $n = \pm 1$ to $n = \pm l$ terms by the set of $2l$ linear equations at each node of the y-grid, where $2l$ is the number of nodes on the grid. The numerical solution can be verified by choosing different grids and mapping ranges on the y axis. Also, we can use a finite number of nodes if $B_n$ vanishes for higher-order terms. That means only several lower-order diffracted waves dominate the grating-coupled surface emission. The numerical solution then converges when $l$ is large enough.

For the grating-coupled surface emission, the coupling efficiency is defined as the Poynting vector ratio of the surface-emitting over the incident, $\eta = \frac{\langle S_a \rangle}{\langle S_0 \rangle}$. From Eqs. (1) and (3), it can be derived that for each diffracted wave, $\eta_n = \frac{n_n^2 \text{Re}(k_{nz})}{n_0^2 k_0^2} |B_n|^2$. The total coupling efficiency is $\eta = \sum_n \eta_n$. The numerical results show that the diffraction coefficients $B_n$ converge quite fast, and including the first ten-order diffracted waves is a good approximation. In the mappings typically 30-60 nodes are used to cover a range of several grating periods.

Figure 3-7 shows the emission coupling efficiency, including all the diffracted waves with different metallic filling factors $f$ ($f = 2a/p$) and for a 2D layer thickness of 3$\mu m$. The most noticeable feature is that emission coupling can occur only within certain ranges of $p/\lambda_s$. This is a result of the grating dispersion relations for emission required by Equations 3.35-37. For example, if $n_0 = 1$ is chosen for air and $n_0' = 3.4$ for the semiconductor (GaAs), then Equations 3.35 and 3.37 can be rewritten for a real $k_{nz}$ (corresponding to a non-evanescent surface-emitting mode) as $1/\lambda_s > 3.4|1/\lambda_s - n/p|$. For $n = 1$, it requires that $0.77 < p/\lambda_s < 1.4$; for $n = 2$, $1.54 < p/\lambda_s < 2.8$; and for $n = 3$, $2.32 < p/\lambda_s < 4.2$, etc.. These ranges of $p/\lambda_s$ correspond correctly to the emission windows (where $\eta > 0$) shown in Figure 3-7. Contrary to the grating coupling for detections (see Appendix A), where higher filling factors ($f \geq 0.6$) yield a better coupling, here lower filling factors ($f \leq 0.4$) yield a higher coupling efficiency. This is understandable because the $E$ field from the intersubband transitions already satisfies the boundary conditions at the metallic regions ($E_y = 0$). It is the aperture
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Figure 3-8: 2D-layer-thickness-induced resonances in a grating coupling of emission with three different filling factors. Coupling efficiency and coupling loss drop to zero when the layer thickness matches the wavelength of the diffracted waves. In this example, $p/\lambda_s = 0.8$. The frequency of the light is 5 THz.

part of the grating that bends the field, since it reinforces a continuous tangential $\mathbf{H}$ component.

Because of the standing waves formed in the 2D layer, the thickness $t$ may introduce some resonant structures in the grating coupling efficiency for a given $p/\lambda_s$. Figure 3-8 shows, for an example, when $t$ matches the wavelength of a diffracted wave ($t = \pi/k'_{nz}$), the coupling efficiency is minimized due to the resonance of a Fabry-Perot cavity. The thickness of the 2D layer thus plays a role as important as the grating parameters (i.e., period and metallic filling factor) for the grating coupling.

By using Equation 3.29, the absolute spontaneous emission power coupled out of the device is determined by the ratio of the coupling loss over the device's total cavity loss. From the definition of the emission coupling efficiency, the grating coupling loss per unit length is $\alpha_g = (S_z dw)/(S_0 tw)/d = \eta/t$, where $d$ and $w$ are the device's length and width, respectively. This leads to, if the thickness of MQWs is chosen
to be $t = 3 \mu m$) as an example, a large coupling loss of several hundred cm$^{-1}$, as indicated on the second $y$ axis in Figure 3-7. The emission power coupled out from the surface of the device is then

$$P_{em}^{tot} = P_0 \frac{\alpha_g}{\alpha_g + \alpha_{fac} + \alpha_{dis}} \sqrt{\frac{\alpha_g + \alpha_{fac} + \alpha_{dis}}{\alpha_g + \alpha_{fac} + \alpha_{dis} - G_0}}. \quad (3.41)$$

Clearly if the coupling loss $\alpha_g$ is much greater than the cavity dissipation loss $\alpha_{dis}$, essentially all the photons generated by the radiative intersubband transitions can be coupled out. This is desirable in THz spontaneous emission measurements.

For surface-emitting lasers, however, this large grating coupling loss should be avoided in order to lower the lasing threshold.

$$G_0^{th} = \alpha_g + \alpha_{fac} + \alpha_{dis}. \quad (3.42)$$

According to the calculations, this can be implemented by using gratings with large filling factors ($f > 0.8$). Also, the chosen 2D layer thickness should be close to the coupling resonances to minimize the coupling loss.

Strictly speaking, the results derived in this section only apply to the case of intersubband lasers, which will produce the initial TEM traveling wave in Equation 3.34. For intersubband LEDs, the spontaneous emission does not produce a long-range coherent TEM wave and, therefore, the source term in Equation 3.34 needs to be modified. Because of the lack of long-range coherence, sharp features in the grating efficiencies shown in Figure 3-7 will be smeared. Thus it results in a finite grating efficiency even in the forbidden regions. Nevertheless, results shown in Figure 3-7 could serve as a semiquantitative guideline to estimate grating coupling efficiency for intersubband LEDs.
3.5 THz mode confinement and cavity loss

Cavity dissipation loss for THz frequencies consists of phonon absorption loss, free carrier loss, and plasma confinement loss:

$$\alpha_{\text{dis}} = \alpha_{\text{ph}} + \alpha_{\text{fc}} + \alpha_{\text{pl}}.$$  \hspace{1cm} (3.43)

Phonon absorption loss is caused by photon interaction with transverse optical (TO)-phonon-like polaritons, and is minimized for frequencies far away from the re- strahl region, which is centered at 34 meV (8.5 THz) in GaAs [109, 110]. Figure 3-9 plots the phonon absorption loss at room temperature for GaAs in THz frequency range [111]. Below 6 THz, the loss $\alpha_{\text{ph}}$ is within 10 cm$^{-1}$.

Free carrier loss and plasma confinement loss can be modeled using semiclassical Drude model with an empirical scattering time $\tau$. The frequency-dependent complex dielectric constant $\varepsilon_r(\omega)$ in Drude model can be obtained from simple one-dimensional oscillator, and is expressed as

$$\frac{\varepsilon_r(\omega)}{\varepsilon_\infty} = 1 - \frac{\omega_p^2 \tau^2}{1 + \omega^2 \tau^2} + i \frac{\omega_p^2 \tau}{\omega (1 + \omega^2 \tau^2)},$$  \hspace{1cm} (3.44)

where $\varepsilon_\infty$ is the high-frequency lattice dielectric constant, and $\omega_p^2 = n_e e^2 / m^* \varepsilon_0 \varepsilon_\infty$ is the plasma frequency with free carrier density $n_e$.

The validity of using Drude model in estimating optical properties of free carriers needs to be verified. At near-infrared frequencies which is below the semiconductor’s fundamental absorption edge, the optical absorption of free carriers is $\lambda^3$ wavelength dependent, and needs a quantum mechanical treatment based on time-dependent perturbation theory. At far-infrared frequencies with photon energy below the carrier’s thermal energy, $\hbar \omega < k_0 T$, the quantum mechanical results reduce to $\lambda^2$ dependence which is given by semiclassical Drude model [112]. For III-V and II-VI polar semiconductors, the Drude theory can be extended into the near infrared range by using a frequency-dependent effective electron scattering time. In the far-infrared, this scat-
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Figure 3-9: Phonon absorption loss $\alpha_{ph} \text{ (cm}^{-1}\text{)}$ of GaAs at $T=300$ K in THz frequency range. Data is plotted using $\alpha_{ph} = k\omega/c_0$, where the extinction coefficient $k$ ($\epsilon_r = (n + ik)^2$) is taken from Ref. [109].

Scattering time reduces to a carrier-concentration-dependent but frequency independent constant, which can then be extracted from the dc mobility measurement as a function of carrier concentration. THz reflection/transmission measurements in samples doped in range of $10^{15}/\text{cm}^3 - 10^{18}/\text{cm}^3$ have confirmed this conclusion [75, 76, 112, 113].

Figure 3-10 plots the free carrier loss in THz frequency range in GaAs at different carrier concentrations. The frequency-independent scattering time at 77 K and 300 K is extracted from dc drift mobility data in Ref. [110]. At frequencies above plasma frequency, $\alpha_{fc}$ scales with $\omega^{-2}$. In lower frequency limit, the free carrier loss is constant which can be seen from Equation 3.44. For M10 structure, the equivalent 3D free carrier concentration in the MQW region is $3 \times 10^{16}/\text{cm}^3$. The loss is $\alpha_{fc} = 55 \text{ cm}^{-1}$ at 4 THz using 300 K data in Figure 3-10. This is believed to be the worst-case estimation since the 2D confinement of electron gas in quantum wells doesn't favor the motion of carriers along the $E$ field polarization [114].
Figure 3-10: Drude model calculated free carrier loss for GaAs in THz frequency range at different carrier concentrations, with plasma frequencies indicated. Scattering time at different carrier concentrations and temperatures are extracted from drift mobility measurements [110].

Next in this section, the Drude model is used to calculate the cavity dissipation loss due to plasma confinement. Since the wavelength of THz radiation in semiconductor is typically several tens of microns, for example, $\lambda_s = 21 \, \mu\text{m}$ at 4 THz in GaAs, and the active region thickness, for 100 modules of triple-quantum-wells, is only $t = 3 \, \mu\text{m}$, dielectric waveguide is a very inefficient method to confine the THz photons. Furthermore, for GaAs/AlGaAs system, the dielectric constant of GaAs is higher than that of Al$_x$Ga$_{1-x}$As. Dielectric wave cladding is impossible for active region grown on lattice-matched GaAs substrate. The only feasible solution for making a THz laser cavity is to use plasma confinement; the heavily doped GaAs contact layers sandwiching the active region can serve this purpose. With a doping concentration higher than $10^{18}/\text{cm}^3$, the plasma frequency exceeds 10 THz, which is above the intersubband radiation frequency. The free carriers in the contact layers act as a plasma and shield the electric field. Due to the limitation for doping bulk GaAs,
ideal plasma confinement will be achieved by using metallic waveguides. This can be realized by using additional device fabrication steps. Figure 3-11 shows the cavity structures of a plasma waveguide and a metallic waveguide.

For plasma waveguide, the confinement on bottom side is made by a thick heavily doped GaAs layer (layer-II', 4 µm) grown between the n-type GaAs substrate (layer-III') and the MQW active region (layer-I, 3 µm). From top side, the heavily doped contact layer (layer-II) is thin (0.1 µm) and the confinement is made by a metallic layer (layer-III). For metallic waveguide, both of the two sides are confined by metallic layers (layers-III and III'). The thin heavily doped contact layers (layers-II and II') are necessary for providing ohmic contacts and compensating for the band bendings between the metal layers and MQWs, at the cost of some additional loss.

To calculate the plasma waveguide loss, the Drude model is used to assign dielectric constants to each of the layers. The metallic layers are assumed to be gold and the scattering time is extracted from Au's 77 K conductivity $\sigma = 2 \times 10^8 / \Omega \cdot m$. Due to the dipole selection rule, the $E$ field generated by intersubband transition is normal to the confinement layers and thus the basic mode pattern is a quasi-TEM mode, or the mixture of TM$_1 +$TM$_2$ mode. The $H$ field is polarized along $x$ direction and it

![Figure 3-11: Waveguide structures for plasma confinement and metallic confinement. The gray layers are heavily doped GaAs contacts sandwiching MQW active region. The shallow gray is n-type GaAs substrate. The black layers are metals.](image)
Figure 3-12: Calculated quasi-TEM mode pattern of the plasma waveguide. Solid and dashed lines are the real and imaginary parts of the fields. The origin point $z = 0$ is the middle of the active region. The $E$ field is normalized by the impedance of GaAs, $109 \, \Omega$. The carrier concentration and scattering time in plasma region are indicated. Plasma cavity loss, confinement factor $\Gamma$, and loss due each layer are given at frequency of 4 THz. The active region thickness is 3 $\mu$m. The top and bottom heavily doped plasma regions are 0.1 $\mu$m and 4 $\mu$m thick respectively.
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Figure 3-13: Plasma cavity loss as a function of photon frequency at different carrier concentrations in the plasma region. The scattering time at each carrier concentration is extracted from the room-temperature GaAs drift mobility measurements.

is expressed as

\[ H_x = A_1 \cos(k_z z) e^{ik_y y} + B_1 \sin(k_z z) e^{ik_y y}, \text{(layer - I)}, \]

\[ H_x = A_2 e^{-\alpha_2 z} e^{ik_y y} + B_2 e^{\alpha_2 z} e^{ik_y y}, \text{(layer - II)}, \]

\[ H_x = A_3 e^{-\alpha_3 z} e^{ik_y y}, \text{(layer - III)}. \] (3.45)

By satisfying boundary conditions and the dispersion relations in each layer, E field and H field are obtained as well as the wavevectors. The cavity loss is given by \( \alpha_{pl} = \text{Im}(k_y) \). Loss due to each layer can be calculated from the Poynting vectors:

\[ \alpha_{pl,l} = P_z(z = l) \int_{-\infty}^{\infty} P_y(z) dz. \]

The confinement factor \( \Gamma \) can also be calculated with known field distribution.
Figure 3-14: Calculated mode pattern of the metallic (Au) waveguide. The carrier concentration and scattering time in plasma region are indicated. The thickness of the plasma layers is 0.1 μm. Cavity loss, confinement factor, and loss due to each layer are given at frequency of 4 THz in comparison with the plasma waveguide.
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Figure 3-15: Metallic (Au) waveguide loss as a function of frequency at different carrier concentrations in the plasma layers.

Figure 3-12 plots the calculated basic mode pattern in the plasma waveguide with a carrier concentration of $3 \times 10^{18}$/cm$^3$ and the scattering time of 0.1 ps in layer-II and layer-II'. This plasma cavity provides good confinement for THz photons, i.e., $\Gamma = 0.91$ at 4 THz. The cavity loss is large, however, $\alpha_{pl} = 187$ cm$^{-1}$ at this frequency. It is mostly due to the free carrier loss in the plasma layer-II', where there is large leakage of the $E$ and $H$ fields. This leakage is caused by the relatively low plasma frequency, i.e., $f_{pl}=18.6$ THz, for $3 \times 10^{18}$/cm$^3$, that allows a significant portion of the field to leak into to interact with the free carriers. The phase of $E_z$ field is inverted in the plasma region because of the negative real part of the dielectric constant for frequencies below the plasma frequency. The plasma loss increases at higher frequency simply because the confinement becomes weaker as frequency approaches plasma frequency. The cavity loss can be reduced by using highly doped contact layers. Figure 3-13 plots the cavity loss in THz frequency range at different carrier concentrations in the plasma region. High doping concentration in the plasma region
Figure 3-16: Calculated mode pattern of a metallic waveguide showing surface plasma mode. The carrier concentration and its plasma frequency are indicated. Surface plasma mode is characterized by a large buried $E_z$ field in the thin plasma layers.
is preferred. To achieve the lowest cavity loss, metallic waveguide should be used to confine THz photons. The basic mode pattern of the metallic waveguide is calculated and plotted in Figure 3-14. At 4 THz, the cavity loss is dramatically reduced to 12.1 cm\(^{-1}\) and the confinement factor is improved to \(\Gamma = 0.95\). Poynting vector calculations reveal that the loss due to metallic layers (Au) is 6.6 cm\(^{-1}\). The loss due to the thin contact layers at \(3 \times 10^{18}/\text{cm}^3\) carrier concentration is 5.4 cm\(^{-1}\). This ideal low-loss metallic waveguide, if it can be fabricated, is promising to achieve THz lasing.

In Figure 3-15 the cavity loss of metallic waveguide is plotted as a function of frequency at different carrier concentrations. Analysis using Poynting vectors reveals that the loss due to metallic layers is primarily independent of the frequency, and the increase of loss at higher frequency is caused by the thin plasma layers, which serve as the contact layers between the active region and the metal. Using higher carrier concentration in these plasma layers will reduce the loss. However, if the carrier concentration is low in these layers, the cavity loss will dramatically increase when the frequency approaches the plasma frequency. For \(n_e = 10^{18}/\text{cm}^3\), the plasma frequency is \(f_{pl} = 10.1\) THz. At 8 THz, the cavity loss is several hundred cm\(^{-1}\), making metallic waveguide too lossy to use. The physical mechanism causing this large loss is the development of “surface plasma mode”. In Figure 3-16, the field pattern at 8 THz, with \(10^{18}/\text{cm}^3\) carrier concentration in the plasma layers is plotted. Compared with the mode pattern in Figure 3-14, a large portion of the \(\mathbf{E}\) field exists in the thin plasma layers. This plasma mode occurs due to the vanishing dielectric constant in plasma regions at frequencies close to the plasma frequency. The continuity of the normal components of \(\mathbf{D}\), required by the boundary conditions, enforces a large \(E_z\) in the plasma layers.
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3.6 Conclusion

THz photon confinement can be realized by using plasma waveguide. Large cavity loss due to plasma confinement can be reduced by using highly doped plasma regions. Due to the doping saturation in semiconductor materials such as GaAs, ideal plasma confinement should utilize a metallic waveguide which has much lower cavity loss. However, to provide electrical connection between metals and the semiconductor, doped contact layers are unavoidable in electrically pumped THz emission MQW devices. Depending on the doping levels in these contact layers, extremely large plasma loss can be introduced into the metallic waveguide through the development of surface plasma mode. This occurs if the operation frequency approaches the plasma frequency in the contact layers. Since the plasma frequencies for typical doping levels in GaAs are close to THz frequency range, it imposes additional difficulty in making a low-loss cavity for an electrically pumped THz laser. The doping profile in the contact regions are thus very important. It should be carefully engineered to avoid this lossy surface plasma mode.
Chapter 4

Temperature Effects on Intersubband Scattering

4.1 Introduction

Intersubband scattering in MQW structures can be inelastic and elastic. Inelastic intersubband scattering are acoustic phonon scattering and longitudinal-optical (LO) phonon scattering which dissipate electron's energy. Elastic intersubband scattering include impurity scattering, interface roughness scattering, and electron-electron (e-e) scattering [107, 115]. The THz emission MQW structure is designed in the ideal condition which corresponds to the low-temperature limit. It has been assumed that the temperatures of both the electronic system and phonon system are close to the device’s ambient cryogenic temperature (< 30 K). Under this situation, for M10 device design, intersubband scattering from subband $E_2$ to $E_1$ by LO-phonon emission is a much faster process than the intersubband scattering from $E_3$ subband to $E_2$, where LO-phonon scattering is not available with subband energy separation in the THz frequency range. Subband population inversion can thus be realized between $E_3$ and $E_2$ levels. This low-temperature approximation gives the largest population inversion possible for a given triple-quantum-well design. However, if the electronic temperature
is significantly higher than ambient temperature, the high-energy tail of electrons on $E_3$ level will open up the LO-phonon scattering window, and the intersubband scattering rate between $E_3$ and $E_2$ increases. Also, because the lattice is heated up during the electrical pumping, acoustic phonon branches close to the $\Gamma$-point will be substantially populated. This leads to stimulated intersubband acoustic phonon scattering which will further increase the intersubband scattering rate between $E_3$ and $E_2$. Population inversion will then be reduced due to this "hot electron" effect and "lattice heating" effect. Furthermore, since LO-phonon emission is the major mechanism to dissipate the energy of electrons in intersubband transitions, significant number of non-equilibrium LO phonons will be generated and then accumulate due to the finite LO-phonon lifetime in semiconductors. The extra "hot LO-phonons" can be re-absorbed by electrons on the $E_1$ level through stimulated phonon absorptions. This pumping-back process for electrons from $E_1$ level to $E_2$ level is another important mechanism that degrades the population inversion for a THz emission device, which in reality deviates from the low-temperature limit.

The emphasis of this chapter is on intersubband phonon scattering to reveal temperature effects pertaining to intersubband transitions in THz emission MQWs. Temperature-dependent intersubband scattering is addressed for the triple-quantum-well structure design. Hot electron effect, lattice heating, and non-equilibrium LO-phonons are quantified by discussing the subband populations in M10 device.

### 4.2 Intersubband phonon scattering

In the triple-quantum-well design in M10 structure, the carrier concentrations on subbands are in the $10^{10}/\text{cm}^2$ range. The electron-electron scattering time at this low carrier concentration is on the order of ten picosecond and is temperature insensitive [107, 116, 117]. Ionized donors cause Coulombic impurity scattering [13, 115]. In the triple-quantum-well design, this elastic intersubband scattering is minimized.
by placing the dopants in the buffer well or within the collector barrier. Interface roughness scattering due to defects depends on MBE growth quality and is usually a smaller effect in intersubband transitions than in intrasubband transitions, and in the latter case the scattering can be characterized via subband linewidth broadening [107, 115, 118, 119]. Phonon scattering is a major topic for intersubband transitions and has been extensively studied both theoretically [115, 120, 121, 122, 123, 124], and experimentally [125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135]. Measurements on intersubband scattering times in the mid-infrared range (80 meV $\sim$ 300 meV) fit well the calculated LO-phonon scattering times [125, 126, 127, 128, 129, 130, 131]. More recently, intersubband scattering times for subband energy separations below the LO-phonon energy were measured by a number of techniques [132, 133, 134, 135]. The reported results vary over a large range and depend on the measurement conditions such as pumping intensity. Nevertheless, effects such as carrier heating were revealed as important factors in determining intersubband scattering time below LO-phonon energy, which is in the THz frequency range.

In the following discussions of the temperature effects on intersubband scattering in the triple-quantum-well design, electrons, LO phonons, and acoustic phonons are treated as three separate subsystems with electronic temperature $T_{ei}$ on i-th subband, LO-phonon temperature $T_{ph}$, and lattice temperature $T_l$ respectively [136]. As an approximation to simplify the analysis and considering the relatively small subband separation ($\leq 36$ meV), the Fermi-Dirac function is used to describe the electron distribution on each subband with quasi-Fermi level $\mu_i = \mu_i(n_i, T_{ei})$, although this assumption can be controversial [137, 138]. In calculating the intersubband scattering times for the three-level system in the triple-quantum-well design, as stated in the rate equation 2.5 in Chapter 2, $E'_1$ and $E_3$ subbands are considered to be at the anti-crossing, and the intersubband scattering times for $E'_1$ and $E_3$ are treated as the same using one wavefunction from $E_3$ level. The combined electron population on the $E'_1$ and $E_3$ is $n_3$, and electron population on the $E_2$ level is $n_2$. 
4.2.1 LO-phonon scattering and hot electron effect

The perturbation Hamiltonian of electron-phonon coupling is [139]

\[ H'_{\text{e-phonon}} = \sum_q \alpha(q)(e^{iq\tau}b_q + e^{-iq\tau}b_q^\dagger). \] (4.1)

By the Fermi’s Golden Rule, the phonon scattering rate between electronic state \( k_i \) on initial subband \( i \) and state \( k_f \) on final subband \( f \) is

\[ W_{k_i \rightarrow k_f} = \frac{2\pi}{\hbar} |< f, k_f | H' | i, k_i >|^2 \delta(E_i(k_i) - E_f(k_f) - \hbar\omega(q)), \] (4.2)

where \( k_i \) and \( k_f \) are in-plane wavevectors for initial state and final states respectively, and \( q = q_1 + q_2 \hat{z} \) is phonon’s wavevector. For electron-LO-phonon interaction,

\[ |\alpha(q)|^2 = \frac{\hbar\omega_{LO}e^2}{2\epsilon_p\epsilon_0 V q^2}, \] (4.3)

where \( 1/\epsilon_p = 1/\epsilon_\infty - 1/\epsilon_s \). \( \epsilon_\infty \) and \( \epsilon_s \) are the high-frequency and static dielectric constants respectively. The wavefunctions of initial and final states have the same expressions as in Equation 3.7. The matrix element of the interaction Hamiltonian is then

\[ < f, k_f | H' | i, k_i > = \alpha(q)A_{i \rightarrow f}(q_z)\delta_{k_i - k_f,q_z}, \] (4.4)

where the form factor \( A_{i \rightarrow f} \) is

\[ A_{i \rightarrow f}(q_z) = \int_{-\infty}^{+\infty} dz \psi_f^*(z)\psi_i(z)e^{iq_zz}. \] (4.5)

Then the scattering rate for an electron from initial state \( |i, k_i > \) to the final subband is, by summing all possible states \( k_f \) on the final subband,
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\[ W_{k_i \rightarrow f} = \frac{2\pi}{\hbar} \sum_{k_f} \sum_{q_z} |\alpha(q)|^2 |A_{i \rightarrow f}(q_z)|^2 \delta(q_z - q_{k_f}) \delta(E_i(k_i) - E_f(k_f) - \hbar \omega(q)). \] (4.6)

By taking into account \( E_i(k_i) = E_i + \hbar^2 k_i^2/2m^* \) and \( E_f(k_f) = E_f + \hbar^2 k_f^2/2m^* \), and approximating LO-phonon energy as \( \hbar \omega(q) = \hbar \omega_{LO} \), the above equation can be expressed as

\[ W_{k_i \rightarrow f} = \frac{e^2 \hbar \omega_{LO} m^*}{4\pi^2 \varepsilon \varepsilon_0 \hbar^2} \int_0^{2\pi} d\varphi \int_0^\infty dq_z \frac{|A_{i \rightarrow f}(q_z)|^2}{q^2} \theta(\varepsilon_i), \] (4.7)

where \( \theta(\varepsilon_i) = \theta(\varepsilon_i + \Delta E_{if} - \hbar \omega_{LO}) \) is the step function requiring energy-allowed electron-phonon scattering. By the momentum conservation \( q_z = k_i - k_f, \ k_{i//} = k_i^2 + k_f^2 - 2k_i k_f \cos \varphi \), and \( q^2 = q_{i//}^2 + q_{z//}^2 \). \( \varepsilon_i = \hbar^2 k_i^2/2m^* \) and \( \varepsilon_f = \hbar^2 k_f^2/2m^* \) are the in-plane kinetic energy of initial and final subbands, respectively. \( k_f \) is given by the energy conservation: \( \varepsilon_f = \varepsilon_i + \Delta E_{if} - \hbar \omega_{LO} \). On the left-hand side of Equation 4.7, \( k_i \) is replaced by \( k_i \) since scattering rate \( W_{k_i \rightarrow f} \) is independent of the direction of \( k_i \).

Equation 4.7 is applied to calculate the LO-phonon scattering time for the three-level system in M10 triple-quantum-well structure. Figure 4-1 plots the picosecond-level LO-phonon scattering time for an electron from \( E_3 \) to \( E_2 \) and from \( E_2 \) to \( E_1 \) as a function of its initial kinetic energy. Since \( \Delta E_{32} \) is about 15 meV at designed bias, an electron needs 21 meV kinetic energy to be scattered by LO-phonon from \( E_3 \) subband to \( E_2 \). For electrons scattered from \( E_2 \) to \( E_1 \), very little kinetic energy is needed since \( E_{21} \) is close to LO-phonon energy. The scattering time gets longer for larger momentum transfer, and increases approximately linearly with the in-plane \( k \) vector, because the denominator \( q^2 \) in Equation 4.7 only contains a first order \( k_i \) term.

For a subband occupied with electrons, assuming a finite temperature and a Fermi level \( \mu_i = \mu_i(n_i, T_{ei}) \), the electron distribution on each subband is given by the Fermi-Dirac function:
Figure 4-1: For M10 structure, $E_3 - E_2 = 15.3$ meV, $E_2 - E_1 = 34$ meV, the calculated LO-phonon scattering time for an electron from $E_3$ to $E_2$ (a) and from $E_2$ to $E_1$ (b) as a function of its initial in-plane k vector (kinetic energy).
\[ f(\varepsilon_i) = \frac{1}{e^{(\varepsilon_i - \mu_i)/kT_i} - 1}, \quad (i = 2, 3) \] (4.8)

By considering the Pauli exclusion principle, and phonon mode population \( N_{LO}(q) \), the electron scattering rate due to spontaneous and stimulated LO-phonon emission is

\[ W_{k_i \rightarrow f}^{LO, em} = \frac{e^2 \omega_{LO} m^*}{4\pi^2 \epsilon_p \epsilon_0 h^2} \int_0^{2\pi} d\varphi \int_0^{+\infty} dq_z (1 - f_f(\varepsilon_f)) \frac{|A_{i \rightarrow j}(q_z)|^2}{q^2} (N_{LO}(q) + 1) \theta(\varepsilon_i), \] (4.9)

where \( N_{LO}(q) \) is the LO-phonon population which is determined by the LO-phonon temperature \( T_{ph} \):

\[ N_{LO}(q) = \frac{1}{e^{\hbar \omega_{LO}/kT_{ph}} - 1}. \] (4.10)

In thermal equilibrium, \( T_{ph} = T_i \). Assuming the lattice temperature \( T_i \) is brought down low (< 200 K) by the device's heatsink which is usually at cryogenic temperature, \( N_{ph} \) is then negligible. This means that the scattering is dominated by spontaneous LO-phonon emission process. However, for non-equilibrium conditions which occur under certain kinds of pumping, \( N_{LO}(q) \) will be given by phonon rate equations, which results in non-equilibrium LO phonon population. Effectively, the LO-phonon temperature \( T_{ph} \) can be much higher than the lattice temperature. This hot LO-phonon issue and the consequent stimulated LO-phonon emission/absorption processes in intersubband transitions will be addressed in the next section. In case of non-zero LO-phonon population, the intersubband absorption rate for \( E_i < E_j \) is

\[ W_{k_i \rightarrow f}^{LO, ab} = \frac{e^2 \omega_{LO} m^*}{4\pi^2 \epsilon_p \epsilon_0 h^2} \int_0^{2\pi} d\varphi \int_0^{+\infty} dq_z (1 - f_f(\varepsilon_f)) \frac{|A_{i \rightarrow j}(q_z)|^2}{q^2} N_{LO}(q) \theta(\varepsilon_i). \] (4.11)

The intersubband scattering time, used in the rate equations in 2.5 to determine
subband populations, is the averaged scattering time of all the electrons on that subband,

\[ W_{i \rightarrow f}^{LO,em} = \frac{1}{n_i} \sum_{k_i} 2f_i(\varepsilon_i) W_{k_i \rightarrow f}^{LO,em}, \tag{4.12} \]

\[ W_{i \rightarrow f}^{LO,ab} = \frac{1}{n_i} \sum_{k_i} 2f_i(\varepsilon_i) W_{k_i \rightarrow f}^{LO,ab}, \tag{4.13} \]

where the factor of 2 accounts for spin degeneracy.

For the three-level system in M10 structure, if the electron temperature of \( E_3 \) level is low, most of the electrons will occupy lower \( k_i \) states so that LO-phonon scattering is not allowed. Thus the intersubband scattering time \( \tau_{32}^{LO,em} \) will be slow.
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However, if the electron temperature is sufficiently high, a portion of the electrons on $E_3$ will be scattered by LO-phonons and intersubband scattering time $\tau_{32}^{LO,em}$ will be reduced. Using Equation 4.13, Figure 4-2 presents the intersubband scattering time as a function of electron temperature. Here it is assumed that $T_{e3} = T_{e2} = T_e$, although this is not generally true. The electron population on $E_3$ is $n_3 = 6 \times 10^{10}/\text{cm}^2$. The solid line corresponds to the case that electron population on $E_2$ is half that of $E_3$. Dash-dotted line corresponds to the case that there are same number of electrons on $E_2$ as on $E_3$ level, and dashed line corresponds to zero electron population on $E_2$ level. The effect of Pauli exclusion principle is profound for $\tau_{32}^{LO,em}$ at low electron temperatures. With more electrons on final state $E_1$ ($E_3$), the scattering rate is reduced due to state blocking. The dramatic decrease of scattering time $\tau_{32}^{LO,em}$ at elevated electron temperatures will reduce the population inversion between $E_3$ and $E_2$. To prevent $\tau_{32}^{LO,em}$ from approaching $\tau_{21}^{LO,em}$ at high temperatures, in which case the population inversion diminishes, the subband separation between $E_3$ and $E_2$ should be well below the LO-phonon energy. Figure 4-3 shows the intersubband scattering time $\tau_{32}^{LO,em}$ as a function of energy separation between $E_3$ and $E_2$. In M10 design, $\Delta E_{32} = 15.3 \text{ meV}$, and this should minimize the degradation of population inversion due to the hot electron effect.

It should be noted that the hot electron effect is characteristic for intersubband lasers, including mid-infrared quantum cascade lasers. For mid-infrared frequency, the energy spacing between the two radiative-transition subbands is several LO-phonon energy, and the intersubband scattering is dominated by LO-phonon scattering for each subband. There is then slight influence of hot electron effect on intersubband scattering time. For THz intersubband lasers, however, with subband spacing below one LO-phonon energy, the intersubband scattering is sensitive to the electron temperature and thus the hot electron effect. To understand the origin of hot electron effect, the acoustic phonon scattering needs to be discussed.
Figure 4-3: For M10 structure, intersubband scattering time $\tau_{s2}^{LO,em}$ as functions of subband energy separation $\Delta E_{32}$ at two electron temperatures $T_{e3} = T_{e2} = 100$ K and 200 K.
4.2.2 Acoustic phonon scattering and lattice heating

Compared with the LO-phonon scattering, acoustic phonon scattering occurs at any subband spacing due to the dispersion relations of acoustic phonon branches. In contrast to mid-infrared quantum-cascade lasers, acoustic phonon scattering is an important issue for THz intersubband lasers, because the radiative intersubband energy spacing only allows acoustic phonon scattering if the electrons on the upper subband are cold. For polar semiconductors such as GaAs, acoustic phonon scattering includes both deformation potential coupling with longitudinal acoustic (LA) phonons and piezoelectric acoustic phonon scattering.

The electron-LA-phonon coupling through deformation potential is [139]

\[
|\alpha(q)|^2 = \frac{D^2 \hbar}{2 \rho c_s V q}.
\]

(4.14)

Here, \( D \) is the deformation constant, \( \rho \) is the density, and \( c_s \) is the velocity of sound. Using the Fermi’s Golden Rule, the intersubband scattering time from an initial state \( |i, k_i > \) to the final subband, by summing all possible states of \( |f, k_f > \), is

\[
W_{k_i \rightarrow f}^{\text{def}} = \frac{D^2 m^*}{4 \pi^2 \rho c_s \hbar^2} \int_0^{2\pi} \int_0^{+\infty} dq_z (1 - f(q))(1 - f(q_z))q |A_{i \rightarrow f}(q_z)|^2 (N_{ac}(q) + 1).
\]

(4.15)

By energy conservation and momentum conservation, using acoustic phonon dispersion relation \( \omega(q) = c_s q \), the phonon wavevector in the above integral needs to satisfy:

\[
\epsilon_f - \epsilon_i + \hbar c_s q = \Delta E_{ij} \quad \text{and} \quad q^2 = q_z^2 + k_i^2 + k_f^2 - 2k_i k_f \cos \varphi.
\]

\( N_{ac}(q) \) is the acoustic phonon mode population determined by the lattice temperature \( T_l \),

\[
N_{ac}(q) = \frac{1}{e^{\hbar \omega(q)/kT_l} - 1}.
\]

(4.16)

The deformation acoustic phonon scattering rate, by averaging over the initial subband, is
\[ W_{i \rightarrow f}^{\text{def}} = \frac{1}{n_i} \sum_{k_i} 2f_i(\varepsilon_i)W_{k_i \rightarrow f}^{\text{def}} = \frac{m^*}{\pi \hbar^2 n_i} \int_0^\infty d\varepsilon_i f_i(\varepsilon_i)W_{k_i \rightarrow f}^{\text{def}}. \quad (4.17) \]

Unlike LO-phonon scattering, the energy transferred from an electron to an acoustic phonon is proportional to the phonon's wavevector. To gain insight into the acoustic phonon scattering, it is necessary to know per scattering event, the average energy loss of a scattered electron to the acoustic phonon. This average energy loss per scattering can be expressed as

\[ \Delta \varepsilon_{i \rightarrow f}^{\text{def}} = \frac{\sum_{k_i} 2f_i(\varepsilon_i)(\varepsilon_i - \varepsilon_f + \Delta E_{if})W_{k_i \rightarrow f}^{\text{def}}}{n_i W_{i \rightarrow f}^{\text{def}}}. \quad (4.18) \]

The calculation of piezoelectric phonon scattering is similar to the deformation acoustic phonon scattering, except that the coupling Hamiltonian between electron and acoustic phonon by piezoelectric interaction [120] is

\[ |\alpha(q)|^2 = \frac{c^2 h_{14}^2 \hbar A}{2 \rho c_a V q}. \quad (4.19) \]

Here, \( h_{14} \) is the piezoelectric tensor component. \( A \) is a dimensionless anisotropy factor that depends on the direction of phonon wavevector: \( A = 18\lambda^2 \mu^2 \nu^2 + 2(\lambda^2 \mu^2 + \mu^2 \nu^2 + \nu^2 \lambda^2) \), where \( \lambda, \mu, \nu \) are expressed as [140]

\[
\begin{align*}
\lambda &= q_z/q, \\
\mu &= (k_i + k_f \cos \varphi)/q, \\
\nu &= k_f \sin \varphi.
\end{align*} \quad (4.20)
\]

Both the deformation and piezoelectric acoustic phonon scattering times between
Figure 4-4: For M10 structure, (a) acoustic phonon scattering time between subbands $E_3$ and $E_2$ as a function of lattice temperature $T_l$, including deformation and piezoelectric scattering. (b) Energy loss per scattering event for deformation and piezoelectric scattering. $T_{e3} = T_{e2} = 100$ K, and $n_3 = 2n_2 = 6 \times 10^{10}$/cm$^2$. 
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$E_3$ and $E_2$ subbands for M10 structure are calculated and plotted in Figure 4-4(a), as functions of the lattice temperature. Compared with LO-phonon scattering, acoustic phonon scattering is a much slower process, typically several hundred picoseconds at low lattice temperatures. Acoustic phonon scattering is sensitive to lattice temperature but does not show much dependence on electron temperature. This behavior is exactly opposite to LO-phonon scattering, because acoustic phonon scattering does not require a threshold subband spacing, and on the other hand, acoustic phonon branches are relatively easier to be populated at elevated lattice temperatures. At $T_l = 200$ K, $\tau_{32}$ drops to 17 ps for M10 device. Lattice heating has comparable influence on subband population inversion with the hot electron effect discussed in the previous section. Figure 4-4(b) gives the energy loss per scattering event for both deformation and piezoelectric acoustic phonon scattering. The energy loss is small, typically within approximately 1 meV, regardless of the lattice temperature. This observation demonstrates a distinctive feature for acoustic phonon scattering from LO-phonon scattering, in that it is quasi-elastic. Similar to other intersubband scattering including electron-electron scattering, impurity scattering, and interface roughness scattering, which are all elastic, electrons lose little energy during an acoustic phonon scattering and most of the potential energy $\Delta E_{32}$ is transferred into the kinetic energy on $E_2$ subband.

It is helpful to further understand this issue in the momentum space. The momentum of a phonon generated in an electron-phonon scattering consists of $\hbar q_z$ and an in-plane momentum $\hbar q_{\|}$. For electrons with kinetic energy of 10 meV, the corresponding in-plane wavevector is $\sim 2 \times 10^8$/m. Considering that the wavevector at Brillouin zone edge, for GaAs for example, is $\sim 10^{10}$/m, the momentum that an electron carries is very small. $q_z$ stems from the form factor $A_{i\rightarrow j}$ in the integrals of electron-phonon scattering rate, Equations 4.7 and 4.15. This form factor $|A_{3\rightarrow 2}|^2$ is given in Figure 4-5(a) as a function of $q_z$ for M10 structure. Again, $q_z$ is in the $10^8$/m range. This is not surprising because $q_z$ is approximately the inverse of sub-
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Figure 4-5: (a) Calculated form factor $|A_{32}|^2(q_z)$ in phonon scattering using M10 structure as an example. (b) Schematics showing for both acoustic-phonon scattering and LO-phonon scattering, only the phonons in the vicinity of $\Gamma$ point can participate the intersubband transitions.
band wavefunction's feature size, and this feature size is defined by the quantum well width $W_{QW}$ that is typically several tens of lattice cell size $a_{cell}$. This scenario is illustrated in Figure 4-5(b), showing that only the phonon modes close to $\Gamma$ point can be excited in an electron-acoustic phonon scattering. The same statement also holds for electron-LO-phonon scattering because of similar reasons. It should be noted that this property, that electrons only interacts with acoustic phonons and LO phonons in the vicinity of $\Gamma$ point, is only characteristic for THz frequency range. In mid-infrared intersubband transitions, electrons are energetic enough to transfer a momentum far away from $\Gamma$ point.

The observation that acoustic phonon scattering is quasi-elastic-type has two-fold impact on THz emission device performance. Firstly, the hot electron effect is proven to be intrinsic to electron transport in MQWs with subband spacing below LO-phonon energy. For the three-level system of M10 structure for example, if the electrons are
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cold on upper subband $E_3$, they can only be scattered to $E_2$ level by either elastic intersubband scattering or quasi-elastic acoustic phonon scattering. Electrons thus gain kinetic energy on $E_2$ and become hot. As illustrated schematically in Figure 4-6, with $\Delta E_{21}$ at one LO-phonon energy, electrons scattered to $E_3$ level of next module by LO-phonon scattering keep the kinetic energy and become hot. This hot electron effect reduces the intersubband scattering time $\tau_{32}$. The second impact of quasi-elastic-type of acoustic phonon scattering is the sensitivity of $\tau_{32}^{ac}$ on lattice temperature as revealed by Figure 4-4(a). Since electrons transfer small energy to the acoustic phonons, shown in Figure 4-5, only the acoustic phonons close to the $\Gamma$-point participate intersubband scattering. These low-energy acoustic phonon modes can be easily populated with elevated lattice temperature and leads to stimulated acoustic phonon scattering. Using the Bose-Einstein distribution, it is estimated that

$$\frac{1}{\tau_{32}^{ac}} \propto \frac{1}{e^{\hbar \omega_q - \Delta E_{21}/kT} - 1} \propto T_l. \quad (4.21)$$

4.3 Non-equilibrium LO phonons

Since acoustic phonon scattering is a slower process, with small energy loss per scattering event, LO-phonon emission is the only efficient mechanism of dissipating electron energy in electrically pumped MQWs. For a steady-state pumping condition, excess LO phonons, i.e., non-equilibrium LO phonons, can be generated and maintained because of a finite rate to be decomposed into acoustic phonons through anharmonic lattice interactions. These non-equilibrium LO-phonons will stay in the active region because of the negligible group velocity of optical phonon modes at $\Gamma$ point. The non-equilibrium LO phonons can be reabsorbed by electrons and consequently, electrons will be scattered back from lower subband to higher subband. This phonon bottleneck phenomenon will reduce the subband population inversion.

Hot LO phonons have been a subject of study in bulk polar semiconductors in the
course of hot carrier cooling by electron-LO-phonon scattering or hole-LO-phonon scattering [141, 142, 143]. This issue is important for device applications such as developing high-modulation-rate semiconductor diode lasers [144]. Non-equilibrium LO phonons generated by intersubband scattering have been observed in superlattice structures [145]. For electrically pumped MQW structures, a non-equilibrium LO-phonon population can have an impact on device performance by affecting the subband populations and thus subband population inversion [146].

4.3.1 Intersubband LO-phonon emission and absorption

The rate of one electron scattered from state $k_u$ on upper subband to state $k_l$ on lower subband by LO phonon emission is the same rate as generating one LO-phonon at wavevector of $q_\parallel = k_u - k_l$. From Equation 4.2, this rate is expressed as

$$W_{k_u \rightarrow k_l} = \frac{\pi \omega_{LO} e^2 |A_{u \rightarrow l}(q_\parallel)|^2}{\epsilon_p \epsilon_0 V} \frac{q_\parallel^2}{(N_{LO}(q) + 1)}$$

$$\times \delta_{k_u - k_l, q_\parallel} \delta(E_u(k_u) - E_l(k_l) - \hbar \omega_{LO}). \quad (4.22)$$

When integrating the above expression with $dq_\parallel$, the LO-phonon population $N_{LO}(q)$ in 3D $q$ space can be transferred into the equivalent LO-phonon population $N_{LO}(q_\parallel)$ in 2D $q_\parallel$ space. This can be done by making the following identity,

$$\int_0^\infty dq_z \frac{|A_{u \rightarrow l}(q_\parallel)|^2}{q^2} (N_{LO}(q_\parallel, q_z) + 1) \equiv \left( \int_0^\infty dq_z \frac{|A_{u \rightarrow l}(q_\parallel)|^2}{q^2} \right) (N_{LO}(q_\parallel) + 1). \quad (4.23)$$

In this way, the scattering rate Equation 4.22 can be considered as a collective LO-phonon generation rate in $q$ space with $q_\parallel$ component. By summing over $k_u$ and $k_l$ states, and integrating with $dq_z$ on the right side of Equation 4.22, the LO-phonon generation rate is
\[ \dot{N}_{LO}(q_{||}) = \sum_{k_u} \sum_{k_l} \sum_{q_z} W_{k_u \rightarrow k_l} \]
\[ = \frac{\omega_{LO} e^2}{4\pi^2 \epsilon_0 \epsilon \hbar} \int_{0}^{+\infty} k_u dk_u \int_{0}^{2\pi} d\varphi \int_{0}^{+\infty} dq_z \frac{|A_{u\rightarrow l}(q_z)|^2}{q^2} \left( N_{LO}(q_{||}) + 1 \right) \delta(E_u(k_u) - E_l(k_l) - \hbar\omega_{LO}) \]
\[ = \frac{\omega_{LO} e^2 m^*}{4\pi^2 \epsilon_0 \epsilon \hbar^2} \int_{0}^{2\pi} d\varphi \int_{0}^{+\infty} dq_z \frac{|A_{u\rightarrow l}(q_z)|^2}{q^2} (N_{LO}(q_{||}) + 1). \] (4.24)

Considering the electron occupation on upper subband and lower subband, the complete expression for LO-phonon generation rate by intersubband scattering is

\[ \dot{N}_{LO}^{gen}(q_{||}) = \frac{\omega_{LO} e^2 m^*}{2\pi^2 \epsilon_0 \epsilon \hbar^2} \int_{0}^{2\pi} d\varphi \int_{0}^{+\infty} dq_z \frac{|A_{u\rightarrow l}(q_z)|^2}{q^2} f_u(\epsilon_u)(1 - f_l(\epsilon_l))(N_{LO}(q_{||}) + 1). \] (4.25)

To satisfy both momentum conservation and energy conservation, the kinetic energy of upper state and lower state, \( \epsilon_u \) and \( \epsilon_l \), are expressed in terms of \( q_{||} \) as

\[ \epsilon_u = \frac{\xi - \eta \sin^2 \varphi + \sqrt{\xi^2 - \eta^2 \sin^2 \varphi} \cos \varphi}{2 \sin^2 \varphi}, \]
\[ \epsilon_l = \frac{\xi + \eta \sin^2 \varphi + \sqrt{\xi^2 - \eta^2 \sin^2 \varphi} \cos \varphi}{2 \sin^2 \varphi}, \] (4.26)

where \( \xi \) and \( \eta \) are

\[ \xi = q_{||}^2 \hbar^2 / 2m^* \]
\[ \eta = \Delta E_{ul} - \hbar\omega_{LO}. \] (4.27)

Both \( \epsilon_u \) and \( \epsilon_l \) should be real and positive for the intersubband transition to occur.

The LO-phonon population \( N_{LO}(q_{||}) \) on the right side of Equation 4.25 gives the
stimulated phonon emission rate. It also gives stimulated LO-phonon absorption rate by scattering electrons from lower subband back to upper subband. The LO-phonon annihilation rate by this reabsorption process is

\[ \dot{N}_{\text{ann}}^{\text{LO}}(q_\parallel) = \frac{\omega_{\text{LO}}e^2m^*}{2\pi^2\epsilon_\parallel\epsilon_0\hbar^2} \int_0^{2\pi} d\varphi \int_0^{+\infty} dq_z \frac{|A_{\text{u} \rightarrow \text{i}}(q_z)|^2}{q^2} f_i(\varepsilon_i)(1 - f_u(\varepsilon_u))N_{\text{LO}}(q_\parallel), \quad (4.28) \]

where \( \varepsilon_u \) and \( \varepsilon_i \) satisfy the same equations in 4.26. The electron distributions on upper subband \( f_u(\varepsilon_u) \) and lower subband \( f_i(\varepsilon_i) \) could make the LO-phonon generation and annihilation rates differ significantly from each other. For example, in the M10 three-level system, if the upper subband is \( E_2 \), which is populated by fewer electrons than the lower subband, which is \( E_1 \) (\( E_3 \) of next module), then there will be more electrons being scattered back from \( E_1 \) subband to \( E_2 \) subband than those scattered downward from \( E_2 \) to \( E_1 \).

### 4.3.2 Non-equilibrium LO-phonon population

LO phonons are generated by intersubband emissions, and annihilated through two processes: intersubband absorption and decay into acoustic phonons through anharmonic phonon interaction [147, 148]. Under static pumping conditions, the non-equilibrium LO-phonon population is determined by the following rate equation,

\[ \frac{dN_{\text{LO}}(q_\parallel)}{dt} = \dot{N}_{\text{gen}}^{\text{LO}}(q_\parallel) - \dot{N}_{\text{ann}}^{\text{LO}}(q_\parallel) - \frac{N_{\text{LO}}(q_\parallel)}{\tau_{\text{LO} \rightarrow A}} = 0, \quad (4.29) \]

where \( \tau_{\text{LO} \rightarrow A} \) is the decay time of a LO-phonon into two acoustic phonons. Since LO phonons are located at the zone center, the two acoustic phonons have opposite \( q \) vectors and equal energy, \( 0.5\hbar\omega_{\text{LO}} \). For a finite lattice temperature, acoustic phonon modes are populated and leads to stimulated decay process [149],
where $\tau_{LO\rightarrow A}^0$ is the LO-phonon decay time at lattice temperature $T_l = 0$ K. $\tau_{LO\rightarrow A}$ can be measured by experiments and $\tau_{LO\rightarrow A} = 7 \pm 1$ ps has been reported for GaAs at $T_l = 77$ K by Raman spectroscopy measurements [148]. Theoretically, the decay time $\tau_{LO\rightarrow A}^0$ can be calculated using perturbation theory and related to the Grüneisen constant $\gamma_G$ and other material parameters [150, 151],

$$\frac{1}{\tau_{LO\rightarrow A}^0} = \frac{\gamma_G^2 \hbar \omega_{LO}^5}{64\pi \rho c_s^2 c_{LA}^2},$$

(4.31)

where $c_s$ is the average sound velocity $3/c_s = 2/c_{TA} + 1/c_{LA}$, and $c_{TA}$ and $c_{LA}$ are TA and LA phonon velocities.

Equation 4.31 suggests a temperature-dependent $\tau_{LO\rightarrow A}^0$, because Grüneisen constant $\gamma_G$ is generally a function of temperature. Data are lacking on Grüneisen constant as a function of lattice temperature in GaAs. Literature search only found measured values at low temperatures ($< 30$ K) [152]. To obtain temperature-dependent $\tau_{LO\rightarrow A}$, experimental data are suggested to be used. Figure 4-7 plots $\tau_{LO\rightarrow A}$ as a function of lattice temperature $T_l$ using Equation 4.30. The experimentally measured LO-phonon decay times found in literatures are indicated by the solid circles at several temperatures [148, 153]. The $\tau_{LO\rightarrow A}^0$ in Equation 4.30 is taken as 7.5 ps.

Under steady-state pumping condition, the non-equilibrium LO-phonon population $N_{LO}(q_{ii})$ should be a self-consistent solution between the stimulated emission/absorption equations 4.25 and 4.28, and the phonon rate equation 4.29. For the three-level system in M10 structure, to get a first estimate of the LO-phonon population due to $E_2 \rightarrow E_1$ intersubband scattering, assuming this is a spontaneous phonon emission process, the non-equilibrium LO-phonon population is then given by
Figure 4-7: Decay time of non-equilibrium LO phonons into acoustic phonons in GaAs as a function of lattice (acoustic phonon) temperature $T_l$. The solid circles are measured values by Raman spectroscopy taken from Refs. [148] and [153].
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Figure 4-8: (a) LO-phonon mode population due to $E_2 \rightarrow E_1$ LO-phonon emission process in the three-level system in M10 structure. (b) The LO-phonon mode temperature $T_{ph}$ corresponding to (a), showing hot LO-phonon effect due to finite decay time of the optical phonons.

\[ N_{LO}(q_{||}) = \tau_{LO\rightarrow A} \dot{N}_{\text{gen,21}}^{LO}(q_{||}), \quad (4.32) \]

The vector on $q_{||}$ is dropped because it is symmetrical along all directions. Using $\tau_{LO\rightarrow A} = 7$ ps in Equation 4.33, the LO-phonon mode population as a function of $q_{||}$ is calculated and given in Figure 4-8(a). The subband populations used in the calculation are $n_3 = 2n_2 = 6 \times 10^{10}$/cm$^2$, and the electron temperatures are $T_{e3} = T_{e2} = 100$ K.

It should be pointed out that this LO-phonon mode population is approximately linearly dependent on the electron population on the upper level $n_2$ and inversely proportional to the LO-phonon decay time $\tau_{LO\rightarrow A}$ which is a function of the lattice temperature $T_l$. It is also noted that the relative distribution of non-equilibrium...
Figure 4-9: (a) LO-phonon mode population due to $E_3 \rightarrow E_2$ LO-phonon emission process by hot electron effect on $E_3$ level in M10 structure. (b) Total LO-phonon mode population due to both $E_2 \rightarrow E_1$ and $E_3 \rightarrow E_2$ LO-phonon emissions.

LO phonons in $q_\parallel$-space is sensitive to the subband energy separation $\Delta E_{21}$, since it determines the momentum that electrons transfer to phonons. The LO-phonon mode temperature $T_{ph}$, corresponding to the mode population, is plotted in Figure 4-8(b). The temperature at $q_\parallel = 0.6 \times 10^8$/m, which has peak LO-phonon population of $N_{LO} = 0.44$, is approximately 350 K, higher than the electron temperature $T_e$ and the lattice temperature $T_l$.

Besides the LO-phonon emissions from $E_2 \rightarrow E_1$ intersubband transitions, the $E_3 \rightarrow E_2$ transition also emits LO phonons due to hot electron effect, and contributes to the total non-equilibrium phonons,

$$N_{LO}(q_\parallel) = \tau_{LO \rightarrow A}[\dot{N}_{LO}^{gen,21}(q_\parallel) + \dot{N}_{LO}^{gen,32}(q_\parallel)].$$  \hspace{1cm} (4.33)
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Figure 4-10: Using non-equilibrium LO-phonon mode population in Figure 4-9(b), (a) reduced LO-phonon population due to $E_1 \rightarrow E_2$ stimulated absorption process in M10 structure; (b) reduced LO-phonon population due to $E_2 \rightarrow E_3$ and $E_3 \rightarrow E_2$ stimulated LO-phonon absorption process.

Using the LO-phonon generation rate Equation 4.25, the LO-phonon population due to $E_3 \rightarrow E_2$ transition is calculated for M10 structure with $n_3 = 2n_2 = 6 \times 10^{10}/\text{cm}^2, T_{e3} = T_{e2} = 100$ K. This is plotted in Figure 4-9(a). The total non-equilibrium LO phonon population, by combining $E_3 \rightarrow E_2$ and $E_2 \rightarrow E_1$ intersubband transitions, is given in Figure 4-9(b). Compared with LO-phonon emissions from $E_2$ to $E_1$ transition, the $E_3 \rightarrow E_2$ intersubband scattering by LO phonons is due to hot-electron effect and results in much less LO-phonon population using $T_{e3} = 100$ K subband temperature and $\Delta E_{32} = 15.3$ meV energy spacing. In Figure 4-9(a), the generated LO-phonon population due to $E_3 \rightarrow E_2$ transitions peaks at much higher $q_{||}$, approximately $1.9 \times 10^8/\text{m}$, because of the small subband separation below LO-phonon energy.
Figure 4-11: For M10 structure, the non-equilibrium LO-phonon population obtained by the self-consistent solution among LO-phonon generation rate through intersubband emission, LO-phonon annihilation rate through intersubband absorption, and LO-phonon decay rate into acoustic phonons. The subband electron populations and temperatures are indicated. The decay time of LO-phonons into acoustic phonons is 7 ps for a lattice temperature of 100 K.
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The non-zero phonon mode population will lead to stimulated LO-phonon absorption processes. A portion of the non-equilibrium LO phonons generated by intersubband emission can be reabsorbed which reduces the number of non-equilibrium LO phonons. The number of reduced phonons can be calculated using the LO-phonon annihilation rate Equation 4.28. Using the phonon population given in Figure 4-9(b), the corresponding reduced number of LO phonons due to both $E_1 \rightarrow E_2$ and $E_2 \rightarrow E_3$ stimulated absorptions are given in Figure 4-10(a) and (b) respectively for M10 structure. Again in the calculation $n_3 = 2n_2 = 6 \times 10^{10}/\text{cm}^2, T_{e3} = T_{e2} = 100$ K is used.

$$N_{LO}(q||) = \tau_{LO \rightarrow A}[\dot{N}_{LO}^{\text{gen}, 21}(q||) + \dot{N}_{LO}^{\text{gen}, 32}(q||)],$$  \hspace{1cm} (4.34)

For intersubband energy separations close to LO-phonon energy, such as $E_2$ and $E_1$ in M10 structure, both LO-phonon emission and absorption processes are allowed for all the electrons on the subbands. For energy separations well below the LO-phonon energy, such as $\Delta E_{32}$, only part of the electron on the upper subband in the hot electron tail can be scattered by LO-phonon emissions, whereas all the electrons on the lower subband can absorb one LO phonon and be scattered back.

The non-equilibrium LO-phonon population, obtained by subtracting the original mode population in Figure 4-9 with the reduced number of LO phonons by intersubband absorption in Figure 4-10 (a) and (b), should re-enter LO-phonon generation rate Equation 4.25, annihilation rate Equation 4.28, and phonon rate Equation 4.29 to iterate, until a self-consistent solution is achieved among these three equations. This is the non-equilibrium phonon mode population for a given subband electron populations and temperatures. For M10 structure, with $n_3 = 2n_2 = 6 \times 10^{10}/\text{cm}^2, T_{e3} = T_{e2} = 100$ K, the calculated non-equilibrium LO-phonon population is presented in Figure 4-11.
4.3.3 Modified subband populations

In this section, the effect of hot LO phonons on intersubband scattering and electron transport will be addressed. This is the issue under concern since, for a THz emission MQW structure, it affects the subband electron population and thus population inversion.

First, with the presence of the non-equilibrium LO-phonon population obtained in Figure 4-11 in previous section, the intersubband back-scattering time \( \tau_{12} \) and \( \tau_{23} \) by LO-phonon absorption processes is calculated using Equations 4.11 and 4.13 for M10 structure. Electron temperatures \( T_{e3} = T_{e2} = 100 \text{ K} \) are assumed in the calculations to take into account the hot electron effect.

With the presence of intersubband back-scattering by LO-phonon absorptions, the expression for subband populations in Equations 2.6-8 should be modified as

\[
\begin{align*}
    n_3 &= \frac{\tau_{32}\tau_{12}/(\tau_{32} + \tau_{12})}{\tau_{32}\tau_{12}/(\tau_{32} + \tau_{12}) + \tau_{21}\tau_{23}/(\tau_{21} + \tau_{23})} N_D, \\
    n_2 &= \frac{\tau_{21}\tau_{23}/(\tau_{21} + \tau_{23})}{\tau_{32}\tau_{12}/(\tau_{32} + \tau_{12}) + \tau_{21}\tau_{23}/(\tau_{21} + \tau_{23})} N_D, \\
    \Delta n_{32} &= \frac{\tau_{32}\tau_{12}/(\tau_{32} + \tau_{12}) - \tau_{21}\tau_{23}/(\tau_{21} + \tau_{23})}{\tau_{32}\tau_{12}/(\tau_{32} + \tau_{12}) + \tau_{21}\tau_{23}/(\tau_{21} + \tau_{23})} N_D.
\end{align*}
\]

Table 4.1 gives intersubband scattering times and population inversions for the M10 structure with and without hot LO-phonon effect for comparison.

For the M10 structure, without hot LO phonons, the population inversion is 83% of total carrier density per module \( N_D \) due to the hot electron effect. With the presence of hot LO-phonon effect, the population inversion is reduced to 57% \( N_D \), mostly
Figure 4-12: For M10 structure, (a) intersubband scattering times as functions of the non-equilibrium LO-phonon population which is indicated by the peak phonon population. The phonon distribution in $q_{\parallel}$ space is assumed to be the same as in Figure 4-11. (b) Corresponding subband population and population inversion as functions of LO-phonon population.
due to the back-scattering of electrons from $E_1$ level to $E_2$ level. This back-scattering process can be a serious problem which degrades population inversion in THz emission MQW structures, especially when the non-equilibrium LO-phonon mode population is large. To evaluate the effect of hot LO phonons on subband population, the dependence of intersubband scattering times on the LO-phonon population needs to be obtained. For a fixed LO phonon decay time into acoustic phonons, the non-equilibrium LO-phonon population should be proportional to the pumping of the MQW structure, i.e., the total free carriers in the structure that give LO-phonon emissions. As an approximation, for M10 structure, the non-equilibrium LO-phonon population is linearly proportional to the total free carriers per module, i.e., the sheet doping density $N_D$. In Figure 4-12(a), the intersubband scattering time is calculated for M10 structure as a function of peak value of non-equilibrium LO phonons, and the profile of LO-phonon population is assumed to be the same as Figure 4-11. This peak value of LO-phonon population is proportional to the total carrier density.
per module, $N_D$. Phonon peak value of 0.36 corresponds to $N_D = 9 \times 10^{10}/\text{cm}^2$ in M10 structure. It is seen that $\tau_{21}$ and $\tau_{23}$ drop quickly with increasing LO-phonon population since intersubband absorption processes are directly proportional to the LO-phonon population, whereas $\tau_{32}$ and $\tau_{21}$ change slowly because phonon emission is a combination of spontaneous processes and stimulated processes. The change of intersubband scattering times will effect the subband populations and thus population inversion between $E_3$ and $E_2$, and this is given in Figure 4-12(b) by Equation 4.37. With the peak LO-phonon population around one, the degree of population inversion, $\Delta n_{32}/N_D$, decreases to less than half of the ideal case without non-equilibrium LO phonons.

The above estimate of the effect of non-equilibrium LO phonons on population inversion gives a guideline on the design of MQW structures for THz intersubband lasers. Increasing the total carriers per module will reduce the degree of population inversion, thus push the inverted population to a diminishing point. The absolute population inversion as a function of total free carriers per module, $N_D$, is given in Figure 4-13. It is suggested that, for M10 structure for example, the sheet doping per module should be within $3 \times 10^{11}/\text{cm}^2$. Further increasing the carriers per module does not improve population inversion significantly, but instead will draw large current density through the structure and cause device heating.

4.3.4 Numerical modeling of electron transport

In the previous subsection in calculating intersubband scattering times due to hot LO-phonon effect, the non-equilibrium LO-phonon population is given and is independent of the subband populations. In an more accurate numerical model, once the subband population is obtained by the rate equations, one should iterate to re-calculate the non-equilibrium LO-phonon population as it has been done in subsection 4.3.2. The iteration then proceeds until a self-consistent solution is achieved between the subband populations and non-equilibrium LO phonons. Within the framework of device
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Figure 4-14: Modeling of intersubband scattering of M10 structure incorporating phonon systems. Self-consistent solutions need to be achieved among subband populations, intersubband scattering, and non-equilibrium LO phonons using numerical iterations.

modeling presented in Figure 2-1 of Chapter 2, a more complete numerical model incorporating hot electron effect, lattice heating, and hot LO-phonon effect is given in Figure 4-14 by adding a chain of temperature-dependent intersubband scattering times. This model needs an input of lattice temperature $T_l$ and estimation of the subband electron temperatures $T_{ei}$. For M10 structure as an example, it calculates subband population inversion for a given sheet doping per triple-quantum-well module, by treating electron system and phonon system in a self-consistent manner. The numerical crunching is albeit a heavy one even for this simple three-level system.

4.4 Discussions

The temperature-dependent intersubband scattering times presented in this chapter can be used to interpret the current densities measured for several M10 structures listed in Table 2.4 in Chapter 2. At designed bias, the current density of M100 device, which has 100 modules of the triple-quantum-well structure, is almost twice of the
current density of M10 device, which has only 10 triple-quantum-well modules. This result indicates that heating speeds up the intersubband scattering rates because M100 device dumps 10 times more electrical power than M10 device in the active region. Current densities of M10p and M10pp devices, which have the same triple-quantum-well structures but more carriers in active region, confirm this point by extracting the effective scattering time $\tau_{eff}$ which is defined as the ratio of the current density with total carriers per module. From the expression of current density in Equation 2-9, the effective scattering time is

$$\tau_{eff} = \frac{(\tau_{32} + \tau_{21})\tau_{31}}{\tau_{32} + \tau_{31}} \approx \frac{\tau_{32}\tau_{31}}{\tau_{32} + \tau_{31}}.$$  \hspace{1cm} (4.38)

For the M10 structure, $\tau_{31}$, which is the direct LO-phonon scattering time of electrons from $E_3$ level to $E_1$ level through middle barrier and collector barrier, is calculated to be $\tau_{31} = 43$ ps. Considering $\tau_{21}$ is much shorter compared with $\tau_{32}$ and $\tau_{31}$, it thus can be ignored in the expression of $\tau_{eff}$.

From the measured $\tau_{eff}$ in Table 2-4 and calculated $\tau_{31}$ for M10 structures, the current density bottleneck $\tau_{32}$ is calculated and given in Table 4.2. By referring to the intersubband scattering time $\tau_{32}$ due to lattice heating in Figure 4-4 and hot electron effect in Figure 4-2 respectively, the lattice temperature and electron temperature, which give rise to a reduction of $\tau_{32}$ if it is due to purely lattice heating or hot electron effect, are given in this table. In real devices, this reduced $\tau_{32}$ can be a result of the combination of these two effects. It should be noted that full-ionization of the $\delta$-doping per module is assumed in calculating $\tau_{eff}$, which may overestimate $\tau_{eff}$. Thus the actual $\tau_{32}$ can be shorter and the temperatures can be higher than the numbers listed in Table 4.2. Electron temperature and lattice heating in the range of 50 K ~ 100 K or higher is a reasonable estimate.

The presence of hot LO phonons in affecting current density is not included, although this effect can change the subband population significantly. To make an independent evaluation of the hot phonon effect on current density, intersubband
scattering times presented in Table 4-1 with and without non-equilibrium LO-phonon population are used to calculate the M10 structure's current density in these two cases to compare. With back-scattering from lower subband to higher subband, the device's current density is expressed as

\[
J_o = \frac{n_3}{\tau_{31}} + \frac{n_2}{\tau_{21}} - \frac{n_3}{\tau_{12}}
= \frac{n_3}{\tau_{31}} + \frac{n_3}{\tau_{32}} - \frac{n_2}{\tau_{23}},
\]  

(4.39)

By plugging in \(\tau_{32}, \tau_{21}, \tau_{23}\), and \(\tau_{12}\) in Table 4-1, \(\tau_{eff} = 16\) ps and \(\tau_{eff} = 19\) ps are obtained respectively for without and with the non-equilibrium LO-phonon population given in Figure 4-11. It is thus seen that the presence of hot-phonon effect does not affect the current density significantly. The \(\tau_{eff}\) obtained here is shorter than the measured \(\tau_{eff}\) for M10 and M100 devices, simply because higher electron temperatures \(T_{e3} = T_{e2} = 100\) K have been assumed in calculating the intersubband scattering times in Table 4-1.

To summarize, in M10 structure design, hot electron effect and lattice heating do not significantly affect subband populations and thus population inversion, but they affect the device’s current density. In contrast, hot LO-phonon effect does not affect current density as much as the lattice heating or hot electron effect, but it can degrade the population inversion severely.
Chapter 5

Measurement Setup and Device Fabrications

5.1 Introduction

Measurement of far-infrared or THz is not a trivial task since it is usually featured with weak emission signal, lack of appropriate detectors, and cryogenic temperature operations. Other problems need to be circumvented for a successful measurement in this spectral region include: possible overwhelming blackbody radiation caused by device heating, water absorption, and right window materials which need to be both transparent to the frequency of interest and compatible with the cryogenic equipment. All the previous spectral measurements of far-infrared emissions from 2D electron gas in Si-inversion layers and GaAs/Al_xGa_{1-x}As heterostructure interface used a set-up developed by Gornik and coworkers [154, 155]. In their setup, both the emission device and the detector were mounted in a light pipe with closed ends so that all the emitted radiation can be collected onto the detector. A filter, made of a magnetic-field-tunable n-type InSb cyclotron resonance absorber [156], is placed between the emission device and detector, and the whole system is placed in a liquid helium cooled superconducting magnetic dewar. This measurement facility has been
successfully used to resolve the first intersubband emission from a superlattice structure by Helm et al. [8, 9]. Very recent spectral measurements of far-infrared emissions from hot quasi-one-dimensional quantum wires and parabolic graded quantum wells also employed this set-up [157, 158]. High optical collection efficiency makes this type of set-up very suitable for weak far-infrared or THz emission signal measurements. However, the intrinsic linewidth of the cyclotron resonance in InSb filter limits the resolution of the resolved emission spectra to 2-3 meV [9, 157]. For laser device development, spectral measurement set-up with higher resolution must be available in order to see the stimulated emission and narrowed lasing linewidth.

Spectral resolution ($< 1 \text{ cm}^{-1}$ or 0.125 meV) can only be achieved by using external spectrometers, and a Fourier Transform Infrared spectrometer (FTIR) is a suitable tool for this frequency range. The emission light needs to be brought out of the device dewar and fed into the spectrometer. In this research project, an FTIR set-up has been developed and demonstrated for THz spectral measurements. To the author's knowledge, this is the first set-up of this kind that has been established in the field.

5.2 THz spectral measurements

In this section the experimental set-up for THz spectral measurements is described. Successful measurement of THz spontaneous emission depends on other experimental conditions, especially the blackbody radiation due to device heating. Such measurement issues will be quantified to give necessary measurement parameters.

5.2.1 Measurement set-up

Figure 5-1 gives the schematic description of the measurement set-up. The THz emission MQW device is mounted in a cryostat and immersed in liquid helium at 4.2 K during the measurement. The cryostat has a glassfiber isolated liquid nitrogen
Figure 5-1: Measurement set-up for revolving THz emission spectrum
shield, and depending on the electrical power dumped to the device, will hold liquid helium for 3-6 hours during measurements. A vacuum jack separates the 4.2 K helium chamber from room temperature. There are therefore two windows that the emission light has to pass through to get out of the cryostat. The emission light is collimated by an off-axis paraboloid mirror coated with 1 μm thick gold and fed to the FTIR, a Magna 850 from Nicolet Instruments. The light coming out of the FTIR is then focused by a second paraboloid mirror to a THz detector, either a composite silicon bolometer or a gallium-doped germanium photon detector. The total distance from the emitter to the detector through the FTIR system is approximately 0.9 meter. For emission measurements, the FTIR is operated at step-scan mode. The position of the Michelson interferometer’s moving mirror is controlled by solenoids through a digital signal processing module in the FTIR. The interference pattern of a build-in Ne:He laser in the optical path is used to calibrate the mirror’s scan position. A personal computer records the interferogram, which is the emission power received by the detector as a function of the position of the moving mirror, and performs a fast Fourier transform to give the emission spectrum. Since the THz detectors, both the Si-bolometer and the Ge:Ga photon detector, are capacitance-coupled differential detectors, the emission signal needs to be modulated at certain chopping frequency by applying pulsed bias on the device. The signal from the detector is demodulated by a lock-in amplifier.

Device mounting

Processed wafers containing emission devices are diced into smaller dies by cleaving along the [1 1 0] or [1 1 0] crystal orientation. To allow easy changing of the device from measurement to measurement, the die is mounted with substrate side down onto a down-cavity ceramic chip carrier using silver epoxy. The chip carrier is pinned to a chip-carrier socket on the measurement rack of the cryostat. The silver epoxy should provide strong adhesion, good electrical conductivity, and reasonable thermal
conductance. The epoxy used is H20E from Epo-Tek, and needs to be cured at 130 °C for ~ 5 minutes. Each die usually has many emission devices and the one to be tested is wire-bonded to the leads of the chip carrier. For grating-coupled surface emission, a condensing cone with inner surface coated with 1 μm thick gold is placed directly above the device shown in Figure 5-2(a); for facet-coupled edge emission, shown in Figure 5-2(b), a copper reflection triangle is mounted by silver epoxy with its 45°-reflection mirror facing the the cleaved emission facet, and the emission light is reflected up to the condensing cone. In the cryostat, the condensing cone is mounted on the same measurement rack as the chip-carrier socket and is looking at the windows of the cryostat.

**THz window materials**

The inner window and the outer window of the cryostat for THz transmission have different requirements. The inner window is cold at 4.2 K and in direct contact with liquid helium. Thus the material should be both transparent to THz frequency and also should guarantee a good seal to prevent small helium molecules from escaping into the cryostat’s vacuum jack. The outer window, however, is kept at room temperature and does not experience thermal recycling. Thus it only needs to be highly transmissive to the THz frequency. To find appropriate window materials which can cover
Figure 5-3: Transmissivities of the THz window materials. (a) 0.1 mm polypropylene measured by FTIR. (b) 2 mm high-density polyethylene measured by FTIR. (c) 1 mm sapphire with antireflection coating (solid line) and without (dashed line), provided by Infrared Laboratory.
the THz frequency range, different crystalline and plastic materials have been tested for both the THz transmissivity and vacuum sealing capability, including polypropylene, polyethylene, sapphire, quartz, and some other plastic materials. The outer window is chosen to be a 0.1 mm thick polypropylene film because it has the highest THz transmissivity. Its transmission spectrum is shown in Figure 5-3(a) measured by FTIR. Attempts to use thick (1 mm) polypropylene as the inner window failed. Due to its large thermal contraction coefficient, this plastic material does not hold the indium-sealed inner window at 4.2 K. The inner window was finally chosen to be a 1 mm thick sapphire crystal covered with a 10 μm thick low density polyethylene thin film as the antireflection coating, shown in Figure 5-3(c) by the solid line. The dashed line is the transmission without the antireflection coating. Sapphire strongly absorbs infrared radiation from 1 THz to 30 THz at room temperature [159], and becomes transparent in the 1 THz \(-9\) THz range at low temperatures. Quartz is an alternative material for the inner window at lower THz frequency but not very transparent beyond 4 THz. The drawback of using these ionic crystals as the inner window is that they have TO-phonon-active reststrahlen band absorption beyond 10 THz. Sapphire at 4.2 K completely cuts off at 11.5 THz (46 meV) [160]. It seems the only possibility to extend the window’s working frequency is to use plastic materials such as polypropylene for both the inner and outer windows. These types of materials can cover frequency from far-infrared to mid-infrared. Figure 5-3(b) is the transmission spectrum of 2 mm thick high-density polyethylene (HDE) material. FTIR measurements reveal that it remains transparent to approximately 20 THz (80 meV) and is more rigid than polypropylene for making the indium-sealed low-temperature window. Efforts have been made to install this material as the inner window. Unfortunately, after a several measurements, it couldn’t withstand the thermal cycling and was broken by aging. The present cryostat, with sapphire as the inner window, cannot be used to measure intersubband emissions above 46 meV.
THz detectors

The silicon composite bolometer is a broad band thermal detector, which is restricted to work in the THz frequency range by using long-wavelength cut-on filters. The model used in this research is made by Infrared Laboratory at Tucson, Arizona. The silicon element has an area of $3 \text{ mm} \times 3 \text{ mm}$ and is mounted on a diamond substrate. The resistance of the silicon element is modulated by radiation heating. The corresponding voltage change on a current sensing resistor is capacitance-coupled to a cold-stage transconductance amplifier and then a preamplifier with a gain of 200. The detector module is mounted on the cold-plate of a dewar’s helium bath, and is optimized to operate at 1.6 K by pumping the helium bath. After the preamplifier stage, the voltage responsivity is $S = 1.1 \times 10^8 \text{ V/W}$ at the output. The noise equivalent power is $NEP = 4.1 \times 10^{-14} \text{ W/Hz}$. The cut-on frequency of the filter can be chosen to be 18 THz, 6 THz, 3 THz, and 1 THz by a filter wheel. The bolometer’s response time is about 1 ms, leading to a roll-off frequency around 150 Hz.

A THz photonconductive detector is also used majorly for the purpose of fast
CHAPTER 5. MEASUREMENT SETUP AND DEVICE FABRICATIONS

detection. It turns out that this fast detection capability plays a key role in resolving intersubband THz emission from the designed MQW structures, and this issue will be addressed later. Due to the small photon energy of THz frequencies, intrinsic photon detectors that utilizes cross-band photon absorption are impossible even using Hg$_x$Cd$_{1-x}$Te material. Extrinsic photon detectors that use doped impurities to set up narrow energy separation between the impurity states and valence band (or conduction) are the only option. The p-type gallium-doped germanium and indium-doped germanium are the materials that have been found suitable for THz frequencies [161]. The photon detector used in this research is a gallium-doped germanium detector made by Infrared Laboratory and operated at 4.2 K. The current responsivity of the detector is 65 A/W measured by using a 770 K blackbody radiation source. The feedback resistor is 1 kΩ, leading to voltage responsivity of $S = 1.6 \times 10^6$ V/W by including the preamplifier stage with gain of 25. The noise equivalent power of the photon detector is $1.7 \times 10^{-13}$ W/$\sqrt{\text{Hz}}$, and the response time is $\sim 1 \mu$s. This fast response time leads to a greatly improved roll-off frequency around 5 kHz, which is primarily limited by the detector’s electronic $RC$ time constant. Compared with the bolometer, a photon detector is a narrow band detector. The relative response of this detector is provided by Infrared Laboratory and is plotted in Figure 5-4. The peak frequency of the detector’s responses is $f_0 \sim 3$ THz. Below $f_0$, detector rolls off quickly because of the forbidden energy transition from valence band to the impurity states; above $f_0$, the detector slowly rolls off according to $1/(f - f_0)$ due to the joint density of states for interband optical transitions.

5.2.2 Emission measurement issues

This subsection discusses several experimental issues that are related to THz emission measurements. Understanding these issues is necessary to interpret the measurement data and ensure correct experimental results.
Figure 5-5: Water vapor absorption lines, by measuring the transmission of a 300 K blackbody radiation through air using FTIR and Si-bolometer. The resolution is 0.015 THz. The dashed line indicates the roll-off of the blackbody radiation power.

**Water absorption**

Water vapor absorption is present over the entire THz frequency region. Figure 5-5 gives the water absorption lines obtained by measuring the transmission of a 300 K blackbody radiation through the free-space FTIR set-up using the Si bolometer. Water absorption lines are discrete and cause sharp features on the emission spectrum if a fine resolution below 1 meV (0.25 THz) is used. The water absorption lines are stable and not sensitive to the weather's humidity condition or the length of the optical path. It seems the only way to remove the water absorption is by using vacuum optical bench which joins the cryostat, FTIR, and the detector together. Purging the optical path with dry N\textsubscript{2} gas has been tried. It only reduces the water absorption strength by about 30% \(\sim\) 50% but still cannot completely remove the sharp features. This method is not recommended for emission measurements because the purge flow of N\textsubscript{2} gas often drifts during the data collection of step-scan and causes unreliable interferograms. However, if the spectrum is collected at low resolutions,
such as 0.5 THz, the fine features caused by water absorption lines will be averaged out and won’t appear in the spectrum.

**Blackbody radiation caused by device heating**

Blackbody radiation power in the THz frequency range due to possible device heating needs to be estimated, to be compared with the power level of intersubband emission signal. Depending on the cut-on frequency $f_c$ of the THz detector, device temperature $T_D$-dependent blackbody radiation power is given by $P_b(T_D) = A \int_0^{f_c} df \epsilon(f)p(f)$, where $A$ is the device emission area, $\epsilon(f)$ is the emissivity and $p(f)$ is 3D photon power density as a function of $T_D$. The absolute emission power with cut-on frequency of $f_c = 18$ THz and $f_c = 6$ THz is calculated using frequency dependent emissivity of GaAs [110], and is given in Figure 5-6 for a 100 $\mu$m $\times$ 100 $\mu$m emission area.

It has been found in measurements that this blackbody radiation power due to device heating, on the order of several tens of nW, has overwhelmed the THz emission
signal. In order to directly “see” the intersubband THz emissions from MQW structures, an effective solution is proposed. It overcomes this problem by increasing the chopping frequency of the device’s bias, so that the slower thermal radiation power is rolled off, and leaves the intersubband THz emission as the dominant signal. Here is the brief analysis of this measurement method.

The thermal equation governing the device temperature change, in the presence of electrical power $IV$, can be written as

$$c_v \frac{dT_D}{dt} + (T_D - 4.2)\kappa = P_{IV}$$

(5.1)

where $c_v$ is the heat capacitance of the device in unit of Joule/K and $\kappa$ is the thermal conductivity between the device and liquid helium in unit of Watt/K. If the device bias is modulated by square-wave voltage pulse with frequency $\omega$, the electrical power dumped to the device can be written into a dc term plus a time-dependent harmonic term: $P_{IV} = P_{IV}^0 + P_{IV}^\prime e^{i\omega t}$. Correspondingly, the device’s temperature is also a superposition of a dc term and a time-dependent harmonic term, $T_D = T_D^0 + T_D^\prime(\omega)e^{i\omega t}$. From Equation 5.1, these temperature terms are expressed as

$$T_D^0 = \frac{P_{IV}^0}{\kappa}$$

(5.2)

$$T_D^\prime(\omega) = \frac{P_{IV}^\prime / \kappa}{i\omega \tau_T + 1}$$

(5.3)

where the thermal time constant is $\tau_T = c_v / \kappa$. Since in emission measurements, the lock-in amplifier is only looking at the detector’s output with the frequency component at $\omega$, the detected blackbody radiation power is then $P_b \propto T_D^\prime(\omega)$. Clearly, by going to high chopping frequencies, $\omega \gg \omega_T = 1/\tau_T$, $T_D^\prime(\omega)$ then diminishes according to Equation 5.3 and the detected blackbody radiation power will roll off, even though the device’s static temperature $T_D^0$ can be significantly high. In principle, this measurement technique can be used to detect very weak intersubband THz emissions
in the presence of severe blackbody radiation due to device heating, provided that the device's thermal time constant is much longer than the intersubband transition time. It will be shown in next chapter that it is necessary to use fast Ge:Ga photon detector to resolve the THz emission spectrum, even though the Si bolometer is a more sensitive detector.

The thermal time constant $\tau_T$, which gives the roll-off frequency $\omega_T$ of black-body radiation, is generally a function of temperature because both $c_v$ and $\kappa$ are temperature dependent. This roll-off frequency can be conveniently determined in experiment, and from which, $\kappa$ is given with the well-known $c_v$ value of GaAs. The device's operation temperature $T_D^0$ can then be inferred from Equation 5.2.

5.2.3 Optical power collection efficiency

Based on the above descriptions of the spectral measurement set-up with FTIR, the optical power collection efficiency $\eta_{cl}$, defined as the ratio of the power received by the detector to the power emitted by the device, is rather low. $\eta_{cl} = 1 \sim 2\%$ has been estimated by including the following factors.

Water absorption in the optical path gives about 30% power transmission. This is based on comparing the emission power received by the detector between with and without purging the optical path with dry N$_2$ gas. The FTIR's Michelson interferometer reflects 50% optical power back when the moving mirror is generally away from the centerburst position. The reflector for He:Ne laser beam on the far-infrared beam splitter will block some light and gives about 20% power reduction. For the window materials used in the cryostat, polypropylene gives about 85% transmission, and the sapphire window gives about 70% transmission. Considering the condensing cone's flaring angle, the diameters of the cryostat's windows, and the size of the paraboloid mirrors, it is estimated that only $20 \sim 40\%$ of the optical power can be collected depending on the alignment condition of the optics.
5.3 Device fabrications

The GaAs/Al$_{0.3}$Ga$_{0.7}$As MQW structures grown on GaAs substrate are processed into grating-coupled surface emission devices and bar devices for edge emission. Different masks have been designed with various grating periods, emission areas, and different widths of the bar structures. Device processing for spontaneous emissions generally involve two or three mask steps. A special processing technique to fabricate metallic waveguide devices has been developed for the first time in this research project, which involves wafer bonding and selective etching techniques.

5.3.1 Device processing for spontaneous emission

Figure 5-7 shows the three-mask processing sequence of THz emission devices using Micro-Lab's facility in Building 13. Major steps are listed below, and processing details are given in Appendix B.

1. Wafer cleaning using solvent.

2. First photolithography step defining device mesas by wet etching or reactive-ion-etching (RIE).

3. Second photo step defining active region and deposit SiO$_2$ or Si$_3$N$_4$ for insulation on side wall and bonding path.

4. Third photo step defining grating stripes for surface emission devices and top metal layers for edge emission devices, using lift-off technique. The metal is Ni/Ge/Au alloy deposited by electron-beam system.

5. Rapid thermal annealing (RTA) to make ohmic contacts to devices.

Figure 5-8 is a top view picture of part of a processed wafer showing grating emission devices and bar devices. Each device has a bonding path. There are different grating periods and metallic filling factors for grating-coupled surface emission devices, to provide different coupling loss for emission measurements. There are also
Figure 5-7: Schematic showing three-mask processing sequence of THz emission devices. (a) MBE-grown MQW wafer. (b) Device mesa formed by wet chemical etching or RIE. (c) Side wall and bonding path covered with SiO₂ or Si₃N₄ for insulation. (d) Grating definition for surfacing emission. (d') Edge emission device with top covered by metal.
different widths for the edge emission bar devices. For effective lateral mode confinement, the width of the bar device should be larger than half of the THz wavelength in semiconductor [100].

5.3.2 Metallic waveguide fabrication for THz laser devices

As discussed in Chapter 3, plasma waveguide possesses large cavity dissipation loss if used for THz confinement. This loss can be greatly reduced by using a metallic waveguide, with two metal layers sandwiching the MQW active region. Fabrication of a metallic waveguide is thus critical in achieving THz intersubband lasing. Since the several-micron-thick MQW thin film is MBE-grown on lattice-matched semi-insulating GaAs substrate, substrate removal and wafer bonding are inevitable steps and need to be developed. The majority of the loss for a metallic waveguide is caused by the 0.1 μm ~ 0.3 μm heavily doped contact layers which are necessary to make ohmic contacts between GaAs and the metals. A recently developed non-alloyed
ohmic contact technique for GaAs can eliminate this heavily-doped region, and thus can further reduce the metallic waveguide loss. In this subsection, a non-alloyed contact, wafer bonding, and selective etching to remove substrate are described. First metallic waveguide devices have been successfully fabricated by combining these techniques. By calibrating the processing parameters, the fabrication results have been quite reliable.

Figure 5-9 is the schematic showing major steps in fabricating the metallic waveguide. The end side of the MBE-grown MQW wafer has non-alloyed ohmic contact
Figure 5-10: The making of non-alloyed ohmic contact. (a) MBE-grown layers of a thin heavily doped n++ GaAs region, capped by non-doped LTG GaAs. (b) Schematic band diagram showing electron tunneling from n++ region to mid-gap states in the LTG cap layer.

with a low-temperature-grown (LTG) GaAs cap layer. A Ti/Au metal layer is deposited on this side of the MBE wafer and directly forms an ohmic contact to the GaAs/Al0.3Ga0.7As MQW structure without alloying. Meanwhile, another bare n+ GaAs wafer is deposited with Ni/Ge/Au alloy and annealed to form ohmic contact. This wafer will be the “new substrate” hosting the MQW thin film after the original semi-insulating substrate for MBE growth is removed. The two wafers both with Au layers on top are bonded to each other by thermal-compression method. Substrate removal can then be performed by first polishing to lap off most of the thickness of the substrate. The remaining part of the substrate is removed by selective etching, so that the MQW active region remains unattacked. At this point, the thin film of MQW structure is bonded on another n+ GaAs wafer, with a metal layer beneath it. The device processing using mask steps described in previous subsection can then start. For bar devices, finally an alloyed metal layer is deposited on top of the thin film. This forms a metallic waveguide as shown in Figure 5-9(4).
Non-alloyed ohmic contact

For n-type bulk doping of Si in GaAs, the doping level saturates at \( n = 5 \times 10^{18}/\text{cm}^3 \), above which, Si replaces As as acceptors and donor concentration stops to increase with the doping density [162]. Since MBE growth usually involves excessive As flux, the stabilization of As produces mid-gap states and causes the Fermi-level pinned at mid-gap at the surface. Electrons are thus depleted from the surface. This allows, in thermal equilibrium condition, that essentially all the Si dopants replace Ga as donors. Thus the n-type doping level can reach as high as \( 10^{20}/\text{cm}^3 \) at the surface of a MBE-grown GaAs wafer. Such a high doping level leads to a thin Schottky barrier and thus non-alloyed ohmic contact between the semiconductor and metal can be formed [162, 163]. However, this surface layer with high doping concentration is only several nanometers thick. If the wafer is exposed to air for days, this thin surface layer becomes oxidized and will be removed during subsequent wafer processing. This non-alloyed ohmic contact seems only possible for in-situ condition. To allow for an ex-situ non-alloyed ohmic contact, Prof. Melloch’s group at Purdue University developed a method using low-temperature-grown (LTG) GaAs cap layer to preserve and passivate this highly doped surface layer [164]. The MQW wafer used for metallic waveguide fabrication in this research also adopts this method for making a non-alloyed ohmic contact on the end-side of the MBE wafer. Its schematic description is given in Figure 5-10. The MQW structure and the \( n^{++} \) contact region is grown at \( \sim 600 \) °C normal MBE growth temperature. The top several nanometers of the \( 5 \times 10^{19}/\text{cm}^3 \) Si-doped contact region will have donor concentration approaching the doping density and forms highly-doped surface layer. The 35 Å thick intrinsic GaAs cap layer is grown at 250 °C, resulting in excessive As scattered in the volume causing numerous mid-gap states. The wafer oxidization will remove partially this LTG cap layer and the highly doped surface layer can be preserved. The mid-gap states in the remaining GaAs cap layer facilitate electron transport by defect-assisted tunneling. Contact resistances as low as mid-10\(^{-7}\) \( \Omega \text{ cm}^2 \) have been achieved. This LTG cap is also more resistant to
oxidization \[165, 166\] and can survive 400 °C annealing temperature in the following device processing [167]. However, the other side of the MQW thin film, i.e., the beginning side for MBE growth, cannot use this non-alloyed ohmic contact technique and an alloyed Ni/Ge/Au ohmic contact is used on the top of the finally processed metallic waveguide, shown in Figure 5-9(4).

Wafer bonding

The wafer bonding is accomplished by Au-Au metal bonding using thermal compression method [168]. Another alternative is solder bonding by using metal alloys with low melting temperatures, such as In [169, 170], Sn, or Pb/Sn [171]. In the metallic waveguide fabrication, Au-Au bonding is chosen because it offers several advantages: i) Au has higher electrical conductivity and thus less waveguide loss; ii) Au has much higher melting temperature that can survive subsequent device processing temperatures such as annealing of the top alloyed ohmic contact at \(\sim 380 \, ^\circ C\), whereas solder alloys, such as Sn, have melting temperatures below 300 °C; iii) Solder alloys tend to oxidize when exposed to air whereas Au is chemically stable. The surface condition is critical for a successful wafer bonding.

The Au-Au metal bonding is performed using MTL/TRL facilities. Its recipe and steps are listed below:

1. E-beam deposit Ti/Au: 200 Å/10000 Å on the MBE-grown MQW wafer to form non-alloyed ohmic contact.
2. E-beam deposit Ni/Ge/Au/Ni/Au: 50 Å/660 Å/1330 Å /400 Å/10000 Å on the n⁺ GaAs bare wafer to form alloyed ohmic contact.
3. Inspect the two wafers under microscope. Blow wafers with N₂ gun to make sure there are no visible dust particles on the surfaces, especially those left by wafer scribing and cleaving.
4. Perform ozone cleaning of the two wafer surfaces for 2 minutes.
Figure 5-11: Schematic description of GaAs substrate removal by polishing and selective etching.

(5) Place the two wafer pieces together with Au sides face-to-face. Align crystal orientations of the two wafers. Place them on a hot plate. Heat up the hot plate to 380 °C.

(6) Apply pressure of 20 psi using tweezers on the top wafer with a duration of 2 minutes. Remove the bonded wafers after the hot plate is cooled down.

The very thick Au layers of 10000 Å are necessary for successful wafer bonding. The wafer surfaces should be very clean to give good quality and yield of the bonding. Otherwise, the bonded interface will not survive subsequent thermal recycling during device processing. Especially after the final RTA step at 380 °C, some of the wafers may have small bubbles developed under the thin film, indicating that the bonding interface has peeled off.

**Substrate removal by selective etching**

Figure 5-11 describes the semi-insulating GaAs substrate removal technique using selective etching. First the 400 μm thick substrate is thinned to about 100 μm by polishing, using the lapping facility in CMSE. The sand paper used for polishing has grain size of 30 μm. The lapping chuck has a meter with 25 μm division, so that the
Figure 5-12: SEM micrographs of fabricated metallic waveguide devices. The viewing angle is 45° with respect to the [1 1 0] cleavage facet of the MQWs thin film where the THz radiation is coming out.
polished thickness can be well controlled. The remaining GaAs substrate is selectively etched by a petri-dish mixture: NH$_4$OH:H$_2$O$_2$=1:19. Etching rate of this petri-dish mixture is very selective between GaAs and high mole AlGaAs. It takes about 30 minutes to etch away the remaining GaAs substrate then the etching stops at the 5000 Å thick Al$_{0.5}$Ga$_{0.5}$As etching stopper grown by MBE. During petri-dish etching, H$_2$O$_2$ oxidizes As, and NH$_4$OH dissolves the oxide. If the wafer turns black, more NH$_4$OH should be added. When GaAs is gone, a shining mirror-like surface appears and gradually spreads out to the whole area, indicating that Al$_{0.5}$Ga$_{0.5}$As etching stopper has been reached and etching of GaAs substrate is finished. When exposed to air, this etching stopper can quickly become oxidized and is turned into deep blue color with reflection fringes, another distinctive feature from GaAs. To protect the MQW structure and the host n$^+$ GaAs wafer to which the MQW thin film is bonded, before this petri-dish etching, the edge and bottom of the bonded wafers are sprayed and covered with Shipley 1813 photoresist. The photoresist is then hard-baked at 130 °C to become solidified, which leaves it very resistant to the etchant. After the etching is complete, this photoresist can be removed by acetone. By taking the advantage of extremely selective etching ($10^7$) for Al$_x$Ga$_{1-x}$As between $x > 0.4$ and $x < 0.4$ using hydrofluoric acid [108, 172], the 5000 Å thick etching stopper is removed by 48% HF acid in 30 seconds to 1 minute, leaving the n$^{++}$ contact layer as the surface.

**Fabricated metallic waveguide devices**

Figure 5-12 are micrographs taken by scanning-electron-microscope (SEM) showing the fabricated metallic waveguide devices. These pictures are top views with a 45° tilted angle looking at the [1 1 0] cleavage facet of the bar structure, where the THz radiation is coming out. The cleaving is done by diamond scribing and subsequent cleaving of the GaAs host substrate. The top metal, which is alloyed Ni:Ge:Au for making an ohmic contact, looks rough due to the thermal annealing processing and formation of eutectics. The partial sticking-out of this metal layer after crystal...
cleaving shouldn’t affect device’s performance. The facet of the MQW thin film looks flat and smooth, indicating that the cleavage of the GaAs host substrate can result in a good reflection mirror for the MQW thin film, even though they are separated by a 2 \( \mu \text{m} \) thick metallic layer. The bonding interface of the two Au layers is indicated by a white line, due to the electron charging effect at the interface under SEM operation condition. The Au-Au bonding interface is very irregular, as a result of the bumpy surface of the n\(^+\) GaAs host substrate which is chemically etched and polished. This explains the fact that a very thick Au layer (\( \sim 1 \mu\text{m} \)) needs to be deposited on each wafer and is critical for successful wafer bonding.

**I-V of metallic waveguide device**

The dc I-V of the THz emission MQW structure is measured at 4.2 K after the metallic waveguide fabrication and device processing are completed. The emission MQW structure, named LSN80, has a similar design as the three-level system in M10 triple-quantum-well structure with designed bias around 50 mV/module. It contains 80 modules so that the required operation bias is \( \sim 4 \) V. The dc I-V is measured using the 100 \( \mu\text{m} \times 100 \mu\text{m} \) diode patterns on the processed wafer, with the top metal of the MQW thin film and the bottom side of the host n\(^+\) GaAs wafer as two terminals. Figure 5-13 presents two typical I-V curves measured from different diodes on the same wafer. Curve-(a) has a predicted I-V relation as designed, with current peak and subsequent NDR appearing at approximately 4 V, which corresponds to the \( E'_1 \rightarrow E_3 \) subband level alignment. Curve-(b) has similar current density as (a) where the current clamping occurs at a much higher voltage of 12.5 V. The transmission line measurement (TLM) structure adjacent to the measured diodes are used to characterize the alloyed ohmic contact, and indicate that Curve-(b) is caused by the non-ideally alloyed contact resistance. This behavior is attributed to the non-uniform annealing temperature distribution during the RTA process, due to the inhomogeneous metal bonding interface between the MQW thin film and the
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Figure 5-13: Measured two typical dc-IV curves at 4.2 K of LSN80 MQW structure processed into metallic waveguide devices. The device areas are 100 μm x 100 μm. The designed bias is 4 V.

host GaAs wafer. The inhomogeneity of the bonding interface is probably due to the variations in surface cleanness of the bonding wafers, or caused by the thermal expansion which is inevitable during the temperature ramping-up period in the RTA process.

Issues about the alloyed ohmic contact

In present metallic waveguide fabrications, the need for an alloyed ohmic contact on one side of the device sets up a hurdle to achieve high quality metallic waveguide. The reasons are summarized below:

(1) Compared with a non-alloyed ohmic contact, an alloyed ohmic contact has thicker n+ doped region which will give additional plasma loss for THz confinement.

(2) In subsequent device processings after wafer bonding and selective etching, the highest thermal recycling temperature is 90 °C for soft-baking of the photoresist, except the RTA process which needs to reach 350 °C ~ 380 °C [173].
The possible bubbles developed during RTA will bend the metallic waveguide, leading to useless devices.

(3) As discussed above, alloyed ohmic contact resistance may not be uniform due to the inhomogeneous bonding interface and consequently the non-evenly distributed annealing temperature.

Future work to replace this alloyed ohmic contact will help to solve these issues and improve the quality of the metallic waveguides [174].
Chapter 6

THz Intersubband Emission

6.1 Introduction

Measuring the THz spontaneous emission from a designed MQW structure is an initial and critical step in developing an intersubband THz laser. Emission frequency, linewidth, power level, and its spectrum need to be obtained as feedback information to evaluate MQW structure design, transport modeling, and cavity properties. Electrical measurements such as I-V characteristics provide valuable but limited information. Several THz emission MQW structures have been designed, grown, and processed. For the first time, THz intersubband emissions from electrically pumped MQW structures at designed frequencies have been observed. The measurement results of these structures are provided in this chapter, as well as the analyses and discussions. THz emission from MQW structure fabricated into metallic waveguide is also measured. Lasing action has not been achieved so far. Besides emission measurements, absorption measurement is a complimentary method, which can also be used to verify the subband levels and MQW structure simulation [7].
6.2 Mid-infrared absorption measurement

Since the MQW structures designed for THz spontaneous emission measurements are grown on n+ substrate which is electrically conductive to provide a backside terminal, absorption measurement of these structures using a light transmission scheme is impossible due to the heavily absorptive substrate. The LSN80 structure is an exception, however. It has 80 triple-quantum-well modules and is grown on semi-insulating substrate which is removed later for metallic waveguide fabrication. Thus the LSN80 MBE wafer allows for transmission measurement. The Nicolet Magna 850 FTIR spectrometer provides facility for mid-infrared spectrum measurement. It has a KBr beamsplitter covering mid-infrared from 40 meV to 900 meV, and a liquid nitrogen cooled HgCdTe detector with long-wavelength cutoff at 80 meV. A sample-holder stage with focusing optics can be installed between the Michelson interferometer and the detector for transmission measurement. The mid-infrared broad band radiation is provided by a globar blackbody source with a temperature at 1250 °C. A metal-grid polarizer is used to select the incident light’s polarization. The beam is focused by a paraboloid mirror into the sample to enhance the transmission signal.

Measurement principle

Figure 6-1 shows the MQW sample processed into a wedge waveguide structure for transmission measurement. Its two facets are polished into 45° angle, so that the transmitted light experiences several bounces within the waveguide to maximize interactions with the thin MQW active region. Due to the intersubband selection rule, only the photons with polarization normal to the quantum wells can be absorbed by intersubband transitions. Assuming the light is incident along the wafer plane, the effective interaction length $l$ is thus given by

$$ l = \frac{2Nt \sin^2 \theta}{\cos \theta} $$

(6.1)
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Figure 6-1: Wedge waveguide used for absorption measurement. $t$ is the MQW region thickness, $w$ is the semi-insulating substrate thickness. $\theta$ is the angle between the $E$ field polarization and quantum well planes.

where $N$ is the number of bounces within the waveguide, and it is expressed as

$$N = \frac{L}{2w \tan \theta} + 1$$  \hspace{1cm} (6.2)

The $\theta$, which is the bouncing angle indicated in Figure 6-1, is calculated to be $\theta = 57^\circ$. The length of the wedge waveguide $L$ used in the experiment is over 5 mm long; and the semi-insulating substrate thickness is 0.4 mm, which results in 5 bounces. For the LSN80 structure, the active region thickness is $t = 2.56 \mu m$. From Equation 6.1, the effective interaction length is $l = 3.3 \times 10^{-5} \text{ m}$. Intersubband absorption coefficient $\alpha(f)$ is simply the negative gain $-G(f)$ without subband population inversion. By measuring the transmission of light with polarization satisfying the selection rule $T_{90}$, and the transmission of light that does not interact with intersubband transitions, $T_0$, to ratio out the background absorption caused by non-intersubband transition mechanisms, the intersubband absorption coefficient has the following expression,

$$e^{-\alpha(f)l} = \frac{T_{90}}{T_0}$$  \hspace{1cm} (6.3)

The absorption spectrum $\alpha(f)$ can thus be obtained. The absorption peak gives the intersubband transition energy $h\nu_0 = E_j - E_i$ and linewidth broadening $\Delta f$. From the gain expression in Equation 3.20, an absorption intensity $S$ is defined as the area beneath the absorption peak, and it is related to the dipole moment for intersubband transition according to the following relation,
Figure 6-2: Mid-infrared intersubband absorption spectrum of LSN80 structure on semi-insulating substrate at room temperature, obtained by transmission measurements using FTIR linear scan. The dashed line indicates the least-square Lorentzian fit of the two peaks.

\[
S \equiv \int_{-\infty}^{+\infty} \alpha(f)df = \frac{\Delta N_{ij} e^2 \omega_0 z_{ij}^2}{2n\epsilon_0 c_0 \hbar}
\]  

(6.4)

Dipole moment \( z_{ij} \) can thus be obtained from the absorption measurement [51, 55].

**LSN80 mid-infrared absorption spectrum**

Figure 6-2 is the measured mid-infrared intersubband absorptance (\( \equiv \log_{10}(T_{90}/T_0) \)) of LSN80 structure at room temperature obtained from transmission measurement. The second \( y \)-axis gives the absorption using the expression in Equation 6.3 and the calculated effective interaction length \( l \). The triple-quantum-well parameters of LSN80 structure is listed in Table 6.1
Table 6.1: LSN80 triple-quantum-well structure parameters

<table>
<thead>
<tr>
<th>$W_3$</th>
<th>$W_2$</th>
<th>$W_1$</th>
<th>$B_3$</th>
<th>$B_2$</th>
<th>$B_1$</th>
<th>$N_D$ (in collector barrier)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23 ML</td>
<td>22 ML</td>
<td>31 ML</td>
<td>20 ML</td>
<td>10 ML</td>
<td>7 ML</td>
<td>$0.6 \times 10^{11}/\text{cm}^2$</td>
</tr>
</tbody>
</table>

Figure 6-3: Numerically simulated energy levels and square magnitude wavefunctions of the subbands in LSN80 triple-quantum-well structure at zero bias. The arrows indicate intersubband absorptions at mid-infrared. The simulation does not include nonparabolicity. The height of the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ barrier is 245 meV.
Table 6.2: Comparison of simulated values with results obtained from absorption measurement for LSN80 structure

<table>
<thead>
<tr>
<th></th>
<th>$E_{41}$(meV)</th>
<th>$\Delta f_{41}$(meV)</th>
<th>$z_{41}$(Å)</th>
<th>$E_{52}$(meV)</th>
<th>$\Delta f_{52}$(meV)</th>
<th>$z_{52}$(Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>simulated</td>
<td>109.6</td>
<td>11.2</td>
<td>148.6</td>
<td>9.0</td>
<td>101.5</td>
<td>10.7</td>
</tr>
<tr>
<td>(nonparabolicity)</td>
<td>(101.5)</td>
<td>(10.7)</td>
<td>(134.1)</td>
<td>(8.7)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>measured</td>
<td>110.9</td>
<td>14.5</td>
<td>135.9</td>
<td>11.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lorentzian fit</td>
<td>110.8</td>
<td>6.5</td>
<td>139.1</td>
<td>13.1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The absorption spectrum in Figure 6-2 reveals two intersubband absorption peaks. At room temperature with zero bias, the electrons from ionized donors will occupy the lowest state in the buffer well and partially the second lowest state in the emitter well. These two peaks are identified as the intrawell intersubband absorptions from the ground state to the first excited state in these two quantum wells respectively.

Figure 6-3 shows the numerically simulated subband levels and square magnitude wavefunctions in LSN80 structure at zero bias. The arrows indicate the intersubband transitions from $E_1$ to $E_4$ and from $E_2$ to $E_5$, to compare with the absorption spectrum in Figure 6-2.

In calculating the dipole moments of these two intersubband transitions, the electrons occupations on subbands $E_3$, $E_2$, and $E_1$ are assumed to obey Maxwell distribution $n_3 : n_2 : n_1 = e^{-\Delta E_{31}/kT} : e^{-\Delta E_{21}/kT} : 1$, where at room temperature $T=300$ K. From the simulated subband energy levels in Figure 6-3, this ratio is $n_3 : n_2 : n_1 = 0.31 : 0.49 : 1$. From charge neutrality condition $n_1 + n_2 + n_3 = N_D$, subband populations $n_1, n_2$, and $n_3$ are obtained. Other higher subband levels are assumed to be empty. Dipole moments $z_{41} = 14.5$ Å, $z_{52} = 11.6$ Å are then deduced by measuring the areas beneath the absorption peaks, to be compared with the numerically simulated values.

The numerically simulated subband levels, dipole moments, and measured results from absorption spectrum for LSN80 device are summarized in Table 6.2. The simulated numbers in parentheses are obtained from a modified SEQUAL code which incorporates GaAs conduction band nonparabolicity [36, 175]. This is based on
the argument that for electrons with subband energy in mid-infrared range, band-nonparabolicity effect should be taken into account when calculating subband levels. The fact, that the simulated subband energy separation $E_{41}$ without band nonparabolicity is exactly the measured absorption peak around 110 meV, should be considered as a coincidence. In SEQUAL code, conduction band offset is taken as $\Delta E_c/\Delta E_g = 0.64$ for GaAs/Al$_x$Ga$_{1-x}$As heterostructure with $x = 0.3$; this can be an uncertainty [176]. The simulated $E_{41}$ with band-nonparabolicity is about 9 meV lower than the measured peak position. This can possibly be explained by the lower barrier height used in the SEQUAL simulation code. The ground state levels are less sensitive to barrier height, compared with the first excited states. The linewidth of $E_{41}$ transition is only 6.5 meV from Lorentzian fit at room temperature. Such a narrow linewidth at mid-infrared benefits from the intrawell type of intersubband transition, and also indicates the good quality and module-uniformity of the MBE growth. The linewidth of $E_{52}$ transition is much wider, 13.1 meV from Lorentzian fit, which can be explained by the fact that $E_5$ subband is closer to the barrier edge, thus extends more in space and experiences interface roughness scattering. The measured dipole moments agree with simulated values within 20 $\sim$ 30%, considering the accuracy of measurement condition and deviation of sheet doping per module by MBE growth.

In general, for LSN80 triple-quantum-well structure design, the simulated subband energy separations and dipole moments match well with the results obtained from mid-infrared absorption measurement.

6.3 THz emission results

6.3.1 Blackbody radiation vs. intersubband emission

As discussed in Chapter 5, measurement of THz emission can be difficult due to the strong blackbody radiation in the THz frequency range caused by device heating. First, the THz intersubband emission power needs to be estimated from grating-
coupled M100 structure as an example, to compare with the thermal radiation power. The emission measurements need to be carried out at much higher chopping frequency if the signal is dominated by the blackbody radiation, as discussed in Section 5.2.

By applying the formula developed in Chapter 3, Equation 3.11 for 3D radiative transition lifetime, Equation 3.21 for peak gain expression, Equation 3.28 for intersubband THz radiation power, and Equation 3.41 for emission power coupled out of the device, the device emission power at designed frequency for M100 structure is calculated as a function of electron population on \( E_3 \) level for different cavity dissipation loss, and is plotted in Figure 6-4. The grating coupling loss of \( \alpha_g = 300 \text{ cm}^{-1} \) is assumed for \( p = 15 \text{ \mu m} \) grating period and filling factor of \( f = 0.5 \) by referring to Figure 3-7. Emission linewidth of 1 THz is used in the calculation. In Figure 6-4, the nonlinearity of the power increase with subband population \( n_3 \) is due to the increased population inversion and thus the optical gain. Considering the relative large cavity loss due to substrate plasma which is \( \alpha_{pl} \approx 400 \text{ cm}^{-1} \) using Figure 3-13 for substrate doping around \( 1 \times 10^{18}/\text{cm}^3 \), \( P_{em} \sim 35 \text{ nW} \) is estimated for \( n_3 = 7 \times 10^{10}/\text{cm}^3 \) electrons on the upper level. Compared with the result of blackbody radiation in Figure 5-6, the THz intersubband emission power is comparable to or smaller than that of the thermal radiation for device heating up to 80 K.

Emission measurements have confirmed this scenario. In early spectral measurements using Si bolometer, essentially all the emission spectra obtained from different devices and MQW structures show broad band blackbody radiation. Results obtained from Ge:Ga detector are similar if using low chopping frequencies in the hundred Hertz range. Figure 6-5 shows several blackbody emission spectra measured from grating-coupled M100 devices with emission area of 200 \( \text{\mu m} \times 400 \text{ \mu m} \). The 1.6 K spectra are obtained by pumping the cryostat’s helium bath to lower the helium temperature. The helium is in superfluid phase at this temperature, and has infinite large thermal conductivity which provides better cooling of the device. All these spectra are measured at 100 Hz chopping frequency and with 100 \( \mu s \) pulse width (duty cycle
CHAPTER 6. THZ INTERSUBBAND EMISSION

40

35-

100

lm x 100

m

300cm-'

200cm

1

30

25

400cm-

20

15-

600c

800cm

-1

10

5

0 1

2

3

4 5 6 7

n 3 (10^10/cm^2)

Figure 6-4: Estimated THz spontaneous emission power from grating-coupled M100 structure as a function of the electron population on E3 subband for different cavity dissipation loss. The device area is 100 μm x 100 μm. The grating coupling loss is assumed to be α_g = 300 cm⁻¹.

of 1%). The bias voltages for these spectra are near the designed value of 5.0 V. The filter of the bolometer has cut-on frequency at 18 THz. The device emission power is estimated by using the following formula,

\[ P_{em} = \frac{V_s}{S\eta_d r_d} \]  \hspace{1cm} (6.5)

where \( V_s \) is the detector's signal output voltage measured by the lock-in amplifier, \( S \) is the responsivity of the detector, \( \eta_d \) is the optical collection efficiency of the FTIR measurement system, and \( r_d \) is the duty cycle of the bias.

Figure 6-5(a) is a typical blackbody emission spectrum at 4.2 K using Si-bolometer. The total emission power is about 200 nW, which indicates a device heating temperature around 70 K by referring to Figure 5-6. The spectrum obtained by the Ge:Ga photon detector in (b) is similar, and the narrower-band emission compared with (a) is due to the spectral response of Ge:Ga photon detector. (c) is the spectrum
Figure 6-5: Emission spectra due to device heating from grating-coupled M100 structure at 100 Hz chopping frequency and with 100 μs pulse width. The device’s emission area is 200 μm \times 400 μm. The spectra are taken using step scan with resolution of 1 THz. Spectra in (d) is a special case which is only obtained when the superfluid helium level close to the device.
measured at 1.6 K. The power level is one order of magnitude lower than that in (a), because of the lower device temperature when placed in the superfluid helium. A dip of the spectrum close to 9 THz is considered to be the TO-phonon-like polariton absorption when the device's surface temperature is cold and possesses reststrahlen band absorption [110]. The spectrum in (d) is an interesting result which only occurs during the measurement when the superfluid helium level is lowered down several centimeters above the device. When this occurs, the emission power is boosted by a factor of 3 \textasciitilde 5. The resolved spectrum in (d) shows this power boost is due to the additional emission peak at 9 THz, making the spectrum in (d) complementary to (c). Possible explanation of this phenomenon is that, when the helium level is close to the device, cooling of the device is not very efficient and causes an increase in surface temperature. The surface region does not function as an absorber but instead emits blackbody radiation. Compared with the blackbody radiation at 4.2 K in (a), the emission in (d) is much sharper and is concentrated at 9 THz, which is the TO phonon energy in GaAs. As a matter of fact, if the spectrum in (a) is considered as blackbody radiation in thermal-equilibrium condition, the sharp emission peak in (d) is more like a non-thermal-equilibrium behavior, which can possibly be explained by the TO-phonon subsystem heating. In superfluid helium, the lattice temperature is colder than that in normal liquid helium, and thus the broad blackbody radiation is reduced. However, the TO-phonon subsystem can be heated up by hot LO phonons during electrical pumping of the MQW structure, as discussed in Chapter 4. TO-phonon modes are then populated through anharmonic lattice interaction by the decay of hot LO phonons. Lowering the lattice temperature in superfluid helium contrasts this non-equilibrium TO-phonon emissions at 9 THz, compared with the emission spectrum at 4.2 K in (a).

Due to the relative strong blackbody radiation, intersubband THz emission has not been observed using the bolometer because the chopping frequency is limited to 1 \textasciitilde 2 hundred Hz. However, the thermal emission spectra obtained by the broad
band bolometer detector shown in Figure 6-5 provide valuable information on device heating and reveal possible TO-phonon subsystem heating and reststrahlen band emission/absorption. Further investigations of these phenomena will help to address issues such as MQW's lattice temperature and non-equilibrium LO-phonon population, which play key roles in analyzing electron transport in THz emission MQW structures.

The intersubband THz emission power is not as strong as expected and is buried in the emission signal caused by device's heating. To be able to see THz intersubband emission, it is necessary to roll off the blackbody radiation by going to a much higher chopping frequency, as discussed in Section 5.2. From this viewpoint, the fast Ge:Ga photon detector becomes the only choice for THz emission measurements.

In later emission measurements of grating-coupled M100 structure using Ge:Ga detector at high chopping frequencies, the dominant thermal emission power begins to
decrease and is rolled off at approximately $4 \sim 8 \text{ kHz}$. In order to completely get rid of the blackbody radiation and leave a clean intersubband THz emission spectrum, chopping frequency has gone up to $20 \text{ kHz}$, which is beyond the Ge:Ga detector’s roll-off frequency of $5 \text{ kHz}$. This chopping frequency is also higher than the roll-off frequency of THz intersubband emission for M100 structure. According to the calculated 3D spontaneous emission lifetime for M100 structure, this frequency is at $1/2\pi \tau_{sp} = 6.3 \text{ kHz}$.

The measured roll-off frequency of blackbody radiation gives thermal time constant of $\tau_T$ in $20 \sim 40 \text{ } \mu\text{s}$, which can be used as another independent method to estimate the device operation temperature. In figure 6-6, the thermal conductance $\kappa$ vs. device temperature $T_D$ is plotted from both $P_{IV} = \kappa T_D$ and $\tau_T = c_v/\kappa$ relations with various electrical power dumped into the active region and thermal time constant. The intersection of these two curves, from given electrical power $P_{IV}$ and measured thermal time constant, determines the device temperature. For a grating-coupled M100 device, the active region has a volume of $400 \text{ } \mu\text{m} \times 400 \text{ } \mu\text{m} \times 3 \text{ } \mu\text{m}$ and the heat capacitance $c_v$ is known using the temperature dependent specific heat data for GaAs from Ref. [110]. The static electrical power dumped to the active region is $P_{IV} = r_d IV$. For a grating-coupled M100 device, at the designed bias of 5 V, the current is 1 A with device area of $400 \text{ } \mu\text{m} \times 400 \text{ } \mu\text{m}$. The duty cycle is 40% for $20 \text{ } \mu\text{s}$ pulse width at $20 \text{ kHz}$ chopping frequency. Therefore $P_{IV} = 2 \text{ W}$. From the measured thermal time constant in $20 \sim 40 \text{ } \mu\text{s}$ range, device temperature of $85 \sim 120 \text{ K}$ is inferred from Figure 6-6, which is higher but consistent with the temperature previously obtained from the blackbody radiation power. The blackbody radiation is primarily determined by the device’s surface temperature, which is expected to be lower than that of the active region.


6.3.2 THz emission from M100 structure

Figure 6-7 presents the THz emission at 3.6 THz from the grating-coupled surface emission M100 structure, compared to the designed intersubband emission frequency at 3.8 THz. The device is submerged in liquid helium. The chopping frequency of the bias is 20 kHz and the pulse width is 20 µs. The Ga:Ge photon detector is used with a lock-in amplifier to demodulate the signal. The spectrum is obtained using step-scan mode with a resolution of 0.5 THz. The inset shows the step-scan interferogram that gives the emission spectrum. The device bias is 4.6 V. Spectra are taken at different biases around the designed bias and all show similar spectra with the emission peak at the same frequency. The device’s emission power, using Equation 6.5, is approximately 1 nW. By referring to the calculated emission power for grating-coupled M100 device, and considering that the measured device has an area of 400 µm × 400 µm, this THz emission power is weaker by two orders of magnitude than estimated. At such a high chopping frequency of 20 kHz, by including the Ge:Ga photon detector’s roll-off at 5 kHz, and intersubband transition roll-off at 6.3 kHz, the emission power is corrected to be 10 nW. Still, there is a factor of 10 difference between the measured and the calculated emission power. Due to the low collection efficiency of the spectral measurement system (~1%), the THz power striking on the detector is at 10 pW level. Because of the relatively large NEP of the photon detector compared with the Si bolometer, a long integration time of 3 ~ 10 seconds is used for the lock-in amplifier to achieve necessary signal-to-noise ratio during the step-scan.

To determine the linewidth of the emission, it is noted that a single Lorentzian function does not fit the spectrum measured in Figure 6-7. According to the designed scheme that uses resonant tunneling to populate electrons on the upper level, because of anticrossing, the intersubband emission at designed frequency should consist of two closely spaced emission peaks, $E_1' \rightarrow E_2$ and $E_3 \rightarrow E_2$, with the peak spacing equal to the anticrossing gap $\Delta_\sigma$. A two-peak Lorentzian fit is made and the result is given in Figure 6-8. Table 6.3 lists the simulated THz intersubband emissions from
Figure 6-7: Resolved THz intersubband emission from grating-coupled M100 structure at 4.2 K using Ge:Ga detector, with spectrum resolution of 0.5 THz. The center frequency is 3.6 THz. The device bias is 4.6 V, with chopping frequency at 20 kHz and pulse width of 20 μs. The grating period is 15 μm with filling factor of 0.5. The device’s area is 400 μm × 400 μm. The inset shows the step-scan interferogram.
Figure 6-8: Two-peak Lorentzian fit of M100 emission spectrum (solid line). The fitted two peaks and their superposition are indicated by the dashed line. $P_1$ and $P_2$ are the heights of the fitted peaks.
Table 6.3: Comparison of simulated M100 THz emission with the Lorentzian fit of the measured emission spectrum.

<table>
<thead>
<tr>
<th></th>
<th>( E_3 \rightarrow E_2 ) (THz)</th>
<th>( E'_3 \rightarrow E_2 ) (THz)</th>
<th>( \Delta \nu ) (THz)</th>
<th>( \Delta f_1 )</th>
<th>( \Delta f_2 )</th>
<th>( z^2 f^3 ) ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>simulated</td>
<td>3.83</td>
<td>4.30</td>
<td>0.48</td>
<td>0.90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>measured (fit)</td>
<td>3.55</td>
<td>4.12</td>
<td>0.57</td>
<td>0.65</td>
<td>1.6</td>
<td>0.69</td>
</tr>
</tbody>
</table>

\( E'_1 \) and \( E_3 \) to \( E_2 \) respectively vs. the measured values obtained by Lorentzian fit.

The spontaneous emission power for each peak is the emission peak height multiplied by the linewidth, which is determined by \( z^2 f^3 \) according to the spontaneous emission lifetime expression in Equation 3.11. The emission power ratio of \( E'_1 \rightarrow E_2 \) to \( E_3 \rightarrow E_2 \) transitions is given for simulated and measured respectively, assuming electron temperature on \( E_3 \) level is high that electrons population on \( n_3 \) is half-half divided between \( E'_1 \) and \( E_3 \) levels according to Equations 2.10 and 2.11. The emission frequencies fit well the designed THz intersubband transitions. The linewidth of the main peak is 0.65 THz, or equivalently 2.6 meV, which is narrow considering the spectral resolution is 0.5 THz or 2 meV. The fact that the linewidth of the second peak is much broader is not expected. The explanation of impurity scattering in the buffer well to \( E'_1 \) level is less feasible. Since strictly speaking, at anticrossing, the two wavefunctions of \( E'_1 \) and \( E_3 \) are 50 – 50% distributed in the buffer well and the emitter well, and therefore they should sense the same amount of impurity scattering.

In THz emission measurements, the polarization of the emitted light is checked by using a wire-grid polarizer to verify the selection rule. However, the birefringence of sapphire as the inner window of the cryostat will scramble the polarization of the emitted light. At 4 THz, the difference of refractive index between the ordinary ray and extraordinary ray is \( n_o = 3.6 \) vs. \( n_e = 4.3 \) at liquid helium temperature [177]. This leads to 90° phase shift between the two rays in 15 \( \mu \)m distance within the sapphire crystal. The sapphire window used in the experiment is 1 mm thick and is randomly cut. Polarization-dependent emission power is not observed on experiment.

In far-infrared or THz measurements, optical transitions of shallow impurity states
in bulk GaAs and quantum wells fall in this frequency range, and need to be carefully ruled out. In bulk GaAs, the 2p-1s transition of hydrogenic dopants is at 1.1 THz [178]. Due to the confinement effect in quantum wells, this 2p-1s transition splits into $2p_{xy}$-1s and $2p_z$-1s transitions with raised energy. The 2p-1s transitions in quantum wells have been well studied and there are both theoretical calculations and experimental data available [179, 180, 181, 182]. For quantum wells narrower than 150 Å, $2p_z$-1s has transition energy above 40 meV which is in the mid-infrared range. The $2p_{xy}$-1s transition energy is insensitive to quantum well width, and is below 6 meV in quantum wells with width from 0 to 150 Å [179].

Figure 6-9 shows the measured emission power using the Ge:Ga photon detector for M100 structure as a function of device bias. The error bar indicates the noise.
level during the measurement. The chopping frequency is 20 kHz, and therefore all the emission power is considered to be due to intersubband emission with the thermal radiation power completely rolled off. The emission power increases approximately linearly with the bias voltage to the designed operation bias at 4.9 V. Emission spectra have been resolved at different biases within the linear region. These spectra are essentially the same as the one shown in Figure 6-7 at 4.6 V, and show no visible voltage-dependent shifts. This behavior is expected since, as described in Section 2.4 in Chapter 2, the bias voltage will be non-uniformly distributed among the modules by means of high-field domain development. As the bias is increased, the designed $E_r \rightarrow E_3$ alignment sequentially develops from one side of the multi-module structure to the other side with increasing the device bias, to give out THz intersubband emission. Thus the emission power increases linearly with the bias, and the emission spectrum remains the same.

Finally, from the resolved emission spectrum, using a linewidth of 0.65 THz, the peak optical gain at center frequency $f_1 = 3.55$ THz is estimated to be 110 cm$^{-1}$ by referring to the gain curve in Figure 3-2. The dipole moment used in the calculation is the simulated value of 25 Å. The subband population inversion used is $1.6 \times 10^{10}$/cm$^2$, or 18% of the sheet doping per module. This is due to the hot LO-phonon limited population inversion of $\Delta n_{32}/N_D = 0.57$ for M100 structure according to the theoretical calculations in Table 4.1. Also remember that $n_3 = n_3^{(3)} + n_3^{(1')}$ from Equations 2.10 and 2.11. The real population inversion contributing to the peak gain at $f = f_1$ should be $n_3^{(3)} - n_2$, which equals to 0.18 $N_D$ in the case of $n_3^{(3)} = n_3/2$.

For grating-coupled M100 structures, the THz emission power is approximately one order of magnitude lower than the calculated. This can be possibly explained by several reasons. First, the grating coupler is separated from the MQW active region by a 0.4 μm thick $n^+$ doped contact layer. The skin-depth of this plasma layer is estimated to be approximately 1 μm using the Drude model. Intersubband emission will be partially shielded by this plasma layer and the coupling of THz photons by
the metallic grating is not as efficient as the ideal case with a perfectly-conducting grating directly covering the MQW structure. Second, the cavity dissipation loss can be greater than the number calculated in Chapter 3. This extra loss is possibly due to additional TO-phonon absorption loss in the presence of non-equilibrium TO phonon population, and extra loss caused by surface plasma mode developed in the graded doping regions at the contact/MQW junctions.

### 6.3.3 THz emission from A10 structure

One of the MQW structures designed for THz emission is named A10. It has ten triple-quantum-well modules and its structure parameters are specified in Table 6.4. Compared with the M10 structure, the A10 structure has a much thicker injector barrier so that the anticrossing gap for $E'_3 \rightarrow E_3$ alignment is smaller. The most pronounced change is the thinner middle barrier and the narrower collector well. As a result, $E_3$ and $E_2$ will be anticrossed to each other at the designed bias. The initial intention for the A10 design was to minimize the emission linewidth broadening, because at anticrossing $E_3 \rightarrow E_2$ transition is more like a intrawell-type with both subbands sensing the same interface roughness scattering [119]. At the designed bias, the wavefunctions of $E_3$ and $E_2$ are 50 - 50% distributed in the emitter well and the collector well. Their energy separation is insensitive to bias and it is primarily set by the anticrossing gap, which is determined by the middle barrier thickness. The thinner this middle barrier is, the larger the anti-crossing gap will be, and less sensitive of the energy separation $E_3 - E_2$ to the bias [13]. The sheet doping per module is higher than that of the M10 structure, $N_D = 1.5 \times 10^{11}/\text{cm}^2$, and is placed in the collector barrier. This modification is expected to minimize the impurity scattering to $E_3$ and

<table>
<thead>
<tr>
<th>$W_3$</th>
<th>$W_2$</th>
<th>$W_1$</th>
<th>$B_3$</th>
<th>$B_2$</th>
<th>$B_1$</th>
<th>$N_D$ (in collector barrier)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25 ML</td>
<td>20 ML</td>
<td>30 ML</td>
<td>21 ML</td>
<td>6 ML</td>
<td>10 ML</td>
<td>$1.5 \times 10^{11}/\text{cm}^2$</td>
</tr>
</tbody>
</table>
CHAPTER 6. THZ INTERSUBBAND EMISSION

$E_2$ states, so that the emission linewidth broadening due to impurity scattering can be reduced. The structure was grown by MBE and processed into grating devices for THz emission measurements.

Figure 6-10(a) shows the self-consistent simulation of A10 structure under designed bias at 51 mV/module, which corresponds to the anticrossings of the three subbands, $E_1'$, $E_3$, and $E_2$. Due to the thick injector barrier, the calculated anticrossing gap between $E_1'$ and $E_3$ is small, $\Delta_o = 0.9 \text{ meV}$. $E_3 - E_2 = 20.5 \text{ meV}$ which corresponds to 5.1 THz radiation, and $E_2 - E_1 = 29.7 \text{ meV}$ corresponding to 7.4 THz. The dipole moments are $z_{32} = 29.6 \text{ Å}$, $z_{1'2} = 29.2 \text{ Å}$ and $z_{21} = 12.6 \text{ Å}$ respectively. Figure 6-10(b) is the measured dc I-V curve of A10 structure at 4.2 K, which is similar to the M10 dc I-V in Figure 2-10. A current bump in 0.5 V - 0.7 V range is observable, indicating the resonant tunneling from $E_1' \rightarrow E_3$ to $E_1' \rightarrow E_4$ alignment when bias voltage is higher than the designed operation point. The NDR region for bias above 1 V corresponds to high-field domain development of $E_1' \rightarrow$ above-barrier state.

Figure 6-11 is the resolved emission spectrum of A10 device at 4.2 K, with bias at 0.6 V. The emission power level is small compared with M100 device, in 0.1 nW range for only 10 modules in device. Resolution of 1 THz is used in collecting the interferogram for necessary signal-to-noise ratio. Two main emission peaks, the first at 3.4 THz, the second at 7.5 THz, are present in the spectrum and are repeatable at different biases. The presence of the second emission peak is considered to be the intersubband emission from $E_2$ to $E_1$ and its emission frequency fits the simulated value well. The first emission at 3.4 THz is lower than the simulated intersubband transition of $E_3 \rightarrow E_2$ at 5.1 THz. Since the $\Delta E_{32}$ is essentially determined by the middle barrier thickness, the only possible explanation is that the actual Al$_{0.3}$Ga$_{0.7}$As barrier is higher than the value used in the simulation, in which $\Delta E_c/\Delta E_g = 0.64$ and gives 245 meV barrier height. A higher barrier will decouple $E_3$ and $E_2$ wavefunctions, and thus reduce the anticrossing gap and the energy separation between $E_3$ and $E_2$. 
Figure 6-10: (a) Self-consistent simulation of A10 structure, showing subband energy levels and square-magnitude wavefunctions. At designed bias of 51 mV/module, $E_1'$, $E_3$, and $E_2$ are anticrossed with one another. (b) Measured dc I-V curve of A10 structure at 4.2 K.
Figure 6-11: THz emission spectrum of A10 device at bias of 0.6 V, coupled by 10 μm period grating. The device area is 400 μm × 400 μm. The chopping frequency is 20 kHz, and the pulse width is 20 μs. The inset shows the step-scan interferogram. The spectral resolution is 1 THz.
Figure 6-12: Simulated intersubband separation of $\Delta E_{32}$ and $\Delta E_{21}$ as functions of the Al$_{0.3}$Ga$_{0.7}$As barrier height at the designed bias for A10 structure. $\Delta E_{32}$ is determined by the barrier height, due to anticrossing.

The energy separation between $E_2$ and $E_1$ is well above their anticrossing gap. This anticrossing gap is simulated to be 7 meV due to the thick collector barrier, 10 ML, used in the A10 structure. $E_2 - E_1$ is then primarily determined by the voltage drop across the collector well and the buffer well. Thus $\Delta E_{21}$ is insensitive to the barrier height. Figure 6-12 shows for A10 structure at designed bias, the simulated $\Delta E_{32}$ and $\Delta E_{21}$ as functions of the barrier height. The fact that the actual barrier is higher than the value used in the numerical simulation is also suggested by the absorption measurement of LSN80 structure, in which case a higher barrier is needed to explain the absorption peak of the $E_1$ to $E_4$ transition. The linewidth of the first emission peak is rather broad, 1.6 THz. Narrower emission linewidths than this value are not observed in measurements by taking spectra at different biases. This can be attributed to the thickness variation of the thin middle barrier during MBE growth, which is only 6 monolayer (17 Å). This thickness variation then causes fluctuation
of the anticrossing gap between $E_3$ and $E_2$ states among different modules, thus
broadens the transition energy of $E_3 \rightarrow E_2$.

The presence of a second emission peak is indicative of significant electron popu-
lation on the $E_2$ level and thus leading to $E_2 \rightarrow E_1$ intersubband emission. From the
calculated dipole moments of $z_{32}$ and $z_{21}$, and the ratio of the measured areas under
the two emission peaks (peak height corrected by the Ge:Ga photon detector spectral
response in Figure 5-4), by using Equation 3.28 it is estimated that $n_3/n_2 = 0.3$, where
$n_3$ is the combined electron population on $E'_1$ and $E_3$ levels since the first peak at 3.4
THz is considered to be one emission peak in the calculations. This result means that
there is no population inversion between $E_3$ and $E_2$ but rather a reversed population
inversion between $E_2$ and $E_1$ levels. By checking the electron-temperature-dependent
intersubband scattering times $\tau_{32}$ and $\tau_{21}$, it is not surprising to see that more elec-
trons are on the $E_2$ subband. Figure 6-13 presents the calculated hot-electron effect
induced LO-phonon intersubband scattering times using the formalism developed in
Section 4.2. The electron temperatures are assumed to be the same for the two sub-
bands. It is shown that $\tau_{32}$ is much faster than $\tau_{21}$ at any given electron temperatures.
There are primarily two reasons that leads to this unintentionally-designed situation.
Firstly, the anticrossing between $E_3$ and $E_2$ at the designed bias maximize the overlap
of these two wavefunctions, making $\tau_{32}$ extremely fast like an intrawell intersubband
transition. Secondly, in the A10 structure, the large sheet doping in the collector
barrier significantly bends the conduction band downward which is shown in Figure
6-10(a), and thus brings closer the energy levels of $E_2$ and $E_1$. $\Delta E_{21}$ is then well
below the LO-phonon energy at designed bias. $\tau_{21}$ is thus much longer than $\tau_{32}$, due
to the thick collector barrier that decouples these two states.

The absence of the $E_2 \rightarrow E_1$ emission peak in the resolved M100 emission spectrum
in Figure 6-7 doesn't mean that it is a good indication that for M100 (or M10) design,
there is no significant electron population on $E_2$ level. Considering the fact that the
roll-off of Ge:Ga detector' spectral response only gives about one-tenth signal at 8.5
THz compared to the peak response, and an extremely large TO-phonon absorption right at this frequency, the $E_2 \rightarrow E_1$ emission might not be observable from the resolved spectrum even though there are electrons populating the $E_2$ level.

### 6.3.4 THz emission from metallic waveguide LSN80 structure

The THz emission structure LSN80 is similar to M100 structure. It is processed into metallic waveguide as described in Section 5.3 in previous chapter. It has 80 modules and the structural parameters are specified in Table 6.1. The self-consistent simulation of LSN80 structure is given in Figure 6-14 at designed bias of 51 mV/module. The sheet doping is $6 \times 10^{10}$/cm$^2$ in the collector barrier, relatively low compared with A10 structure and M100 structure. The band bending is thus small as shown in Figure 6-14. At the designed bias, $\Delta E_{32} = 15.2$ meV and $\Delta E_{21} = 35.7$ meV which is...
right at LO-phonon energy. The anticrossing gap between $E'_1$ and $E_3$ is 1.1 meV, due to the thick injector barrier of 20 ML. The simulated dipole moments are $z_{32} = 21.9$ Å and $z_{21} = 19.6$ Å respectively. The dc I-V curve of the processed LSN80 structure in metallic waveguide is shown in Figure 5-13 in previous chapter. The NDR at 4 V confirms the designed bias of 51 mV/module where $E'_1$ and $E_3$ levels are aligned for resonant tunneling.

For the LSN80 device, from the above calculated dipole moment, a peak optical gain of $\sim 100 \text{ cm}^{-1}$ is estimated at the designed frequency, 3.8 THz, using a population inversion of $2 \times 10^{10}/\text{cm}^2$ as a result of lattice heating, hot electron, and non-equilibrium LO-phonon effects. The linewidth is assumed to be 0.5 THz. The LSN80 structure is processed into metallic waveguides, and a number of the bar devices are tested for THz emission. The loss of the metallic waveguide, as calculated in Chapter 3, is a sum of the facet coupling loss, phonon absorption loss, free carrier
loss, and the plasma loss at the n+ doped contact region between metal and semiconductor. The facet coupling loss is 10 cm\(^{-1}\) for 1 mm long cavity by using Equation 3.33. The TO-phonon absorption loss is estimated to be 5 cm\(^{-1}\) from Figure 3-9. \(\alpha_{fc} = 40\) cm\(^{-1}\) is used for the free carrier loss as a conservative estimate from the 3D Drude model result in Figure 3-10. The plasma cavity loss is calculated to be 12 cm\(^{-1}\) assuming perfect conducting metal and 0.1 \(\mu\)m thin contact plasma regions. The total cavity loss is then estimated to be \(\sim 70\) cm\(^{-1}\). However, in emission measurements, THz lasing action has not been observed from these bar devices.

Figure 6-15 shows the resolved THz emission spectrum of the LSN80 structure at 6.0 V, from a metallic waveguide bar structure with device area of 1 mm \(\times 25\) \(\mu\)m. The first emission peak, at 3.6 THz, fits the simulated \(E_3 \rightarrow E_2\) intersubband transition. The second emission at 5.8 THz, however, cannot be explained by an \(E_2 \rightarrow E_1\) transition, since \(\Delta E_{21}\) is at one LO-phonon energy which corresponds to 9 THz. The presence of the second peak is not well understood. The most plausible explanation is that it is due to \(E_3 \rightarrow E_2\) intersubband emission at higher bias voltage of 110 mV/module. Simulation reveals \(E'_1\) is aligned with \(E_4\) at this bias and the corresponding energy separation between \(E_3\) and \(E_2\) is 28 meV, or 7 THz. At device bias of 6 V, about half of the modules are aligned with \(E'_1 \rightarrow E_4\), and the other half with \(E'_1 \rightarrow E_3\) alignment.

The spontaneous emission power measured from typical 1 mm \(\times 25\) \(\mu\)m bar devices is about 10 nW after being corrected for the detector's response time. To compare with theoretical calculations, the 2D spontaneous radiative lifetime \(\tau_{sp} = 3.2\) \(\mu\)s is used in estimating the emission power. The intersubband radiation power \(P_o = A\Delta E_{32} N_m n_3 / \tau_{sp}\), for 1 mm \(\times 25\) \(\mu\)m device area, 80 modules, and \(n_3 = 4 \times 10^{10}/\)cm\(^2\) upper level population, is then calculated to be 610 nW. Compared with grating-coupled emissions, the facet coupling loss for edge emission is well defined and this clears the ambiguity in calculating the coupling efficiency. By using the expression of Equation 3.29 for emission power coupled out of the device, total cavity loss of
Figure 6-15: Emission spectrum of LSN80 structure at 6.0 V from facet-coupled edge emission metallic waveguide device using Ge:Ga photon detector. The chopping frequency is 40 kHz, and voltage pulse width is 10 μs. The length and the width of the bar are 1 mm and 25 μm respectively. The inset shows the step-scan interferogram. The spectral resolution is 1 THz. The power level is not corrected by the detector’s response time.
\( \sim 700 \text{ cm}^{-1} \) is suggested to explain such a low emission lower level. Considering for spontaneous emission, the facet coupling loss from lateral sides, due to the 25 \( \mu \text{m} \) bar width, is as big as 400 \( \text{cm}^{-1} \), a cavity dissipation loss of 300 \( \text{cm}^{-1} \) is inferred for the metallic waveguide. This cavity loss is much greater than the estimated number, which can be used to explain the fact that lasing threshold is not achieved, and also the low spontaneous emission power.

### 6.4 Discussions

THz emission measurements, from both grating-coupled surface emissions, and facet-coupled edge emissions, have not shown any indications that lasing threshold is approached. The weaker-than-expected spontaneous emission power reveals that the THz cavity loss is much larger than the previous theoretically calculated value. This indicates that there is a large margin to push before the designed MQW structure can reach the THz lasing threshold. Identifying the cavity loss mechanisms and reducing the cavity loss by appropriate measures are the next major research steps before a THz laser can be realized. Here are some issues that the author believes to be important:

1. For metallic waveguide fabrication, the top alloyed ohmic contact which needs to be annealed is detrimental to THz optical cavity. The rough surface introduces additional scattering loss which has not been included in the loss calculations. Plasma loss, resulting from annealing process to drive the dopants into semiconductor and MQW region, can be much larger compared with the bottom side which has a non-alloyed ohmic contact. Surface plasma mode can be formed due to the graded dopant distribution resulted from the diffusive process during the thermal annealing. This can give large cavity loss according to the loss calculations in Section 3.5.

2. Experimental methods to measure the cavity loss at THz frequencies, such as pump-probe measurements, will be very valuable to characterize the cavity loss and
identify the loss mechanisms. New device fabrication techniques can also be introduced to reduce the cavity loss due to the alloyed ohmic contact. For example, the top side electrical connection to the MQWs could be provided by a highly conductive 2DEG made by a GaAs/Al$_x$Ga$_{1-x}$As heterostructure. Annealed ohmic contacts only need to be made at the edge of the bar to this 2DEG. In this way, the electrical connection is separated from the optical confinement in device design and fabrication.

(3) Extra cavity loss can possibly be caused by additional reststrahlen band absorption due to hot TO phonons. Theoretically, hot TO phonons can be generated by the decay of hot LO phonons through anharmonic lattice interactions. This is a topic that needs to be studied, since the author is not aware of any relevant literatures. So far, the only experimental evidence of hot TO phonons is the emission peak at TO phonon energy, which is much higher than the thermal radiation background which is shown in Figure 6-5(d).
Chapter 7

Conclusions

The research presented in this Thesis is a pioneering work in this field. Based on systematic studies, this work attempts to provide a coherent picture by addressing both fundamental and practical issues in developing a compact solid-state THz laser based on intersubband transitions using multiple-quantum-well structures. Appropriate triple-quantum-well structures have been proposed and designed to realize THz gain media. Intersubband THz emissions at designed frequency have been observed from the MQW structures. A THz laser cavity has been implemented by using a metallic waveguide to reduce the large cavity loss caused by plasma confinement, which is the major obstacle in achieving THz lasing action. The key theoretical and experimental accomplishments and conclusions can be summarized as follows:

- Possible schemes to realize intersubband population inversion have been discussed, which are related to transport design. Local k-space population inversion is an attractive concept and has been successfully employed in mid-infrared quantum cascade lasers and superlattice lasers. However, at THz frequency range, this concept is impractical due to the small energy separation. Global subband population inversion is the most viable way by engineering intersubband scattering rates.
A conduction band three-level system in GaAs/Al_{x}Ga_{1-x}As heterostructures, implemented by a triple-quantum-well design, has been proposed and designed to realize THz radiative transitions. This design has a simple scheme to achieve global subband population inversion by utilizing the difference of intersubband scattering rates between acoustic-phonon scattering and LO-phonon scattering. This design seems to be a natural option, because the fast LO-phonon scattering is not favored for intersubband energy separation corresponding to THz frequencies.

1. A numerical code is modified and implemented to give correct simulation of the electrically pumped MQW structures and subband levels. Intersubband rate equations are incorporated into the simulation model.

2. The triple-quantum-well structures are designed and simulated by this numerical code. THz radiative transitions occur between $E_3$ and $E_2$ levels. Energy separation between $E_2$ and $E_1$ is comparable to one LO-phonon energy so that $E_2$ level can be emptied by fast LO-phonon scattering.

3. Inter-module connections of the triple-quantum-well structures under bias are realized through resonant tunneling by directly placing two modules together, instead of through a classic Fermi reservoir made of a heavily doped GaAs buffer region. This all-quantum-mechanical treatment of the MQW design is motivated by early design failures, with the purpose of avoiding tremendous free carrier absorption, and the nonlinear band bending which exists at the junction of the classic region and MQW active region. Numerical modeling of this nonlinear band bending is critical in designing subband levels with THz-energy accuracy, but may take years of effort to develop a working code by taking care of both the classic transport and quantum transport. On the other hand, however, the present resonant tunneling scheme cannot avoid the hot electron effect, and is subject to developing high-field domains in certain conditions.
4. The THz emission device consists of many modules of such triple-quantum-well structure, to spread out the necessary population inversion. In this way, sheet doping per module is kept low, which makes design and simulation more controllable by using a linear band bending approximation. The low subband population also helps to avoid electron-electron scattering, and reduce the possibility of high-field domain development.

5. Measured dc I-V curves of the THz emission MQW structures at cryogenic temperature confirm the MQW structure design and the operation bias.

- Device modeling is established for such THz emission MQW structures, which is used to calculate the subband population inversion. Electron transport is governed by temperature-dependent intersubband phonon scattering. Major discoveries are:

1. The hot electron effect is an important issue in realizing subband population inversion. The original design expectation in differentiating intersubband scattering rates for subband energy separations above and below LO-phonon energy may not be valid if the electron system is hot. Due to this effect, the high energy distribution tail will open up LO-phonon scattering, which greatly speeds up the intersubband scattering rate between the \( E_3 \) and \( E_2 \) levels. Population inversion for THz radiative transitions is thus reduced.

2. Intersubband phonon scattering usually involves very small momentum transfer compared with the Brillouin zone. As a result, acoustic phonon scattering, which is the dominant scattering mechanism for electrons not energetic enough to emit an LO phonon, only dissipates a small amount of energy. Electrons thus undergo quasi-elastic-type intersubband scattering and become hot on the next subband. Since intrasubband acoustic phonon scattering is also a slow process, hot electron effect is inevitable. Acoustic
phonon scattering is very sensitive to the lattice temperature and has comparable effect as hot electrons in degrading subband population inversion.

3. In the GaAs/Al_{1-x}Ga_{x}As material system, non-equilibrium LO phonons play a key role in determining subband population inversion. Non-equilibrium LO phonons are generated by intersubband LO-phonon scattering and have a finite lifetime before they decay into acoustic phonons. The phonon rate equation is used to calculate the non-equilibrium LO-phonon population. The existence of LO phonons leads to stimulated LO-phonon absorption processes which pump electrons from lower subband back to the upper subband. This hot LO-phonon effect will severely degrade the subband population inversion. According to the quantified study of M10 structure, population inversion is reduced approximately by half compared to without hot LO-phonon effect. Generally, increasing the pumping of the THz emission MQWs, such as increasing the sheet doping per module, has a limited effect on improving the population inversion.

- THz mode confinement is investigated by using a plasma cavity which is formed by heavily doped contact layers. The Drude model is used to assign dielectric constants to the plasma regions. Cavity loss is calculated as well as the basic mode pattern within the waveguide. Due to the limited doping level in GaAs, a plasma cavity possesses loss as large as several hundred cm^{-1}. Additionally, if the plasma frequency of the heavily doped layers is close to the THz intersubband radiation frequency, a surface plasma mode will build up and give extremely large cavity loss.

- To achieve THz lasing, the ideal cavity should be made by using metallic waveguide to significantly reduce the cavity loss. Such a metallic waveguide has been fabricated for the first time using wafer bonding and selective etching techniques. From measured dc I-V data and device inspection under SEM, the
fabrication is judged to be successful. A non-alloyed ohmic contact is made on one side of the waveguide. However, on the other side of the waveguide, the electrical connection has to be provided by alloyed ohmic contact. This alloyed ohmic contact degrades the optical performance of the metallic waveguide, due to the poor metal quality after annealing and additional diffused dopants between the metal and semiconductor, which form a plasma region and give extra cavity loss.

- The formalism of THz emission power coupled out of the device is developed using sub-threshold photon rate equation. The spontaneous emission power and the emission linewidth are dependent on the coupling loss, cavity dissipation loss, and optical peak gain. This general treatment can provide guidelines for THz emission device design and measurements.

- A metallic grating coupler is used to couple out the THz emission power. Compared to edge coupling, a much larger emission signal can be obtained by using gratings. Sufficiently large emission power is desirable in emission measurements to resolve the spectrum. The concept of grating coupling loss is proposed and quantified with the aid of a numerical method. Depending on the grating parameters, grating couplers can be made to offer large coupling loss for spontaneous emission measurements, and small coupling loss for surface emission THz lasers.

- A major part of the research effort is devoted to developing a measurement system for resolving the intersubband THz emission spectrum, including:

1. A free space spectral measurement set-up using a Fourier Transform Infrared spectrometer was established. The optical collection efficiency of this system is rather low, estimated to be in the 1% range.

2. Found appropriate window materials for device cryostat and right THz
detectors were used.

3. It was found that in THz emission measurements, the device bias has to be chopped at high frequencies to avoid the dominant blackbody radiation signal due to device heating. From this information, the device operation temperature can be inferred.

4. A bolometer is inappropriate for THz emission measurements. A fast Ge:Ga photon detector is the only option as a THz detector.

- Mid-infrared absorption measurements have been performed on a THz emission MQWs structure grown on a semi-insulating substrate. The absorption spectrum reveals intersubband energy separations in mid-infrared range, dipole moments, and linewidths, which verify the triple-quantum-well structure design, simulation, and MBE growth.

- Intersubband THz emission spectra have been successfully resolved from grating coupled devices and metallic waveguide device, and show good agreement with the designed frequencies. Emission linewidth as narrow as 0.65 THz (2.5 meV) has been observed using a spectral resolution of 0.5 THz. The device emission power, however, is in the 10 nW range and is one order of magnitude lower than the calculated value. THz lasing action has not been observed using metallic waveguide devices.

The facts that the lasing threshold is not achieved and that devices emit very low spontaneous emission power suggests larger-than-expected THz cavity loss. Further systematic work needs to be done regarding this issue. The invention of the first THz intersubband laser will rely on a low-loss cavity. Subjects and research suggested in future work include:
CHAPTER 7. CONCLUSIONS

- Perfect metallic waveguide fabrication. The major obstacle in making a high-quality metallic waveguide is the alloyed ohmic contact on one side of the device, as discussed in Section 6.4 in the previous chapter. Possible solutions are:

  1. Modify the device fabrication. The top-side electrical connection can be provided by a highly conductive 2DEG from lateral side. In this way, the annealed metal layer can be avoided to be used as an optical waveguide.

  2. Use different material system, such as InP based quaternary heterostructures to design the THz emission MQW structures. The doping level in such a material system can be sufficient high so that the alloyed ohmic contact is not necessary.

- Besides the alloyed ohmic contact, subjects under concern to possibly explain the larger-than-expected cavity loss are: surface plasma mode development due to graded doping profile at the metal/semiconductor contact region; 2DEG free carrier loss in the active region, which needs to be calculated using a quantum-mechanical treatment; extra reststrahlen band absorptions due to possible hot TO phonons. These losses can be quantified by some theoretical means.

- A valuable approach to resolve the uncertainty in cavity loss is an experimental set-up to directly measure the THz loss. Especially the pump-probe types of measurements can not only give the cavity loss, but also bring information on optical gain and transient behaviors such as intersubband scattering times. A high power THz laser, such as a free electron laser or a molecular gas laser, seems to offer this possibility.
Appendix A

Grating coupling for detection

For grating coupling for detection, the light is incident normal to the surface and is coupled into the MQWs. Using the coordinate system in Figure 3-6, only the light with H field polarized along the x direction can be scattered by the grating. The total field on both sides of the grating is

\[ H_x = e^{-ik_0z} + A_0 e^{ik_0z} + \sum_{n=\pm 1}^{\pm \infty} A_n \cos\left(\frac{2\pi n}{p} y\right)e^{ik_n z}, \quad z > 0, \]
\[ H_x = B_0 e^{ik'_0z} + \sum_{n=\pm 1}^{\pm \infty} B_n \cos\left(\frac{2\pi n}{p} y\right)e^{-ik'_n z}, \quad z < 0, \]  
(A.1)

In the above expressions, \( e^{-ik_0z} \) is the incident wave with a normalized amplitude. \( k_0 = n_0\omega/c \) and \( k'_0 = n'_0\omega/c \), where \( n_0 \) and \( n'_0 \) are the refractive indices of the air and semiconductor respectively. \( k_n \) and \( k'_n \) are wavevectors for the n-th diffracted waves toward \(+z\) and \(-z\) directions, respectively. They obey the following grating dispersion relation,

\[ k_n^2 + \left(\frac{2\pi n}{p}\right)^2 = k_0^2, \]
$k_n'^2 + \left(\frac{2\pi n}{p}\right)^2 = k_0'^2$, \hspace{1cm} (A.2)

The $E$ field is given by Equations 3.38-39. For detection, the coupling efficiency $\eta$ is defined as the ratio of the energy density of the $z$-polarized waves at $z < 0$ over the energy density of the incident wave. From Equation A.1, the $n$-th wave's coupling efficiency is $\eta_n = \frac{|B_n|^2}{2n_0^2}(\frac{\lambda_s}{p})^2$, where $\lambda_s$ is the wavelength in semiconductor and $p$ is the grating period. The total coupling efficiency is then $\eta = \sum_n \eta_n$. It is important to notice that from Equation A.2, the diffracted wave may be evanescent in the semiconductor, with a decay length $\delta_n = p/(2\pi\sqrt{n^2 - p^2/\lambda_s^2})$. For coupling the radiation into MQWs with a finite thickness $t$, an averaged effective coupling efficiency is defined as $\eta_{neff} = \eta_n(1 - e^{-2t/\delta_n})\delta_n / 2t$.

The amplitudes $A_n$ and $B_n$ of the diffracted waves are determined by the boundary conditions at the incident medium and semiconductor interface: at metallic regions $E_y$ vanishes on both sides, at aperture regions both $E_y$ and $H_x$ are continuous. $A_n$ can then be related to $B_n$ by: $(1 - A_0)/n_0 = B_0/n_0'$, and $-k_n A_n/n_0^2 = k_n'B_n/n_0'^2$. Since the total field is a periodic function of the grating period $p$ along the $y$ direction, it is sufficient to determine the coefficient $B_n$ by considering the boundary condition in only one period. The equation to determine the wave coefficients is

$$\sum_{n=0}^{\infty} \frac{k_n'}{k_0} B_n \cos\left(\frac{2\pi n}{p} y\right) = 0, \hspace{1cm} -a < y \leq a,$$

$$\sum_{n=0}^{\infty} \left(1 + \frac{n_0^2 k_n'}{n_0'^2 k_0}\right) B_n \cos\left(\frac{2\pi n}{p} y\right) = 2, \hspace{1cm} a < y \leq p - a. \hspace{1cm} (A.3)$$

The above equation is solved numerically by a mapping method to give the wave coefficient from zero to high-order terms, for an arbitrary value of $p/\lambda_s$. Previous results on grating coupling for detection are done by analytic method. However, they can only give solutions in the range of $0 < p/\lambda_s < 1.8$, in which case only the first 2 order waves can be included [102-105].
Figure A-1: Detection coupling efficiency of the 1st-, 2nd-, and 3rd-order diffracted waves and total effective coupling efficiency $\eta_{eff}$, including all the diffracted waves, with 3 different filling factors. $n_0 = 1$ for air and $n'_0 = 3.4$ for semiconductor (GaAs). The active region thickness is 3 $\mu$m.
The numerically calculated coupling efficiency of the 1st-, 2nd-, and 3rd-order diffracted waves and the total coupling efficiency are presented in Figure A-1.

It should be noted that, for detection, higher filling factors of the grating yield better coupling efficiencies, whereas for the emission, lower filling factors will give better coupling. This is because for emissions, it is the aperture part of the grating that bends the field since it reinforces a continued tangential $H$ component. The reciprocity should not be simply used to relate detection optimization of grating coupling to that of the emission cases.
Appendix B

Device processing

B1. Wafer degreasing

(1) 1,1,1-trichloroethane (TCE): boil at 70 °C-90 °C for 5 minutes.
(2) 1,1,1-trichloroethane (TCE): ultrasound for 5 minutes.
(3) Acetone: ultrasound for 5 minutes.
(4) Methanol: ultrasound for 5 minutes.
(5) Methanol rinsing for 30 seconds.
(6) Blow dry with N₂ and inspect under microscope.

B2. Mask cleaning

(1) Mix NH₄OH : H₂O₂ : H₂O in ratio of 1:1:5 for 1 liter.
(2) Heat mixture slowly to 80 °C.
(3) Boil items for 15 minutes in liquid.
(4) Rinse in DI water for 5 minutes and blow dry with N₂.

B3. First and second photosteps

(1) Wafer prebake at 200 °C for 30 minutes in oven, then cool to ambient.
(2) Deposit HMDS, spin at 4000 rpm for 40 seconds.
(3) Deposit Shipley 1813 photoresist. Spin at 4000 rpm for 40 seconds.

(4) Wafer softbake at 90 °C for 30 minutes in oven.

(5) Karl-Suss exposure for 8 seconds (8 mW/cm², 365 nm).

(6) Develop in Shipley MF319 for 40 seconds.

(7) Rinse in DI water for 2 minutes and blow dry with N₂.

(8) Inspect patterns under microscope.

**B4. Third photostep (lift-off)**

(1) Wafer prebake at 200 °C for 30 minutes in oven, then cool to ambient.

(2) Deposit HMDS, spin at 4000 rpm for 40 seconds.

(3) Deposit Shipley 1400-27 photoresist. Spin at 4000 rpm for 40 seconds.

(4) Wafer softbake at 90 °C for 30 minutes in oven.

(5) Chlorobenzene (poisonous, handle carefully) soak for 100 seconds, blow dry.

(6) Softbake at 90 °C for 5 minutes for drive out solvent.

(7) Karl-Suss exposure for 12 seconds (8 mW/cm², 365 nm).


(9) Inspect patterns under microscope.

*When lift-off:*

(1) Soak wafer in acetone or PRS-3000. Ultrasound for 5-10 minutes.

(2) Rinse with methanol and blow dry with N₂.

(3) Inspect under microscope.

**B5. Wet chemical etching recipe**

Mix NH₄OH : H₂O₂ : H₂O in ratio of 10:5:240 for 500 ml. The etching rate is approximately 0.25 μm/minute. Calibrate it with a dummy wafer each time.
B6. RIE dry etching recipe

BCl$_3$ flow rate 30 sccm, SiCl$_4$ flow rate 20 sccm. Chamber pressure 20 mTorr. RF: 300 Volts (power typically 215 W). Heat exchange at 60 °C. The etching rate is 0.15 μm/minute.

B7. Low-stress Si$_3$N$_4$ PECVD recipe

Flow rates: NH$_3$, 3 sccm; He, 1200 sccm, SiH$_4$/N$_2$, 300 sccm. Pressure: 900 mTorr. RF power: 75 W. Substrate temperature set to 250 °C. The deposition rate is 90 Å/minute. BOE etching rate varies, typically 800 Å/minute.

B8. SiO$_2$ sputtering recipe

Target SiO$_2$ at Position-3. Argon flow of 5 μm. RF power of 300 W. The deposit rate is 80 Å/minute. BOE etching rate is typically 1000 Å/minute.

B9. RTA recipe for alloyed ohmic contact

E-beam deposited alloy: Ni/Ge/Au/Ni/Au: 50 Å/660 Å/1330 Å/400 Å/1000 Å. The ramping temperature is 250 °C for 30 seconds. The annealing temperature is 370-380 °C for 30 seconds. The resulting contact resistance $R_c$ is in 0.1 ~ 1 Ωmm range from TLM measurement.
Appendix C

MBE-growth sheets of MQW structures

This appendix attaches the MBE growth sheets of the THz emission MQW structures.
M100 structure MBE growth

<table>
<thead>
<tr>
<th>Layer</th>
<th>Composition</th>
<th>Doping</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs</td>
<td>doped $2 \times 10^{18}$ cm$^{-3}$</td>
<td>0.2 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $1.2 \times 10^{18}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $8 \times 10^{17}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As</td>
<td>undoped</td>
<td>7 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>centered Si plane $9 \times 10^{10}$ cm$^{-2}$</td>
<td>31 ML</td>
<td></td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As</td>
<td>undoped</td>
<td>17 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>undoped</td>
<td>24 ML</td>
<td></td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As</td>
<td>undoped</td>
<td>9 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>undoped</td>
<td>23 ML</td>
<td></td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As</td>
<td>undoped</td>
<td>7 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>centered Si plane $9 \times 10^{10}$ cm$^{-2}$</td>
<td>31 ML</td>
<td></td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As</td>
<td>undoped</td>
<td>17 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $2 \times 10^{17}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $4 \times 10^{17}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $2 \times 10^{18}$ cm$^{-3}$</td>
<td>0.2 micron</td>
<td></td>
</tr>
</tbody>
</table>

n+ GaAs substrate [1 0 0]
### A10 structure MBE growth

<table>
<thead>
<tr>
<th>Layer</th>
<th>Composition</th>
<th>Doping Density ($n_e$)</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs</td>
<td>doped $2 \times 10^{18}$ cm$^{-3}$</td>
<td>0.2 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $1.2 \times 10^{18}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $8 \times 10^{17}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>$\text{Al}<em>{0.3}\text{Ga}</em>{0.7}\text{As}$</td>
<td>undoped</td>
<td>10 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>centered Si plane $1.5 \times 10^{11}$ cm$^{-2}$</td>
<td>30 ML</td>
<td></td>
</tr>
<tr>
<td>$\text{Al}<em>{0.3}\text{Ga}</em>{0.7}\text{As}$</td>
<td>undoped</td>
<td>21 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>undoped</td>
<td>25 ML</td>
<td></td>
</tr>
<tr>
<td>$\text{Al}<em>{0.3}\text{Ga}</em>{0.7}\text{As}$</td>
<td>undoped</td>
<td>6 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>undoped</td>
<td>20 ML</td>
<td></td>
</tr>
<tr>
<td>$\text{Al}<em>{0.3}\text{Ga}</em>{0.7}\text{As}$</td>
<td>undoped</td>
<td>10 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>centered Si plane $1.5 \times 10^{11}$ cm$^{-2}$</td>
<td>30 ML</td>
<td></td>
</tr>
<tr>
<td>$\text{Al}<em>{0.3}\text{Ga}</em>{0.7}\text{As}$</td>
<td>undoped</td>
<td>21 ML</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $1.7 \times 10^{17}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $4 \times 10^{17}$ cm$^{-3}$</td>
<td>0.1 micron</td>
<td></td>
</tr>
<tr>
<td>GaAs</td>
<td>doped $2 \times 10^{18}$ cm$^{-3}$</td>
<td>0.2 micron</td>
<td></td>
</tr>
</tbody>
</table>

n+ GaAs substrate [1 0 0]
### LSN80 Structure MBE Growth

<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs LTG (250°C) cap layer</td>
<td>35 Å</td>
</tr>
<tr>
<td>GaAs doped $5 \times 10^{19}$ cm$^{-3}$</td>
<td>100 Å</td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As undoped</td>
<td>20 ML</td>
</tr>
<tr>
<td>GaAs undoped</td>
<td>31 ML</td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As centered Si plane $6.0 \times 10^{10}$ cm$^{-2}$</td>
<td>7 ML</td>
</tr>
<tr>
<td>GaAs undoped</td>
<td>22 ML</td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As undoped</td>
<td>10 ML</td>
</tr>
<tr>
<td>GaAs undoped</td>
<td>23 ML</td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As undoped</td>
<td>20 ML</td>
</tr>
<tr>
<td>GaAs undoped</td>
<td>31 ML</td>
</tr>
<tr>
<td>Al$<em>{0.3}$Ga$</em>{0.7}$As centered Si plane $6.0 \times 10^{10}$ cm$^{-2}$</td>
<td>7 ML</td>
</tr>
<tr>
<td>GaAs doped $1 \times 10^{19}$ cm$^{-3}$</td>
<td>500 Å</td>
</tr>
<tr>
<td>Al$<em>{0.5}$Ga$</em>{0.5}$As undoped (etching stopper)</td>
<td>5000 Å</td>
</tr>
</tbody>
</table>

Repeats 80 times

Semi-insulating GaAs substrate [1 0 0]
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