SILICON-GERMANIUM QUANTUM-CASCADE LASERS

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The prospects and advantages of silicon germanium quantum cascade lasers are discussed, from both physical and technological perspectives. A range of Si/SiGe intersubband laser configurations are discussed, for both edge and surface emission. Recent experimental activity on mid- and far-infrared devices is reviewed, and the value of detailed theoretical tools for heterostructure design is highlighted. Steps towards silicon optoelectronic integration are also considered.

Keywords: Silicon optoelectronics, intersubband, terahertz, virtual substrate.

1. Introduction

This chapter explores the techniques and prospects for Si-based SiGe/Si intersubband lasers that emit within the 3 to 10 THz spectral range, a region where photonic approaches to the creation of THz sources are appropriate. Today, SiGe intersubband lasers stand at the threshold of realization, and when these miniature solid state THz sources become actualized, they will open up a new Group IV-IV application area within quantum cascade laser (QCL) technology. Our laser-wavelength range of interest is 30 to 100 µm, also known as the far infrared (FIR) region. In this chapter we discuss innovative FIR device designs, simulation, theory, experiment, and the unique benefits of monolithic optoelectronic integration on a silicon substrate. The devices examined here are strained-layer superlattice and multi-quantum-well (MQW) heterostructures.

As discussed in the previous chapter of this book, QCLs in the InGaAs/InAlAs and GaAs/AlGaAs materials systems have been tremendously successful in the mid infrared (MIR) waveband and are presently moving towards the FIR or THz range. Generally, when the emission wavelength of a QCL is extended from MIR to FIR various difficulties are encountered, such as an increased free-carrier absorption loss which adds to the laser waveguide attenuation, thereby increasing the required gain and pumping. Also, the waveguide dimensions become larger and the modes become "leakier"; a problem which can be alleviated by substituting a metal-clad semiconductor structure for an all-dielectric THz waveguide. In addition, there is a perceived need to lower the operating temperature to approximately 20K, although, as we argue in this chapter,
operation at 77K or above appears possible for SiGe/Si lasers. We believe that the FIR technical hurdles can be surmounted in the IV-IV heterosystem.

2. Advantages and disadvantages of SiGe for intersubband lasers

Silicon is an excellent platform for monolithic integration of THz sources, THz detectors, and high-speed Si or SiGe electronic integrated circuits. Such optoelectronic (or “tera-electronic”) integration could be used to create a miniaturized THz transceiver, for example. Silicon has a higher thermal conductivity than GaAs, thus providing better thermal management, which is a key issue in any active optoelectronic system. Silicon and the SiGe alloys also have the advantage of a relatively large radiative-to-nonradiative branching ratio for the intersubband laser transition. In the covalently bonded SiGe/Si heterosystem the non-polar optical phonon scattering is weaker than the polar optical phonon scattering found in III-V heterostructures. This implies stronger branching in IV-IV vis-a-vis III-V lasers. Between 4 and 77K, the alloy disorder scattering in SiGe dominates the optical phonon scattering, as discussed below. The indirect bandgap of SiGe, Si and Ge presents no disadvantage for quantum cascade laser operation because the radiation is generated by intersubband transitions, rather than interband recombination. The IV-IV heterostructures also offer a simple buried-mirror technique for vertical-cavity surface-emitting laser (VCSEL) construction. Unique to IV-IV is the fabrication of a WSi₂ or CoSi₂ layer buried beneath the surface of a Si substrate; a layer that is highly reflective at THz frequencies. The SiO₂ layer in a silicon-on-insulator (SOI) substrate may also be used as a buried THz reflector.

Unlike the conduction intersubband transitions employed in III-V QCLs, all current attempts to realize SiGe/Si quantum cascade lasers are based on valence intersubband transitions in p-type heterostructures. There are various reasons for this. For growth of pseudomorphic Si/SiGe heterostructures directly on silicon, substantial band offsets can only be achieved in the valence band. The standard method of obtaining usable conduction band offsets is to grow the heterostructure on a relaxed SiGe buffer (or ‘virtual substrate’): even then the offsets obtained are generally not as large as those available in the valence band (up to 740meV for pure Si on pure Ge [1]). Realisation of a surface-normal emitting cascade laser (described in section 5 below) cannot be achieved in an n-type system (except by the use of a surface grating), but requires light hole to heavy hole transitions in a p-type heterostructure. That said, there is still potential for an n-type edge-emitting Si/SiGe cascade laser, as discussed in section 6 below.

One disadvantage of the p-type SiGe system is that the hole masses are significantly larger than the III-V electron masses. Consequently, the hole wavefunctions in SiGe heterostructures are quite well localized in individual quantum wells, hence interwell coupling is weak, and delocalised superlattice type states cannot be formed unless the barrier layers are very thin. For the same reason, the device currents in p-SiGe QCLs will be lower than in III-V devices for the same external bias. Also, both heavy hole and light
hole subbands are always present in p-SiGe heterostructures. Whilst this is an essential feature of surface-emitting QCLs, it is an added complication in the design of edge emitting lasers based on heavy hole to heavy hole transitions, and it makes the design of any interstitial injector regions more difficult.

Another difference between p-type Si/SiGe heterostructures and n-type III-V systems appears in plots of subband energy versus the wavevectors $k_x$ and $k_y$ (the in-plane dispersion). The valence subband dispersions are both anisotropic and non-parabolic, while the conduction subband dispersions in III-V materials are isotropic and almost parabolic (for the range of wavevectors typically encountered in cascade lasers). This feature of p-Si/SiGe systems clearly complicates device design; however, the non-parabolicity can be engineered to produce features which may be favourable for local-in-k-space population inversion, as discussed in section 5. The THz electric dipole matrix elements (the oscillator strength of the lasing transition) are comparable in the p-Si/SiGe and n-III-V cases.

3. Advantages of the relaxed SiGe-on-Si virtual substrate

The 4% lattice mismatch between Si and Ge can be viewed as a problem or as an opportunity for beneficial "strain engineering". Lattice matching to a silicon substrate is feasible for the special case of a SiGeC/SiGe superlattice wherein the Ge to C atomic ratio is chosen as 9 to 1 and the ternary SiGeC alloy layers are quantum wells. However, the carbon concentrations available with today's technology are < 2%, so the SiGeC strategy is limited to shallow quantum wells [2]. Generally, SiGe superlattice devices will require strained-layer epitaxy, unlike the unstrained III-V superlattices matched to GaAs or InP. Perhaps 98% of all the SiGe/Si photonic devices grown during the past decade have been grown directly upon an Si wafer and have been coherently but unsymmetrically strained; i.e., the SiGe quantum wells have had compressive in-plane strain with respect to the Si substrate, and the Si barriers have been unstrained. Because strain builds up across the asymmetrically strained MQW stack, the maximum permissible stack height is typically no more than 50 nm (the critical thickness for stable strain [3]), otherwise, dislocations will nucleate to relieve the strain in the stack. Therefore, the "unbalanced" strain approach is not a satisfactory solution to the problem of "thick" (0.1-10 µm) MQW growth. Strain symmetrization is the solution to this problem.

During the past three years, a strain-balanced MQW growth technique has been developed that allows stack thicknesses of several micrometers; beneficial for Si/SiGe lasers, detectors, modulators, resonant tunneling diodes, etc.[4]. First, a relaxed Si$_{1-x}$Ge$_x$ buffer or "virtual substrate" is grown upon silicon. The virtual substrate has a larger lattice parameter than Si and becomes a new "template" for subsequent SiGe/Si epitaxy. Next, the MQW is strain-engineered so that the compressive in-plane strain of the Si$_{1-x}$Ge$_x$ quantum wells opposes and balances the tensile in-plane strain of the Si$_{1-x}$Ge$_x$
barriers \(x > y > z\). For sufficiently high precision growth, the net strain across the whole MQW stack is reduced to zero.

Experimental data for SiGe/Si virtual substrate heterostructures reported to date shows excellent interface flatness and smoothness. [5]. The buffer concentration \(x\) offers another degree of freedom in device design that supplements the engineering of wavefunctions. SiGe buffer technology was pioneered at the Massachusetts Institute of Technology [6]. In most approaches, the SiGe buffer is typically \(\sim 3\)\(\mu\)m thick, but new techniques are being developed (primarily for application in n-SiGe FETs) for growth of stable, strain-relaxed sub-0.1\(\mu\)m buffer layers [7]. Two additional virtual substrate techniques are available today for device implementation. The first is the use of an SGOI substrate (SiGe on insulator) in which a thin crystalline layer of Si\(_{1-x}\)Ge\(_x\) rests atop a 500 nm layer of SiO\(_2\) upon silicon[8-9]. The second is to base the devices upon a single-crystal Si\(_{1-x}\)Ge\(_x\) wafer (with 0<x<0.2), although the present surface quality of such wafers needs improvement [10].

We believe that virtual substrate methods are likely to revolutionize the crystal-alloy layer quality and the performance of IV-IV MQW and superlattice devices. The virtual substrate appears essential for a silicon based cascade laser, since the number of periods usually required in such a device would require a total thickness of strained material well in excess of the critical thickness when grown directly on silicon. On the other hand, the success obtained so far with the virtual substrate approach implies that it may be possible to grow SiGe cascade heterostructures with a similar number of periods to the largest reported for III-V QCLs.

4. Theory and simulation techniques

Given the complexities of the Silicon-Germanium system, detailed modeling work is an important aid to understanding the electronic and optical processes involved in SiGe heterostructures, and to successful device design. The valence subbands in the SiGe system are strongly anisotropic, and significantly warped in in-plane \(k\) space due to mixing of heavy, light and spin-split-off hole states. Therefore, the one-band effective mass theory commonly used to model the electronic states of n-type cascade lasers is not sufficiently accurate here. However, for heterostructures involving reasonably low Germanium mole fractions (< 0.5, which appears sufficient for THz photon emission), the \(k.p\) method has been shown to give results in very good agreement with pseudopotential bandstructure calculations [11,12], and hence provides a relatively fast means of calculating subband dispersions and carrier wavefunctions. The \(k.p\) method can be used for complex multiplayer structures, and a Fourier Transform based implementation provides substantial improvements in efficiency [11]. The \(k.p\) approach can also be combined self-consistently with a solution of the Poisson equation to account for internal electric fields and space charge. Once the electronic states of a given cascade
structure have been obtained, the intersubband optical absorption spectra can then be calculated, for both edge and surface-normal propagating modes.

In both the III-V and IV-IV materials systems, the non-radiative intersubband transition rates are considerably faster than the radiative rates. Therefore, population inversion – and hence and laser gain – are determined primarily by the relative non-radiative transition rates in the system, and so accurate calculations of these rates are required for laser design and optimisation. In III-V heterostructures, polar optical phonon scattering is the dominant non-radiative intersubband transition process. In the non-polar SiGe system there is no polar carrier-phonon interaction, but there is a deformation potential optical phonon interaction which can give significant intersubband scattering. Several vibrational modes are present: Silicon-like phonons, Ge-like phonons, and new alloy phonon modes, all of which give intersubband scattering. For SiGe heterostructures designed for THz emission, the subband energy gaps are smaller than all the optical phonon energies (the 37.4meV Ge phonon being the smallest), and hence the intersubband phonon scattering rates are strongly suppressed at low temperatures (∼10^9 s⁻¹). At room temperature, the optical phonon scattering rates are typically ∼10^11 s⁻¹ – which is about an order of magnitude lower than the polar phonon scattering in III-V systems. The deformation potential interaction with acoustic phonons in SiGe is stronger than in n-type III-V systems, due to the larger effective masses involved, and the rates are generally comparable with those for optical phonon scattering [13]. Alloy disorder scattering in the SiGe quantum wells can also give rise to intersubband transitions. This process is virtually temperature independent, and hence is dominant in heterostructures with closely spaced subbands at low temperature [14]. Consequently, the intersubband lifetimes are relatively insensitive to temperature, in marked contrast to the case of polar III-V systems. This has been confirmed experimentally by pump-probe experiments on p-SiGe heterostructures using a free electron laser [15,16]. The measured intersubband lifetime for p-type modulation doped Si_{0.75}Ge_{0.25} quantum wells grown on a Si_{0.75}Ge_{0.22} virtual substrate was found to be ∼10^11 s throughout the temperature range 4.2-80K.

Another potentially important non-radiative scattering process is carrier-carrier scattering. In n-type III-V cascade lasers this process is important for transitions between closely spaced states, such as the lowest injector and highest active region states, and the lowest active region and highest collector states [17]. Relatively little theoretical work has been done on hole-hole scattering in quantum well structures. Our own calculations show that the LH1-HH1 hole-hole scattering rate in a Si_{0.7}Ge_{0.3}/Si quantum well is about 10^11 s⁻¹ at 4.2K for a carrier density of 10¹⁵ cm⁻² (in otherwords, commensurate with the alloy disorder scattering rate), and is only weakly dependent on temperature [18].

More detailed studies of carrier dynamics require vertical transport models, using, for example, rate equation [17] or Monte Carlo methods [19]. Whilst the rate equation approach generally uses subband lifetimes which are averaged over a given carrier distribution, the Monte Carlo method can be programmed to account for the full k-space
dependence of scattering, and hence generate in-plane \( k \)-space carrier distributions which are essentially a solution of the semi-classical Boltzmann equation. This level of detail may be valuable, for example, in designs where local-in-\( k \)-space population inversion, rather than global subband population inversion, is sought, but obviously requires a much more extensive software development effort. We have developed a cellular Monte Carlo scheme in which scattering rates are tabulated on a relatively coarse 2-dimensional \( k \)-space mesh, and then interpolation is used to determine the exact transition rate between a specific pair of states\cite{19}. This approach reduces the computer storage requirement to practical levels, and also ensures that the correct angular dependences for each scattering process are implicitly included in the model. The algorithm uses periodic boundary conditions to enable modeling of vertical transport through multi-period quantum cascade structures. Whichever of the rate equation or Monte Carlo methods is used, the task of modeling vertical carrier transport is simplified by the assumption that inter-well transitions are dominated by incoherent (intersubband scattering) processes, rather than coherent tunneling \cite{20}. We have found that, for \( p \)-type heterostructures, the in-plane \( k \) dependence of the inter-well scattering rates is an important factor in determining the device current\cite{21}. The inter-well transition rates can vary strongly across \( k \)-space, and subbands in adjacent wells which appear resonant at the zone center are not necessarily resonant at finite \( k_{\parallel} \). Consequently, models based solely on the zone center transition rates, or on thermal equilibrium carrier distributions, can substantially underestimate the device current.

5. Surface emitting SiGe QCLs

All existing III-V \( n \)-type QCLs are edge-emitting devices, as a consequence of the symmetry rules which govern the radiative intersubband transitions. The optical matrix element is non-zero only for interaction with an electric field dipole oriented perpendicular to the quantum well layers (TM polarization), hence the emitted radiation propagates parallel to the layers – and thus emerges from the edges of the heterostructure. Collection of radiation from the surface of such a device can be achieved by fabricating a diffraction grating on the surface, although this is not a very efficient approach. Design of a QCL based on \( p \)-type Si/SiGe heterostructures allows the possibility of realizing a true surface-emitting device, without the aid of any grating. For transitions between pure heavy hole subbands, the symmetry rules restrict the interaction with radiation in the same manner as for electron intersubband transitions, resulting again in edge-emission. However, transitions between light hole and heavy hole subbands can also couple to in-plane electric field dipoles (TE polarization), resulting in surface-normal propagating radiation. For pairs of subbands in which the quantum well envelope functions have the same parity (e.g., LH1 and HH1), surface-normal emission only occurs for states with non-zero in-plane wavevectors (in the limit of zero electric field), but where the envelope functions have different parity (e.g., in the HH2 and LH1 subbands), strong surface emission can be obtained even at the Brillouin zone center.
The design of a QCL based on light hole – heavy hole transitions raises various challenges. For p-type Si/SiGe heterostructures the SiGe alloy layers represent the quantum wells, whilst the Si layers act as the confining barriers. In strain-balanced structures the energy gaps between different heavy hole subbands depend primarily on quantum well width, whereas the energy gaps between light hole and heavy hole subbands depend primarily on strain – and hence alloy composition – and are relatively invariant with well width. Therefore, engineering of heavy and light hole subband energies in a 3 or 4 level intersubband laser system requires simultaneous tuning of both layer widths and layer compositions.

For FIR laser design, the energy gaps between subbands are necessarily much smaller than in MIR devices (e.g., a 50µm (6THz) FIR device has a photon energy of 25meV, compared to 138meV for a 9µm (33THz) MIR device). Considering also that most MIR cascade lasers utilize optical phonon-mediated depopulation of the lower laser subband (with a phonon energy of ~36meV), the total energy difference between adjacent periods is at least 174meV for a 9µm device (there is also a small amount of energy loss in the injector region). The much lower energy drop per period in the FIR devices means that alternative design strategies must be considered. One attractively simple possibility is the ‘quantum-staircase’ design first proposed by Soref and co-workers [22,23]. Figure 1 shows a quantum staircase system based on LH1-HH1 intersubband transitions.

These transitions occur within each quantum well, and the carriers are transported from well to well by non-radiative HH1-LH1 transitions. The electric field is chosen to achieve near-resonance between the HH1 subband in one well, and the LH1 band in the following (‘downstream’) well. Clearly, non-radiative intra-well LH1-HH1 transitions will occur in addition to the desired radiative transitions and, in order to attain population inversion, the total inter-well HH1-LH1 transition rate must be faster than the total intra-well LH1-HH1 rate (which will be dominated, as in all intersubband lasers, by the non-radiative transition rate). Optimisation of the inter-well HH1-LH1 rate in such a system is rather difficult. As mentioned above, the interwell transition rates in QCLs are
generally dominated by the incoherent scattering processes, rather than coherent tunneling. This will certainly be the case in the p-type Si/SiGe system, where the effective masses in the Si barriers are much larger than those in the n-type III-V systems, leading to slow tunneling times. The large effective masses result in strong localization of the wavefunctions, which also reduces the matrix elements for all incoherent scattering processes. Obviously, reducing the barrier widths helps to increase the matrix elements, but this remedy is limited, in practice, by available growth technology. Furthermore, at the zone center, the heavy hole and light hole subbands are completely decoupled, therefore there is no transition matrix element between such states, even when they are exactly resonant. Thus, the interwell coupling is dependent on off-zone center states – which contain an admixture of heavy hole, light hole and spin-split off character (within the k.p representation).

One possible means of improving upon the basic LH1-HH1 quantum staircase design is by utilizing the inverted mass feature which can be engineered in the LH1 subband. An LH1-HH1 subband pair then form the basis of a 4 level unipolar laser, as shown in figure 2. Carriers are injected into the LH1 subband at the zone center, and then

![Diagram showing THz quantum staircase design based on HH2-LH1 optical transitions.](image)

Figure 2. THz quantum staircase design based on HH2-LH1 optical transitions (wide arrows). The electric field is set such that carriers tunnel/scatter from HH1 into the HH2 subband in the following well (narrow arrow).

relax to the (off-zone-center) subband minimum, from which radiative transitions to HH1 occur. These holes then relax towards the zone center in the HH1 subband, before being scattered into an adjacent well [22-24]. One advantage of such a system is that a ‘global’ population inversion between the LH1 and HH1 subbands is not necessary: it is sufficient to attain a local (in k-space) inversion, in the vicinity of the LH1 subband minimum, and this local inversion is can be more readily achieved due to the favourable band curvature of LH1 and HH1 respectively. Unfortunately, it is difficult to achieve a strong inverted mass feature in the LH1 subband in strain-balanced Si/SiGe structures:
the typical energy difference between the LH1 zone center and the subband minimum is of the order of 1-2meV. However, even for negligible energy differences, the fact that many of the LH1 carriers can access off-zone-center states is advantageous in itself, since the optical matrix element at the off-zone-center subband minimum is much larger than at the zone center. It should be mentioned that the inverted mass heterostructures are very difficult to realize in practice due to the sensitivity of the bandstructure to growth tolerances. Engineering of the inverted mass feature in the LH1 subband requires bringing LH1 into close proximity with HH2, at the zone center. This, in turn, requires accurate control of quantum well thickness, quantum well composition, and virtual substrate composition. Any error in any of these parameters can shift one or other of the subbands enough to destroy the inverted mass feature.

Another potential laser design based on the quantum staircase concept is the HH2-LH1 laser. A schematic diagram is shown in figure 3. In this device, there are three active subbands in each quantum well. The FIR optical transition is the intrawell HH2-LH1

![Figure 3. Local-in-k-space population inversion scheme based on an inverted (negative) effective feature in the LH1 subband of a SiGe quantum well](image)

transition. Depopulation of the lower laser subband (LH1 in this case) is achieved by non-radiative LH1-HH1 scattering. The electric field is chosen to attain near-resonance between HH1 and the HH2 subband in the following (downstream) well. This design offers two advantages over the LH1-HH1 quantum staircase. Firstly, the optical transition (HH2-LH1) is fully allowed at the zone center, whereas the LH1-HH1 zone-center optical transition is almost forbidden (the electric field serves to break the symmetry of the confining potential and hence allow weak coupling). Secondly, the inter-well coupling is much stronger, since it relies upon HH1-HH2 transitions rather
than HH1-LH1. True anticrossing behaviour can be observed between HH1 and HH2 in adjacent wells, for sufficiently thin barriers, with good delocalisation of wavefunctions across both quantum wells [18]. Although population inversion can be achieved between the HH2 and LH1 subbands, in the steady state a substantial percentage of the carriers reside in the HH1 subbands in each quantum well, which represents a loss in quantum efficiency. However, the situation is probably not much worse than that in typical MIR III-V cascades, where the total population in the many non-lasing states in the injector region, as well as that of the ground state in the active region, is quite substantial [19].

One way of improving the prospects of population inversion in SiGe quantum staircase devices is to design the structure to operate via inter-well, rather than intra-well, optical transitions. In such a device, the HH1 subband then becomes the upper laser level, whilst the lower laser level is an excited subband (LH1 in the simplest scheme) in the next ‘downstream’ quantum well, as shown in figure 4. The staircase must be biased such that

![Quantum staircase designed for inter-well THz photon emission](image)

Figure 4. Quantum staircase designed for inter-well THz photon emission

the HH1 and the ‘downstream’ LH1 subbands are separated by the required THz photon energy at the zone center. Hence, the structure is readily field-tunable. In such a design, obtaining population inversion is relatively easy, since the majority of carriers generally occupy the HH1 subbands. A further advantage of this design is that the HH1-LH1 inter-well transition is fully allowed at the zone center, because the wavefunctions of the two states do not have the same parity relative to the two-well potential function. The main remaining design criterion is then to reduce the thickness of the Si barriers which separate the wells sufficiently to obtain a reasonably large optical matrix element for the inter-well transition. A barrier thickness of ~15Å is required to obtain optical matrix elements of a similar magnitude to those obtained for intrawell transitions [19].

A common problem for all the quantum staircase devices is the possibility of thermionic emission over the silicon barriers. The barrier height for low Ge composition wells with
Si barriers, grown on a silicon substrate, is relatively modest (~0.74 eV) where x is the Ge mole fraction. For strain-balanced heterostructures grown on a SiGe virtual substrate, the barrier height is somewhat lower for the same quantum well alloy composition, since the tensile strain (Si on relaxed Si$_{1-x}$Ge$_x$) results in a smaller shift in the bulk band edge than does the compressive strain (Si$_{1-x}$Ge$_x$ on Si or Si$_{1+y}$Ge$_y$ on Si$_{1-y}$Ge$_y$) [1] (the valence band offset for Si$_{0.7}$Ge$_{0.3}$ wells and Si barriers grown on a Si$_{0.3}$Ge$_{0.7}$ virtual substrate is approximately 120 meV). The best way, in theory, to increase the valence band offset is to raise the quantum well Ge composition as high as possible, whilst keeping the virtual substrate composition as low as possible, but the strain balance criterion then dictates either very narrow wells – which will push the confined states closer to the top of the wells in any case – or very thick barriers – which will make inter-well coupling very weak. Of course, an alternative remedy for the thermionic emission problem is the design of a superlattice injector layer which acts as a DBR for the carrier wavefunctions, in a similar manner to that employed in n-type III-V cascades. However, injector design is more difficult for p-type cascades, since both light hole and heavy hole states are present; creating a ‘minigap’ in the energy spectrum therefore requires engineering of both layer thicknesses and compositions, within the limits of the strain-balance requirement.

Irrespective of the exact active region layer design, the generation of surface-normal propagating THz radiation from light hole – heavy hole transitions allows for the possibility of designing a vertical cavity surface emitting quantum cascade laser (VCSEQCL). As mentioned above, the Si/SiGe materials system offers an important advantage over III-V materials in this respect, in that the technology for buried reflector layers already exists. Si/SiGe multiple quantum well detectors which included silicon dioxide [25,26] or tungsten silicide [27] buried reflector layers, have both been demonstrated for operation at mid-infrared wavelengths. Cobalt disilicide is another possible choice of reflector material. New growth techniques are also emerging to enable preparation of a buried SiO$_2$ layer above a SiGe virtual substrate without the need for wafer bonding [28]. The envisaged VCSEQCL device geometry is shown in Figure 5.
For the upper reflector, a distributed Bragg reflector (DBR) stack comprising alternate layers of amorphous silicon and SiO₂ is proposed. Of course, for operation at THz frequencies, the layer thicknesses required for the laser cavity and Bragg stack are unusually long. For 6THz operation, a λ/2 cavity requires a total Si/SiGe thickness of 7.6μm, which should be possible using chemical vapour deposition (CVD) for epitaxial growth, but not molecular beam epitaxy (MBE). Each silicon layer in the DBR must also be ~3.8μm thick. Fortunately, there is a large refractive index between the silicon and SiO₂ layers, which means that a relatively small number of periods will be required in the DBR compared with those in visible-wavelength GaAs/AlGaAs VCSELs (at 6THz, only 6 periods are required for >99% reflectivity).

6. Edge emitting Si/SiGe QCLs

Edge-emission occurs for THz laser light polarized along the superlattice growth axis Z, the polarization that excites the TM₁ laser waveguide mode. The optical selection rules for SiGe/Si valence intersubband transitions say that Z polarized radiation is strongly allowed for a transition between HH2 and HH1, hence this HH transition becomes the basis of edge-emitting QCLs. The University of Delaware and Sarnoff Corporation, under an Air Force contract funded by DARPA, are investigating edge-emitting SiGe/Si THz QCLs and have proposed a microdisk laser resonator that is discussed in another chapter of this book. This is a novel alternative to the ridge waveguide geometry which is used for MIR quantum cascade lasers and which should also be viable for FIR edge-emitting devices. The team is pursuing an FIR SiGe/Si QCL well-and-barrier design that
contains MQW injector regions as well as 3-well or 4-well active regions, similar to the p-Si/SiGe MIR-emitting cascade structure reported by Dehlinger et al [29].

Simulations performed at AFRL and The University of Leeds have shown that there are two good possibilities for HH2-HH1 quantum staircase THz lasers [30]. The first technique is to engineer an inverted effective mass for the HH2 dispersion at \( k_x k_y \) values of \( \sim 0.02 \) Å\(^{-1}\), which allows the same type of local-in-k-space population inversion proposed for the LH1-HH1 laser. The second technique is to engineer the HH2 subband dispersion to be flat, or even parabolic near \( k_z = 0 \). When that is done, a zone center laser results. It has a global rather than local k-space population inversion. The zone center approach uses the anti-crossing of subband levels in adjacent quantum wells of the quantum staircase, wells coupled by a thin Si barrier. The level separation as a function of the applied electric field bias, known as the Stark ladder, reaches an anti-crossing condition at a field \( F = F_{ac} \). Slightly above \( F_{ac} \), HH1 and HH2 each form \( \sim 1 \) meV doublets in most quantum wells of the staircase, yielding a 4-level laser scheme at the zone center with a photon energy smaller than the lowest optical phonon energy. Such a scheme was first discussed by Harrison and Soref for the CB2 and CB1 subbands of an GaAs/AlGaAs MQW [31] but the principle applies equally well to the HH2 and HH1 subbands in a p-type system.

The HH2 and LH1 dispersion shapes are governed by the proximity of the HH2 and LH1 subbands. We have observed the HH2-LH1 repulsion or anti-crossing in k,p simulations. For example, we examined a series of eight related, unbiased, free-standing Si\(_{0.7}\)Ge\(_{0.3}\)/Si superlattices grown upon a (100) Si\(_{1-x}\)Ge\(_x\) buffer, where \( y \) is chosen in each case to give overall strain balance. Taking the barrier thickness \( l_b = 40\)Å with \( T = 77\)K and \( k_z = 0.5 \), we varied the quantum well thickness \( l_w \) from 80Å up to 150Å. As \( l_w \) was increased, we first found an inverted effective mass for LH1 at \( l_w \sim 100\)Å. Then at \( l_w \sim 120\)Å, the levels exchanged positions and an HH2 inverted mass appeared. This was followed by a nearly parabolic HH2 dispersion at \( l_w \sim 140\)Å. So, the desired negative mass can be engineered generally by fixing \( x, y, l_b \) and varying \( l_w \).

Terahertz gain in a p-Si/SiGe quantum staircase design based on a negative-mass feature in the HH2 subband has recently been modeled in detail by Soref and Sun [32,33]. The subband dispersions for a structure comprising 90Å Si\(_{0.8}\)Ge\(_{0.2}\) quantum wells with 35Å Si barriers on a (100) Si\(_{0.9}\)Ge\(_{0.1}\) virtual substrate are shown in Figure 6. The desired radiative transition occurs between the two doublets in each well, as indicated in Figure 7, and has a calculated spontaneous emission lifetime of 77 µs at \( T = 77\)K.
Figure 6. The (1,1) dispersion curves for a 5-layer SiGe/Si quantum staircase at the $F_0$ resonant tunneling bias.

Figure 7. Dispersion of the two doublet levels that appear in each central QW of an extended quantum staircase structure.

(The hole/acoustic-phonon scattering lifetime at this temperature was 1.0 ns.) The dipole matrix element between the doublet states was 20Å. For an applied field of 30 kV/cm (which is 3.6 kV/cm above $F_{ac}$), and a hole current density $J = 1.7$ kA/cm$^2$ selectively injected into the upper HH doublet, a gain of 450 cm$^{-1}$ at a wavelength of 41 μm is predicted. The zone center laser with parabolic subbands has not yet been examined in detail.
There are also possibilities for n-type unipolar SiGe THz lasers, which await investigation. The conduction band offset in SiGe/Si superlattices (which determines the quantum well depth in the n-type laser) can be adjusted to some extent with the virtual substrate method. The quantum wells will be shallow for conduction subbands, yet deep enough for THz laser operation. Although the CB1, CB2...CBN subbands have their energy minima in the X-Δ region of the Brillouin zone, they have largely parallel $k_x$ dispersion curves, and strong THz radiative transitions are indeed expected between curves at the X valley; e.g., the X2 to X1 transition is allowed. The selection rules for the X subbands are affected by virtual substrate crystallographic orientations because band mixing comes into play [34]; thus a TE-polarized n-i-n VCSEL may be feasible for nonstandard substrate orientations such as (110). One advantage of the n-type Si/SiGe system is that the Si layers act as the quantum wells for electron confinement, hence there is no alloy disorder scattering in the wells.

Low-loss waveguide design is an issue not fully resolved in FIR edge-emitting lasers. The issue arises in the electrically pumped lasers discussed here, and in the phonon-pumped laser discussed in Section 7. Undoped semiconductor layers may be considered as dielectrics at THz frequencies, and an all-dielectric THz waveguide, either a ridge guide or a strip guide, will be feasible in a semiconductor heterostructure. However, the height of such waveguides is generally about $\lambda/2$, so for a typical wavelength of 60 $\mu$m (in air) this would imply semiconductor epitaxy $\sim10$ $\mu$m thick. As discussed above for the case of vertical cavity devices, epitaxial growth of this thickness is probably not practical using solid-source MBE, but should be achievable using CVD, and possibly gas-source MBE. An alternative solution is a metal-clad semiconductor waveguide (ridge or strip) in which the waveguide height is a small fraction of the wavelength such as $\lambda/20$. The results reported by Colombelli et al for III-V quantum cascade lasers operating at wavelengths of 21$\mu$m and 24$\mu$m [35] indicate that the metal-clad structure, known as a surface plasmon waveguide, should be practical at FIR wavelengths. The electromagnetic mode does not penetrate deeply into the metal film due to skin effect, ensuring low loss, and the TM$_0$ mode can be supported for deep sub-wavelength waveguide thicknesses. Recently, THz laser action has been reported from an n-type GaAs/AlGaAs quantum cascade device [36,37]. A key feature of this device was apparently the low loss waveguide design. A ridge waveguide geometry was used, but incorporating adjacent n+ and undoped semiconductor layers such that the dielectric constant changes sign across the interface, providing confinement of surface plasmon modes without the need for a metal layer. This approach could also be used in the SiGe system.

7. **Superlattice SiGe QCLs and quantum-parallel lasers**

A 1997 paper from AFRL and more recent works [38-41] propose a SiGe/Si quantum-parallel laser (QPL); a device still awaiting implementation. The superlattice is in a nearly flat-band condition, and the laser transition is between superlattice minibands.
Recent papers from the Lucent group report innovative superlattice interminiband lasing in III-V heterostructures. The structure was a cascade of superlattice active regions in which interminiband lasing occurred “in parallel”[42]. Thus, this cascade was a series arrangement of parallel lasers. They investigated a cascade in which miniband transport was used within each superlattice injector in each period. They also studied an injectorless cascade in which the lower miniband of one active period resonated with the upper miniband of the next period[43].

We believe that analogous IV-IV cascades could be constructed using the valence minibands in a Si/SiGe superlattice. Rather than presenting those cascades designs explicity, we have chosen here propose a new and more speculative QPL: a flat band p-i-p SiGe/Si superlattice electrically pumped with holes. This QPL would have a very simple well-and-barrier structure. The ideas behind the QPL are: firstly, to use a low field \( F \) that is below the Wannier-Stark localization field \( F_{n_0} \), implying that the shared miniband levels are not decoupled from one quantum well to the next, and secondly, to inject holes from a p\(^+\) contact selectively into an upper miniband, giving rapid transport of carriers along that miniband to all quantum wells in the superlattice. Then the carriers in all quantum wells make simultaneous radiative transitions to the to a lower miniband, giving FIR emission. The quantum well pumping and emission are in parallel rather than in series.

The QPL lasing scheme -- comprising, in effect, four levels - can be seen by looking at the valance subband curvatures as a function of superlattice normalized wavevector \( \Omega \), over the superlattice minizone bounded by \( k_z=0 (\Omega_z = 0) \) and \( k_z = \pi P \ (\Omega_z = 1) \) where \( P \) is the period (Figure 8). The upper and lower ends of a curve define the miniband width. We propose that a new THz QPL VCSEL could be created in SiGe/Si by utilizing a HH2 miniband to LH1 miniband radiative transition at the edge of the minizone. The dispersion diagram shown in figure 8, engineered at AFRL, was obtained after several \( k_p \) trials; the final design being a strain balanced 70Å Si\(_{0.7}\)Ge\(_{0.3}\)/ 20Å Si superlattice on (100) SiGe virtual substrate. Selective pumping into HH2 is done at the superlattice zone center. Those holes relax rapidly via acoustic phonons to the HH2 minizone edge where the 22 meV TE-polarized vertical HH2-to-LH1 radiative emission occurs.
Figure 8. SiGe/Si superlattice dispersion for the QPL example listed in text.

Note that Z-polarized photon emission from HH2 to HH1 is also feasible. For a QPL designed for TE emission, the cavity geometry would be engineered to suppress the TM mode (HH2-HH1) emission. However, an alternative QPL bandstructure design may also be conceived, in which HH2-HH1 is the desired radiative transition, with a ridge-waveguide geometry used as a resonator.

In the silicon rich superlattice of the QPL there are very few 37meV Ge-Ge mode optical phonons. Thus, in effect, the lowest-energy optical phonon modes are the Si-Ge alloy modes, with a phonon energy of approximately 52meV. We have engineered the superlattice so that the energy of the diagonal-in-$Q_z$ optical phonon emission path from the populated HH2 band at $Q_z=1$ to the relatively empty HH1 band at $Q_z=0$ is 50.8 meV - less than the Si-Ge phonon energy. By that technique, the non-radiative phonon emission at $Q_z=1$ that competes with the laser radiation is not energetically allowed, giving an enhanced ratio of radiative to nonradiative intersubband transitions, as desired. Hole/phonon scattering is a very rapid intrasubband process that provides the necessary relaxation processes for this QPL, and acoustic phonons also help to empty the lower LH1 level, as needed for HH2-LH1 population inversion, by scattering holes from LH1 to HH1 at the zone center. More generally, the QPL design could also be implemented in III-V superlattices and in n-i-n devices that use the CR2 and CR1 minibands.

8. Other SiGe laser ideas: the phonon-pumped laser (PPL)

A revolutionary kind of SiGe/Si superlattice interminiband THz laser - the "phonon-pumped laser" (PPL) - has been invented and analyzed by Sun, Soref, and Klurgin [44].
The PPL does not employ optical pumping or electrical pumping. Only a temperature difference across the superlattice, from 77K to 300K for example, is required to pump up the carriers from the lowest miniband into the excited miniband. The scheme has been described in recent publications [44,45]. A semiconductor layer called the heat buffer layer (a Ge-rich alloy) is deposited atop the superlattice to confine most of the optical phonons within the superlattice while acoustic phonons escape. Thus the optic phonons have a "hotter" temperature profile over a portion of the superlattice than the acoustic phonons as shown in Figure 9. This allows optical phonon absorption to create a hole population inversion between upper and lower minibands locally at the $Q_z=1$ zone edge. For example, the flat-band dispersion curves of a 68Å p-Si$_{0.94}$Ge$_{0.06}$/Si superlattice strain balanced on an SiGe virtual substrate when plotted versus $Q_z$ look similar to those described above in Figure 9 for the QPL, and the opposed curvature of adjacent minibands is used in a 4-level phonon pumped scheme. Here the 52 meV Si-Ge phonon energy is greater than $E(\text{HH}2, Q_z=0) - E(\text{HH}1, Q_z=0)$, not less as in Figure 8. The quantum wells of the superlattice are p-doped, or remotely doped, to a density $N_p \approx 1 \times 10^{18}$ cm$^{-3}$ in order to populate the lowest miniband. It is also feasible to phonon-pump at the center of the Brillouin zone if the superlattice shows an inverted mass vs $k_x$ or $k_y$. In practice, the superlattice chip would be bonded to a cold finger of an optical dewar at 77K (or at 20K in closed-cycle cooler) that has a THz-transparent window situated near the chip end where the TM-polarized edge emission from the laser chip transmits through the window. To maintain the upper surface of the chip at about 300K, a thin-film NiCr electrical resistance heater (in the form of a stripe) would be deposited atop the superlattice as shown in Figure 10.
This heater strip would have the same form as the line-shaped THz waveguide employed in the PPL. Then a dc current would be passed through the resistive strip and local Joule heating would give the desired temperature gradient across the superlattice stack. The required amount of electrical power dissipated in the strip depends upon the thermal conductivity of the superlattice, the superlattice thickness, and the width and length of the strip. For representative values, this power is about 0.2W.

9. Experimental progress to date

A consortium led by the University of Leeds (UK), and including Cambridge, Sheffield and Heriot-Watt universities, and the UK company QinetiQ, have been working towards the development of surface-emitting THz Si/SiGe quantum cascade lasers under DARPA/AFRL funding. P-type Si/SiGe heterostructures have been grown by low pressure CVD at QinetiQ using an industry standard Applied Materials Epi-Centura reactor. SiH₄ and GeH₄ sources were used, with a hydrogen carrier, whilst B₂H₆ was used to provide p-type dopants. The team have focused on strain-balanced heterostructure designs, as described in section 3, grown on SiGe virtual substrates, which typically comprise 3μm of linearly graded SiGe, followed by a 1μm strain-relaxed buffer at the target composition. Buffer compositions in the range 20-30% have been grown. Figure 11 shows a TEM image of a 10 period multiple [46].
quantum well structure grown using this method. The buffer composition is 22% and the quantum well Ge composition is 28%. Each quantum well has Si barriers and the wells are separated by thin $\text{Si}_{0.78}\text{Ge}_{0.22}$ spacer layers. The TEM image clearly shows that, whilst misfit dislocations exist in the linear graded region of the sample, the vast majority terminate within the buffer layer, with no significant propagation into the quantum well layers.

The Leeds-led team has recorded a number of notable achievements in THz emission from Si/SiGe heterostructures. They have observed the first THz intersubband electroluminescence in Si/SiGe heterostructures (in both edge- and surface-propagation geometry)[46,47], and the first surface-normal electroluminescence in a quantum-cascade device in any materials system[5,48]. The quantum cascade devices grown by the team follow the quantum staircase design described in section 5. 30 period heterostructures comprising $\text{Si}_{0.7}\text{Ge}_{0.3}$ quantum wells and Si barriers have been grown, nominally strain balanced on a $\text{Si}_{0.77}\text{Ge}_{0.23}$ virtual substrate. Short (30nm) linearly graded (23-30% Ge composition) injector and collector layers were grown at either end of the quantum well stack to improve carrier injection and collection efficiencies. Figure 12 shows a TEM image of the 30 period quantum well stack, displaying the excellent uniformity and planarity of the layers, and again confirming the absence of any significant dislocation density in the heterostructure region.

![TEM image of a 30 period Si/Si$_{0.7}$Ge$_{0.3}$ quantum cascade structure, nominally strain balanced on a Si$_{0.77}$Ge$_{0.23}$ virtual substrate.](image-url)

**Figure 12.** TEM image of a 30 period Si/Si$_{0.7}$Ge$_{0.3}$ quantum cascade structure, nominally strain balanced on a Si$_{0.77}$Ge$_{0.23}$ virtual substrate [5].
Additionally, figure 13 shows the Germanium composition profile across the graded injector layer and the first few quantum well layers obtained using both electron energy loss spectroscopy (EELS) and energy dispersive X-ray analysis.

![Fractional Ge Concentration vs Nanometres](image)

Figure 13. Germanium composition profile across the graded injector layer and the first few quantum well layers of the quantum cascade structure shown in figure 12. The solid line shows data obtained from energy filtered TEM (electron energy loss spectroscopy), whilst the individual points (squares) mark data obtained from energy dispersive X-ray analysis [48].

Devices were fabricated by reactive ion etching into 180 μm x 180μm and 360 μm x 360μm mesas, with Al ohmic contacts, and were analysed by Fourier transform infrared spectroscopy using a Bruker 66V spectrometer with a liquid helium cooled Si bolometer detector. The spectrometer was used in step-scan mode with a lock-in amplifier, and the vertical bias applied to the cascade structures was pulsed (at 413Hz) to provide a lock-in reference. Figures 14 and 15 show typical spectra obtained for a sample mounted in edge-emission and surface-emission geometry respectively.
Figure 14. Edge-emission FTIR spectrum for the quantum cascade device shown in figure 12, taken at 4.2K, with a 7V bias pulsed at 413Hz with a 10% duty cycle [48].

Figure 15. Surface-emission FTIR spectrum for the quantum cascade device shown in figure 12, taken at 4.2K, with a 7V bias pulsed at 413Hz with a 50% duty cycle [5].

Both heavy hole – heavy hole and heavy hole – light hole optical intersubband transitions give rise to edge-propagating radiation, and figure 14 clearly shows features corresponding to the LH1-HH1 and HH2-HH1 transitions, as deduced from the agreement with the theoretically calculated intersubband absorption spectra, also shown. On the other hand, only the light hole – heavy hole transitions give rise to surface-normal emission, and, indeed, figure 15 shows that the HH2-HH1 emission is absent in surface-emission geometry, but the LH1-HH1 feature remains. THz power levels of up to 10nW have been measured in surface-emission mode at 4.2K, which is over 3 orders of magnitude higher than that reported for any other THz quantum cascade emission. When translated to a power efficiency, for the 15meV photon energy and 1mA current, this
device gives a figure of $2.4 \times 10^5$, which compares remarkably favourably with the $4.4 \times 10^{11}$ figure of merit obtained for spontaneous emission from a GaAs/AlGaAs THz cascade [49].

A consortium led by the Paul Scherrer Institute in Switzerland has reported electroluminescence from a prototype Si/SiGe quantum cascade structure at mid-infrared wavelengths [29]. The photon energy was $\sim 130 \text{meV}$, corresponding to HH2-HH1 transitions in their structure[50]. The MIR (edge-emission) power output was approximately 20pW, for a current of 800mA, giving a power efficiency of $\sim 10^{-11}$. The much higher efficiencies obtained for the SiGe THz cascade, compared to both the GaAs/AlGaAs THz cascade and the SiGe MIR cascade may be due, in part, to the reduced non-radiative scattering which results from use of a non-polar system (compared to the case of GaAs/AlGaAs) and from working at photon energies below the optical phonon energy (compared to the SiGe MIR device). Certainly, for a 130meV subband separation, strong deformation potential optical phonon scattering may be expected, compared to the SiGe THz device. The high efficiencies obtained may also be due to a higher collection efficiency in surface emission mode, compared to the edge emission mode.

10. Prospects for Si-based optoelectronic THz chips

Optoelectronic integration is a key motivation for choosing SiGe/Si. We envision a wafer-scale or chip-scale Si or Si-virtual substrate platform serving as “motherboard” for a complete THz system including lasers, detectors, active switching components, Si and SiGe electronic drivers and amplifiers, and passive photonic components such as a planar network of THz waveguides, filters, couplers, splitters, combiners, add/drop wavelength multiplexers, and THz antennas. When THz radiation makes a transition from free space to-or-from the Si chip, Si gratings or undoped silicon lenses (transparent at THz) can aid this transition. (The assumption is that semi-insulating Si will be transparent because its free carrier absorption will be low.) SGOI and SOI are valuable THz substrates as well. We mentioned earlier the buried silicide and buried oxide possibilities for the lower mirror of a THz VCSEL. Another intriguing possibility being investigated at the University of Delaware under AFOSR sponsorship is THz waveguiding and switching in a photonic bandgap (PBG) lattice of posts or holes that are e-beam etched into an SOI substrate[51]. Simulations by FDTD indicate that a network of THz waveguide components and 2 x 2 electrically controlled THz switching components can be created in a 2D or 3D PBG SOI structure. Sharkawy et al [52] have modeled an SOI low-loss, low-crosstalk 2 x 2 PBG THz directional coupler switch in which the conductivity of the coupling region is controlled by carrier injection.
11. Summary

It is clear from the above description that much remains to be done in the area of SiGe quantum cascade lasers, and Si-based THz optoelectronics in general. However, there has certainly been an acceleration in activity. After several years existing as a theoretical proposal only, the SiGe quantum cascade laser is now being actively pursued in at least 4 experimental programmes worldwide. Although the SiGe materials system does pose some different challenges from those originally faced by the III-V quantum cascade laser community, none of these appear fundamental, and the example set by that community indicates that, with sufficient ingenuity, expertise and effort, a SiGe cascade laser can also become a reality.

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References

18. Z Ikonic, unpublished


32. R. A. Soref and G. Sun, "Terahertz gain in a SiGe/Si quantum staircase utilizing the heavy-hole inverted effective mass" Appl. Phys. Lett. 79 3639-3641 (2001)


37. A Trediciucci et al, unpublished


44. G. Sun and R. A. Soref, "Phonon-pumped terahertz gain in n-type GaAs/AlGaAs superlattices", Appl. Phys. Lett. 78 3520-3522 (2001)

50. MIR luminescence due to HH2-HH1 transitions in Si0.35Ge0.45/Si quantum cascade structures has also been reported by: I. Borman, K. Brunner, H. Riedhl, G. Abstreiter, S. Hackenbuchner, G. Zandler, P. Vogl, S. Schmelt, W. Meindr and W. Wegsneider, "Mid-Infrared Intersubband Electroluminescence of Si/SiGe Quantum Cascade Structures", presented at the Sixth International Conference on Intersubband Transitions in Quantum Wells (ITQW'01), Asilomar CA, (10-14 Sept 2001).
51. D Prather, "Photonic band gap structures for terahertz photonics" paper IMB1-2, Optical Society of America, Integrated Photonics Research Conference, Digest, pp 2-4, Monterey, CA (11 June 2001)