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**Published paper**
Simulated [111] Si–SiGe THz Quantum Cascade Laser

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The prospect of developing a silicon laser has long been an elusive goal, mainly due to the indirect band-gap and large effective carrier masses. We present a design for a THz intersubband laser grown on the [111] crystal plane, and simulate performance using a rate equation method including carrier–phonon and Coulombic interactions. We predict gain greater than 40 cm⁻¹ and a threshold current density of 70 A/cm².

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Quantum cascade lasers (QCLs) have undergone much development over recent years and are now commercially available as compact semiconductor sources of THz radiation. A Si-based THz QCL would potentially reduce fabrication costs because of the mature processing technology.[1] Intersubband electroluminescence has been demonstrated in Si–SiGe systems,[2, 3] however, an Si-based QCL has yet to be realized.

Investigation of Si–SiGe QCLs has so far focused on p-type systems grown on [100] Si substrates. The most commonly stated reasons are that valence band offsets are larger than conduction band offsets, that n-type dopants cannot be localized within individual barriers, and that hole masses are lower than the electron masses.[4] however, we will show that none of these cited drawbacks are an issue for [111] oriented n-type systems. Firstly, conduction band offsets were calculated to be 160 meV for Si–Si₀.₅Ge₀.₅ on [111] strain-symmetrized virtual substrates, which is certainly large enough for THz intersubband transitions. Secondly, the calculated ionized impurity scattering for uniformly distributed dopants does not significantly affect the carrier dynamics. Finally, the quantization mass for the [111] orientation is approximately equal to the heavy-hole mass.

Designs have emerged for n-type Si-based QCLs exploiting L-valley transitions in Ge–SiGe systems,[5, 6] however these require very high Ge fraction virtual substrates which are difficult to grow on an Si substrate. Some progress has been made towards an n-type QCL using Si–SiGe in the [100] orientation,[7] but the many-valley band structure causes problems. The conduction band minima are in the six degenerate Δ valleys in bulk materials. However, strain and effective mass anisotropy split the degeneracy in QCLs into a pair of Δ⊥ valleys with quantization effective mass, \( m_q = 0.916 \) (the longitudinal effective mass) and a quartet of \( \Delta \parallel \) valleys with \( m_q = 0.19 \) (the transverse effective mass). In [111], the quantization effective mass, \( m_q = 0.26 \), is the geometric mean of the longitudinal and transverse effective masses[8] (c.f. heavy-hole masses of 0.29 in Si and 0.21 in Ge).[9]

In [100], the \( \Delta\perp \) band offset is larger, and the subband energies lower than the \( \Delta\parallel \) case.[10] The \( \Delta\parallel \) states are effectively unconfined for quantum wells (QWs) on length scales that strongly confine the \( \Delta\perp \) states. A similar situation exists with light-hole states in [100] p-type systems. In these anisotropic mass systems, the energy range for intersubband transitions is limited by strain-splitting to avoid populating the low mass states. Using thicker barriers increases the splitting but reduces the dipole matrix element between QWs. Growth in the [111] orientation preserves the \( \Delta \) valley degeneracy, and thus avoids these constraints. Although the band offset is lower than those of the high mass states in [100] systems, the usable energy range for intersubband transitions increases as it is no longer restricted by the presence of low mass states. Conduction band offsets were calculated using the model solid approximation.[11] \( \Delta \) minima were located for unstrained alloys by interpolation of elemental \( \Gamma \rightarrow \Delta \) band...
enhance depopulation, it would require an increased electric transition at 15 meV and a depopulation transition of 30 meV. Although a larger depopulation energy would dominate.

The electron probability densities at the design bias are shown in Fig 2. The design exploits the dependence of scattering on subband separation by having a radiative transition at 15 meV and a depopulation transition of 30 meV. Although a larger depopulation energy would enhance depopulation, it would require an increased electronic field and hence give rise to a larger current and higher electron temperatures. 30 meV was chosen as a compromise between these factors.

Electron temperatures were calculated self-consistently to be 150 ± 10 K at the design bias and at a lattice temperature of 4 K. The doping was 2 × 10^16 cm^-3 throughout the system, giving 7.8 × 10^10 cm^-2 sheet density, which is low enough to avoid significant band-bending due to space-charge.

The carrier lifetimes were calculated as 6.11 ps for the upper laser level and 2.74 ps for the lower laser level, and the population inversion was 17.9% of the sheet doping density. The gain peak at 3.6 THz corresponds to the designated laser transition, and the additional peak at 4 THz corresponds to stimulated transitions into the subband just below the lower laser level. Absorption below 2 THz is due to intra-miniband transitions and at 6–8 THz due to transitions across the large population well. Spontaneous emission occurs at the same frequencies as stimulated emission and at energies corresponding to the depopulation transitions in the large well.

To gain insight into the carrier dynamics in the Si–SiGe heterostructure carrier-dynamics is given in our related publication.

State populations were calculated by solving a set of rate equations for the quantum confined states, accounting for alloy disorder, interface roughness, intervalley acoustic phonon scattering, electron–phonon, and carrier–carrier scattering. Gain and electroluminescence were then calculated using the subband populations obtained from the solutions of the rate equations. Further detail on the Si–SiGe heterostructure is given in our related publication.

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FIG. 4: Current density as a function of applied electric field. $z_{av}$ is the current calculated according to the difference in $z$-expectation values between states, whereas $r.p$ is calculated by considering only inter-period scatterings across a ‘reference plane’ with an effective displacement of one period length.

The gain exceeds this at around 12 kV/cm, from which we can infer that the threshold current density will be approximately 70 A/cm$^2$. For a device area of 200 $\mu$m by 3 mm this corresponds to a current of 0.4 A, and for an active region height of 10 $\mu$m (and hence an applied bias of 12 V) we have a total dissipated power of 5 W assuming negligible contact resistance.

In conclusion, the [111] $n$-type system removes the design constraints imposed by the presence of low mass strain-split states in [100] systems, and as such is a more attractive candidate for Si-based QCLs. We have simulated Si–SiGe heterostructures on the [111] crystal plane using a rate equation approach which includes scattering due to phonons, interface roughness, alloy disorder and Coulombic interactions. Using this, we have developed a 3.6 THz Si–SiGe QCL design, with gain of over 40 cm$^{-1}$ and a threshold current density of around 70 A/cm$^2$.

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