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Terahertz gain in a SiGe/Si quantum staircase utilizing the heavy-hole inverted effective mass

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Modeling and design studies show that a strain-balanced $Si_{1-x}Ge_x/Si$ superlattice on $Si_{1-y}Ge_y$-buffered Si can be engineered to give an inverted effective mass HH2 subband adjacent to HH1, thereby enabling a 77 K edge-emitting electrically pumped $p-i-p$ quantum staircase laser for THz emission at energies below the 37 meV Ge–Ge optical phonon energy. Analysis of hole-phonon scattering, lifetimes, matrix elements, and hole populations indicates that a gain of $450\,\mathrm{cm}^{-1}$ will be feasible at $f=7.3$ THz during $1.7\,\mathrm{kA/cm}^2$ current injection. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1421079]

Previous work on electrically injected SiGe/Si quantum-well (QW) THz lasers[1–3] has centered on the light-hole-1 to heavy-hole-1 (LH1 to HH1) intersubband transition that is suitable for XY polarized vertical-cavity surface emitting lasers. In this letter we propose a hole-injected Z-polarized edge-emitting THz laser that employs the HH2 to HH1 transition in which an inverted effective mass (IEM) is engineered for the HH2 subband near the zone center. Assuming an operating temperature of 77 K, we calculate the well-and-barrier parameters that yield the HH2 IEM, a local band curvature produced by repulsion of nearby LH1 and HH2 subbands at $\mathbf{k}_{\parallel}=\mathbf{0}$. We determine the critical electric field bias F_0 that gives 3 meV spaced HH doublets in two neighboring active QWs that comprise the proposed quantum staircase laser (QSL). The population distribution between the HH doublets follows the Boltzmann function because of the small energy separation and strong envelope-function overlap, which leads to a population inversion between HH2 and HH1 in the two neighboring doublets. Hole-acoustic-phonon intersubband scattering rates are calculated along with the THz spontaneous emission rates to establish a relationship between the total hole population and injected current density. Then a rate-equation analysis predicts the total population inversion. The gain in the staircase is estimated as a function of the selectively injected current density J. Our proposed QSL is intended to be a useful adjunct to the LH1-HH1 SiGe/Si THz laser being developed by the University of Leeds, Cambridge University, in conjunction with DERA and Heriot-Watt University.[4,5] Unlike the quantum cascade laser (QCL), the QSL does not contain chirped superlattice injectors or wide/narrow coupled-well active regions. Thus, the QSL is a simpler alternative to the SiGe/Si THz QCL being developed by the Swiss group[6] and by the University of Delaware and Sarnoff Corporation.[7]

The SiGe/Si superlattice (SL) is assumed to be strain balanced, that is, the compressively strained $Si_{1-x}Ge_x$ QW layers and the tensile strained Si barrier layers are grown on a relaxed $Si_{1-y}Ge_y$ buffer layer-on-⟨100⟩ Si (a virtual substrate), where y is chosen to give zero net strain for the specific x, l_w, and l_b being studied (l_w=QW thickness, l_b =barrier thickness). For SLs with (or without) an electric field applied, we determined the subband energies, subband dispersion in (k_x, k_y) space, wave function amplitudes, and band mixing among HH, LH, and SO using the 6×6 band $\mathbf{k\cdot p}$ commercial software from Quantum Semiconductor Algorithms, Inc., Northborough, MA. The software includes strain effects and it uses a 0.68 eV Ge/Si valence band offset. The IEM exists over several regions in x, l_w, l_b space. For example, using the SL boundary condition at $q_z=0.5$, $F=0$, $x=0.3$, and keeping l_b fixed at 40 Å, we find a LH1 IEM when $98\,Å<l_w<105\,Å$. An increase in l_w produces a HH2 IEM over the range of $105\,Å<l_w<112\,Å$. Increasing l_w to more than 112 Å leads to quasiparabolic HH2 dispersion. The changeover from the LH1 IEM to the HH2 IEM as l_w widens is general behavior. The quasiparabolic F_0-biased HH2 structures appear to be feasible for QSLs, but at higher-J thresholds than IEM SLs.

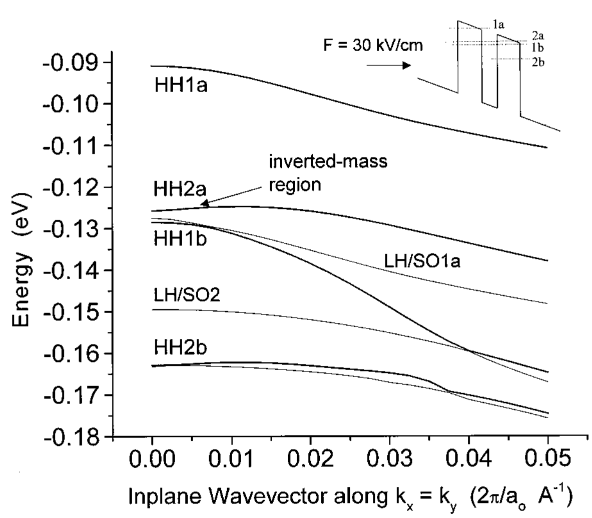

FIG. 1. Dispersion of a strain-symmetrized $Si_{0.8}Ge_{0.2}/Si$ 2QW at bias of F_0 just above the anticrossing value.

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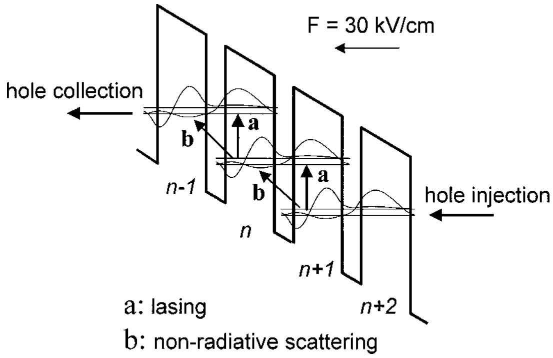

FIG. 2. Band diagram of the proposed SiGe/Si HH2/HH1 QSL at F_0. The labels $(n-1,n,n+1,...,)$ represent the QWs in which the wave functions are localized.

We want to eliminate optical phonon emission from the upper laser state and make the radiative-to-nonradiative branching ratio as large as possible. Since the QWs contain Si–Si, Si–Ge and Ge–Ge lattice vibration modes (with optical phonon energy $\hbar\omega_0=64.5$, 50.8 and 37.2 meV, respectively), we engineer the SL so that the laser photon energy $(\hbar\omega_L)$ is less than the lowest-energy Ge–Ge phonons. This requires small values of x. We then analyze a model system consisting of two QWs under electric field bias, knowing that the easily computed two-well results for the lowest-two HH states would give the essential behavior of a similarly biased N-well staircase, the actual laser. After several (l_w, l_b) trials, the five-layer strain-symmetrized 2QW for $x=0.2$ of 250 Å Si/90 Å SiGe/35 Å Si/90 Å SiGe/250 Å Si was found to exhibit a LH1 state 2 meV higher than HH2 at $\mathbf{k}_\parallel=0$, as desired for HH2 IEM. Figure 1 shows the calculated in-plane (1,1) dispersion of this biased structure, where the Stark-split levels are labeled HH1a, HH1b, HH2a, and HH2b. An anticrossing of HH1b and HH2a occurs at the field $F_{ac}=\delta E_{hh}/P$ where δE_{hh} is the 33.1 meV zero-field separation and the P is the 90 Å + 35 Å period, yielding $F_{ac}=26.4$ kV/cm. The operating field of the laser F_0 is made larger than F_{ac} to produce a 3 meV spacing between HH2a and HH1b, namely, $F_0=30$ kV/cm. The resulting QSL $(\hbar\omega_L=30$ meV), illustrated in Fig. 2 for the case of four QWs, has two active doublets per QW, that is, a four-level system discussed previously for GaAs/AlGaAs.[8] In Fig. 2, the laser transitions are indicated by the vertical arrows. The

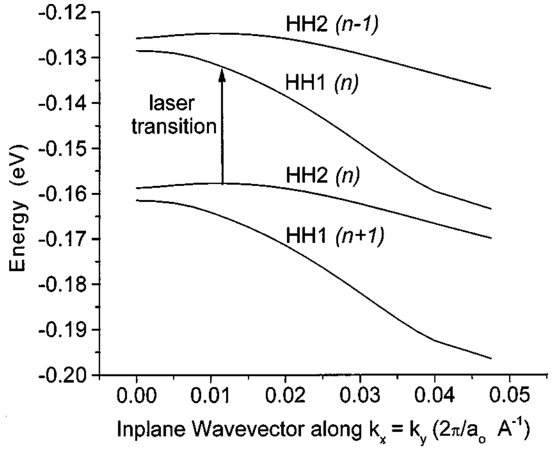

FIG. 3. Dispersion of the four active levels in Fig. 2.

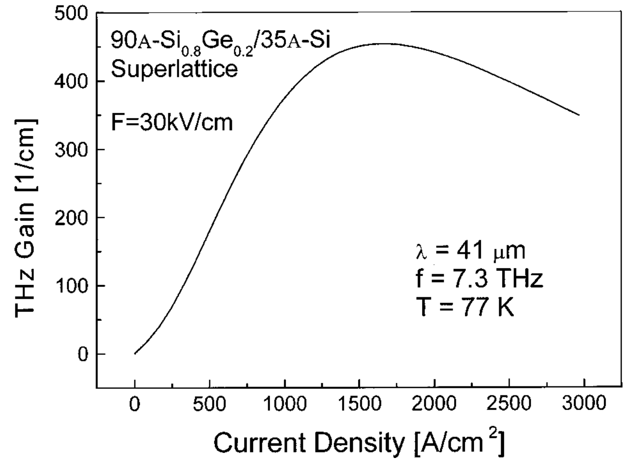

FIG. 4. Calculated gain in the Fig. 2 QSL as a function of the hole current density injected into the upper laser states.

transitions within the doublets are rapid. Figure 2 illustrates the wave functions found at this bias. Figure 3 shows the four-level system in $\mathbf{k}_\parallel$ space.

The total concentration N of holes injected into the doublets is $N=N_1+N_2$, and when quasiequilibrium is reached in the doublets, the Boltzmann relation gives $N_1=N_2\exp(-\delta E/kT)$, where δE is the 3 meV energy separation within the doublets. This relation holds for all doublets. Also, the injected current density can be related to the total population as $J=eNP/\tau_{eff}$, where τ_{eff} is the effective lifetime $1/\tau_{eff}=1/\tau_{sp}+1/\tau_{ph}$, in which τ_{sp} is the spontaneous emission lifetime in the Fig. 3 level-3-to-level-2 laser transition, and τ_{ph} is the nonradiative lifetime on that transition. In turn, τ_{ph} is governed by the hole-acoustic-phonon scattering rate, which we have determined for the Fig. 1 2QW using the formalism given by in Sun *et al.*[9] Our calculations give $\tau_{ph}=1.0$ ns. The dipole matrix element of the vertical in $\mathbf{k}$ space lasing transition is the overlap integral between two HH wave functions (upper and lower laser states) which, according to Fig. 2, are localized in the same QW. We performed this integration numerically and found that $\langle HH_u|z|HH_l\rangle=20$ Å in Fig. 2. This result in turn implies that $\tau_{sp}=77\,\mu$s. We used these two lifetimes together with the Boltzmann distributions to estimate hole populations, which showed a total inversion of the Fig. 3 HH2(n) population relative to HH1(n), as desired. Finally, with the aid of Eq. (5) in Ref. 3, we estimated the gain as a function of J with the result presented in Fig. 4. The peak gain of 450 cm^{-1} at 7.3 THz is expected to be larger than the QSL cavity losses such as free carrier absorption.

In conclusion, we have designed and simulated a 3–9 THz, 77 K strain-balanced Z-polarized SiGe/Si $p-i-p$ laser in a simplified form of the quantum cascade that we call the quantum staircase. The x, l_w, and l_b are selected to give the IEM for HH2, which optimizes the THz gain. The staircase is biased above the anticrossing field, creating two active HH doublets per QW, a four-level system. The first p^+ contact injects holes selectively into the doublets of the first QW, while the second p^+ contact collects holes from the doublets of the last QW in this high-gain superlattice.

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