

The Design and Operation of TeraHertz Sources Based on Silicon Germanium Alloys

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Abstract—During the past few years, vigorous studies have begun on semiconductor devices that generate and detect frequencies from 0.3 - 10 TeraHertz (1000 - 30 μm). Previous THz sources were based on electrical methods using transistor oscillators (to 0.5 THz), diode frequency multipliers (to 2.5 THz), and femtosecond optical pulse switches. Infrared emitters such as the Quantum Cascade Laser in the III-V semiconductors have been difficult to extend to THz frequencies due to reststrahlen absorption by polar phonons. In contrast, Si has lower absorption and devices may be able to operate over a broader THz range than the III-V semiconductors. This report describes the fabrication and characterization of THz sources based on three different design approaches: intersubband transitions in Silicon Germanium quantum wells, resonant state transitions in boron-doped strained SiGe quantum wells, and dopant impurity transitions in doped Si layers.

Index terms—TeraHertz, Intersubband devices, Silicon Germanium, Quantum wells, Impurity transitions

I. INTRODUCTION

Imaging, communication, and spectroscopic applications in the mid- and far-infrared regions have underscored the importance of developing reliable sources and detectors operating in the frequency range from 0.3 to 10 TeraHertz (1000 to 30 μm wavelength). Recent studies suggest that THz interactions can enable a variety of new applications on a wide range of solids, liquids, gases, including polymers and biological materials such as proteins and tissues[1, 2]. Compared to microwaves, the far-infrared or TeraHertz frequency range has significant reductions in antenna sizes, and greater communication bandwidth. Commercial applications comprise thermal imaging, remote chemical sensing, molecular spectroscopy, medical diagnosis, fire and combustion control, surveillance, and vehicle driver vision enhancement. Military applications comprise night vision,

rifle sight enhancement, missile tracking, space-based surveillance, and target recognition [3].

Quantum cascade lasers (QCLs) fabricated from III-V materials have demonstrated light emission at wavelengths typically shorter than 10 μm over large temperature ranges. However, III-V compound semiconductor devices may have limitations due to the strong reststrahlen phonon absorption at THz frequencies. The silicon-germanium material system is an established technology offering monolithic circuit integration with powerful signal processing algorithms, and polar phonons are absent offering low-loss guiding capability and reduced free-carrier absorption. The quantum-mechanical selection rules of bandgap engineered silicon germanium predict both in-plane and out-of-plane photon polarizations. This could potentially allow vertical incidence without the need for grating couplers to convert the electric field to be perpendicular to the plane of the quantum wells, as required in conventional III-V quantum well devices. A silicon based design allows easy integration and better thermal conductivity to the substrate and device packages [4]. Few results have been published on silicon-based devices, however, due to the challenges of making high-quality strained silicon-germanium multiple quantum wells on silicon substrates.

In this talk, we describe the fabrication and characterization of sources based on three types of design approaches: SiGe quantum well intersubband transitions, boron doped resonant state transitions in strained SiGe, and impurity transitions in doped Si.

II. QUANTUM WELL INTERSUBBAND TRANSITIONS IN SiGe

Electroluminescence has been reported from structures based on intersubband transitions between confined states in SiGe quantum wells. The observed emission was typically at the upper limit of the THz range, with emission reported at for instance 30 THz [5] and 34-37 THz [6]. Recently, there have been reports on longer-wavelength emission at 2.9 and 6 THz [7]. In the SiGe material system, the band gap difference manifests itself mainly as an offset in the valence band. Quantum well devices fabricated from SiGe alloys typically employ the confinement of holes in the valence band.

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Several factors complicate theoretical calculations for SiGe structures. The valence band quantum wells can confine heavy holes, light holes, and spin-orbit split-off holes. The spin-orbit interaction splits the valence bands into four-fold, and two-fold degenerate bands. SiGe alloys on Si substrates are typically strained, resulting in additional splitting of the band, and coupling between different valence bands. For the calculations to be accurate, these effects must be taken into account [8]. The intersubband transition approach described here used multiple periods of SiGe wells (typically 2 to 3 nm thick) with Si barriers (typically 1.4 to 3 nm thick) [9]. The layer thickness and compositions were designed using software that solves the Schrödinger equation based on an 8 band k·p model (FemB software from QSA).

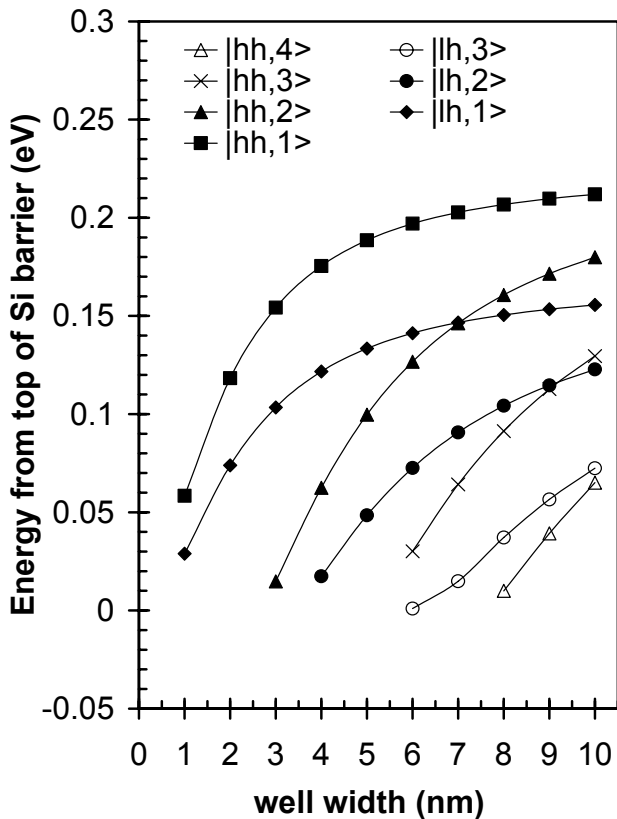


Figure 1. Calculated eigenenergies of confined states in a Si/Si_{0.7}Ge_{0.3}/Si quantum well vs. well width for zero applied electric field. Energy is referenced to the heavy hole/light hole band edge in the Si barrier. The bottoms of the quantum wells for the heavy hole and light hole occur at 223 meV and 167 meV, respectively.

The subband energies for a Si_{0.70}Ge_{0.30} quantum well as a function of the quantum well width are given in Figure 1. For small quantum well widths, there are only two confined states; a heavy-hole state; and a state with both spin-orbit and light-hole character. For 30 % Ge content, we have selected well widths for separations in energy corresponding to transitions slightly below 12 THz.

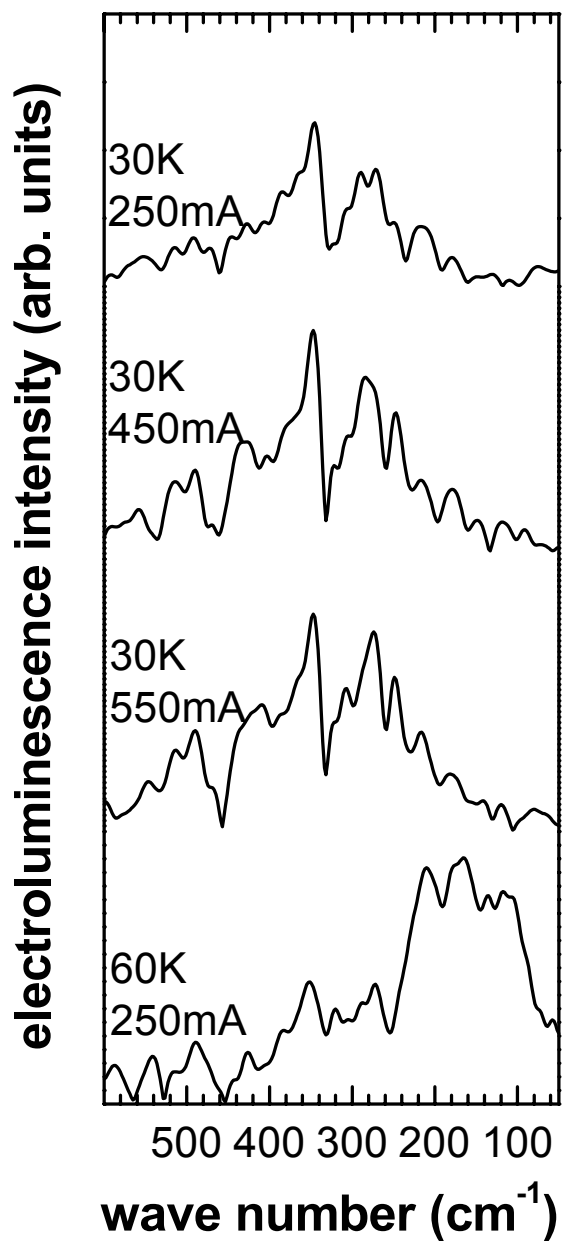


Figure 2. Dependence of electroluminescence intensity (relative units) on wavenumber for a 16-period superlattice of 2.2 nm Si_{0.7}Ge_{0.3} QWs, with 3 nm Si barriers (SGC 437) at temperatures of 30K and 60 K, showing a peak at 350 cm⁻¹ (10.5 THz). The peaks of the drive current pulses are indicated near the curves, which are offset in the vertical scale for clarity. The shift of the peak to smaller wavenumbers at the temperature of 60 K was attributed to the dominance of a different subband transition.

Mesa shaped devices with typical areas of 200 μm x 200 μm were fabricated using photolithography with dry etching. The emission spectrum of a typical device is shown in Figure 2, measured by Fourier Transform Infrared Spectroscopy (FTIR) in the step-scan mode using a 0.5 % duty cycle with 500 ns pulses at a 413 Hz repetition rate, to avoid device heating that produces black body emission and much broader

spectra. The FTIR instrument was a ThermoNicolet Nexus 870 with a solid-state beamsplitter and liquid-helium cooled silicon bolometer detector. The devices operated to temperatures above 20 K, with some devices giving weak emission up to 150 K. The emission frequency agreed with quantum well simulations.

III. RESONANT STATE TRANSITIONS IN SiGe

The second type of THz source was based on resonant state transitions between boron acceptor states that are split by the built-in strain in SiGe quantum wells [10]. The upper level of the acceptor state is resonant with the valence band. For 15 % Ge in the well, the strain splits the boron dopant levels by about 31 meV, which is sufficient to move the upper levels of the boron acceptor (with ionization energy = 45 meV for Si, 10 meV for Ge) from the gap state into the valence band, producing state resonance and population inversion. Devices were fabricated using standard processing with lateral contacts on the top surface, and parallel polished facets along the sides. The device was a highly polished bar, approximately 1 mm square by 1 cm in length. THz emission was demonstrated from boron delta-doped sheets located within strained SiGe quantum wells at a wavelength of approximately 100 μm [11]. As shown in Figures 3 and 4, an applied current of tens of mA produces emission near 3 THz with output powers near 0.3 mW at a temperature of 4K. The spectrum was measured using a grating spectrometer and a Ge:Ga photodetector. The device was biased with low duty cycle sub-microsecond pulses to avoid heating.

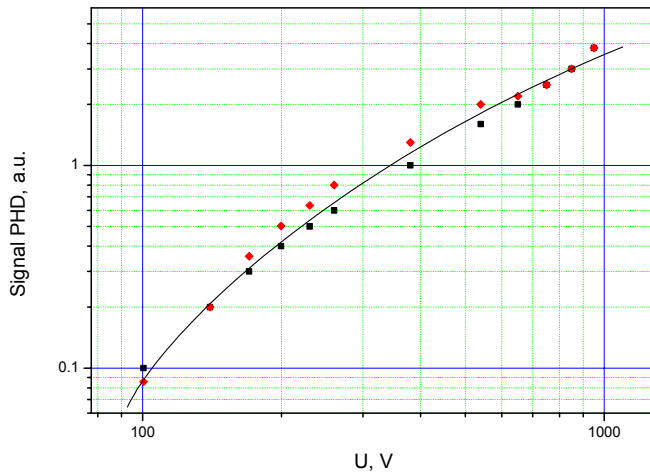


Figure 3. The measured emission signal intensity (arbitrary units) versus applied voltage (Volts) for structure 416, in liquid He. The resonant state device had a boron delta doped plane in a SiGe quantum well on a Si substrate.

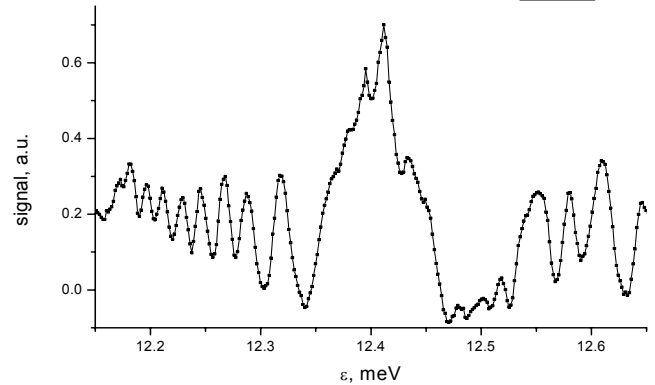


Figure 4. The measured intensity spectrum (arbitrary units) versus emission energy of the resonant state device with a boron delta doped plane in a SiGe quantum well on Si substrate. The emission peak is at 3 THz with 0.3 milliWatt output power at a device temperature of ~ 4 K.

IV. IMPURITY TRANSITIONS IN DOPED SI

Electromagnetic radiation in the THz frequency range can be generated in bulk silicon by electronic transitions in impurities, such as boron. Although the exact mechanism is still unclear, it is attributed to the hydrogenic character of the boron orbitals. To fabricate the devices, p-type boron-doped silicon wafers were cleaned using a multi-step procedure that removed organic and metallic contaminants and produced atomically smooth surfaces. Rectangular mesas (120x190 μm^2 and 17 μm deep) were defined and anisotropically RIE etched using standard photolithography and the lift-off of electron-beam evaporated Ti/Pt/Au (200/200/5kÅ) metal contacts [12]. The backside contact was Ti/Pt/Au (200/200/2kÅ), evaporated without breaking vacuum by rotating the samples. Four 1-mil gold wires were wedge-bonded to the mesa top metal contact to ensure sufficient current carrying capability. The devices were attached to the copper cold finger of a liquid-helium cryostat using low-temperature-compatible two-component silver epoxy that allowed rapid cooling to temperatures between 4.4 and 350 K. Voltage pulse trains of varying duty cycle and pulse numbers were applied to the devices employing a HP 8114A pulse generator. The emission spectra as in Figure 5 were recorded using a Nexus 870 FTIR in the step-scan mode calibrated with a black body source. These emission peaks are attributed to impurities, because they appear in devices fabricated from Si wafers with no SiGe quantum wells. At an applied current of 1.5 Amperes, one device emitted at 8.1 THz with a time averaged spectral power of 11.3 nW/cm^{-1} , corresponding to pulses with a peak power of 3.78 μW integrated over the wavelength spread of the peak. The devices operated up to temperatures of 20 K, above which the intensity rapidly diminished. The emission energies were comparable to the $p_{3/2}$ series of boron dopant levels for samples made from Si with resistivity of 1-10 $\Omega\text{-cm}$, while samples fabricated from undoped Si ($>1000 \Omega\text{-cm}$), and highly doped (0.01 $\Omega\text{-cm}$) bulk silicon did not yield THz

emission. The emitted radiation was not polarized and the intensity increased linearly with pumping current density. This device may be useful as a THz source that can be integrated with Si circuits without the need for SiGe epitaxy.

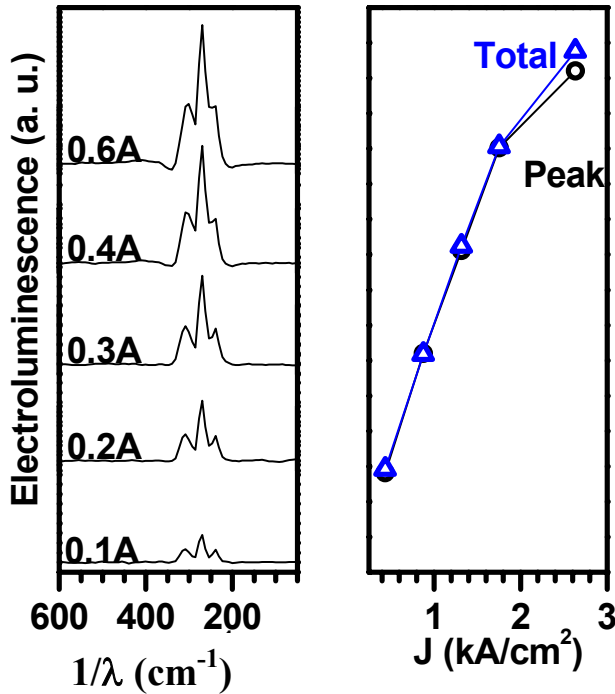


Figure 5. Dependence of electroluminescence intensity (relative units) on wavenumber (left panel) and on current density (right panel) for a doped Si device with resistivity of 1-10 Ω -cm corresponding to $N_A \sim 1e16$ to $1e15$ cm^{-3} , at a temperature of 4K. The vertical scale versus wavenumber is offset to separate the curves; that versus current density is shifted to overlay and compare trends. The peak at 270 cm^{-1} corresponds to 8.1 THz. The electroluminescence intensity versus current density was linear at low currents. The absence of square law dependence of intensity on current, and the sub linearity at higher current densities suggested that thermal blackbody radiation was negligible as a contribution to the observed THz emission. (Open triangles correspond to time averaged intensity; open circles to the peak intensity).

V. CONCLUSIONS

We have demonstrated THz electroluminescence at different frequencies from three different types of device approaches, including SiGe/Si quantum wells and unalloyed doped Si. For these devices, theoretical calculations suggested emission in the THz range, and the emission data agreed well with calculations.

The quantum well intersubband devices and the resonant state devices are being optimized for higher output power and higher temperature operation. Samples with a larger range of quantum well thickness are also under investigation. For the

doped Si emission, the temperature dependence of the emission and its exact mechanism are currently under investigation. These results indicate that THz sources based on silicon germanium nanotechnology are feasible and may be useful for novel applications including biological, chemical and medical imaging and sensing.

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