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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Gernot S. Pomrenke, PhD AFOSR Program Manager - Optoelectronics and Nanotechnology Directorate of Physics and Electronics Air Force Office of Scientific Research; Ballston Common Towers III 4015 Wilson Blvd, Room 713 Arlington VA 22203-1954	10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR
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14. ABSTRACT
We report on the design and fabrication of THz detectors based on silicon germanium nanostructures grown by MBE to obtain intersubband transitions in the energy range from 4.1 meV to 41 meV (1 to 10 THz). The absorption and photoresponse was characterized by Fourier Transform Infrared Spectroscopy (FTIR), and simulated using a 6 band k·p band structure calculation. A multistep SiGe quantum well structure was designed and fabricated to have transitions between two heavy hole (HH) states. The best device, SGC 439, had an absorption spectrum that agreed reasonably with the photocurrent spectrum and showed response peaks at 280 and 360 cm⁻¹ (8.4 THz and 10.8 THz) with the sample temperature at 77 K. It is concluded that SiGe quantum well devices are feasible as THz detectors.

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program manager:

Gernot S. Pomrenke, PhD
AFOSR Program Manager - Optoelectronics and Nanotechnology
AF Nanoscience SRA rep
DoD and AF representative to the Subcommittee
on Nanoscale Science, Engineering and Technology (NSET)
AFOSR/NE
Directorate of Physics and Electronics
Air Force Office of Scientific Research
Ballston Common Towers III
4015 Wilson Blvd, Room 713
Arlington VA 22203-1954

e-mail: gernot.pomrenke@afosr.af.mil

Tel: 703-696-8426

Fax: 703-696-8481

SiGe Intersubband Detectors for Terahertz Communication and Sensing

James Kolodzey
Department of Electrical and Computer Engineering,
University of Delaware, Newark DE, USA 19716-3130

EXECUTIVE SUMMARY

This is the final report of our one year program to study the possibility of THz detection based on SiGe nanotechnology. It is necessary to use quantum wells for this study to obtain intersubband transitions in the desired energy range from 4.1 meV to 41 meV, corresponding to 1 to 10 THz. We are growing silicon germanium quantum wells and nanostructures by molecular beam epitaxy (MBE).

Our interim report described photoresponse at 23 THz (13 μm) that agreed with the theoretical value of 25 THz (12 μm) for transitions from the heavy hole HH1 state to the continuum. Here, we report on further studies with the design and fabrication of a quantum well structure with the thickness and appropriate doping concentration so that the first ground state in the quantum well can be populated by holes. We report on the characterization of this device showing detection at 280 to 380 cm^{-1} (333 $\text{cm}^{-1} \leftrightarrow 1 \text{ THz}$). The SiGe layers were evaluated by high-resolution X-ray measurements, and fabricated into detectors using photolithography and conventional semiconductor processing. The absorption and photoresponse was characterized by Fourier Transform Infrared Spectroscopy (FTIR). Each detector design was simulated using band structure calculations performed with a 6 band $k \cdot p$ perturbation method using FemB software from QSA. A multistep SiGe quantum well structure was designed and fabricated that is expected to produce greater sensitivity with less dark current for transitions between the two heavy hole (HH) states. The THz absorption spectra and the photocurrent spectral response of the detectors were measured by FTIR with the sample temperature at 77 K. The best device, SGC 439, had an absorption spectrum that agreed reasonably with the electrical photocurrent spectrum, and showed response peaks at 280 and 360 cm^{-1} . Simulations indicated the presence of 2 spectral peaks at the same wavelengths as observed in the data. Dark current reached 2 μA at 1 volt bias for a device with area of 0.5 cm^2 . It is concluded that SiGe quantum well devices with structures that are similar to the well known QWIP device are feasible as detectors in the range near 10 THz.

SUMMARY ABSTRACT

We report on the design and fabrication of THz detectors based on silicon germanium nanostructures grown by MBE to obtain intersubband transitions in the energy range from 4.1 meV to 41 meV (1 to 10 THz). The absorption and photoresponse was characterized by Fourier Transform Infrared Spectroscopy (FTIR), and simulated using a 6 band $k \cdot p$ band structure calculation. A multistep SiGe quantum well structure was designed and fabricated to have transitions between two heavy hole (HH) states. The best device, SGC 439, had an absorption spectrum that agreed reasonably with the photocurrent spectrum and showed response peaks at 280 and 360 cm^{-1} (8.4 THz and 10.8 THz) with the sample temperature at 77 K. It is concluded that SiGe quantum well devices are feasible as THz detectors.

I. INTRODUCTION

TeraHertz devices can be useful for a wide range of applications in the areas of communication, imaging and sensing [1, 2]. The strong molecular absorption of TeraHertz radiation (1-30 THz) due to vibrational and rotational transitions makes this frequency regime attractive for chemical and biological sensing and imaging, and military applications, such as ranging [3] and imaging, and free-space communication between spacecraft. The extremely high atmospheric absorption ($>10^3$ dB/km), makes it suitable for short-range, and undetectable applications. Compared to microwave systems, THz-based devices are expected to be smaller and more compact due to the shorter wavelength. To support new applications at THz frequencies, components such as sources, detectors, and couplers must be designed and optimized. Our sources and detectors are based on intersubband transitions in SiGe quantum wells. The resonators and waveguides are based on structures that incorporate photonic crystal elements for frequency selection and mode control [4].

Few results have been published on silicon-based devices due to the difficulty of making high-quality strained silicon-germanium multiple quantum wells on silicon substrates [5]. In the III-V compound semiconductors, the design and fabrication of THz-emitting devices is challenging due to free-carrier and phonon absorption of infrared radiation. The phonon absorption is particularly intense in the reststrahlen bands, near 8 THz in GaAs with absorption coefficients as high as 2×10^4 cm^{-1} . In the SiGe alloy system, however, phonon absorption is mitigated with negligible infrared-active polar lattice vibrations. SiGe offers monolithic integration in the well established Si integrated circuit processing [6].

We have reported on the operation of detectors, and in other programs, we have obtained electroluminescence at frequencies near 10 THz [7, 8]. It is interesting to determine if THz detectors can be made with good performance similar to the QWIP device that works at mid-infrared frequencies [9]. We have grown SiGe layers, quantum wells and nanostructures by the MBE method under various growth conditions, and simulated SiGe devices by using growth parameters with software for band structure calculations. In this report, we describe THz detection from intersubband transitions in multilayer nanostructures of SiGe quantum wells and Si barriers.

II. ANALYSIS

The objectives are to: (a) Develop SiGe Quantum Wells for intersubband THz detectors; (b) Identify techniques to improve detector responsivity by adjusting the device structure, composition, and doping concentrations; (c) Assess the compatibility of the SiGe detector processing steps with Silicon integrated circuit technology; (d) Evaluate the integration of SiGe Terahertz detectors with passive circuit elements including transmission lines, filters, couplers, and antennas; (e) Develop an effective working relationship with members of the technical community.

The relevance of this program is that: (a) the availability of sensitive THz detectors would significantly impact the advancement of THz technology and practical applications; (b) the

applications include high bandwidth communication, remote sensing and chemical - biological detection; (c) we expect that the intersubband THz detectors will outperform alternative detectors, such as bolometers, in terms of sensitivity and speed; (d) the use of SiGe technology is feasible and would render the THz detectors compatible with silicon integrated circuit technology.

The THz detector design approach method was to:

1. Calculate the confined energy states with various well widths and Ge concentrations, find one design which enables us to have a bound to quasi-bound structure, which means we have a state very close to continuum. In addition, we should let the first ground state be very close to the bottom so that it is easy to populate with a convenient doping.
2. Use the calculated well thickness and confinement energy states to find the Fermi level.

The analytical model used was:

$$\frac{N_a}{1+4\exp\left(\frac{E_B - E_F}{kT}\right)} = \frac{4\pi m^* E_{LH}}{h^2} \int_{E_{HH}} f(E) dE$$

Where $f(E)$ is the Fermi-Dirac distribution function. The left hand side represents how many acceptors are ionized, with a degeneracy factor of 4 for holes in the doubly degenerate valence band at $k = 0$. The right hand side represents how many holes are in the confined energy state. There is another contribution of holes, which is the thermally activated electron-hole pairs across the gap, but this is small at our temperature. The results of this analysis will yield the position of the Fermi that is needed for populating a particular quantum sublevel state. Based on this analysis, the following SiGe quantum well layers for SGC 439 were grown in an EPI 620 MBE system. The band diagram for this structure is shown in real space Fig. 2, and in k space in Fig. 3..

Si 50nm contact layer (p-doped, $1E18 \text{ cm}^{-3}$)	} X 10
Si _{0.9} Ge _{0.1} spacer 10nm (undoped)	
Si 1nm undoped	
Si _{0.7} Ge _{0.3} well 1.6nm ($1.2E12 \text{ cm}^{-2}$)	
Si 1nm undoped	
Si _{0.9} Ge _{0.1} spacer 10nm (undoped)	
Si substrate (CZ(001), $\rho=1-10\Omega\cdot\text{cm}$)	

Figure 1. Structure showing MBE growth sequence for the THz detector. The quantum well region is repeated 10 times.

Wavefunctions of SGC439

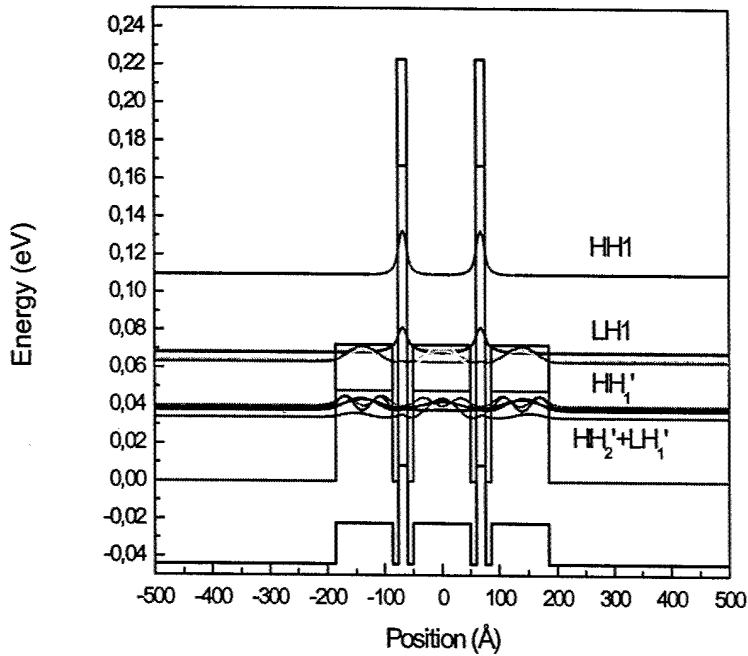


Figure 2. This Quantum well detector was designed with the band diagram shown. It contains a deep quantum well with $\text{Si}_{0.8}\text{Ge}_{0.3}$, $L_w=1.6\text{nm}$ and $N_a=7.5e^{18}\text{cm}^{-3}$, and spacer layers with $\text{Si}_{0.9}\text{Ge}_{0.1}$ $L_{\text{spacer}}=10\text{ nm}$, and barrier layers of unalloyed Si.

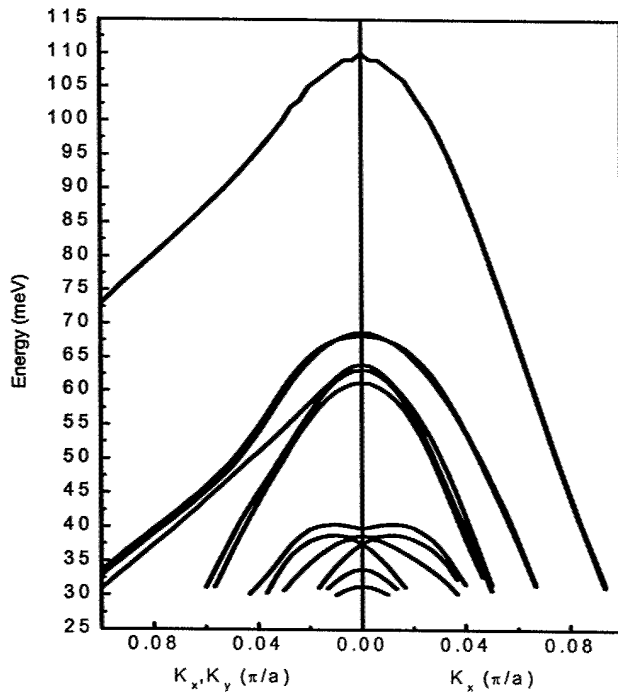


Figure 3. Calculated hole band dispersion curves of the quantum well device with subbands along [100] and [110] directions, showing the range of possible radiative transitions.

III. EXPERIMENTS

A SiGe/Si multiple quantum well structure was grown by molecular beam epitaxy (MBE) on Si(001) substrates at the relatively low growth temperature of 400 °C. The MBE instrument was an

EPI 620 system [10]. The quantum wells are nominally 1.6 nm $\text{Si}_{0.7}\text{Ge}_{0.3}$, and boron doped to have a sheet carrier concentration of $1.2 \times 10^{12} \text{ cm}^{-2}$, sandwiched between 1 nm Si barrier and further separated by 10 nm $\text{Si}_{0.9}\text{Ge}_{0.1}$ spacer layers. High-resolution XRD rocking curve exhibiting the Pendellosung fringes showed the growth of a good quality pseudomorphic structure, as in Figure 4. Reciprocal lattice mapping (not shown) of the (004) reflection was also used to characterize the epitaxial quality. Cross sectional transmission electron microscopy (TEM) was used to study the interfaces, as in Figure 4. Both these techniques indicated the growth of a good quality epitaxial layer.

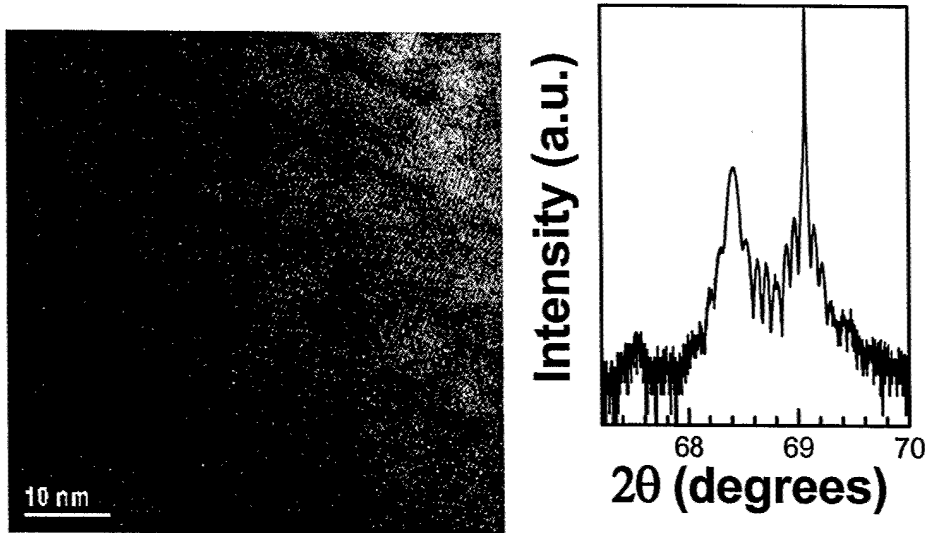


Figure 4. An example of the materials characterization of the SiGe THz detector structure. Left panel shows a cross-sectional TEM view of the SiGe quantum well layers of THz detector sample SGC 439 (TEM by Chaoying Ni, University of Delaware). Right panel shows a high-resolution X-ray diffraction measurement of X-ray intensity versus diffraction angle of sample SGC 439 showing the (004) peak of the SiGe layers (left peak), and of the substrate (right peak).

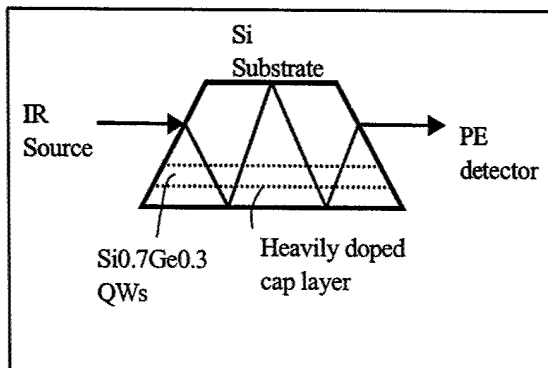


Figure 5. Diagram of the absorption measurement geometry in the multipass waveguide configuration that is used with the FTIR system

We measured the THz absorption of the quantum well layers by Fourier transform infrared spectroscopy (FTIR). The FTIR instrument was a ThermoNicolet Nexus 870 with a DTGS-PE detector. We prepared polished wedge samples for multiple bounce measurements using the

waveguide method as shown in Figure 5. Intersubband absorption at long wavelength ($\sim 30\mu\text{m}$) was observed at cryogenic temperatures, as in Figure 6. The photoconduction mechanism involves intersubband transitions from occupied QW levels to the valance band continuum.

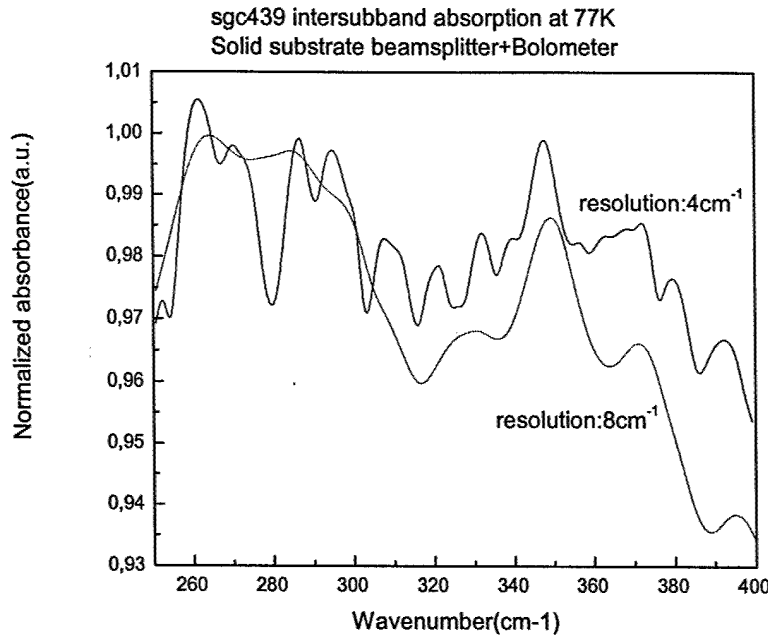


Figure 6. Measurements of the absorption spectrum versus wavenumber ($1/\lambda$) at 77K using FTIR with a solid substrate beam splitter and pyroelectric detector. The measurement geometry is shown in the inset. ($333\text{ cm}^{-1} \leftrightarrow 1\text{ THz}$)

Dark current bias curves as a function of temperatures

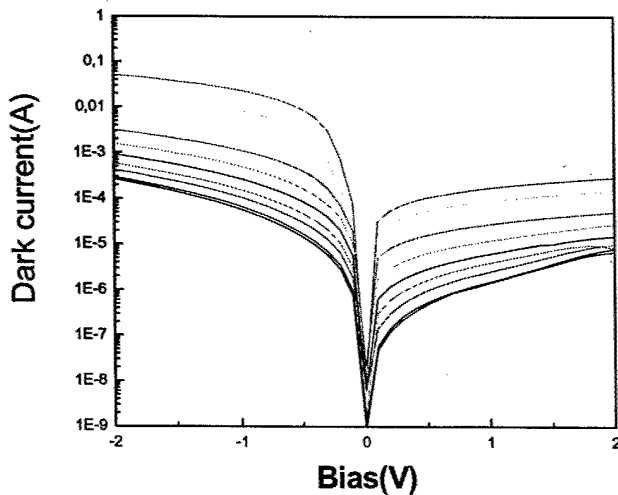


Figure 7. Dark current-voltage measurements over temperature range from 77K to 250K, for device with area 0.5 cm^2 . The current increases with temperature.

A THz detector chip (with area 0.5 cm^2) was fabricated from p-doped SiGe quantum wells on a Si substrate. Devices were fabricated by polishing the structure into waveguides and by the evaporation of metal contacts. Current-voltage measurements without illumination at temperatures ranging from 10K-250K were performed. The current- voltage characteristics in Figure 7 indicated

the presence of thermionic emission with an activation energy of $\Delta E = 31$ meV at a bias voltage of $V_b = 0.1$ V. The activation energy indicated that the Fermi energy lies 10 meV above the ground heavy hole (HH) state, as intended.

III. RESULTS AND DISCUSSION

The band structure was calculated with a 6 band k.p method using FemB software from QSA, based on which the absorption peaks were assigned, as in Figure 8. Theoretical absorption curves were calculated and compared with experimental data, and good agreement was achieved.

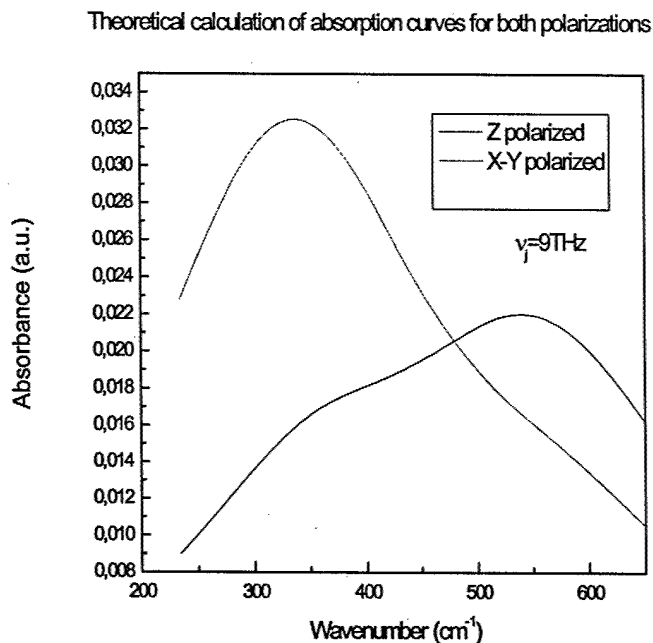


Figure 8. Theoretical calculations of THz absorption for the SiGe quantum well device with both in-pane and perpendicular polarizations. Simulations are based on oscillator strengths, calculated from the matrix elements for the 4 dominant transitions, taking line width $\nu_j = 9$ THz for each transition.

THz photocurrent measurements were performed with a Fourier transform infrared spectroscopy (FTIR). The measured response (Figure 9) agreed with the theoretical values (Figure 8) for the heavy hole HH1 transition from the bound quantum well state to the extended state. The absorption and photocurrent spectrum of the THz quantum well detector showed detection response peaks at 280 and 360 cm^{-1} , corresponding to 8.4 and 10.8 THz [11].

SGC439 Photoresponse at 77K

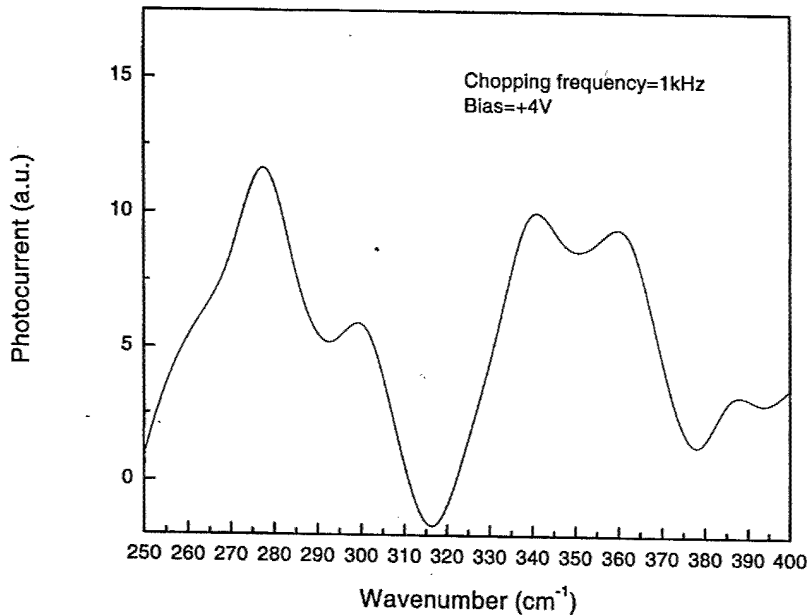


Figure 9. Measured photocurrent spectrum versus wavenumber ($1/\lambda$) at 77K using FTIR with a solid substrate beam splitter. ($333 \text{ cm}^{-1} \leftrightarrow 1 \text{ THz}$). Note agreement with absorption and with simulations of Fig. 8.

IV. CONCLUSIONS

The goal was to design a quantum well structure and find an appropriate doping concentration so that the first ground state in the quantum well can be populated. We demonstrated that SiGe quantum wells grown by MBE have high quality and can absorb THz radiation by intersubband transitions. This means that with proper design and characterization, we can produce high responsivity and high speed THz detectors. Further study is needed to better understand the relation between the quantum well energy levels and the Fermi energy to improve the responsivity and reduce the dark current to enable higher temperature operation. This will be done by considering the relations between the photocurrent and the quantum well layer composition, thickness, strain, and doping levels. These results suggest the possibility of utilizing this device structure as a suitable design for Terahertz detectors.

ACKNOWLEDGMENTS

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SiGe Intersubband Detectors for Terahertz Communication and Sensing

James Kolodzey

University of Delaware, Newark DE, USA 19716-3130
Center For Terahertz Unipolar Structures

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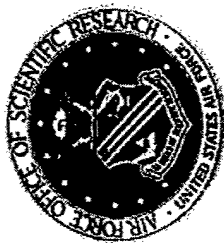
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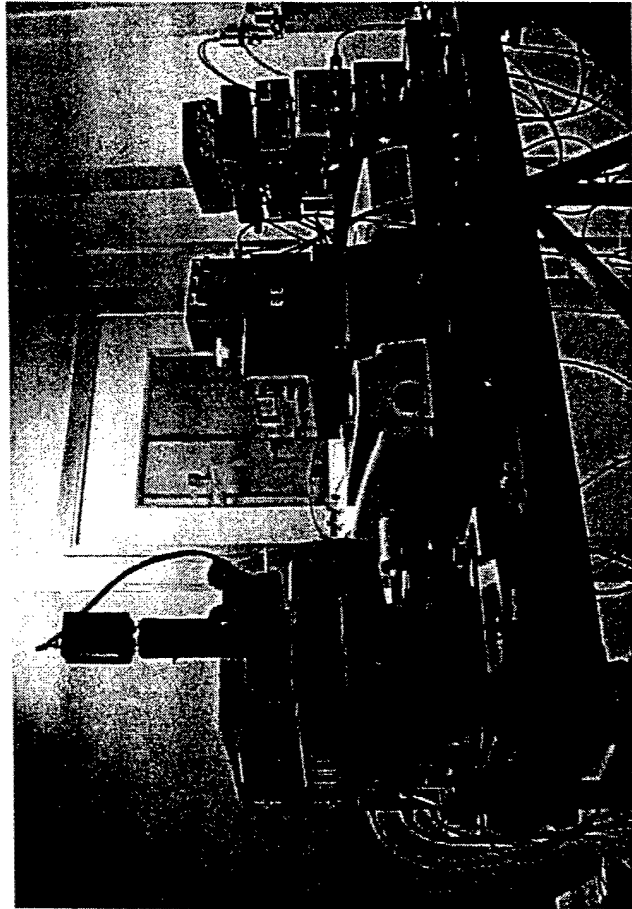
CETUS



Installed new FTIR system at University of Delaware



FTIR system (Thermo-Nicolet 870 used for characterizing SiGe quantum well sources and detectors, purchased with assistance of grant from Sarnoff Corp.



Microscope allows FTIR measurement of individual microdevices

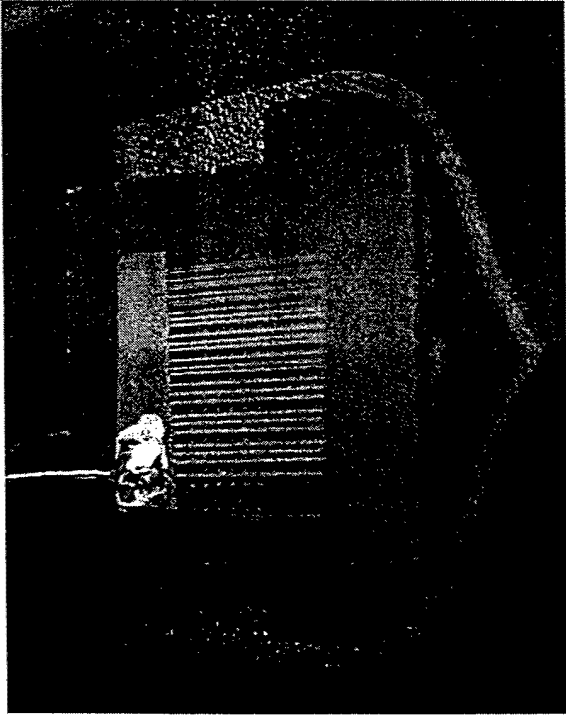


display of interferogram from new FTIR system installed October 2001

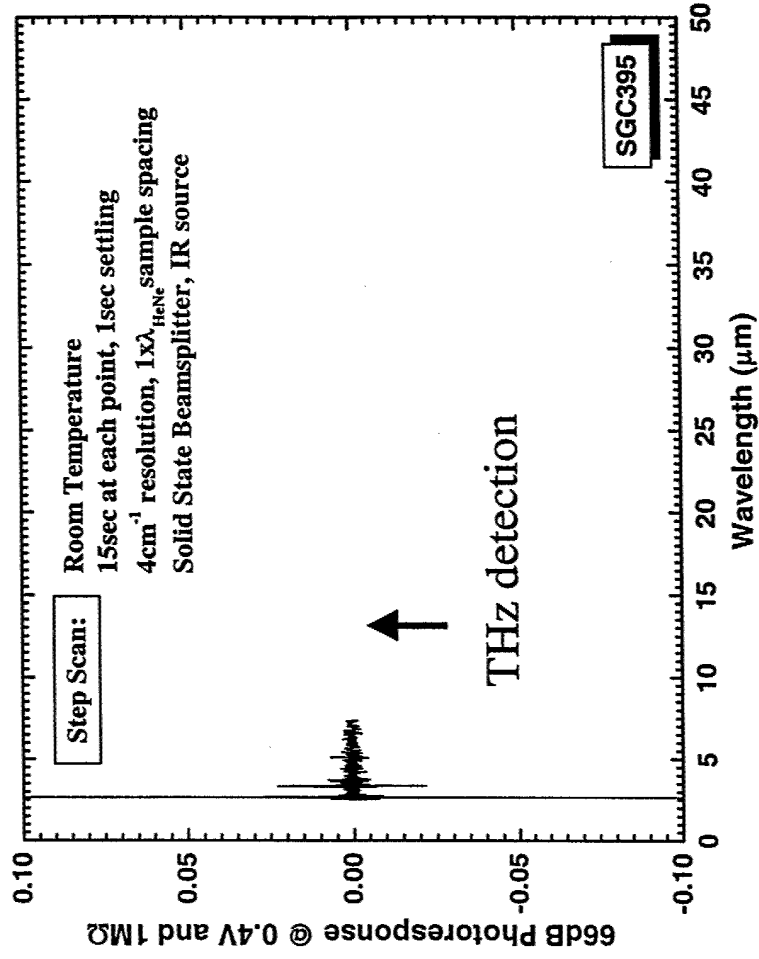


Detected THz signals with MBE-grown SiGe quantum wells

THz detector chip (1 cm²) fabricated from p-doped SiGe quantum wells on Si substrate. Yellow patterns are Gold metal contacts. The photoconduction mechanism involves intersubband transitions from occupied QW levels to the valance band continuum.



FTIR spectrum of THz quantum well detector. Response at 23 THz (13 μm) agrees with the theoretical 25 THz (12 μm) for the heavy hole HH1 state to the continuum, simulated using FemB software from QSA.



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