

Terahertz Sensing Science & Electronic Technology for CB Defense

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ABSTRACT

During the last few years, many new research programs have emerged within the U.S. Army and the Department of Defense (DoD) that have been focused on advancing the state-of-the-art in terahertz (THz) frequency electronic technology and on investigating novel applications of THz frequency sensing. Similarly, there has been a steadily growing interest among the international scientific and technical communities in the unique challenges associated with developing a robust electronics technology and with developing a detailed understanding of the THz frequency sensing science. The U.S. Army has maintained a focused research and development (R&D) program in THz-related Science and Technology for nearly two decades, which has been motivated primarily by the potential of THz sensing to chemical and biological (CB) defense. More recently, the U.S. Defense Threat Reduction Agency (DTRA) and the U.S. Army Research Office (ARO) have established a number of jointly-supported R&D projects that place an emphasis on assessing the practical utility of THz sensing to warfare agents threats, with biological agent detection being the top priority. This paper will present a brief historical overview of the U.S. Army supported THz R&D program and report on the recent progress and future directions of the DTRA-ARO program for point and remote detection of biological warfare agents.

1.0 INTRODUCTION

The mission of the U.S. Army Research office (ARO) has always been to support basic research that seeks scientific and technological discoveries that will enhance Army capabilities (www.aro.army.mil). Furthermore, one of the primary thrust areas of the ARO Electronics Division is *Terahertz & Ultrafast Electronics* which seeks to remove the fundamental limits of power, efficiency and sensitivity of solid-state devices when they are pushed to operate at frequencies approaching 1 terahertz (THz) or at time scales below 1 picosecond. The general benefits of an ever increasing high-frequency electronic capability are exceedingly clear from a general perspective – i.e., higher frequency/faster devices means faster components and systems and this inevitably means superior performance for sensing, communications, computation, data processing, etc. which are all important from a typical military perspective. However, the specific focus areas and investments of the ARO basic research program are always assessed in terms of their scientific and/or technical merit and they are also judged for their relevance and potential payoffs to military applications and needs. Indeed, the *ARO Terahertz & Ultrafast Electronics* program has been established in a manner that is in precise agreement with these previous standards, and this means that the research investments have been guided in the context of the existing state-of-the-art and in the context of the science & technology (S&T)

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challenges that must be overcome to realize military-relevant payoffs in the future. As a result this type of thinking, and a realization of the potential of terahertz frequency sensing and imaging to military defense [1], the ARO research program has had a long-standing commitment to ‘THz-Frequency Sensing Science & Electronic Technology’ related research and development.

The ARO THz-Frequency program presently pursues sensing science investigations and electronic technology development in the portion of the submillimeter-wavelength electromagnetic (EM) spectrum between approximately 1 mm (300 GHz) and 100 μm (3 THz). A few technical points regarding this part of the spectrum may be useful for novices to this area. The THz regime is an almost paradoxical portion, or “gap”, in the EM spectrum located between the traditional radio-frequency (RF) microwave and the infrared (IR) domains – see Fig. 1. Note here that the specific boundaries of the so-called “THz regime” have no officially recognized or widely accepted definition but, in this author’s opinion, have always been defined by “gaps” in the electronic technology capabilities and/or in the scientific insight into related phenomenology. The THz regime inherently offers important technical advantages when compared to RF electronics (e.g., wider bandwidths, improved spatial resolutions, component compactness, etc.) and holds the promise for new and novel sensing modalities (e.g., inspection of sealed packages, concealed weapons detection, chemical and biological agent detection, medical diagnostics, etc.). However, this same THz regime presents significant challenges (e.g., extreme atmospheric attenuation, weak interaction signatures, standing wave interference, etc.) to practical sensor implementation within traditional scenarios and there are fundamental science and engineering problems that have to date either prohibited, or severely limited, the implementation of conventional electronics technology within this far IR quasi-optical regime where EM wavelength is on the order of component size. However, when one makes an objective assessment of the most promising THz Sensing & Imaging (THz-S&I) application areas within the specific context of their particular S&T challenges (see [1]) one can find generous amounts of broad-based THz-S&I opportunities that should fuel entrepreneurs, technologists and researchers for a very, very long time. For example, there appear to be: (i) very near-term technology implementations towards security screening and analysis of highly ordered materials (e.g., explosives and pharmaceuticals); (ii) medium-range technology development for remote (or standoff) detection and characterization of biological (and chemical) agents; and (iii) far-future research-enabling opportunities for architecturally interfacing to, or electromagnetically probing of, molecular or nanoscale systems. Indeed, a review of the information given in [1] shows that there have been practical demonstrations, technology advances and research breakthroughs that justify these general expectations.

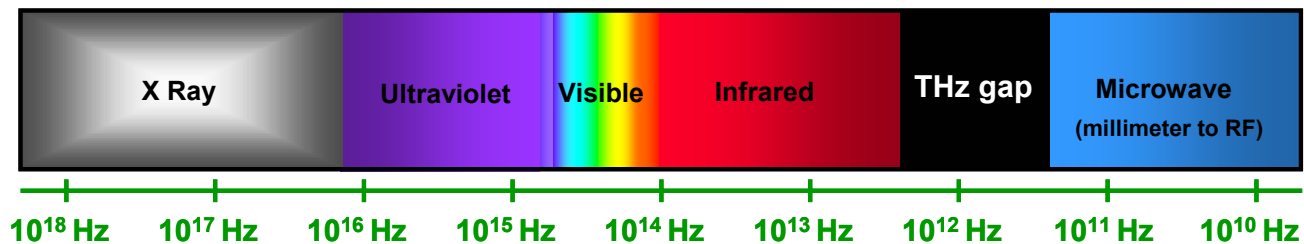


Figure 1: Electromagnetic spectrum illustrating the “THz gap” relative to the microwave and infrared.

U.S. Army basic research programs have recognized the potential of THz-S&I towards chemical and biological defense applications for many years. Furthermore, programs within the U.S. Army and the U.S. Department of Defense (DoD) have been continuously addressing the S&T challenges for nearly two decades. For example, research programs supported by the U.S. Army Research Laboratory, the U.S. Edgewood Chemical Biological Center (ECBC) and the U.S. ARO have been supporting basic research in THz sensing

and sensor technology development continuously since the early 1990's. This program has grown in scope over the years and addresses an array of S&T issues for CB threat agent detection, identification and characterization. Specifically, the U.S. ARO presently supports or co-supports THz S&T research at a rate that exceeds \$10M per year. Here, the U.S. ARO program emphasizes bio-agent sensing sciences but also supports efforts that study the phenomenology associated with THz-S&I of chemical agents and concealed weapons and explosives. The U.S. ARO also has a very expansive THz technology program and supports numerous efforts in the general categories of: (i) engineering enhancements to existing electronics devices and technology, (ii) systems development, and (iii) novel electronic device concepts. This technology component seeks to: (i) increase the capability of THz electronic components and make them available to the community, (ii) advance THz system performance to enable new scientific inquiry, and (iii) discover entirely new device concepts that will remove existing barriers to performance. This ongoing THz program has made many important achievements and has made noteworthy progress in a very challenging S&T area, however one might argue that some of its most important contributions have been to identify the bottleneck challenges to the successful application of THz-S&I to countering bio-threats. Indeed, the U.S. ARO and the U.S. DTRA have recently launched a number of new research projects that seek to build upon these accomplishments. In particular, these projects seek to enable and execute new scientific studies that will focus on assessing the practical utility of THz S&I against CB threats, with a major emphasis on bio-agents. The sections that follow will place this joint program into perspective by giving summaries for some of the pre-existing research efforts, along with a sample of the new research projects.

2.0 THZ WAVE INTERACTION WITH BIOLOGICAL MACROMOLECULES: EXPERIMENT AND SIMULATIONS

Professors Tatiana Globus and Boris Gelmont, of the University of Virginia and Professor Maria Bykhovskaia, of Lehigh University, lead a research team that have been focused on the experimental and theoretical study of terahertz wave interactions with biological molecules during the last four years. This research has been conducted under the U.S. Army Research Office (ARO) managed Multidisciplinary University Research Initiative (MURI) Program on "Science and Technology of Chemical and Biological Sensing at Terahertz Frequencies." This project consists of the focus areas: Experimental Spectroscopy (Prof. Globus), Advanced Theory and Modeling (Prof. Gelmont), and Simulation and Analysis (Prof. Bykhovskaia).

This research project is a spearhead component of the ARO sensing program and it is focused on the generating scientific insight into the molecular structure, dynamical properties, and the THz interaction mechanisms related to biological and chemical agents in order to develop a scientific base for THz-frequency sensing. The primary impact of this research will be to establish the initial foundation for the future use of terahertz spectroscopy in the detection, identification and characterization of biological macromolecules and related materials.

This research includes active collaboration with Dr. D. Woolard (ARO), Dr. A. Samuels and Dr. J. Jensen (Edgewood Chemical and Biological Center), with the group of Prof. T. Crowe (UVA and Virginia Diodes Inc.), groups of Prof. R. Weikle (UVA), Prof E. Fernandez (UVA), Prof. D. Theodoresku and Prof. H. Frierson (UVA), the group of Prof. N. Stewart (the University of Tennessee), with the group of Prof. E. Brown (UCSB), Lowell University in Massachusetts, Goodrich Co., NRAL. Results of characterization are immediately transferred to Edgewood Chemical and Biological Center. The results will be also used in future development of biosensing technology (Virginia Diodes).

This research program has been responsible for many of the pioneering measurements of the terahertz-frequency absorption properties of biological materials which have been performed at the University of

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Virginia using a commercial Fourier Transform Spectroscopy (FTS) along with their theoretical interpretation. Spectral characterization has been performed for thin-film DNA macromolecules, short artificial DNA and RNA, fungal spore samples and some proteins has been analyzed in the 10-25 cm^{-1} spectral range with a spectral resolution of 0.25 cm^{-1} . Computational methods have been developed and applied to predict the low-frequency absorption spectra of short-chained artificial DNA and RNA of known base-pair sequences. Thus, multiple resonances due to low-frequency vibrational modes within biological macromolecules have been unambiguously demonstrated in agreement with the theoretical prediction. It is important to note that the spectroscopic results generated by this program were for a long time relatively exclusive and had been under scrutiny by the general community. However, very recent confirmations of THz frequency resonance modes, in either direct or relative agreement with those of this program, have been demonstrated through the independent technique of a photomixing sweep oscillator as a source of a THz radiation with very high spectral resolution [E.R. Brown, J.E. Bjarnason, T.L.J. Chan, A.W.M. Lee, and M.A. Celis, Optical Attenuation Signatures of *Bacillus Subtilis* in the THz Region, *Appl. Phys Letters*, **84**, pp. 3438-3440 (2004); T. M. Korter and D. F. Plusquellic, Continuous-wave terahertz spectroscopy of biotin: vibrational anharmonicity in the far-infrared, *Chemical Physics Letters*, **385**, Issues 1-2, Pages 45-51 (2 February 2004)]. This project has substantial support and has been extremely productive during the last year, yielding new scientific results across a number of areas including, but not limited to: (1) The successful demonstration of resonant signature phenomena in solid films of DNA, RNA, short-chained oligonucleotides of known base-pair sequences and spores, along with similar demonstrations for proteins, cells and tissues and bio-materials in liquid phase; (2) Application of THz Spectroscopy for biomedical research: characterization of cancer cells and tissue; (3) Developing THz characterization technique for diluted solutions of biological materials for possible future applications in real time monitoring of biological processes on molecular level and detecting water contaminations. Specific summaries for just three of the recent scientific investigations, along with a description of the accomplishments, are given in the subsections that follow.

2.1 THz Characterization of Biological Warfare Agent Simulant Aerosols

The first measurements of BG cell samples in the form of aerosol were conducted using FT spectroscopy which demonstrated very high sensitivity for low material concentration. Our results indicated that the signature of material deposited on the surface of windows and of material in the form of an aerosol is very much the same. Some of the measurements taken in this study are given in Fig. 2(A). Experimental results were used to make preliminary estimates of the spectral absorption coefficient per 1 mg of BG cells in aerosol, α/c , as, $\alpha/c = 2.3 \text{ (A/g) [mg}^{-1}\text{]}$, or $\alpha = 2.3 \text{ (A/d) [cm}^{-1}\text{]}$, where: α is the absorption coefficient of the material; c is the concentration of absorbing material for the unit of length mg/cm ; g is the total amount of material, $[\text{mg}]$; and d is the effective distance that the light travels through the material in cm . Here, absorbance A is determined by Beer's Law, $A = \log_{10}(I_0/I) = \log_{10} 100/\%T$ or $A = 2 - \log_{10} \%T$, where: I_0 is the intensity of the incident light; and I is the intensity after passing through the material. Absorption coefficient for 1 mg material, α/c , is demonstrated in Fig. 3. A comparison with absorption of the material in the form of solid films shows that α is at least an order of magnitude higher in aerosol form. At the same time, our results indicate that aerosol material exhibit much stronger and sharper resonance-absorption spectra as compared to material in the form of solid films or gel, with the magnitude-change in one observed peak $\sim 100\text{-}300\%$ greater. Details of this work can be obtained from references [2-4].

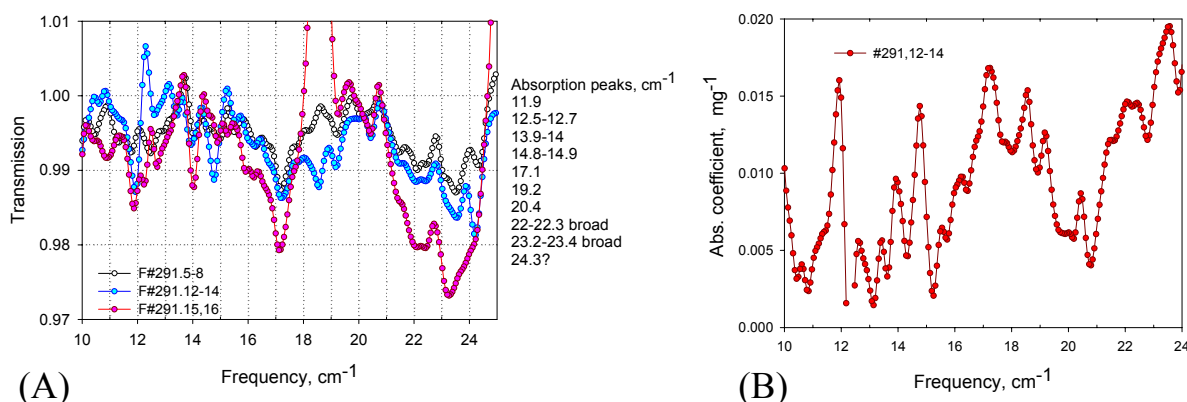


Figure 2: (A) A comparison of three experiment results on BG cell aerosols, (B) Estimated absorption coefficient of BG cell aerosol, α/c , with a concentration less than $5 \cdot 10^{-3}$ mg/ml.

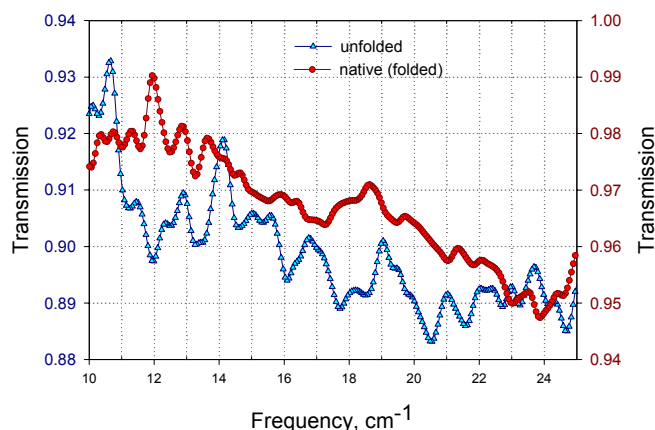


Figure 3: The transmission spectra of folded and unfolded protein lysozyme.

2.2 Characterization of Proteins and Their Conformational States

This research effort has investigated the application of FTIR technique in the low terahertz frequency range of $10\text{-}25 \text{ cm}^{-1}$ to discriminate between different protein conformations with the goal to evaluate possible application of THz spectroscopy for monitoring of protein folding-unfolding process. After many years of study, protein folding-unfolding processes are still not completely understood. Refolding of some classes of proteins, of which lysozyme is an example, involves the transient population of partially folded states (partially folded intermediate or molten globules). Lysozyme is a globular $\alpha+\beta$ protein with approximately 45 % of α -helix type secondary structure and $\sim 20\%$ of β -sheet structure. In addition it has $\sim 25\%$ various turn conformations that generally exist in globular proteins and $\sim 13\%$ of unordered or “random coil” secondary structure. Lysozyme also adopts specific tertiary structure known from X-ray diffraction and nuclear magnetic resonance (NMR).

In this work, thin, air dried protein films were characterized as well as material in the form of gel. Spectra reveal resonance features in transmission which represent vibrational modes in the protein samples. These

results clearly demonstrate resonance features in THz transmission which represent vibrational modes in the protein samples due to weak hydrogen bonds and non-bonded interactions between different functional groups within the molecules. A great variability of spectral features for the different conformational states showed the sensitivity of vibrational frequencies to the three dimensional structure of proteins. The results obtained on liquid (gel) samples indicate that THz transmission spectroscopy can be used for structural characterization of proteins, including secondary structures and probably partially folded intermediate states, and for monitoring folding-unfolding process in a realistic, aqueous environment. Specifically, much higher absorption resonance intensities were observed for protein unfolded with guanidine chloride GuCl compare to the native form - see Fig. 2. The results obtained on liquid (gel) samples indicate that THz transmission spectroscopy can be used for structural characterization of proteins, and for monitoring folding-unfolding process in a realistic, aqueous environment. However, detailed assignments of resonance frequencies to specific structure features will require more detailed studies. Details on this research is given in reference [5].

2.3 Theoretical Analysis of THz Spectral Signatures of Nucleic Acids

The effective application of THz spectroscopy for the detection, identification and characterization of DNA molecules will require robust theoretical capabilities for predicting the associated absorption spectra and for the analysis of the spectral signatures of complex biomolecules. Prior research by our group has utilized the JUMNA & LIGAND (J&L) as developed by Lavery et al., for the potential energy minimization and normal mode analysis of nucleic acids with known three-dimensional structure to determine the frequencies of vibrational modes and their eigenvectors. Here, this approach was extended to allow for the calculation of oscillator strengths and THz absorption spectra. Furthermore, this approach was used successfully to show good correlation with experimental data. However, the experimental polarization dependence of absorption was not reproduced well by these earlier theoretical approaches. More recently, new investigations have been executed to test the feasibility of using the commercial molecular dynamics package AMBER 8 (Assisted Model Building with Energy Refinement) and the corresponding AMBER 99 force field for THz spectral generation, and to assess whether AMBER 8 or J&L better reproduces the experimental data. In these studies, nucleic acid molecules were built based on the structure parameters from X-ray diffraction of fibers, which are included as library files in AMBER. poly(G)-poly(C) RNA (or poly(rG)-poly(rC)) was examined in a canonical double-strand A-form and poly(A)-poly(T), poly(AT)-poly(TA) DNAs (poly(dA)-poly(dT), poly(dAT)-poly(dTA)) or were examined in a canonical double-strand B-form. The total potential energy was minimized in the Cartesian coordinate space. Note that in Jumna and Ligand, internal coordinates for the molecular structure are utilized, which required additional steps to convert to Cartesian coordinates before the normal modes and oscillator strengths in the THz spectra could be calculated. The covalent bond energy, covalent angle energy, proper and improper torsions, non-bonded interactions including electrostatic, and Van der Waals interactions were taken into account using AMBER 99 force field. Then the normal modes of molecular vibration were calculated in the Cartesian coordinate space.

The most significant difference between the JUMNA & LIGAND and AMBER 8 based results was observed for the Z-polarized light (light polarized along nucleic acid axis) analysis. Our current study confirms that multiple resonance modes exist in 2-300 cm^{-1} frequency range and demonstrates the general ability the AMBER 8 package to predict and analyze the light absorption signatures of biomolecules, including the effects of the light polarization. For example, Fig. 4 gives the calculated spectrum of poly(rG)-poly(rC). Here, the oscillator dissipation γ is assigned to 0.5 cm^{-1} , as this assignment gives the best fitted results with the experimental data. In Fig 4(A), the calculated spectrum in the range 10 cm^{-1} to 25 cm^{-1} is compared to the experimental results for XY light polarization (the electric field of radiation is perpendicular to Z direction which points along the RNA axis. Similarly, Fig 4(B) gives the simulated spectra for Z light polarization. The calculated absorption spectra of RNA poly(rG)-poly(rC) reproduce many essential features of the

experimental THz signatures in $10\text{-}25\text{ cm}^{-1}$ range. Note that most of the measured resonance peaks are found in the modeled spectrum. The position of the strongest absorption peak at 15.1 cm^{-1} is reproduced very well by these simulations. The analysis indicated that the optical activity at 15.1 cm^{-1} is localized and is dominated by some phosphate groups and selected base atom contributions. The AMBER 8 based results predict that XY and Z polarizations yield comparable absorption values. The C-G RNA absorption coefficient peaks for Z-polarized light are somewhat smaller but comparable to the peaks for XY-polarization. Most important, these predictions are in the reasonable agreement with the measured data (Figs. 4(A) & (B)) when bulk sample effects are taken into consideration. For example, overall sample misalignment can affect an absorption peak width as well as the relative peak magnitudes and this might explain differences in peak shapes between the theory and the experiment, and this will be a point of study in future investigations. Figure 5 makes a direct comparison between the JUMNA & LIGAND (J&L) and AMBER results for XY polarization. The J&L based approach reproduces XY absorption spectral data reasonably well. However, J&L predicts much smaller relative values for the absorption coefficient peaks for Z orientation as compared to XY orientation that does not agree very well with experimental data [see J. W. Powell, G. S. Edwards, L. Genzel, F. Kremer, A. Wittlin, W. Kubasek and W. Peticolas, "Investigation of far-IR vibrational modes in polynucleotides" *Phys. Rev. A*, vol. 35, no.9, pp. 3929-3939, 1987]. Thus, the polarization dependence produced by Amber is more closely in agreement to the polarization dependence observed experimentally. More details of these studies, and how they are being used to interpret experimental measurements can be found in reference [6].

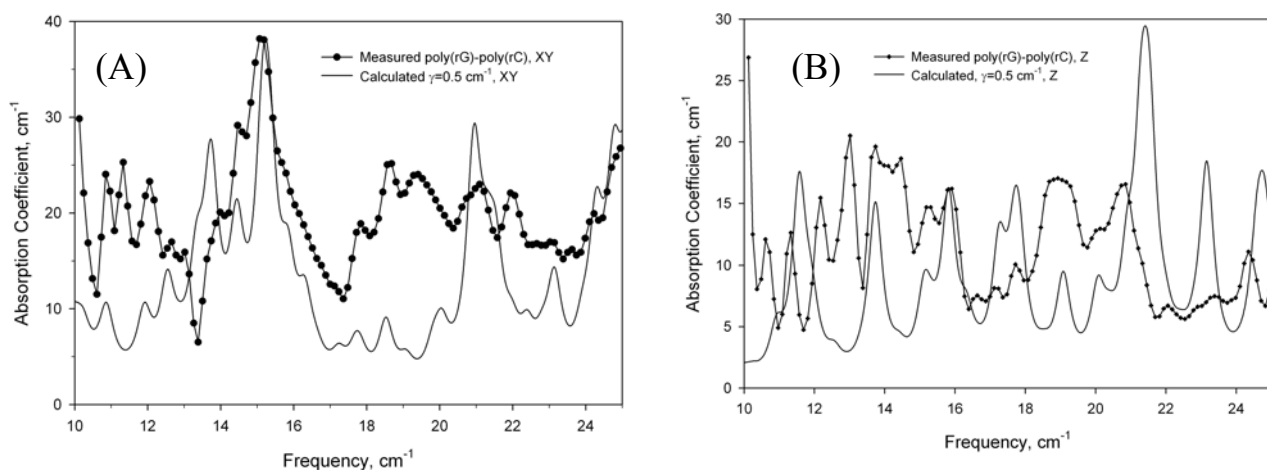


Figure 4: (A) Calculated (AMBER8) and experimental spectra of homopolymer poly(rG)-poly(rC). Light is polarized in the direction perpendicular to the RNA axis (XY). (B) The theory and the experiment for the light polarized along the RNA axis. The scaling factor for the calculated spectrum is the same for (A) and (B).

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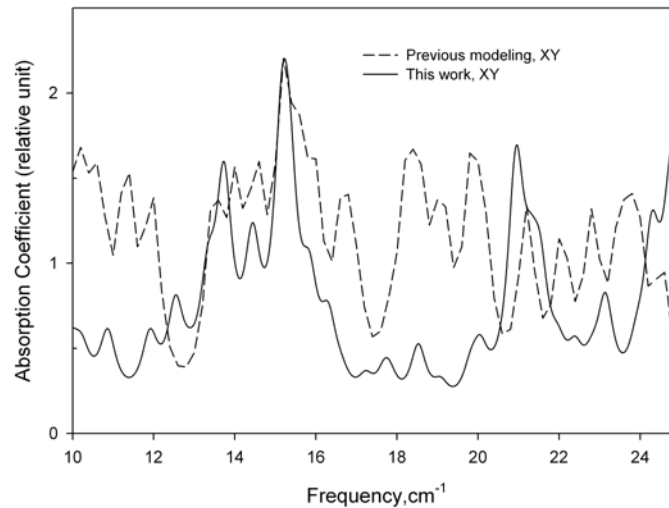


Figure 5: Calculated spectra of poly(rG)-poly(rC) for XY polarization. AMBER - solid line, and JUMNA & LIGAND - dashed line.

3.0 ELECTRONICALLY TUNABLE AND COMPACT SOURCES AND DETECTORS OF TERAHERTZ POWER FOR SPECTROSCOPY

Drs. David Kurtz, David Porterfield and Thomas Crowe, of Virginia Diode Inc., have been in the pursuit of advanced THz sources and detectors under a U.S. Army managed SBIR Phase I and Phase II during the last few years. This project seeks to create compact and reliable sources and detectors of terahertz power and to demonstrate full waveguide band frequency domain terahertz spectrometers. The ultimate goal of this research is to create a militarily viable terahertz technology suitable for use in portable spectrometers for point and/or stand-off detection of explosives and chemical and biological threats. To achieve this goal the technologists from Virginia Diode Inc. are developing a compact and reliable terahertz spectrometer based on nonlinear diode circuits to translate the functionality of microwave electronics into the terahertz frequency band (100 – 3,000 GHz). This technology uses integrated diode circuits to achieve full waveguide bandwidth, exceptional dynamic range and reliable performance in a compact system.

This research has the potential for impacting a number of scientific and technology areas. First, the project is developing and demonstrating improved terahertz sources and receivers that will be applicable to a wide array of scientific, military and commercial applications. Second, a prototype spectrometer will be developed and applied to confirm the spectra of biomaterials previously measured by researchers from the University of Virginia using Fourier Transform Spectroscopy. Finally, the compact nature and inherent reliability of this all-solid-state system will allow the development man-portable spectrometers for future application in the field.

These components and system technology developed under the project will be useful for a host of other applications including compact range radars, atmospheric studies, terahertz test equipment, plasma diagnostics and possibly medical imaging. Government Agencies that are directly benefiting from this research include the U.S. Army National Ground Intelligence Center (ERADS Program), NRL, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, NASA, NOAA, NIST and the National Radio Astronomy Observatory. Also, as terahertz technology improves, numerous new applications are expected. These will span the defense, medicine, communications, industrial and test equipment arenas. The lack of

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compact, cost-effective and reliable sources of electronically tuned terahertz power is the main technological impediment that prevents the terahertz band from being as useful as the microwave and infrared bands are today. Successful completion of this research will greatly accelerate the further investigation and maturation of terahertz related applications.

Some of the recent achievements of this project include:

- The implementation of a diode-based prototype transmitter that was utilized in spectroscopic investigations of various materials (Teflon, mylar, metal mesh, & DNA) in the range 350-450 GHz. Here, tests were performed to define component developmental goals needed for the future realization of a spectroscopic system with adequate capability for collecting bio-signature data.
- The successful development of very broadband, all-solid-state sources and receivers that mitigate critical spectrometer design issues (e.g., adequate power, standing waves, etc), and that are electronically sweep with no moving parts.
- The development of a lower-frequency (210-270 GHz) heterodyne spectroscopic system prototype has demonstrated up to 100dB of dynamic range and a precision less than 1% for solid-samples and high levels of repeatability.
- The development of new class of very broadband, low LO power frequency mixers has been developed. This will facilitate the extension of the first prototype to higher frequency bands.
- The broadband sources and receivers are now being successfully marketed for compact range radars systems that determine the RCS of military vehicles and projectiles, as well as for antenna test ranges

In the subsections that follow, details will be provided on recent sub-component development aimed at the future demonstration of a highly sensitive 350-450 spectrometer.

3.1 Very Broad-Band All-Solid-State Sources

Design and development efforts were successfully employed to realize very broad-band components that will be instrumental in the future implementation of highly-sensitive THz spectrometers. One early accomplishment was the design and test of a new doubler (designated as WR12x2b) that possessed power-input handling capability of over 1 watt – note that this level of input power is readily available from commercial amplifiers in the 26.5-40 GHz range. The new design consisted of an array of 20 GaAs Schottky varistor diodes mounted on a high thermal conductivity substrate and the predicted performance of this component was over 100 mW. Figure 6(a) actually shows the significant increase (i.e., x 2) in output-power performance of the WR12x2b over the initial WR12xb that was obtained from using better GaAs Schottky diodes and heat sinking. This improvement is a direct result of improved input matching of the WR12x2b as indicated by the input-return-loss given in Fig. 6(b). It is also important to note that the WR12x2b can safely handle twice the input-power level (i.e., 1600 mW) as compared to the WR12x2 design.

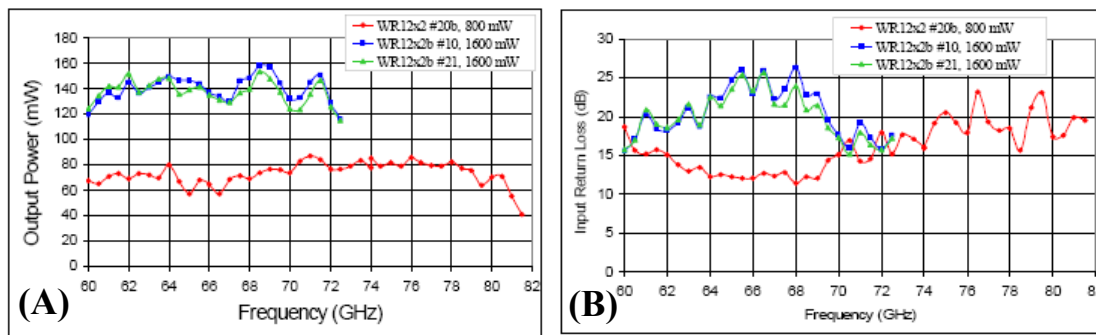


Figure 6: (a) A comparison of the output power, and (b) the input return loss, obtained from the original WR12x2 design and the new WR12x2.b.

3.2 Demonstration of a Lower-Frequency (210-270) Heterodyne Spectroscopic System

A lower-frequency (210-270 GHz) heterodyne spectroscopic system prototype was implemented to enable initial spectroscopic testing and benchmarking of the system optics, sub-stage components for the transmitter and receiver, as well as the data collection protocols. A heterodyne system is attractive because it provides greater dynamic range, faster sweep-times, and allows for the direct measurement of phase. Hence, this work was valuable for assessing the influence of system trade-space performance (absolute power, power stability, dynamic range, etc) on measurement speed, repeatability and accuracy. This heterodyne spectrometer employed a broadband solid-state source to radiate the material samples under test. The source uses a VDI-WR4.3x6 integrated sextupler (doubler and tripler), which is pumped by a 35-45 GHz Spacek Active Quadrupler. Note that the VDI-WR4.3x6 employs the newly developed WR12x2.b doubler discussed above. With computer control this source (see left bottom of Fig. 7) can quickly sweep the RF and yields output power as shown in Fig. 7(A). The receiver uses a VDI-WR3.4SHM (subharmonic mixer) which is pumped by a VDI-WR8x3 and a 35-45 GHz Spacek Active Quadrupler. This receiver (see right top of Fig. 7) can also be rapidly swept across the band giving a conversion loss shown in Fig. 7(B). Due to the fixed, narrow bandwidth of the IF amplifier, the mixer LO is locked to the transmitter. This was accomplished using a sideband upconverter to produce a slightly offset sideband of the signal from the YIG oscillator. This sideband is filtered by a YIG, amplified by a Spacek 35-45 GHz active quadrupler, and multiplied by a VDI tripler (WR-8x3) to provide the LO for the subharmonic mixer so that the IF is set at 1.7 GHz. The resulting frequency-domain spectrometer developed under this effort, which is illustrated in Fig. 7, has demonstrated up to 100dB of dynamic range and a measurement precision of less than 1% for solid-samples with high levels of repeatability. Measurement results taken on common dielectric materials (Teflon & Mylar) and on biological thin films (Salmon DNA) are given in Figs. 8(A) and 8(B), respectfully. Here, frequency averaging and mechanical calibrations were employed to rapidly (~ 5 sec) acquire transmission results with better than 1 % accuracy and measurement repeatability down to 0.1 %. This research will serve as the platform to realizing much higher frequency spectroscopic sensing – see reference [7] for more details.

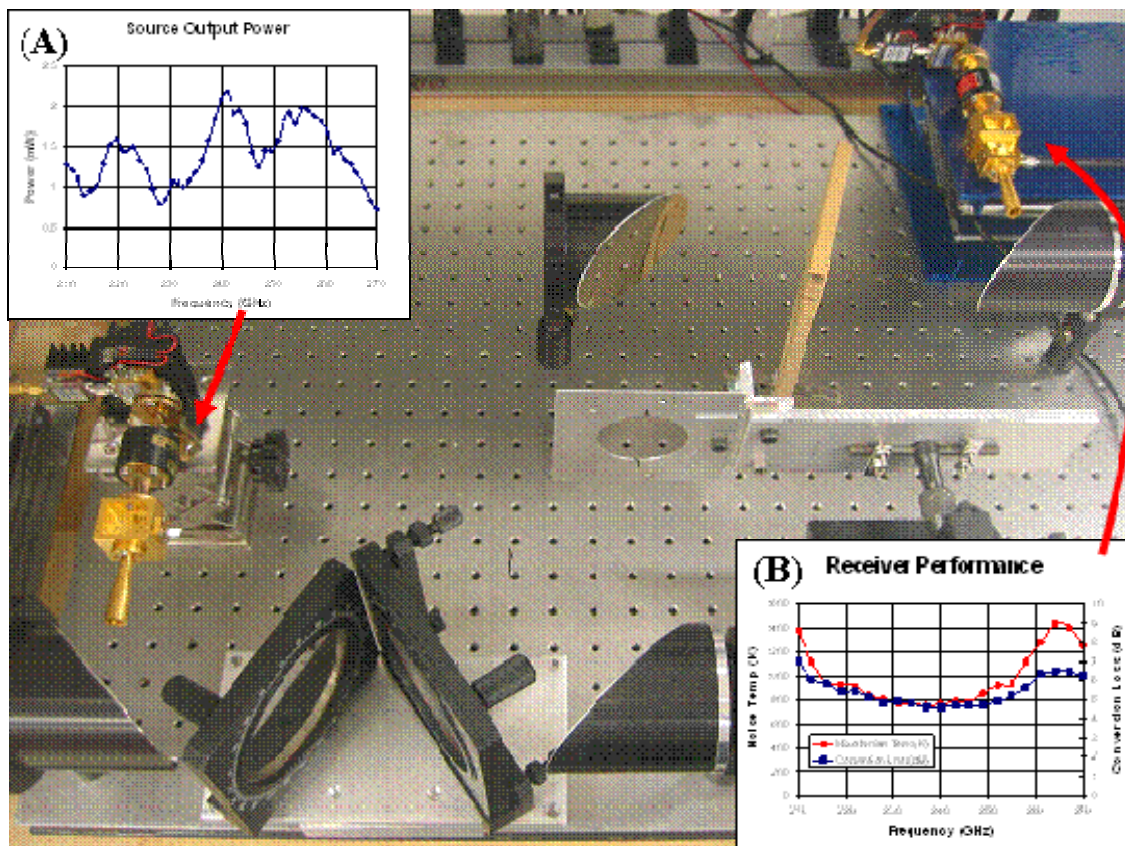


Figure 7: Breadboard Prototype 210-270 GHz Heterodyne-Spectrometer with (A) source output power, and (B) receiver conversion loss, characteristics in the insets.

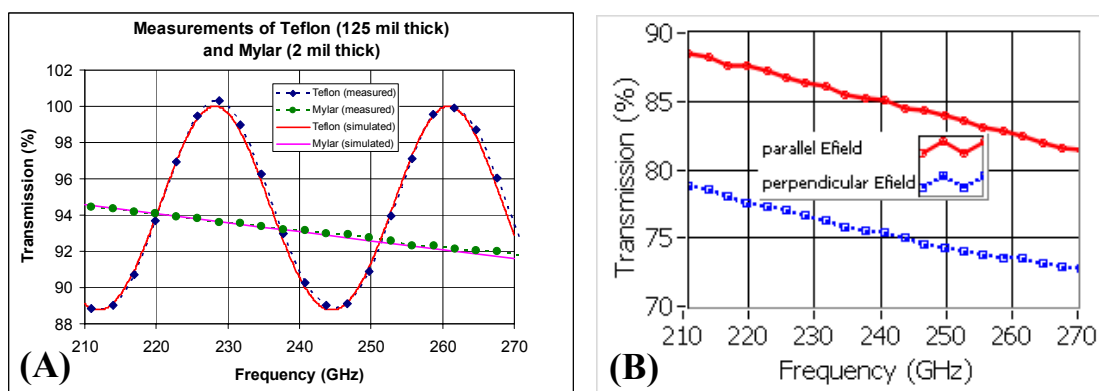


Figure 8: Breadboard Prototype 210-270 GHz Heterodyne-Spectrometer with (A) source output power, and (B) receiver conversion loss, characteristics in the insets.

4.0 INTERBAND RESONANT-TUNNELING-DIODE (I-RTD) OSCILLATOR

Professor Weidong Zhang, of North Carolina State University, Dr. Dwight Woolard of North Carolina State University and U.S. ARO are leading a research study of novel resonant tunnelling structures with the goal of identifying interband-tunneling induced instabilities that will be useful for the generation of terahertz (THz) frequency oscillations. This research is being conducted under the support of a National Research Council (NRC) administered project on “Physics and Modeling of Terahertz Electronic Devices and Nanostructures,” of which Dr. Woolard is the ARO advisor. The primary focus of this research project is nanoelectronic physics-based model development and high-frequency simulation. This project also includes past and present collaborative contributions from Prof. Boris Gelmont, of the University of Virginia, on the subject of semiconductor physics, and from Prof. Elliott Brown, of the University of California at Santa Barbara, on the the subject of electro-optical devices and systems. The primary goal of this project is to conduct detailed investigations of the physics and transport dynamics associated with resonant-tunneling-diode (RTD) structures that allow for interband-tunneling induced instability processes. Here, the engineering research is focused on the identification of nanoscale devices and processes that lead to THz-frequency oscillations. Specifically, the project is applying advanced device models and circuit analysis to optimize the performance of Interband RTDs (I-RTDs) that are implemented as oscillator sources at THz frequencies.

This research seeks to discover new and innovative approaches for producing THz-frequency output-power using solid-state based approaches at room temperature. Here, the goal is to utilize novel nanoelectronic concepts that allow for inventing approaches that avoid the long-standing technological limitations to output power levels and efficiency. This research has merit because the THz-frequency regime continues to be extremely technology-limited from the perspective of robust and powerful solid-state room-temperature sources – i.e., deep into the THz regime (i.e., > 500 GHz) the output powers are limited to milliwatt levels and below, and efficiencies drop well below 10%. Since solid-state device performance within the THz regime is limited by fundamental factors, there is motivation to search for entirely new physical mechanisms that lead to instability and oscillations. Specifically, this research seeks to investigate interband tunnelling processes as a means for realizing nanoscale feedback mechanisms that can be used to induce intrinsic instability processes. This is important because one of the limitations to conventional RTD-based oscillators is their extrinsic mode of operation – i.e., they resonant with the external circuitry to produce the oscillation and this leads to power-limiting design constraints because the devices are broadband unstable. Hence, this research seeks to discover new avenues for producing intrinsic oscillations in solid-state devices that could lead to higher powers and efficiencies. Therefore, this research has merit in terms of its contributions to fundamental device physics and merit in that it has the potential to significantly advance high-frequency source technology. Furthermore, improved THz power sources of this type would facilitate the study of THz frequency phenomenology in laboratories and enable more compact and cost-effective devices for field sensors and systems. Therefore, these studies have the potential to impact a broad range of THz applications related to sensing science and sensor technology. This The two subsections that follow will provide summaries for recent achievements in this research area.

4.1 An Interband-Resonant-Tunneling-Diode (I-RTD) Based High-Frequency Oscillator

A novel concept as been investigated for realizing a very high-frequency oscillator through the use of interband tunneling found to be present in type-II AlGaSb/InAs/InGaSb double-barrier heterostructures. This concept was developed specifically to circumvent power restrictions associated with conventional implementation of RTDs as oscillation. The basic concept is to utilize the interband tunnelling and the resulting charging in a manner that can lead to strong oscillations. As illustrated in Fig. 9(A), at large applied biases where occupied hole-levels in the valence (VB) well come into alignment with unoccupied electron

states in the collector region, an interband tunneling process (i.e., electron transport) is available to charge the VB-well. This positive charging of the localized barrier within the I-RTD obviously has the ability to electrostatically influence the resulting potential profiles of the entire device and alter electron conduction in the conduction-band (CB) well. Hence, the possibility exists that an I-RTD might be engineered and implemented where the interband current is used to establish a nanoscale feedback between charge transport processes in the conduction and valence bands. Indeed, this research developed new physical models [8, 9] that were used to study the associated charging and discharging processes, and to successfully demonstrate a new type of “intrinsic” instability process [10].

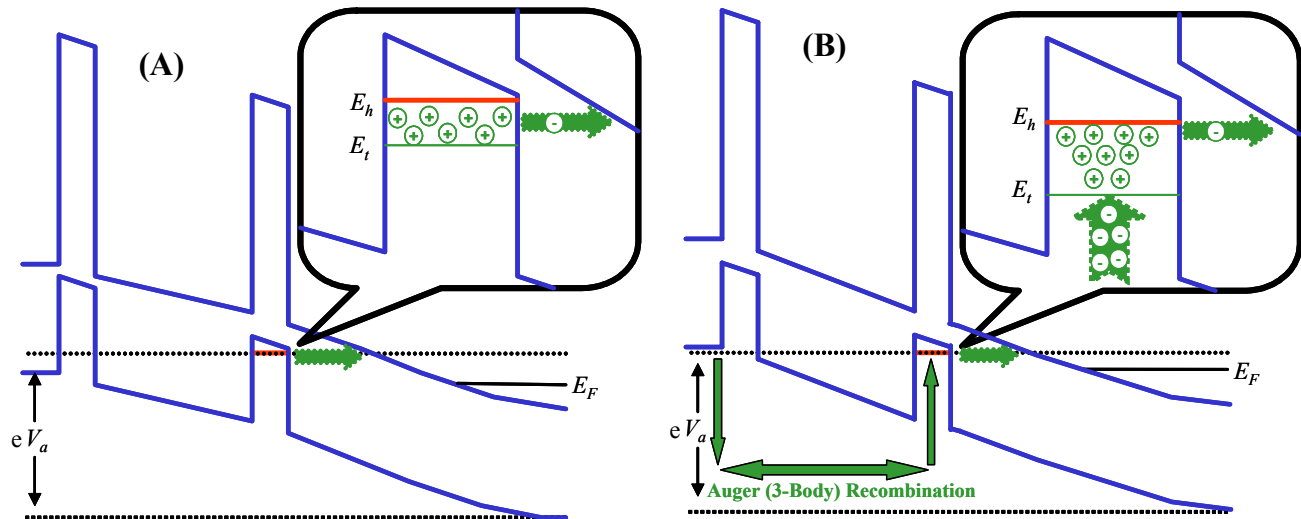


Figure 9: Two phase oscillation process with (A) interband tunnelling induced charging phase, and (B) Auger recombination induced discharging phase.

These prior studies consider room-temperature operation of the I-RTD subject to significant DC biases such that the initial band structure is approximately as shown in Fig. 9(A). Subsequently, an instability process is discovered that consists of two phases which can be summarized as follows. The first phase of the oscillation is produced by the interband charging of the VB well by holes which are generated by an electron interband tunneling current. Here, the positive increase in VB well charge lifts the energy-bands (EBs) in the emitter-end relative to the VB well region. The holes trapped in the VB well can be characterized by a hole-state band which is defined from the quasi-bound transverse energy-level (i.e., denoted by E_h) to a total energy-level (i.e., denoted by E_t) which defines the maximum energy of the entire hole ensemble that arises due to in-plane hole motion. For sufficiently large applied biases, this process must continue until a portion of this hole-state band dips below the VB edge of the emitter. This is true because for very large biases the interband tunneling current can not saturate due to the alignment of E_h with the Fermi energy of the collector on the right. Once a portion of the hole-state band assumes a position below the VB edge of the emitter (i.e., $E < eV_a$) then all holes with energies less than $E < eV_a$ are subject to annihilation by Auger recombination. Hence, the second phase of the oscillation occurs when Auger recombination leads to a rapid discharging of the VB well as illustrated in Fig. 9(B). Note that there are quantum mechanical effects that ideally prevent the occurrence of a balance at the Auger-induced discharge point – see reference [10]. This work is noteworthy because it demonstrates a new instability process that arises as a result of Zener type tunneling and defines a new approach for realizing a very high-frequency oscillator based upon an I-RTD.

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Time-dependent numerical simulations were performed to study the dynamical operation of an AlGaSb/InAs/AlGaSb double-barrier structure. This analysis led to high-frequency relaxation-oscillation condition that produced quasi-sinusoidal variations for both current and voltage. The time-dependent results for I-RTD emitter-to-collector terminal voltage and current density are given in Fig. 10 (a) and (b). Here, an oscillation frequency of 285.7 GHz was obtained and significant variations both in device current and voltage were observed. The power estimates for this non-optimized I-RTD structure indicate that 2.2 mW is available for a diode with a $100 \mu\text{m}^2$ cross section, and this is comparable to the power available from a Gunn diode at a much lower frequency. Hence, these initial figures of merit for oscillation frequencies (e.g., ~ 300 GHz) and output powers (e.g., > 2 mW) suggest that the I-RTD is a promising new device for implementation as a terahertz (THz) frequency oscillator. Furthermore, these studies suggest that strategic engineering of the interband tunneling and charge accumulation processes may allow for significant latitude in controlling the performance of this oscillator concept at very high frequencies. This work also immediately suggests alternative approaches where hybrid implementations (e.g., I-RTD combined with optical emission devices) could be utilized to artificially induce the charging/discharging cycles. This mode of operation will be discussed in the next section.

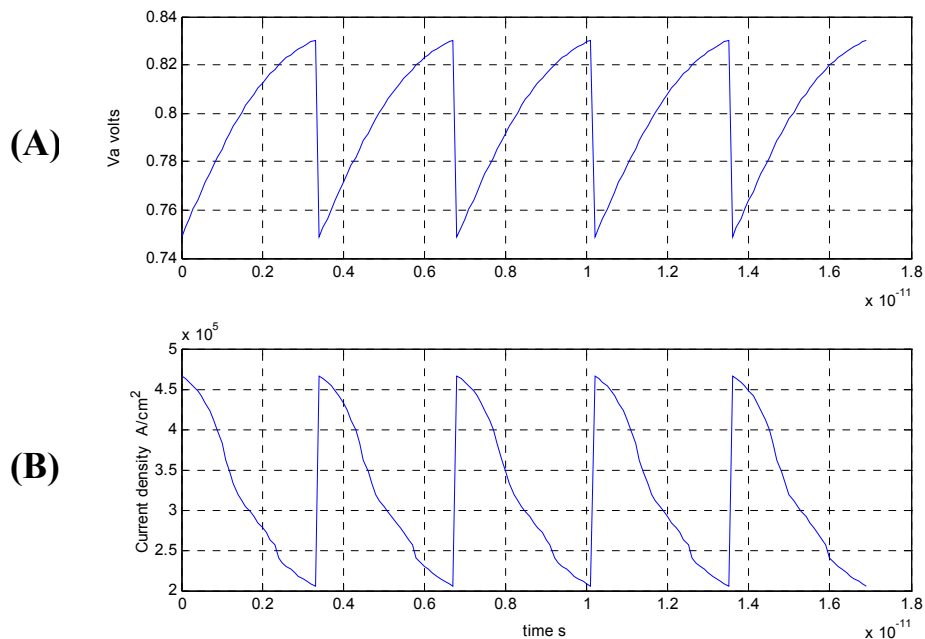


Figure 10: Resulting voltage (A) and current (B) dynamics associated with the I-RTD relaxation oscillation.

4.2 A Novel Optically-Triggered I-RTD Oscillator Concept

As shown in the last section, the double-barrier AlGaSb/InAs/AlGaSb heterostructure with staggered bandgap alignment can admit significant interband tunneling current in addition to the conduction band electron transport. The resulting positive hole-charge accumulation in the right valence-band (VB) well will electrostatically modify the spatial potential profile across the device structure, thereby effectively altering the conduction of conduction-band electron transport. Recent investigations have been used to show that a sequentially triggered optical discharging process can be used to annihilate, or substantially reduce, the

trapped holes that are generated from the interband tunneling process. Hence, an artificially induced electro-optic interaction can be used to return the device to its initial state and to produce a two-cycle oscillation process – i.e., one with a interband-induced charging transient followed by a optically-induced discharging transient to the initial state. These charging-discharging cycles obtained from this hybrid type of interband resonant-tunneling-diode (I-RTD) device constitute steady-state oscillatory behavior at very high frequency and produce alternating-current (ac) power as long as very short (i.e., sub-picosecond) and intense far-infrared laser pulses are presented to the diode. Initial studies of non-optimized structures and designs predict impressive figures of merit for oscillation frequencies (e.g., ~ 300 -600 GHz) and substantial output powers (e.g., ~ 10 mW) for very modest device areas (i.e., $100 \mu\text{m}^2$).

In particular, simulation results were generated for an optically-triggered (OT) I-RTD hybrid oscillator operating at 555.6 GHz and subject to idealized embedding impedances – i.e., short-circuited higher harmonic modes [11,12]. At $t=0$, hole charge accumulation is zero and the Zener tunneling process begins. At $t=1.5$ ps, an optical pulse with duration 0.3ps is applied to the device. The optical intensity is $3.5 \times 10^7 \text{W/cm}^2$ (transmission losses are ignored) and the wavelength is $\lambda=4.77 \mu\text{m}$ (0.26 eV). After one charging-discharging cycle is completed the diode resumes its initial state. The simulation results at the room temperature (300K) for bias voltage and current densities are plotted in Fig. 11. Note that the interband current is at a maximum ahead of the peak value of bias voltage. This is attributed to the exhaustion of available valence electrons in the right VB well as the Zener process proceeds. The peak CB current density is $3.7 \times 10^5 \text{A/cm}^2$ while the valley current density is $1.8 \times 10^5 \text{A/cm}^2$ (PVC_R= 2.1). The peak value of interband current density is $8.2 \times 10^4 \text{A/cm}^2$. The first-harmonic output power density is $9.7 \times 10^4 \text{W/cm}^2$. Hence, the total output power is 9.7mW for the assumed diode area of $100 \mu\text{m}^2$. In the lumped-circuit diode model, the negative R_D is calculated to be -3.2Ω while the capacitance C_D is 0.25 pF. Similar simulations at different frequencies of operation were carried out for the same device structure and bias conditions as above. For 330GHz, the obtained ac output power was 10.4 mW and equivalent circuit elements are $R_D = -3 \Omega$ and $C_D = 0.31 \text{pF}$. For 500GHz, the ac power output is 9.9mW and equivalent circuit element are $R_D = -3.14 \Omega$ and $C_D = 0.26 \text{pF}$. These results clearly show the superiority of this novel oscillator concept which demonstrates a very broadband output power capability over a significant portion of the THz regime. In fact, this device will only be limited by its power handling capability (i.e., thermal heating) and future studies are planned for analyzing this issue. The OT-I-RTD power efficiency (P_i/P_0 , P_0 is the dc power dissipation) is 4.4% if laser losses are ignored. Note that issues associated with the required laser technology are addressed in reference [12].

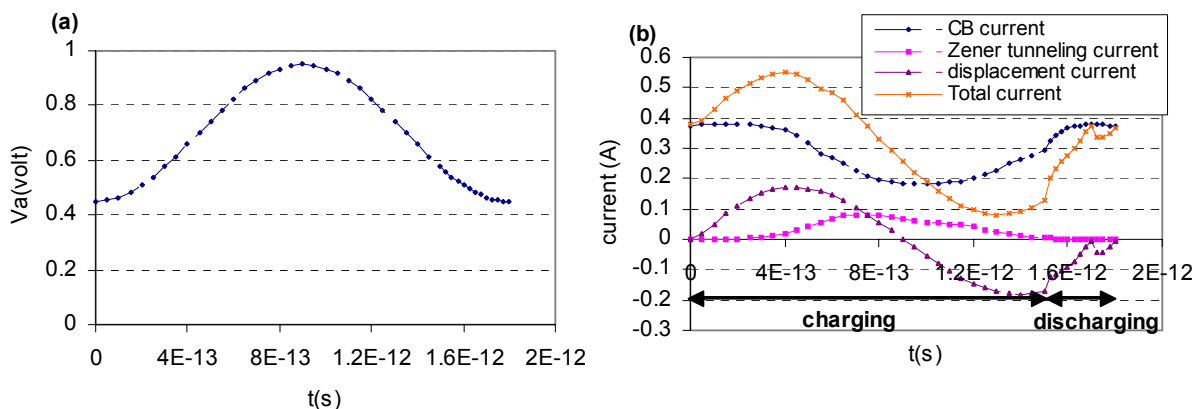


Figure 11: OT-I-RTD (a) bias voltage & (b) current.

5.0 NEW CONCEPTS FOR DETECTION OF BIOLOGICAL TARGETS: TERAHERTZ SIGNATURE DATABASE

Professors Tatiana Globus, Alexei Bykhovski and Boris Gelmont, of the University of Virginia, lead a research effort that is defining new experimental and theoretical techniques for accurate interpretation of terahertz (THz) frequency spectroscopic signatures so as to assess their utility in biological, and possibly chemical, agent detection, identification and characterization. This research has been conducted under the support of the U.S. Defense Threat Reduction Agency (DTRA) Program for CB Detection and is managed by the U.S. Army Research Office (ARO). This project consists of the focus areas: Experimental Spectroscopy (Prof. Globus), HPC-based Simulation and Analysis (Prof. Bykhovskaia), and Advanced Theory and Modeling (Prof. Gelmont). The number one goal of this project is to establish a realistic and credible scientific foundation for the future use of terahertz-frequency spectroscopy as a technique for the detection of biological agents in aerosol and liquid form. This will be achieved through the application of theoretical modeling and experimental characterization towards the development of a new database for terahertz (THz) spectral signatures of select biological materials and their fundamental molecular components.

This research will address the major challenges to collecting and interpreting THz-frequency spectral characteristics from biological materials and agents. Here the goal is to define experimental techniques for preparing samples and executing measurements that will lead to accurate and repeatable collection of the THz absorption characteristics and to establish accurate physical models that can be used to properly interpret the spectral results and how they related to the microscopic dynamics of the associated biological molecules. Hence, this research will make important contributions to the knowledge base in the area of bio-molecular science and provide valuable insights into the utility of THz spectroscopy as a detection, identification and characterization technique for biological materials and agents. This research includes active collaboration with Dr. D. Woolard (ARO), Dr. A. Samuels and Dr. J. Jensen (Edgewood Chemical and Biological Center), with the group of Prof. T. Crowe (UVA and Virginia Diodes Inc.), groups of Prof. R. Weikle (UVA), Prof T Khromova (UVA) and with the group of Prof. E. Brown (UCSB). Results of characterization are immediately transferred to Edgewood Chemical and Biological Center. The results will be also used in future development of biosensing technology (Virginia Diodes).

This research has high merit both in the basic sciences and in practical applications. In particular, the theoretical models and experimental procedures developed under this project will be a strategically important enabler to an array of activities in the biological and medical sciences. For example, these models and procedures will allow for new studies on the microscopic biological function and therefore has the potential to impact the medical sciences. This research will also establish reliable THz signature data for biological stimulants that will be critically important for developing new techniques for achieving early warning capabilities for biological threat agents. Here, the research will correlate the physical properties of the targets to their spectral signatures and this will be useful in defining the technical specifications needed for early-warning monitoring systems. For example, once reliable spectral signatures are established it will be possible to define the performance specifications (source power, receiver sensitivity, bandwidth, etc) and sensing modalities that will be required to field a useful bio-agent detection system. Therefore, this research will contribute to basic bio-molecular science and to practical sensing systems development. Summaries for two very recent scientific investigations, along with a description of the associated accomplishments, are given in the subsections that follow.

5.1 THz Signature Studies on Bacillus Subtilis 168 (BG) – Chromosome DNA

In order to make useful scientific interpretations of the THz signatures acquired experimentally from biological materials, it will be crucial to utilize physical models that reflect the underlying physics of the bio-

systems accurately without placing excessive demands on the computational resources. In addition, simulation results for THz absorption have been shown to be very sensitive to the choice of the model for the molecular structure and the associated physical parameters. In an effort to develop new insights into how structure influences THz signatures in complex bio-systems, this research effort has recently implemented a new model for *Bacillus subtilis* 168 (BG) chromosome DNA using its full sequence data (over 4,000,000 base pairs). The BG DNA has a (C+G) to (A+T) base pair ratio approximately equal to 0.43, which is lower than in *E. coli* DNA (0.5), but higher than is expected in anthrax DNA strains. The research also considered the base-pair statistics for the *Bacillus subtilis* 168 chromosome DNA, including base pair concentrations, the frequencies of appearance of different cluster types (A, C, G, T, AA, CC, GG, TT, etc), the average separations between the nearest neighbors of the same cluster type (A-A, AA-AA, AAA-AAA, C-C, CC-CC, CCC-CCC, etc), and different cluster types (A-C, A-T, A-G, A-AA, A-CC, A-TT, A-GG, AA-CC, AA-TT, etc) for the entire 4.2 million base pair *Bacillus subtilis* 168 sequence. The standard deviations for these separations were calculated as well. In order to simplify the initial computational analysis of the THz absorption, a representative 20 base pair sequence (AAGTACTGCTTTCAGACATG) with approximately the same (C+G)/(A+T), C/G/A/T ratios and base pair distributions as in the *Bacillus subtilis* 168 strain was considered. The effect of a solvent (water) was taken into account implicitly and Sodium ions were included as they are usually present. The covalent bond energy, covalent angle energy, proper and improper torsions, non-bonded interactions including electrostatic, and Van der Waals interactions were taken into account using AMBER 99 force field. Also, a higher effective dielectric constants (ϵ) as compared to the intrinsic ϵ for a DNA itself were used in sodium-DNA Coulomb interaction terms to account for the effect of water loading. The resulting structure was optimized using the conjugate-gradient algorithm for the potential energy minimization until a convergence in atomic forces was reached. The calculated BG THz signature reproduces many features of our experimental signature (see Fig. 12) and is useful for determining base-pair sub-chain contributions to the THz spectral characteristics. This research is important because when it is combined with more extensive investigations of base-pair sub-chains it may define completely new methods for identifying certain classes of bio-agents.

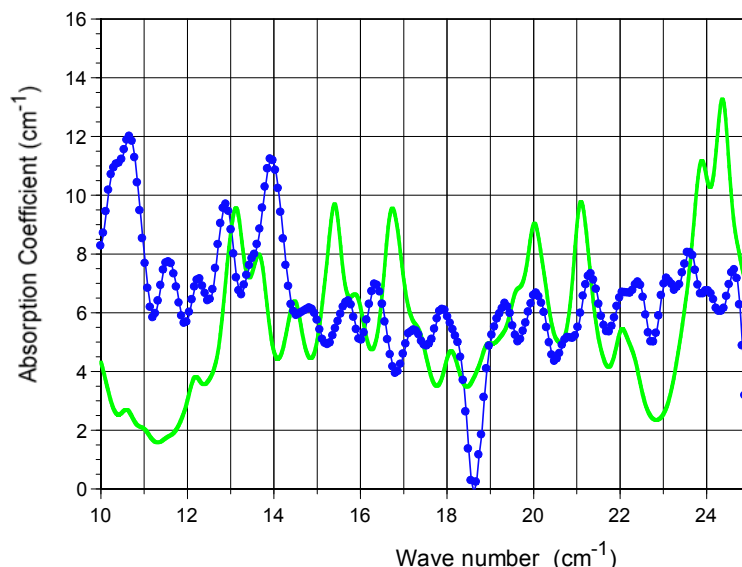


Figure 12: Theoretical predictions (green line) and experimental results (blue dotted line) for the THz spectrum of *Bacillus subtilis* 168 (BG) chromosome DNA.

5.2 THz Characterization of E-Coli DNA Strains in Diluted Solutions

In previous work, specific methods have been developed for performing measurements on diluted solutions of biomaterial in water have been developed. Here, optimum thickness and concentration of samples trapped between two polycarbonate substrates were determined to minimize standing-wave and lens effects when control samples of pure water are measured as the background. These methods permitted the suppression of most of the artificial spectral structure and enabled the measurement of very low concentrations – 0.1 to 3 mg/ml which corresponds to 0.01 to 0.3 % of biomaterial. These previously developed techniques have been applied to study of diluted solutions of E-coli DNA. Here, spectra for two different strains of E-coli DNA was collected and compared to the results obtained from BG DNA. It is very important to note that DNA samples can tend to form ordered patterns both in solid and gel (i.e., diluted solutions) form and this makes the resonant absorption structure sensitive to the orientation of the samples relative to the polarization of the incident THz radiation. This can lead to situations where measurement generates significantly different spectral characteristics for two different samples of the same material. Such an example is illustrated in Fig. 13 which shows transmission measurements on samples of the same E-coli solutions that possess spectral characteristics of opposite phase.

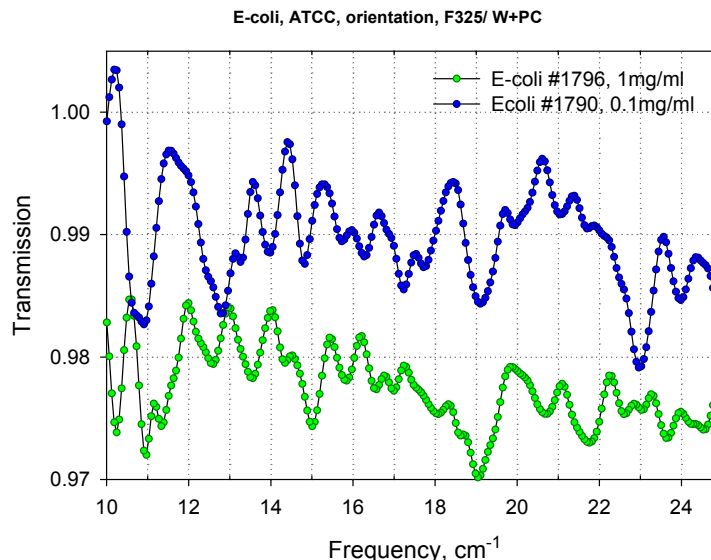


Figure 13: Spectra of two identical E-coli DNA samples presumably having different orientation.

Studies from earlier experiments have shown that even a relatively small shift in the frequency of the strong absorption peak (transmission minimum) around 14 cm^{-1} can be used as an experimental indicator of the sample orientation and provides an effective technique for correlating spectra taken from identical and similar (i.e., ones that contain a strong common line) biomaterial samples that possess regular structure. [T. Globus, D. Theodorescu, H. Frierson, T. Kchromova, and D. Woolard, "Terahertz spectroscopic characterization of cancer cells", Progress in Biomedical Optics and Imaging, Vol 6, No7, p 233-240, 2005]. Using this indicator as an experimental tuning key it is possible to accurately compare spectra taken from different samples in order to examine the similarities and differences. Figure 14 compares spectra from the two strains of E-coli DNA and BG DNA after the samples are correlated for orientation effects. Although frequencies of many resonance absorption peaks are reproduced in both type of DNA, there are notable differences that are useful for discrimination. In particular, there are uniquely resolvable absorption peaks at 12.3 cm^{-1} and 23.6 cm^{-1} in

BG DNA spectra. It is also noteworthy that E-coli DNA has a much stronger background absorption in the range $15\text{--}20\text{ cm}^{-1}$ as compared to the BG DNA. Note that the difference at 18.6 cm^{-1} is due to spurious water absorption from the varying humidity of the air and must be ignored. This is an important result, since after orientation correlation these results show similar spectra for the two strains of the E-coli DNA as should be expected because their base-pair composition is relatively close.

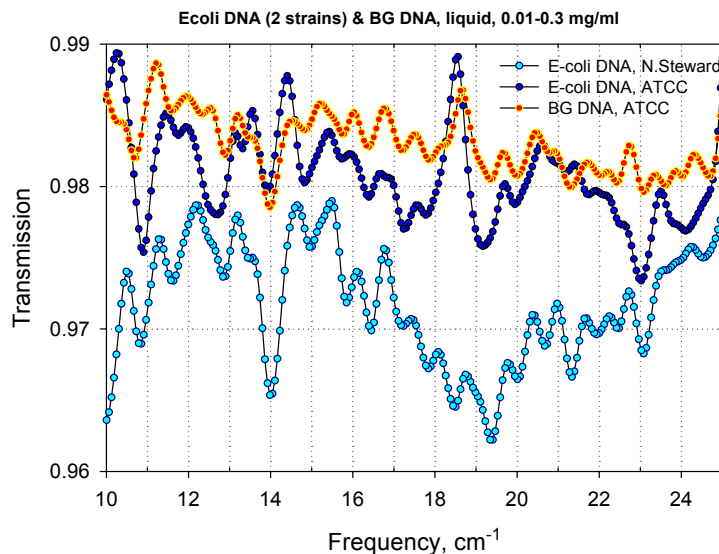


Figure 14: Comparison of the THz spectra from BG DNA and E-coli DNA, all in liquid.

6.0 TERAHERTZ FREQUENCY-HOPPING SPECTROMETER FOR BIOLOGICAL DETECTION

Professor Elliott Brown of the University of California at Santa Barbara and Professor Timothy Korter, of Syracuse University are collaborating on a new research project that will develop highly accurate and fast acquisition THz spectrometer and apply it to the study of synthesized bio-molecules to study spectral signature dependence on microscopic structure. This research has been conducted under the support of the U.S. Defense Threat Reduction Agency (DTRA) Program for CB Detection and is managed by the U.S. Army Research Office (ARO). This project consists of the focus areas: Spectrometer development and experimentation (Prof. Brown) and molecular chemistry and characterization (Prof. Korter). The specific goals of this project are: (1) to make radical improvements to the state-of-the-art in photomixer-based terahertz (THz) frequency spectroscopic instrumentation to allow for accurate and rapid acquisition of the spectral signatures associated with biological and chemical agents, and (2) to qualify this new capability through advanced spectroscopic studies conducted on an array of naturally occurring and strategically synthesized biomaterial targets.

This research seeks to implement a novel type of photomixer-based hopping-spectrometer where sensitivity will be increased by orders of magnitude through the use of both a coherent transmitter and a coherent receiver. Here, the main new innovation is to achieve coherent detection by using a second photomixer as the receiver and driving it with the same two diode-lasers that are used in the transmitting photomixer. The goal is to achieve measurement capabilities that can be rapidly tuned in discrete steps ($\sim 1\text{ GHz}$) across the entire

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THz band (i.e., ~ 100 GHz to 2 THz) while maintaining the high amplitude stability and frequency precision that is traditional with the photomixer-based approach. Hence, the technological impact of this project is significant because it will define a new capability for the rapid identification of spectral signatures across the entire THz band. In addition, through a joint multidisciplinary collaboration, this project will apply this new technology to the study of numerous biological materials, which will include naturally occurring bio-agents (e.g., *Bacillus Subtillis* spores) and carefully synthesized materials (e.g., proteins). The study on synthesized materials is particularly important as it will allow for studies on peptides of known composition that will be methodically increased in size and complexity to provide inside to the specific source of particular resonant features. Therefore, this project will provide unique insights to the microscopic dynamics and associated THz spectra of known biological materials and this will help to guide the application of THz spectroscopy to detection applications. These studies will also consider the performance advantages of the new photomixer-based spectrometer through direct comparison to existing more traditional time-domain spectroscopy techniques. This research includes an active collaboration with Goodrich Corporation that is developing new photomixer technology under the support of a Congressional program and is linked to a parallel research effort with Pegasus Inc. (Dr. Hong-Liang Cui) and the U.S. Army's Dugway Proving Grounds testing center to execute future spectroscopic studies on live Anthrax.

This research has extremely high merit in that the new technology that is to be developed will be an important enabler to scientific inquiry and in that it seeks to facilitate the assessment of THz spectroscopy as a detection methodology for biological and possibly chemical agents. In particular, the primary goal is to establish a spectrometer that is extremely accurate and fast in acquiring spectral data and one that is cost-effective and compact to allow for scientific studies within difficult testing environments – e.g., as in protective containment areas at the U.S. Army's Dugway Proving Grounds. The project also has merit in that it has incorporated a chemistry expertise for engineering/synthesizing molecular systems for investigating the dependence of spectral signature on material structure and composition and for dual performance testing against more traditional spectroscopic systems. Hence, this project will be a major facilitator for acquiring new scientific information and for enabling unique experimental inquiries in the future. The next section will summarize some of the preliminary developments that have already occurred in this very new project.

6.1 Preliminary Photomixer-based Spectrometer Development & Testing

While the project to develop and test a "THz Frequency-Hopping Spectrometer for Biological Detection" is in its initial stages, it is important to note that good quality photomixer-based spectroscopic instrumentation has already been established under prior U.S. Army support and that capabilities of this type have already been applied to scientific inquiries. Also note that the specific goals of this new project are to refine existing THz spectrometer capabilities such that they will possess enhanced sensitivity and data collection capabilities. In addition, while the details of such a system development proposal are quite technically involved, the new "frequency-hopping" implementation will integrate two major innovations that have already been investigated under prior programs – hence this project is developmental in nature and of moderate risk. Specifically, prior research and development conducted partially under the support of the ARO-managed Multidisciplinary University Research Initiative (MURI) program on Sensing Science & Electronic Technology at Terahertz Frequencies has been used to develop breadboard-type photomixer-based spectrometers that have been applied in numerous investigations of important THz-related phenomenon. For example, previously developed photomixer-based spectrometers have been employed to demonstrate that isolated bioparticles exhibit unique (i.e., enhanced) spectral signature phenomenon (see Fig. 15), and are actively being employed to study newly theorized phonon-localization effects in dilute polyethylene powders which may help to explain observed enhancement in the spectral absorption characteristics of aerosols. For details on some of these experimental studies see reference [2].

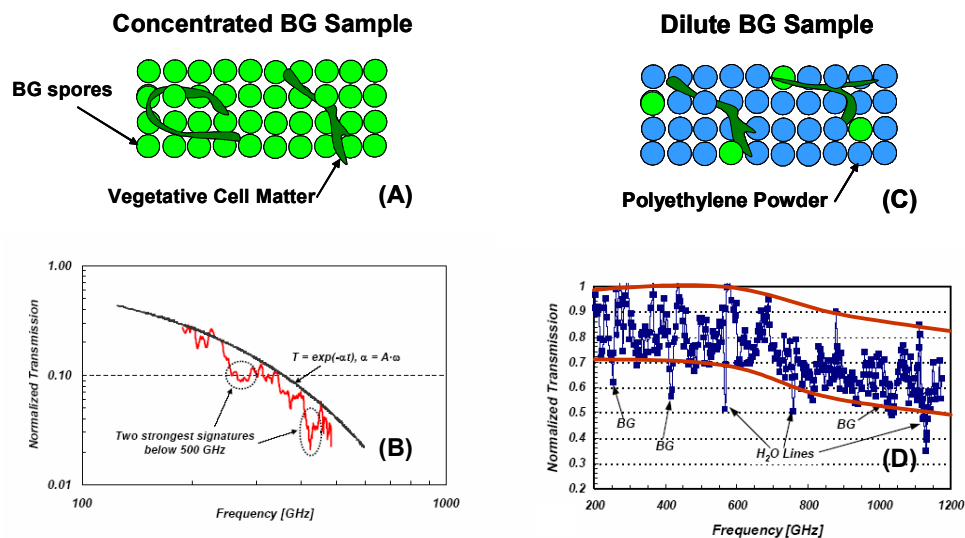


Figure 15: (A) Illustration of concentrated BG samples showing spores and vegetative cell matter, (B) Absorption spectra for concentrated BG samples, (C) Illustration of dilute BG samples showing spores, vegetative cell matter and polyethylene matrix material, and (D) Absorption spectra for dilute BG samples.

While the existing breadboard systems have been effective in spectroscopic studies, they require the utilization of large commercial systems as components and they are slow and cumbersome in data collection because they typically use direct detection (i.e., bolometer or Golay cell). Hence, innovations will be incorporated into the new frequency-hopping system that leverages recent technological breakthroughs. The primary innovations to be used in the new spectrometer will be the use of: (1) a recently demonstrated 780-nm-based ErAs:GaAs coherent photomixing transceiver, and (2) thin-film high-Q dielectric filters, which when combined with distributed Bragg reflector (DBR) laser diode with < 10 MHz linewidths lead to 1 GHz hopping capability, to replace a large and expensive optical spectrum analyzer that is used for detection. In regards to the later, commercially available broadly tunable DBR laser diodes are available from Sacher Lasertechnik [13] that lock to a single thermally-stabilized multi-layer thin-film dielectric filter and provide for frequency tracking (i.e., to within 100 MHz) and synchronous detection. In regards to the former, a photomixing transceiver has been previously demonstrated that utilizes both a photomixer source and a receive photomixer to provide for coherent detection with outstanding signal-to-noise (S/N) while operating at room temperature. In fact, as was reported already in [14], implementations of ultrafast ErAs:GaAs (lifetime 0.3 ps) photoconducting material into devices as illustrated in Fig. 16 have yielded S/N ratios approaching 60 dB/Hz^{1/2} at 86 GHz, and the performance at higher frequencies will increase substantially because the dominant noise sources (e.g., trap-induced 1/f noise) will contribute much less there. If this facts were not compelling enough, another research group from Europe (i.e., Teraview Ltd) has just recently reported a commercially available continuous-wave THz imaging system with 60 dB dynamic range at 0.53 THz using this same basic technique – and this represented a significant increase in S/N ratio (350/1 as compared to 300/1) as compared to pulsed time-domain imagers. Hence, preliminary technology achievements suggest that a THz frequency-hopping spectrometer is well within reach and that this research will be an important enabler in the near-future to new and novel scientific investigations into molecular level dynamics and signature phenomenology.

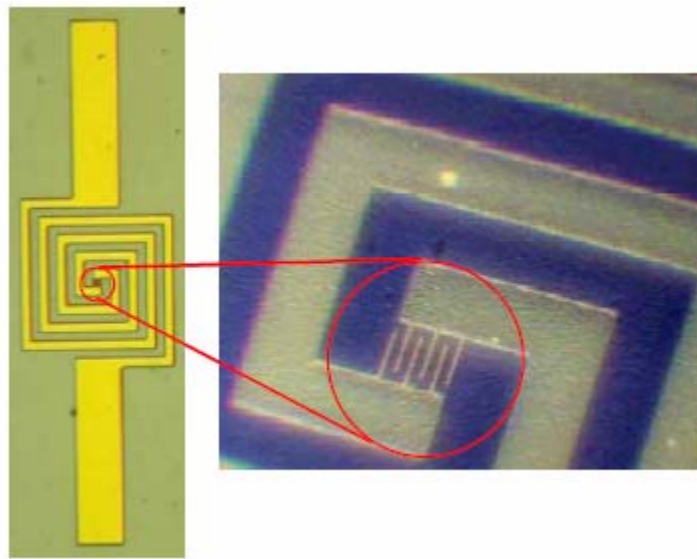


Figure 16: Top view of ErAs:GaAs photomixer device showing two-turn, self-complimentary square spiral antenna, bias lines, and exploded view of interdigital active region.

7.0 TERAHERTZ-FREQUENCY DEEP SUB-WAVELENGTH SPECTROSCOPIC IMAGING (THZ-DSSI) FOR BIOLOGICAL AGENT DETECTION

In light of many of the difficulties of collecting THz-frequency spectral signatures from bulk samples of biological materials, and in order to facilitate the study of the structure of microscopic biological systems, the U.S. ARO and U.S. DTRA has plans for new research initiatives that we seek to enable novel THz characterization methodologies. One of these newly launched initiatives is in the area of THz-frequency deep sub-wavelength spectroscopic imaging (DSSI). This program will support the study of viable approaches for collecting THz-frequency spectroscopic images from microscopic biological molecules. Here, the general problem is how to realize a very sensitive method that can be used to successfully measure spectroscopic absorption across the surfaces of bio-molecules. This is essentially the problem of performing very long wavelength microscopy, and since the features of interest have dimensions on the orders of 100's of nanometers or less, THz-DSSI will require resolution capability of 100x or better below the wavelength. A program has been implemented to support a number of seed investigations in the area of THz-DSSI, where each will explore a slightly different technique to assess its viability for success. At this point, new efforts have been launched in the following areas:

Pump-Probe Spectroscopy for Sub-Wavelength-Resolution THz Spectroscopic Imaging

This project will be conducted by the research team: Prof. Elliott Brown, of the University of Virginia, and Prof. Steven Brueck, of the University of New Mexico. This approach will consider the use of the nonlinear response associated with stimulated emission (i.e., in analogy to stimulated emission depletion microscopy which has already demonstrated 50x at optical frequencies) to achieve resolutions below the diffraction limit. Here, the use of IR-pump and THz-probe can be used to introduce a nonlinearity that changes the threshold associated with the spatial resolution. In the proposed technique, an IR-pump will be used to establish a diffraction-limited spot-size (i.e., which is much under the probe wavelength) which then is used to search for the much longer-wavelength spectral absorption phenomenon that is enabled only by the nonlinear THz-

probing. This technique, which can be considered as a nonlinear synthetic aperture approach, will be applied to the imaging of fluidic chips that possess nanoscale channels that are also being used to develop orienting sensing platforms for THz spectroscopic analysis.

Integrated Resonant THz Nanosensing Probes

This project will be conducted by the research team: Prof. Peter Harng Bolivar, of the University of Siegen, Germany, and Prof. Boris Mizaikoff, of Georgia Institute of Technology. This research will consider the feasibility of developing resonant nanoscopies sensors operating in the THz frequency regime. Here the goal is to reduce the required quantities for analyzing bio-molecules, by reducing the analyzed volume beyond the diffraction limit using near-field THz sensing probes. Research will also be performed to develop integrated resonant probes to attempt to compensate for the extremely small apertures and resulting limits to spectroscopic sensitivity.

Near-Field Microscopy and Code Aperture Arrays for Sub-Wavelength Terahertz Imaging

This project will be conducted by the research team: Prof. Judy Wu, of the University of Kansas, and Prof. Robert Weikle, of the University of Virginia. This research will explore alternative strategies for THz EM wave transport and detection as it applies to near-field spectroscopic imaging. Here, studies will be performed to assess the performance of a probe chip that contains a thin-film dipole antenna integrated with a thin film planner waveguide. This research project will also investigate the promise of coded aperture techniques as a means of directly generating two-dimensional spectroscopic images with nanoscale resolution. Here, the multiplexed properties of encoded masks will be studied for their ability to yield image resolution below the diffraction limit. The main challenge of this approach is to devise methods for making encoded masks that allow for switching the individual pixels.

The seed-projects described above, along with a number of others, will be developing a technology roadmap that assesses the viability of various techniques for achieving THz-DSSI in the future. It is expected, that one or more of the most promising techniques will receive support in the future to enable the development of a THz microscope. If successfully implemented, such a THz microscope would certainly be an important enabler to bio-agent detection and characterization, and that is the primary motivation of this program.

8.0 CONCLUSIONS

This paper has presented an overview of the joint U.S. ARO and DTRA research program on THz Sensing Science and Electronic Technology for CB Defense. This program is focused on the study of sensing science phenomenology and on the development and application of electronic technology for the purpose of assessing the value and effectiveness of THz spectroscopy for applications in CB defense. This program seeks to leverage pre-existing science-based research and device/component development to move towards practical applications in defense, with an emphasis on biological threat detection and identification.

9.0 REFERENCES

- [1] Dwight Woolard, Elliott Brown, Michael Pepper and Michael Kemp, "Terahertz Frequency Sensing & Imaging: A Time of Reckoning Future Applications?" to appear in the *IEEE Proceedings*, October, 2005.
- [2] E.R. Brown, T.B. Khromova, T Globus, D. L. Woolard, J. O. Jensen and A. Majewski, "Narrow THz Attenuation Signatures in Bacillus Subtilis Spores," submitted to *Phys Rev. Lett.*, Jan., 2005.

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- [3] D. L. Woolard, Y. Luo, B. L. Gelmont, T. Globus, and J. O. Jensen, "Bio-Molecular Inspired Electronic Architectures for Enhanced Sensing of THz-Frequency Bio-Signatures," accepted to *International Journal of High Speed Electronics and Systems (IJHSES)*, 2005.
- [4] D. L. Woolard, Y. Luo, B. L. Gelmont, T. Globus, and J. O. Jensen, "A Bio-Molecular Inspired Electronic Architecture: Bio-Based Device Concepts for Enhanced Sensing," in *Proc. SPIE Security and Defense Symp.*, 2005.
- [5] Tatiana Globus, Tatyana Khromova, Rebecca Lobo, Dwight Woolard, Nathan Swami, and Erik Fernandez, "THz characterization of lysozyme at different conformations", Proceedings of SPIE, "Terahertz for Military and Security Applications", v. 5790, p.54-65, Defense and Security Symposium, Orlando, Florida, 28-29 March, 2005.
- [6] Xiaowei Li, Alexei Bykhovski, Tatyana Khromova, Tatiana Globus, Boris Gelmont, Dwight Woolard, Alan C. Samuels, and James O. Jensen. Computational Methods for Analysis of Terahertz Spectral Signatures of Nucleic Acids Nanotechnology, 2005, IEEE Conf. on Nanotechnology, IEEE-NANO 2005, Japan, Nagoya, July 11-15).
- [7] David S. Kurtz, Thomas W. Crowe, Jeffrey L. Hesler, David W. Porterfield, "Frequency Domain Terahertz Spectroscopy," in the Proceedings to IRMM-Wave/THz Meeting, Williamsburg, VA, 2005.
- [8] B. Gelmont, D. Woolard, W. Zhang and T. Globus, "Electron Transport within Resonant Tunneling Diodes with Staggered-Bandgap Heterostructures," *Solid State Electronics* **46**, p.1513, 2002.
- [9] D. L. Woolard, W.R. Loerop and M.S. Shur, "Advanced Theory of Instability in Tunneling Nanostructure" "Chap. 8 in *Terahertz Sensing Technology*": Volume II (World Scientific, Singapore, 2003).
- [10] D. Woolard, W. Zhang, and B. Gelmont "A Novel Interband-Resonant-Tunneling-Diode (I-RTD) Based High-Frequency Oscillator," *Solid State Electronics* **49**, p. 257, 2004.
- [11] Weidong Zhang, Dwight Woolard and Boris Gelmont, "The Physics of Terahertz-Frequency Oscillations in an Optically-Triggered Interband-Resonant-Tunneling-Diode (OT-I-RTD) Device," submitted to *Physical Review B* (2005).
- [12] Weidong Zhang, Dwight Woolard, Elliott Brown and Boris Gelmont, "A Novel I-RTD Based Optically-Pumped Hybrid Device for Generating THz Oscillations," in the Proceedings to the SPIE Optics East, 2005.
- [13] Sacher Lasertechnik, LLC, Buena Park, CA, <http://www.sacher-laser.com/index.php>.
- [14] J. E. Bjarnason and E. R. Brown, "Sensitivity measurement and analysis of an ErAs:GaAs coherent photomixing transceiver," *Appl. Phys. Lett.*, 87, 134105(1-3), (2005).