R2-C.2: Multiplexed Mid-Infrared Imaging of Trace Explosives

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II. PROJECT DESCRIPTION

A. Project Overview

The overall goal of this project is to develop technology to enhance the ongoing work of ALERT by providing lower-cost, wide-bandwidth, mid-infrared (MIR) laser sources and to develop MIR laser-based imaging technology. The end-state of the research will be a new MIR imaging and detection platform that is field deployable (small size, weight, power, and cost) and sensitive to trace explosives (on the order of micrograms per square centimeter). Other ALERT projects are already exploring the MIR region of the spectrum and identifying features unique to explosives, and ALERT industrial partners are producing commercial MIR laser arrays. However, these other existing efforts are restricted by technological questions such as: (1) How do you perform sensitive spectroscopic imaging in a wavelength range that lacks robust and widely available focal plane arrays and optical components; and (2) How do you combine several high-cost laser chips into a single module for sensitive imaging and detection? This project seeks to answer these questions through novel semiconductor fabrication techniques and laser scanning with the use of time/frequency multiplexed imaging technology. Additionally, this project is now exploring combining multiple MIR imaging techniques with brand-new, commercial, low-cost (<$300) MIR detector arrays for sensitive and specific imaging. Overall, this will enhance ongoing ALERT efforts by enabling lower-cost and higher-resolution imaging technology to detect signatures characterized by other ALERT projects, provide a technology to enhance the commercial offerings of ALERT industrial partners, and provide new low-cost spectroscopic explosive imaging platforms useful throughout the Homeland Security Enterprise (HSE).

Due to the successful development of a low-cost MIR imaging platform, our project overview has expanded a bit to add translation. We are also asking the new research question: (3) Can applying probabilistic models to data acquired using low-cost MIR imaging platforms increase imaging speed, sensitivity, and specificity? Now that we can acquire spectroscopic images of explosives quickly at low cost, we are leveraging advances from “big data” to improve our performance.
B. State of the Art and Technical Approach

This project is investigating three complimentary technical advancements: (1) On chip heterogeneous integration of widely disparate wavelength MIR lasers; (2) a low-cost vanadium oxide bolometer for explosive detection (which superseded the original goal of investigating MIR coded aperture imaging technology due to bolometer array’s superior size, weight, power, and cost profile); and (3) development of optical sensor selection algorithms to improve sensitivity and speed of complete sensor systems.

B.1. On Chip Heterogeneous Integration of Widely Disparate Wavelength MIR Lasers

The most commonly used and commercially available semiconductor MIR light source is a quantum cascade laser (QCL) [1]. QCLs are made into widely tunable devices that can have large ranges over the entire absorption band of explosives residues using external cavity (EC) feedback. These devices, known as EC-QCLs, select wavelength by rotating the incident angle of light on a diffraction grating. Such a system has been of particular interest recently, to detect trace explosives residues on various targets [2-4]. These systems require moving parts and manual assembly; integration would be preferred for simplicity, lower cost, and to improve mechanical reliability. Arrays of lasers can be fabricated in such a way that the lasing wavelength of adjacent lasers is slightly offset, thus producing a discretely tunable source by selectively turning on and off individual lasers [5]. This is the basis of the technology of Pendar Technologies. These lasers have a lateral offset, and thus can use external free space optics to combine the beams into a single output [6]. External beam combining, while not requiring moving parts, requires free space optics and alignment, which adds complexity and renders the devices susceptible to mechanical instability.

The technical approach we are employing is to combine laser arrays on a single chip and on separate chips into a single module using a novel inter-chip alignment and optical coupling technique. In this technique, individual laser chips are fabricated with extending copper nodules. The chip with nodules is combined with similar chips to form a quasi-monolithic “quilt,” from which the name “Optical Quilt Packaging” (OQP) is derived (see Fig. 1).

![Figure 1: Illustration of “Optical Quilt Packaging.”](image)

The proposed OQP leverages advances in electronic quilt packaging, a novel technique developed at the University of Notre Dame (UND) for high-speed electronic interconnections. Electronic quilt packaging integrates diverse electronic device technologies into a quasi-monolithic module by connecting separate die with solid metallic contacts along the vertical faces for both mechanical and electrical connection (see Fig. 2). Research at UND has demonstrated the world-record low inter-die insertion loss of less than 0.1 dB from 50 MHz to 100 GHz [7] with submicron alignment.
B.2. MIR Spectroscopic Imaging of Trace Explosives

To increase signal-to-background detection of trace samples of explosives, we will employ MIR spectroscopic imaging. MIR imaging arrays are prohibitively expensive, so we are exploring time and frequency multiplexed imaging with the laser modules developed in this project to improve speed (frame rate) and sensitivity (minimal detectable concentration) of differential reflection spectroscopy by replacing the relatively high-noise infrared detector array with a more sensitive (and less expensive) single element photodetector. MIR trace explosives imaging systems typically employ bolometer (i.e. thermal) or semiconductor detector (i.e. photonic) Focal Plan Arrays (FPAs). Semiconductor detector arrays exhibit a wavelength dependence on the material; materials useful in the MIR tend to be prohibitively expensive for multipoint distributed sensing. Bolometer-based FPAs can be prohibitively slow for many differential measurement schemes of moving objects; however, recent commercialization of bolometer-based FPAs have drastically reduced system cost by more than 100 fold, opening up new possibilities to investigate using distributed networks of explosive detection systems. To our knowledge, we are the first to explore leveraging these advances and have published the first papers demonstrating hyperspectral chemical imaging using low-cost, microbolometer arrays.

B.3. MIR Chemometric Analysis of Trace Explosives

MIR spectroscopic imaging has been demonstrated to be a powerful tool for trace explosives detection by several groups (e.g. [2-4], [8]RDX, and tetryl), including ALERT researcher, Professor Samuel Hernandez-Rivera of the University of Puerto Rico at Mayagüez (Project R3-C). Professor Hernandez-Rivera employs QCL systems that have been used to deliver high-spectral-energy-density radiation onto highly energetic materials (HEMs) deposited on complex substrates. Through standard preprocessing (second derivative, standard normal variate, and multiplicative scatter correction) and principal component analysis (PCA) or linear regression analysis, pentaerythritol tetranitrate (PETN) and trinitrotoluene (TNT) can be detected on wood, cardboard, and aluminum substrates. An example of an explosive detection signature is shown in Figure 3. We leverage previous advances by employing the successful techniques within our imaging systems. Additionally, we explore extending these techniques to include elipsometry [8] or polarimetric imaging [9].
To improve sensitivity and specificity, we are developing a new trace explosive technique based on imaging the thermal relaxation of chemical film residue. MIR explosive residue detection sensitivity and specificity (and therefore accuracy and speed) are limited by the ability to differentiate between the spectral absorption features; however, in real-world environments, substrate and chemical confusants can dramatically reduce performance. Traditionally, this is overcome by imaging samples at many different illumination wavelengths simultaneously; however, such an approach increases system cost and complexity. Our new approach is to not only image the reflected light spectrum, but to also measure the speed at which thermal energy is dissipated in each point of the image. This added data dimension gives chemical information on the matrix (i.e. binder) of explosive residue, and is different for explosives compared to other compounds. We are, to our knowledge, the first to explore this method. It is based on the PI’s extensive work on biomedical fluorescence lifetime imaging, which is used to quantitatively measure the environment of trace biomedical compounds.

Finally, to assist translation, we have begun developing optical sensor selection algorithm development with Professor Vijay Gupta of the University of Notre Dame. We are exploring both probabilistic detection models and machine learning models to use our hyper-dimensional data to increase detection sensitivity and speed while decreasing system cost and complexity.

C. Major Contributions

C.1. Summary

One student was involved in the project during Year 4: David Benirschke. The project is supported by ALERT funds, a graduate-student fellowship external to ALERT, and internal support from the Notre Dame Center for Nanoscience and Technology.

C.2. Year 5

Two major accomplishments were achieved in Year 5: (1) 5x improvement in imaging speed of our low-cost microbolometer platform while maintaining the same signal-to-noise ratio, and (2) development of a wireless, solar powered, MIR imaging system to leverage the distributable, low-cost microbolometer array imaging platform.

We characterized and published results demonstrating that the low-cost microbolometer arrays are capable of achieving performance required for trace explosive detection [10]low-cost, uncooled vanadium oxide microbolometer array, the Seek Compact, in accordance with common infrared detector specifications: noise-equivalent differential temperature (NEDT. As published, we reported that a ~90x decrease in imaging...
speed was required to achieve the same performance as a system that cost 50x more; however, this decrease in speed was not unreasonable since the resulting frame rate were on the order of 1-3 seconds, and therefore still useful for field applications. Furthermore, we have subsequently improved the imaging speed by a factor of 5 through software and hardware modifications to the commercial microbolometer system. We have increased maximum frame rate from ~7 frames per second to more than 30 frames per second without negatively affecting the signal-to-noise ratio. 

To leverage the low-cost, low-power performance of our imaging system, we collaborated with Prof. Jon Chisum and the Army Research Lab to integrate our MIR imaging platform in wireless, solar-powered, distributable hardware platforms. Real-time spectroscopic data is streamed to custom control software developed by our group for analysis. A flow chart and images of the wireless platforms, and the control GUI are presented in Figure 4. This platform is currently being used as our primary imaging platform in our current work.

![Flowchart of wireless MIR spectroscopic imaging platform](image)

**Figure 4:** Flowchart of wireless MIR spectroscopic imaging platform (top) and resulting representative data (bottom) collected for analysis using custom-built control software.

### C.3. Year 4

**C.3.a. On Chip Heterogeneous Integration of Widely Disparate Wavelength MIR Lasers**

In Year 4 we recorded low array-to-array mid-infrared coupling between chips, and published the results in IEEE Photonics Technology Letters [11]. This work built upon Year 3 results, presented below, and demonstrated a record low 4.1 dB coupling loss for Ge on Si wafers with arsenic trisulfide chalcogenide glass cladding as seen in Figure 5.
C.3.b.  **MIR Spectroscopic Imaging of Trace Explosives**

C.3.b.i.  **New, Low-cost MIR Imaging Platform**

We characterized and published work on using low-cost (<$250) imaging arrays to perform spectroscopic MIR imaging of nitride films with thicknesses of 1-2 μm. Thorough noise analysis and spectroscopic imaging of nitride films were published in Optical Engineering [12] and depicted in Figure 6. These results proved that low-cost MIR imaging arrays are capable of sensitive spectroscopic measurements of trace chemical residues, and we are leveraging these results to develop distributed MIR spectroscopic imaging for explosives detection: low cost complete detection systems that can be used throughout an environment.

![Normalized Coupling Loss Measurement Results](image)

Figure 5: Coupling loss for an array of three waveguides of varying waveguide length coupled using Optical Quilt Packaging (OQP).

![Silicon nitride films in the shape of an “N” (1 μm) and “D” (2 μm)](image)

Figure 6: Silicon nitride films in the shape of an “N” (1 μm) and “D” (2 μm) are deposited on a germanium substrate (left). Differential absorption imaging was performed by using the low-cost MIR imaging arrays as detectors in a Fourier-transform infrared (FTIR) spectrometer (right). Results above show subtle difference in relative transmission through the “N” and “D” due to subtle differences in nitride deposition conditions.
C.3.b.ii. Multiphoton Microscopy Detection of Trace Explosive Particles

In collaboration with Dr. Melissa Sweat, Transportation Security Laboratory (TSL), we have begun investigating the use of multiphoton microscopes to detect trace explosive residues. Specifically, we are looking to aid TSL studies on hand-to-hand and multiple fingerprint transfer of explosive residues. Current techniques have difficulty accurately identifying small, micron-scale explosive particles that are mixed within binder. Our preliminary results show that multiphoton microscopy can resolve particles of energetic material > 1 μm in size, in three-dimensions, inside of binder material.

C.4. Year 3

C.4.a. On Chip Heterogeneous Integration of Widely Disparate Wavelength MIR Lasers

C.4.a.i. Improved Fabrication of OQP Packaged Modules

In the initial OQP fabrication, there is a high risk of surface damage during the chemical mechanical polishing (CMP) process. In a modified fabrication process, copper nodules are fabricated via sputter deposition in order to eliminate the surface damage due to CMP. The aligned Ge-on-Si OQP sample (with sputter deposited copper nodules) is shown in Figure 7 (left). In the OQP sample, where copper nodules are fabricated by sputtering, the inter-chip gap is reduced more from the previously fabricated OQP sample. The inter-chip distance is 1.4±0.3 in the new OQP sample. According to the finite-difference time-domain (FDTD) simulation (see Fig. 7, right), the expected coupling loss for the sample is ~7 dB. In addition to protecting from surface damage, this new process is compatible with fabricating nodules on existing commercial laser arrays.

![Figure 7: OQP sample with sputter deposited copper nodules (left). Coupling loss variation with inter-chip gap for Ge-on-Si to Ge-on-Si OQP structure (for λ=8 μm) (right).](image)

C.4.a.ii. Demonstration of Optical Coupling Between MIR Laser Arrays Using OQP

A QCL source (8.1 μm wavelength) is used to measure the optical coupling loss of the fabricated Ge-on-Si OQP sample. The optical transmission through the Ge waveguide is difficult to distinguish from the optical transmission through the transparent Si substrate in the OQP sample. To overcome this problem, a bend in the waveguide structure after optical coupling is proposed. The OQP sample with sputter deposited copper
nodules is fabricated with a bend in waveguide structure. Coupling loss is measured as the ratio of the light passing through the OQP Ge-on-Si sample and the light passing through an undivided waveguide sample of the same length and shape of the combined Ge-on-Si OQP chip. The optical measurement scheme is shown in Figure 8. The measurement setup with QCL is shown in Figure 9.

![Coupling loss measurement scheme of Ge-on-Si OQP sample with QCL MIR source.](image)

![Optical setup for OQP coupling loss measurement.](image)

In the optical measurement, the QCL beam is focused to the input facet of the first OQP waveguide. The light emitting from the second waveguide is measured with a liquid nitrogen cooled photoconductive mercury-cadmium-telluride (MCT) detector. Then a similar measurement is done with a reference Ge-on-Si waveguide sample of same length and shape of the combined Ge-on-Si OQP waveguide. The linear fitted measured data is shown in Figure 10 on the next page. The coupling loss is measured ~9 dB for the OQP sample fabricated with sputter deposited copper nodules. The loss is nearly the same for each laser in the array, demonstrating highly uniform alignment across the array. The slope of the fitted line is the propagation loss of the Ge-on-Si waveguide. The propagation loss is measured ~3dB/cm for both the samples.
C.4.b. MIR Spectroscopic Imaging of Trace Explosives

C.4.b.i. New, Low-cost MIR Imaging Platform

In the past few years, inexpensive thermal cameras have become commercially available. This is primarily due to advances in uncooled vanadium-oxide microbolometer technology. The limiting factor of this technology is that it suffers from high thermal background noise. This project aims to use one of these inexpensive thermal detectors to detect explosives. The detector chosen for this project is the SEEK Thermal Compact, available off-the-shelf for $250 (see Fig. 11).

In order to predict the minimum detectable quantity of explosives, one must determine the signal to noise ratio (SNR) of the detector. To do this, the Allan Variance was computed for pixels of this camera. The SNR of the camera is shown in Figure 12 for five different pixels. The SNR was calculated by taking images of a room temperature scene and computing the ratio of the mean pixel value to the square root of the Allan variance (i.e. Allan deviation). It is assumed that the temperature of the scene changed negligibly over the course of the experiment. From the plot, we can see that all of the pixels have similar noise characteristics, and starts off with an SNR of ~100. Below 100 frames, the SNR smoothly increases, suggesting that this region is dominated primarily by white noise, which can be averaged away through integration. Beyond 100 frames, the SNR changes rapidly as one increases the number of integration frames. This is common of Allan variances, and shows that the SNR is being affected by the random-walk nature of the flicker noise in a system. The frame rate of the SEEK Thermal Compact is reported as < 9 Hz. Therefore, 100 frames would take ~11 seconds if ran close to 9 Hz. This suggests that, for rapid scan uses, one would not integrate much longer than 100 frames and the flicker...
noise is a non-issue. Using this data, and the following hyperspectral imaging studies, we now can evaluate and predict imaging sensitivity and speed for various targets.

![Figure 12: SNR versus number of frames integrated for low-cost vanadium-oxide microbolometer array.](image)

**C.4.b.ii. New MIR Image Analysis Software Tool**

Application of PCA to discriminate thermal changes seen by the SEEK Thermal camera was tested by imaging a piece of cardboard illuminated by a QCL. Images were taken with the QCL and ran at multiple currents, thus changing the wavelength and power. The results are shown in a tool developed to rapidly investigate the PC space (see Fig. 13). The x and y axes are the first and second PC scores, respectively. The circle selects data having those PC scores and highlights them in the corresponding image. The first PC (PC1) explains ~94% of the variance in the data and, thus, explains almost all the change. PC1 has been attributed to the power change of the QCL, as it very cleanly discriminates the spot from the rest of the scene. The first figure selects the points on the negative side of PC1 and correspondingly highlights all the points outside of the spot. The second figure does the exact opposite, selecting those on the positive side of the axis and highlighting the QCL spot. The third image shows that there is very little change in accordance with the second PC axis. Now that this has been shown to be capable of detecting changes in images, the next step is to apply this to explosives imaging.
C.4.b.iii. Differential Absorption/Diffuse Reflection Imaging with Low-cost Arrays

As a surrogate for explosives residues, petroleum jelly was smeared on a 1 cm² area on a piece of cardboard. Each sample was illuminated by 1192 and 1190 cm⁻¹ QCL laser radiation, and imaged by the low-cost vanadium oxide bolometer array. The ratio of absorption of these two wavelengths is presented in Figure 14. Each figure represents the ratio of diffuse reflection when no laser illumination (left) and laser illumination (right) is incident on a very weak absorption feature of petroleum jelly. The first image shows that at ~175mg, the jelly is almost indistinguishable from the background while the second of ~250mg is visible. While these masses are considerably large, the wavelength of interrogation corresponds to absorption that is ~30x weaker than would be used for explosives imaging. Using this data and the previous SNR experiments, we are now predicting explosives detectivity levels to determine whether this system is feasible. We are also investigating additional surrogate targets with stronger absorption characteristics for higher confidence measurements.

Figure 13: Demonstration of custom image analysis tool. Hyperspectral images of an MIR laser illuminating a piece of cardboard are analyzed; individual pixels can be selected based on PCA components and identified in the image.

Figure 14: Diffuse reflection images of weakly absorbing petroleum jelly taken by the low-cost vanadium oxide microbolometer array system. Each image represents the ratio of 1190 to 1192 cm⁻¹ QC laser illumination. The blue dots on the diagonal are artifacts of the system that do not carry useful readout information.
C.5. Year 2

C.5.a. On Chip Heterogeneous Integration of Widely Disparate Wavelength MIR Lasers

C.5.a.i. Fabrication of OQP Packaged Modules

Ge-on-Si waveguide structures were coupled via OQP with a chip-to-chip distance of ~10 µm. To reduce the chip-to-chip distance, a new design was proposed and Ge-on-Si waveguide OQP modules were fabricated and aligned via OQP with inter-chip distance, and was reduced from 10 µm to 4.6±1.1 µm and lateral misalignment of 920±150 nm (see Fig. 15). Waveguide facets were prepared by deep reactive ion etching (DRIE), which, at the same time, releases the extended part of the Cu nodules used for the alignment. Cu nodules show great stability in the etching process, with 50.2±0.7 µm in width (designed as 50 µm) and 52.9±0.7 µm spacing between nodules (designed as 54 µm).

C.5.a.ii. OQP Characterization

To experimentally determine the optical coupling efficiency of an aligned Ge-on-Si OQP chip, we used a Fourier-transform infrared (FTIR) system as the MIR source of light. The FTIR has a broadband MIR global source, and the emission coming out of it could be coherently guided from one of the side ports of the system. We used ZnSe plano-convex lenses to focus the MIR beam to the facet of the Ge-on-Si waveguides. A 3-axis manual translation stage was used to move the OQP sample so that the FTIR beam can be aligned properly to the facet of the waveguide. An MCT detector was used to collect the light coming out of the other facet of the OQP chip, and the response of the detector was fed back to the FTIR system. The beam we used was a Gaussian, with a full width half maximum spot size of ~350 µm. To ensure we were only collecting coupled light, a 90-degree bend was incorporated in the Ge-on-Si waveguide so that scattered light and guided light exit the waveguide array perpendicular to each other. The bend loss has been modeled (see Fig. 16), and the device is currently under testing to determine OQP coupling loss across arrays of waveguides.

Figure 15: Separate Ge-on-Si waveguide chips aligned via OQP into a quasi-monolithic integrated chip.
C.5.b. MIR Spectroscopic Imaging of Trace Explosives

Last year, we began MIR characterization and spectroscopic imaging of trace explosives samples. To begin developing the MIR imaging system, we first sought to optimize our system for peak sensitivity by performing MIR spectroscopic imaging using FTIR. Spectral analysis of the complete explosive (energetic material, binder, and plasticizer) yields the required laser spectra, tuning ranges, power spectral density, and imaging speeds for a required sensitivity and specificity.

Trace samples (gloved thumbprints) of C4 (91% RDX) and Semtex-1A (76% PETN, 4.6% RDX) were deposited on bare car-body aluminum, car-body aluminum with car paint and clear coat, and low-reflectivity plastic. Samples were provided by ALERT thrust leader Professor Steve Beaudoin of Purdue University (Projects R2-A.1, R2-A.3, and R2-D.1). While the HEM components of C4 and Semtex (PETN and RDX) are commonly characterized in the MIR [4] on similar substrates [13], and C4 is well characterized in laboratory settings [8], we sought to establish performance parameters of composite explosives on realistic substrates.

The experiment was set up so that the sample was illuminated at 45° by the FTIR and collected onto the MCT detector. Alignment was done by maximizing the output of the analog-to-digital converter (ADC) from the MCT. The sample used was C4 on a substrate of aluminum covered in automobile paint. The incoming beam from the FTIR was focused by a 1.5'' lens to an elliptical spot with a major axis length of ~450 μm and minor axis length of ~350 μm. The FTIR spectrum was then obtained for the sample and normalized to bare aluminum. Results were consistent with identical experiments previously published (see Fig. 17), and was the first step towards developing an imaging platform.
C.6. Year 1

C.6.a. On Chip Heterogeneous Integration of Widely Disparate Wavelength MIR Lasers

C.6.a.i. Fabrication Process

In Year 1, we established the fabrication process for MIR OQP; a simplified wafer-scale fabrication flow for alignment only is presented in Figure 16. Deep wells formed at the die boundaries were filled with electroplated copper (see Fig. 18a-b). The copper overburden was removed via chemical mechanical polishing (CMP) (Fig. 18c). Ridge or rib waveguides were lithographically defined and etched (Fig. 18d), and then die boundaries were defined using DRIE (Fig. 18e), exposing metallized contacts protruding from the edge facets (Fig. 18f). A second deep etch pattern forms narrow perforations along which subsequent die cleaving will occur, forming optically flat waveguide facets (Fig. 18g). The cleaving of waveguides is a commonly employed method for forming facets and we expect no special problems with carrying out this step. Use of perforations to guide the cleave line is not commonly done but is not unheard of [14], and has been done successfully at UND. The cleave line was positioned such that the nodules extend past the optical flats, enabling a nearly perfect coupling of the waveguides between sensor components. This was the central innovation of this proposal, and to our knowledge is unique to the UND process.

Sensor die components were then mated to each other for optical coupling and soldered for mechanical stability (see Fig. 18h). All processing steps were compatible with conventional semiconductor processing technologies that were already available at the Notre Dame Nanofabrication Facility (NDNF).
Proof-of-concept devices on Si have been fabricated to determine minimum experimental tolerances. Figure 19a shows a top-down view of two combined OQP modules. Lateral alignment between waveguides on separate chips resulted in a tolerance of ~1 micron. Processing Ge-on-Si waveguides and deep (> 50 micron) etched facets (Alcatel 601E inductively coupled plasma reactive ion etch (ICP-RIE)) has been demonstrated in Figures 19a and b.

**C.6.a.ii. OQP Simulations**

Optical waveguide coupling requires precise lateral, vertical, and axial alignment for high efficiency coupling. Additionally, heterogeneous coupling between QCL waveguides and semiconductor rib waveguides with different mode geometries poses an additional challenge to direct waveguide coupling via OQP. To evaluate the proposed concept, estimate maximum coupling, and develop a research strategy, OQP calculations were performed using the FDTD method [15]. This was achieved using MEEP, a freely available software package [16] a popular free implementation of the finite-difference time-domain (FDTD. The results of these calculations are presented in [17] and summarized further herein.
C.6.a.iii. Dependence of Waveguide Coupling Efficiency on Axial Gap Distance

Transmission between a typical QCL ridge waveguide [18] and a single-mode Ge-on-Si rib waveguide [19] was simulated for \( \lambda = 8 \) μm light. The inter-chip separation varied from 0 (contact) to 10 μm. Coupling efficiency was defined as the ratio of flux at the output of the Ge-on-Si waveguide normalized to that of a continuous QCL waveguide of length equal to that of the two waveguides combined. Simulations include reflections at all interfaces, modal mismatch between waveguides, and beam divergence. The results of the calculations are shown in Figure 20. Transmission, as a function of the inter-chip gap, shows a sharp decrease in coupling efficiency as the waveguide separation increases from 0 to 2 μm. Please note that even with a gap of up to 4 μm, which we expect to be easily achieved, the worst loss will be 6 dB, a value that is at least as good as conventional off-chip coupling schemes that are sensitive to mechanical instabilities and require external free-space optics [20].

Coupling efficiency can be further increased by filling any gap with a material that reduces the air-semiconductor index of refraction mismatch. Arsenic trisulfide (As\(_2\)S\(_3\)) chalcogenide glass (index of refraction of ~2.4 in the MIR [21]) is a popular optical material in the MIR [22-27], and is compatible as a spin-on material. Calculations show filling a 10 μm gap between a QCL and Ge-on-Si waveguide with As\(_2\)S\(_3\) glass results in a 600% improvement in coupling efficiency. As\(_2\)S\(_3\) spin-on glass is compatible with the OQP process and provides a conformal coating on waveguides. Combining these two technologies yields highly-efficient, direct coupling between two different waveguides on separate die.

C.6.a.iv. Dependence of the Waveguide Coupling Efficiency on the Lateral/Vertical Alignment

Conventional QP offers the precise lateral alignment necessary for OQP. Calculations show that the lateral alignment tolerance between a QCL and silicon-on-insulator (SOI) waveguide may be as high as ~3-4 μm and should be similar for other types of waveguides. This is easily within the range of QP, which recent unpublished results at UND have demonstrated alignment on the order of 0.5 μm. Although the alignment tolerance of OQP is already acceptable for the project, waveguide mode shaping can render the coupling efficiency less sensitive to alignment issues. For example, Figure 21 shows simulations of a \( \lambda = 8 \) μm QCL waveguide coupled to a Ge-on-Si ridge waveguide normalized to zero lateral offset. With no mode shaping, a lateral offset of ~2.5 μm would produce 1 dB of loss, while a horn-shaped geometry has a tolerance of 3.5 μm for 1 dB of loss. Both are within the tolerance limits for sensors based on OQP, and waveguide mode shaping serves as a complementary strategy to decrease coupling loss. Vertical alignment is also crucial to high coupling efficiency. Simulations show that vertical alignment tolerance must be < 2 μm for 1 dB insertion loss and is within the tolerance of precision polishing of the chip substrates or epi-down (i.e. “upside down”) packaging.

![Figure 20: Coupling efficiency versus gap distance from a λ=8 μm InP QCL to a Ge-on-Si waveguide.](image)

![Figure 21: Coupling efficiency versus horizontal misalignment for a λ=8 μm InP QCL to a Ge-on-Si waveguide.](image)
D. Milestones

To achieve the project's final objective, we need to demonstrate explosive residue imaging on the order of micrograms per square cm with an acquisition time of less than 10 seconds. To achieve this performance metric, we targeted the following Year 5 milestones as identified in the Year 5 Work Plan for this project:

- A milestone from Year 4 will be addressed in the remainder of Year 4 and in Year 5. We will demonstrate imaging of trace explosives using a MIR bolometer arrays and laser illumination; baseline sensitivity levels will be quantitatively characterized.

- Hyperspectral, thermal emission, thermal time constant, and polarization-based imaging techniques will be characterized to establish improvements over baseline and to evaluate minimum sensitivity levels.

Both Year 5 milestones were accomplished. We demonstrated spectroscopic imaging of trace explosive films using MIR bolometer arrays and laser illumination using hyperspectral, thermal emission, thermal time constant imaging techniques. While performing this analysis, and after communications with both industry partners and review of the academic literature, we decided to pursue our new probabilistic approach to detection since the real-world samples would not be as clean as the baseline measurements in the lab. As such, we did not perform baseline sensitivity measurements but instead performed measurements classifying the distribution of explosive trace residues to act as a Bayesian prior in our new approach.

In Year 6, the major milestone would be the incorporation of probabilistic models in our imaging platform that distinguishes trace energetic material residue from common confusants. This first proof-of-concept demonstration would significantly enhance the value of our imaging platform. Our goal is to perform pre-scanning to identify potential hot-spots to be investigated with established techniques (swab and MS, Raman detection). As such, we aim for image acquisition time of films on the order of 100 microgram/cm² in ~1 second with < 5% Type I and II error rates. These results are intended to be baselines on which further translation work would improve since we are incorporating new algorithms with a new, low-cost imaging platform.

E. Future Plans (Year 6)

The research plan for Year 6 focuses on derisking the existing prototype system to increase the effectiveness of translation as well as investigate and develop innovative detection techniques to further the state-of-the-art of MIR explosive residue imaging. The programmatic risk lies in the ultimate system speed and sensitivity. To address this risk, we are carefully characterizing system performance at each step to ensure the final system will still achieve the required DHS end-user performance levels. We are also pursuing two parallel research tracks: (1) Standard MIR hyperspectral reflection imaging; and (2) new experimental methods for trace detection by imaging thermal time constants. The first track, on its own, will provide a usable chemical imaging system, and the second track is designed to further enhance system speed, sensitivity, and specificity. Both of these tracks will also use probabilistic detection models using both Bayesian and machine learning approaches in collaboration with Professor Vijay Gupta of the University of Notre Dame. We have collected baseline hyperspectral imaging data of various trace explosive films on different substrates using our MIR platform, and are using these dense, multi-dimensional data sets to determine majority-rule criteria for detection and sensor selection as well as to use as training sets within the TensorFlow machine learning framework.

Over the next year, we will investigate additional contrast mechanisms to improve trace explosive detection speed and sensitivity. Nearly all MIR explosive imaging and detection techniques used in the field are based on comparing standard differential reflection measurements to library spectra of known explosive reflection signatures, or by performing principle component analysis on a sample to differentiate energetic materials from background material. Additional contrast mechanisms, such as thermal time constant and polarization sensitive optical activity imaging, have the potential to open up entirely new methods of residue detection. By combining the information obtained using these multiple contrast mechanisms, more selective and sen-
sitive detection is possible. We will modify our current imaging system to incorporate a homodyne detection technique to measure thermal decays in explosive residues. This data will measure thermal time constants with sub millisecond resolution and give extra insight into chemical properties of the films that is currently unavailable for analysis and detection.

The final deliverable is the design and characterization of a complete MIR spectroscopic imaging system using low-cost microbolometer arrays that will enable distributed MIR spectroscopic explosive imaging. The system will incorporate “conventional” hyperspectral imaging techniques as well as be used to explore novel techniques, such as thermal time constant imaging, and be used to generate large data sets for developing advanced probabilistic detection models to increase detection speed and accuracy.

III. RELEVANCE AND TRANSITION

A. Relevance of Research to the DHS Enterprise

Detection of trace explosive residues by hyperspectral imaging: image residues at > 10 distinct wavelengths with a total data acquisition and analysis time faster than 10 seconds/frame. Detectable limits should be evaluated for sample residues to be less than 1 mg/cm². Total system cost should be <$15k and be field-deployable (size, weight, and power restrictions). Our unique position for transition comes from the fact that we are using off-the-shelf commercial components that cost 50-100x less than typical approaches. However, that alone is not enough to successfully translate the technology, as the technology development space is crowded and detection is difficult in complex systems. Our unique tack is to combine the low-cost sensors with new probabilistic detection models that include the complexities: we consider both absorption and sample emissivity, utilizing broadband emitters and detectors, on real substrates that include confusants. To accomplish this, we have just began collaborating with experts in detection and estimation algorithms, and have already made advances by demonstrating that hyperspectral imaging data does not follow the normal distribution, but instead a generalized extreme value distribution (GEVD). Traditional probabilistic models based on normally distributed samples do not work for MIR microbolometer imaging data, but can successfully discriminate samples when considering a GEVD distribution. We have also shown why a GEVD distribution is what should be expected from microbolometers. This work is currently in preparation for publication. Finally, we are developing new ways to increase the available data in order to discriminate samples in complex environments in either machine learning or probabilistic model detection methods. Specifically, we have modified our imaging system to not only image reflectance, absorption, and emissivity, but also the thermal time constant of chemical residue films. This additional information is unique to the environment of the film (e.g., plastic explosive binder, or hand cream surfactant) and therefore give an additional variable to investigate to identify and differentiate residues. The thermal time constant imaging system is currently being evaluated and will be used along with our probabilistic and machine learning models.

B. Potential for Transition

End-user applications include the incorporation of both the laser module and imaging systems in a variety of screening locations. Portable (deployed with security personnel) and fixed devices (e.g., integrated with document scanners, cargo/luggage processing) are being developed to both quickly identify potential threats and to aid in the detailed diagnostic of potential threats.

C. Data and/or IP Acquisition Strategy

Transition is being led by the new Notre Dame IDEA Center, which is filing provisional patents, funding prototype development, and performing initial market research and validation. The IDEA Center is a brand new center started to transition University IP across the technology “valley of death.” The low-cost imaging plat-
form is one of the first technologies to participate in the Notre Dame IDEA center. A patent on the integrated optical laser module has been granted and licensed to Indiana Integrated Circuits, LLC, who is a contractor for AFOR and ARL. The end users would be those maintaining screening points within the security enterprise, and can be used in both field-deployable (e.g., portable inspection of vehicles) or fixed-platform (e.g., document scanning, cargo/luggage processing). This project will be evaluated on the new trace analysis testbeds developed by ALERT at Purdue University. Project staff has been interfacing with two customer-facing companies, Indiana Integrated Circuits (several DoD contracts) and Pendar Technologies (ALERT industrial collaborator), to develop business platforms to transition the project outputs. Project staff have submitted a pending white paper for technology translation to the DHS Standoff Explosives Detection on Vehicles (SED-V) BAA in collaboration with Tanner Research, Inc. Initial imaging platform prototypes have been built, once validated in our lab we will begin external validation in DoD/DHS laboratories (1-2 years).

D. Transition Pathway

Research will reach the end-users through the commercialization of both the MIR laser sources as well as in the MIR imaging platform technology. We are currently collaborating with three commercialization partners that are in the defense and homeland security space: Indiana Integrated Circuits, Pendar Technologies, and Rapiscan Systems. Indiana Integrated Circuits is licensing the OQP technology and has submitted several DoD SBIR/STTR calls to further commercialize OQP for a variety of defense and security applications. We anticipate integration of OQP with the Pendar Technologies laser arrays for MIR characterization of explosives. Because of our existing partnerships, OQP MIR modules can be provided within a relatively short time frame (< 2 years) upon successful demonstration and characterization. Scanning imaging systems require more development and have additional technical risk, and thus require additional time before being available to end-users (>5 years).

Over the past year, the Notre Dame IDEA Center has performed dozens of market-evaluation interviews with stakeholders in airport checkpoint operations, checkpoint security technology vendors to develop a thorough understanding of the market landscape. In the coming months, they will present their report and proposed strategy to pursue translation. Preliminary results indicate a high desire for the technology, but absent regulatory requirements to use our technology, facilities may be less likely to invest in new platforms.

E. Customer Connections

- Jason Kulic (jason.kulick@indianaic.com), Indiana Integrated Circuits, LLC: Monthly meetings.
- Charles Dietlein, Sensors and Electron Devices, Army Research Laboratory: Indirect contact through Professor Jonathan Chisum, Notre Dame Wireless Institute, which consists of preliminary collaboration developing distributed devices
- Kevin Jim, Oceanit, DoD Contractor: New collaboration evaluating MIR imaging systems on aerial drones with Navy contract. We are currently under contract, and have commenced work.

IV. PROJECT ACCOMPLISHMENTS AND DOCUMENTATION

A. Education and Workforce Development Activities

1. Student Internship, Job, and/or Research Opportunities: Two students that have worked on ALERT projects graduated in the past year with PhDs. Genevieve Vigil is now a post-doctoral fellow at NASA Marshall Space Flight Center and Tahsin Ahmed is a process development engineer at Intel.

2. Interactions and Outreach to K-12, Community College, and/or Minority Serving Institution Students or Faculty: In June, 2017, the Howard Research group collaborated with the Wyandanch
Union Free School District (Wyandach, NY) to host two high school students and two teachers to participate in a program to introduce students from under-represented groups to future educational and career opportunities in STEM. Students and teachers worked together on projects learning about optical sensing of chemicals as well as how college admissions and financial aid works. Students and teachers lived in dorms, ate in dining halls, and participated in campus activities available to Notre Dame students to help give a perspective on academic and social life at college. Over the past year, we have continued to follow up and plan the next program with this school, which will occur in the late summer/early fall.

B. Technology Transfer/Patents


V. REFERENCES


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