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 ALERT research programs by providing lower cost, wide-bandwidth, mid-infrared (MIR, \( \lambda = 4-12 \mu \text{m} \)) laser sources, and developing MIR laser-based imaging technology for the detection of trace explosives. 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 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/coded aperture imaging technology. This will enhance ongoing ALERT efforts by enabling higher resolution imaging technology to detect signatures characterized by other ALERT thrusts, providing a technology to enhance the commercial offerings of ALERT industrial partners, and providing new spectroscopic tools that could be useful to the security enterprise as well as other fields where MIR technology is employed, such as medical diagnostics, industrial process control, environmental monitoring, and pharmaceutical process analytical technology.

The MIR region of the electromagnetic spectrum contains unique absorption “fingerprints” corresponding to vibrational modes of molecules. ALERT projects led by Hernández (R3-C), Hoffman (R2-C.3), Rinaldi (R2-B.3), and ALERT industrial collaborator Pendar Technologies, are using MIR light to identify molecular fingerprints corresponding to trace amounts of explosives. For example, two MIR lasers tuned to relevant on-and-off resonant wavelengths (e.g., 1348 cm\(^{-1}\) on and 1370 cm\(^{-1}\) off resonance for trinitrotoluene (TNT)) can be used to measure the differential absorption of light between those two frequencies attributed to the presence of an explosive. The ability to detect explosives with MIR light is limited by the availability of high-performance MIR laser sources and imaging platforms. MIR lasers, especially lasers that can identify many unique explosives simultaneously, are very expensive. Additionally, imaging platforms are difficult to produce since few MIR "cameras" exist (or are very expensive).
This project develops technology that will make it cheaper to produce laser systems that can identify multiple explosives at the same time, as well as a complementary imaging platform. Thus, this project serves as a translation layer between fundamental spectroscopic characterization and deployable detection platforms. This is done through two complimentary efforts: (1) The development of an MIR spectroscopic imaging platform that overcomes the technical limitations in MIR imaging and a lack of cost-sensitive MIR imaging devices; and (2) The integration of low-cost, and highly-robust device geometries with new MIR imaging platforms to form a single, integrated, wide-bandwidth, single-output-port, high-power-spectral-density source.

Sensitive MIR spectroscopic detection platforms have been limited due to a lack of strong signal-to-background detection. This is due to the common use of larger spectroscopy systems (i.e., Fourier transform infrared spectrometers (FTIR)), which have low power-spectral-density at a given wavelength, as well as a lack of MIR imaging systems that require large-area sampling. Thus, systems attempt to detect a narrow trace explosive spectral bandwidth and small sample size amongst an excessively large spectrometer bandwidth and beam spot size. We address these challenges by employing laser spectroscopic and spatial frequency multiplexed imaging to obtain high power spectral density and high resolution imaging, respectively.

To obtain high power spectral density and high resolution imaging, a high spectral power density light source, such as a laser, must be employed. Quantum cascade lasers (QCLs) are ideal devices for MIR imaging; however, widely tunable QCLs require external cavity tuning and are, thus, susceptible to mode-hopping instabilities and mechanical failure, which severely limits performance. Pendar Technologies has overcome these issues by developing QCL arrays where each device in the array has a unique output wavelength. To maintain high signal-to-background contrast with small trace samples on substrates, high resolution imaging is required. In these imaging systems, however, each of the lasers in the array must follow the same beam path, which is not possible from laser waveguide arrays. This project also develops integrated wide-bandwidth single-output-port high-power-spectral-density sources by developing new micro-fabrication techniques to build a system which combines the light out of several expensive MIR lasers together into an inexpensive silicon-based chip. The light can then be used for imaging or possibly for the detection of explosives in small quantities.

Both of these technologies form an integrated MIR explosives imaging platform unlike any that is currently available. Additionally, this platform is modular and can be extended for the rapid development of further advanced screening and detection systems.

**B. Biennial Review Results and Related Actions to Address**

The Biennial Review panels identified the proposed method as "practical, cost effective, and technically defensible". The project was described as addressing a specific and important knowledge gap in developing low-cost MIR sources for sensing and imaging while also developing a compatible imaging platform simultaneously. The weaknesses were identified as not having enough "discussion and progress on the metrics important to standoff detection, namely: sensitivity, selectivity, distance and cost when compared to other approaches". Additionally, they highlighted the need for specifically identifying and engaging Department of Homeland Security (DHS) end-users, and developing a transition plan that includes industry once the proof of concept has been demonstrated.

This important feedback was directly included in the Year 4 workplan. We will continue progress on the low-cost sources and imaging platforms, now with an especial emphasis on quantitative sensitivity and selectivity measurements. We have characterized the detector noise of the new imaging platform and will be performing studies to establish the minimum sensitivity using multiple MIR techniques (differential absorption, polarization sensitive imaging, and transient thermal imaging). From these measurements, the relationship between signal-to-noise ratio (SNR), minimum sensitivity, and speed will be established and directly compared to the security enterprise’s needs and competing technologies. As it is validated, we will evaluate the technology with explosives residues and common confusion materials (e.g., hand creams, motor oils, etc.). Additionally,
cost analysis will be performed. To engage DHS end-users and industry, we will engage with multiple groups that have expressed interest in working together including Rapiscan Systems and Pendar Technologies. Additionally, following the Biennial Review, Edward Donovan, Support Contractor with the DHS Science and Technology (S&T) Explosives Division (EXD), indicated an interest in providing system feedback and evaluation. We also recently collaborated with Tanner Research on a DHS Broad Agency Announcement (BAA) proposal that combines our platform with Tanner’s complimentary Raman spectroscopic imaging technology. We are considering using our technique as a “fast scan” to identify potential explosives residues which can be interrogated by the more sensitive, but significantly slower and expensive, Raman spectroscopy.

C. State of the Art and Technical Approach

This project is investigating two complimentary technical advancements: (1) On chip heterogeneous integration of widely disparate wavelength MIR lasers; and (2) MIR coded aperture imaging technology.

C.1. On chip heterogeneous integration of widely disparate wavelength MIR lasers

The most commonly used and commercially available semiconductor MIR light source is a 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] until recently, small and easy to operate laser sources were not readily available for applications outside the laboratory. The situation changes with the maturation of quantum cascade lasers (QCLs). 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).

![Optical Quilt Packaging](image)

Figure 1: Illustration of “Optical Quilt Packaging”.

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 inte-
grates 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.

C.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). Bolometer-based FPAs can be prohibitively slow for many differential measurement schemes of moving objects. Semiconductor detector arrays exhibit a wavelength dependence on the material; materials useful in the MIR tend to be prohibitively expensive for multipoint distributed sensing. We propose increasing the speed (frame rate) and sensitivity (minimal detectable concentration) of MIR differential reflection spectroscopic imaging by replacing the relatively slow or expensive infrared detector array with a more sensitive and less expensive single element photodetector while intensity modulation multiplexing our differential measurement signal to acquire images at multiple wavelength simultaneously. Spatial information is obtained by scanning the laser spot over the sample or by using a coded aperture scheme. The coded aperture is obtained by fabricating a linear spatial light modulator (SLM), where each point in the line is modulated at a distinct frequency. High modulation rates are required to resolve multiple distinct points along the line. Commercially available linear SLMs with the required pixel numbers cannot modulate at such high speeds. Therefore, we created a free-space optical chopper [8]in vivo [1-2]. Phosphorescence lifetime imaging microscopy (PLIM) (see Fig. 3, top dashed box, on the next page) that can modulate an array of point sources at MHz rates by scanning a line-focused laser beam over a small (10-20 μm period) mirror grating on a photolithography mask (see Fig. 3, right). Each horizontal line on the photolithography mask has a different spatial frequency. The reflected light is then de-scanned by the same mirror, and is imaged onto the sample by the line scanning microscope. Examples of raw and processed data from [8]in vivo [1-2]. Phosphorescence lifetime imaging microscopy (PLIM are presented in Figure 4 on the next page. This technology would allow for MIR spectroscopic imaging without needing MIR detector arrays. Trace explosives imaging and detection will allow for real-time standoff and targeted interrogation of objects of interest to give authorities accurate and specific information on the type and extent of possible threats.
MIR spectroscopic imaging has been demonstrated to be a powerful tool for trace explosives detection by several groups (e.g., [4, 2, 3, 9]), including ALERT researcher Samuel Hernandez-Rivera (R3-C). Prof. Hernandez-Rivera employs QCL systems that have been used to deliver high-spectral-energy-density radiation onto highly energetic materials (HEM) deposited on complex substrates. Through standard preprocessing (2nd derivative, standard normal variate, and multiplicative scatter correction) and principal component analysis (PCA) or linear regression analysis, pentaerythritol tetranitrate (PETN) and TNT can be detected on wood, cardboard, and aluminum substrates. We leverage previous advances by employing the successful techniques within our imaging systems. Additionally, we explore extending these techniques to include polarimetric imaging [10] or elipsometry [9].

We will also participate in the Thrust R2 trace explosives sensing test-bed at Purdue University by developing our imaging platform so that it is compatible with the new conveyor-belt test system. A line-scanning imaging system will interrogate targets passing through a field. Performance (speed, resolution, sensitivity) will be evaluated; results will be used to further optimize system design.
D. **Major Contributions**

D.1. **Summary**

This project has completed its third year. Two students are involved in the project: Tahsin Ahmed and David Benirschke. The project is supported both by ALERT funds, a graduate-student fellowship external to ALERT, and internal support from the Notre Dame Center for Nanoscience and Technology.

D.2. **Year 3**

D.2.a. **On chip heterogeneous integration of widely disparate wavelength MIR lasers**

D.2.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 5, 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. 5, 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.

![Image](image_url)

**Figure 5:** Left: OQP sample with sputter deposited copper nodules. Right: Coupling loss variation with inter-chip gap for Ge-on-Si to Ge-on-Si OQP structure (for λ=8 μm).

D.2.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...
same length and shape of the combined Ge-on-Si OQP chip. The optical measurement scheme is showed in Figure 6. The measurement setup with QCL is shown in Figure 7.

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 8 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.
D.2.b. MIR spectroscopic imaging of trace explosives

D.2.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. 9).

In order to predict the minimum detectable quantity of explosives, one must determine the 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 10 on the next page 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 and benefits from 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 that 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.

D.2.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 below in a tool developed to rapidly investigate the PC space, seen in Figure 11 on the next page. 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.

Figure 10: SNR versus number of frames integrated for low-cost vanadium-oxide microbolometer array.
D.2.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 12. Each figure represents the ratio of diffuse reflection at laser off and 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 11: 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 12: 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.
D.3. Year 2

D.3.a. On chip heterogeneous integration of widely disparate wavelength MIR lasers

D.3.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. 13). 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).

![Waveguide Alignment via OQP](image)

Figure 13: Separate Ge-on-Si waveguide chips aligned via OQP into a quasi-monolithic integrated chip.

D.3.a.ii. OQP characterization

To experimentally determine the optical coupling efficiency of an aligned Ge-on-Si OQP chip, we used an 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. An image of the measurement set-up is shown in Figure 3. 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. 14 on the next page), and the device is currently under testing to determine OQP coupling loss across arrays of waveguides.
D.3.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 Prof. Steve Beaudoin (projects R2-A.1 and D.1) at Purdue University. While the HEM components of C4 and Semtex (PETN and RDX) are commonly characterized in the MIR [4] on similar substrates [11], and C4 is well characterized in laboratory settings [9], 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. 15), and was the first step towards developing an imaging platform.
D.4. Year 1

D.4.a. On chip heterogeneous integration of widely disparate wavelength MIR lasers

D.4.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. 16a-b). The copper overburden was removed via chemical mechanical polishing (CMP) (Fig. 16c). Ridge or rib waveguides were lithographically defined and etched (Fig. 16d), and then die boundaries were defined using DRIE (Fig. 16e), exposing metallized contacts protruding from the edge facets (Fig. 16f). A second deep etch pattern forms narrow perforations along which subsequent die cleaving will occur, forming optically flat waveguide facets (Fig. 16g). 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 [12], 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. 16h). All processing steps were compatible with conventional semiconductor processing technologies that were already available at the Notre Dame Nanofabrication Facility (NDNF).

![Figure 16: Process flow for OQP: (a) Define trenches; (b) Electroplate copper; (c) CMP copper; (d) Lithographically define and etch optical components; (e) Expose nodules via DRIE; (f) Place perforation for cleave with DRIE; (g) Cleave to separate die; and (h) Mechanically combine chips.](image)

Proof-of-concept devices on Si have been fabricated to determine minimum experimental tolerencing. Figure 17a (on the next page) 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 17a and b.
D.4.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 [13]. This was achieved using MEEP, a freely available software package [14]. The results of these calculations are presented in [15] and summarized further herein.

D.4.a.iii. Dependence of waveguide coupling efficiency on axial gap distance

Transmission between a typical QCL ridge waveguide [16] and a single-mode Ge-on-Si rib waveguide [17] was simulated for $\lambda = 8 \, \mu m$ light. The inter-chip separation varied from 0 (contact) to 10 $\mu m$. 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 18. 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 $\mu m$. Please note that even with a gap of up to 4 $\mu m$, 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 [18].

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 [19]) is a popular optical material in the MIR [20–25], and is compatible as a spin-on material. Calculations show filling a 10 $\mu m$ 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-efficiency, direct coupling between two different waveguides on separate die.
D.4.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 19 shows simulations of a λ = 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 19: Coupling efficiency versus horizontal misalignment for a λ=8 μm InP QCL to a Ge-on-Si waveguide.

E. Milestones

To achieve the project’s final objective, we need to demonstrate explosives residues imaging on the order of micrograms per square cm with an acquisition time of less than 10 seconds. To achieve this performance metric, we will target the following Year 4 milestones: (1) Establish a baseline minimum sensitivity level using the new MIR bolometer arrays and simple differential absorption spectroscopy; (2) Evaluate improvements to baseline sensitivity levels using hyperspectral, polarization-sensitive, and thermal imaging; and (3) Evaluate explosives detection performance with confusion residues. Finally, external evaluation of the platform with ALERT collaborators and DHS end-users will be performed to further refine the system and assist and accelerate transition.

The following milestones need to be achieved for the project to reach its objectives.

E.1. On chip heterogeneous integration of widely disparate wavelength MIR lasers

1. Year 3: Demonstration of efficient chip-to-chip coupling of passive MIR waveguide arrays. This milestone has been achieved.
2. Year 4: Demonstration of chip-to-chip coupling of MIR QC laser arrays (from Pendar Technologies) to passive MIR beam combining arrays.
3. Year 4: Characterization of beam quality of integrated modules; proof of concept demonstration as a single on-chip spectrometer suitable for trace explosives detection.
4. Year 5+: Development of translational toolkit for commercialization in collaboration with industrial partners Indiana Integrated Circuits (quilt packaging) and Pendar Technologies (MIR laser manufacturer).

E.2. MIR spectroscopic imaging of trace explosives

1. Year 3: Microspectroscopic imaging of trace explosives using FTIR; PCA to determine spectral
ranges for efficient detection using laser-based system and establish preliminary confidence intervals, sensitivity, and specificity using explosives samples on realistic substrates. This milestone has been achieved.

2. Year 3: Time multiplexed (laser scanning) and frequency multiplexed (spatial frequency scanning) imaging with QCL system using analysis established with FTIR studies. Incorporate frequency multiplexed microscopy [8] and/or spatial frequency modulation for imaging [26]. This may possibly be superseded by the new imaging system.

3. Year 4: Incorporation of OQP MIR laser modules with time and frequency multiplexed imaging system.

4. Year 5: Development of field testing of devices within ALERT.

5. Year 5+: Development of translational prototypes in collaboration with Tanner Research, Pendar Technology, and Morpho Detection.

F. Future Plans

Over the next year, we will undertake the following research plan to achieve the above milestones.

F.1. On chip heterogeneous integration of widely disparate wavelength MIR lasers

1. Publication of MIR waveguide array to waveguide array coupling.

2. For the demonstration of chip-to-chip coupling of MIR QC laser arrays to passive MIR beam combining arrays, the laser arrays provided by Pendar Technologies will continue to be packaged via OQP to Ge-on-Si waveguide arrays using fabrication techniques developed in this project. As begun in Year 3, Beam quality will be characterized, and new output facet geometries will be developed to optimize beam quality for trace explosives imaging (e.g., three-dimensional horn geometry).

F.2. MIR spectroscopic imaging of trace explosives

1. Publication of MIR spectral imaging system based on un-cooled low-cost microbolometer arrays.

2. Evaluation of hyperspectral MIR imaging of trace explosives with un-cooled low-cost microbolometer arrays. Minimum concentrations and speed must meet the below metrics for relevance in the DHS enterprise (detection of trace PETN, RDX, TNT, Semtex, or C4 on the order of 100 microgram/cm² on metal, cloth, or paper substrates).

III. RELEVANCE AND TRANSITION

A. Relevance of Research to the DHS Enterprise

1. Detection of trace explosives 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).

2. Development of electronically tunable, wide bandwidth, narrow spectral line sources for MIR imaging and sensing: single output port span 100 wavenumbers in the MIR with sub 1 wavenumber resolution. Coupling loss should be less than 10 dB (~>10% efficiency) for each laser in the array.
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

No outside data is required, and we have access to the required IP.

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 (< 3 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).

E. Customer Connections

- Indiana Integrated Circuits, LLC- Contact: Jason Kulic. jason.kulick@indianaic.com. Monthly meetings.
- Pendar Technologies (formerly EOS Photonics)- Contact: Mark Witinski, witinski@eosphotonics.com. Semi-annual conference call.
- Rapiscan Systems- Contact: Dan Strellis, dstrellis@rapiscansystems.com. New collaboration, preliminary discussions.

IV. PROJECT ACCOMPLISHMENTS AND DOCUMENTATION

A. Education and Workforce Development Activities

1. Course, Seminar, and/or Workshop Development
   a. EE60568: “Fundamentals of Photonics” has been significantly reworked to include several lectures on the fundamentals of absorption spectroscopy, reflection-based imaging, and polarimetric imaging. Enrollment is now 15 graduate students from several departments including electrical engineering, mechanical and aerospace engineering, chemical engineering, and chemistry. Both ALERT students in this project and the students working with Prof. Anthony Hoffman (project R2-C.3) have taken this course.

2. Student Internship, Job, and/or Research Opportunities
   a. PhD student Tahsin Ahmed attended the ALERT Annual Student Pipeline Industry Roundtable Event (ASPIRE) in April 2016, which established new contacts for collaboration with the project both at Pendar Technologies and Rapiscan Systems.

3. Interactions and Outreach to K-12, Community College, and/or Minority Serving Institution Students or Faculty
a. In the summer of 2015 and for the upcoming summer of 2016, we have hosted an REU student from Indiana Wesleyan University, a local, primarily undergraduate institution. This has provided the student an opportunity to be involved in research he would not have otherwise received.

b. As part of the annual “National Robotics Week” event at the University of Notre Dame, our group has organized and ran an exhibit on infrared remote sensing and spectroscopy for each year of ALERT funding (see Fig. 20). There, we made various musical instruments out of infrared range finders to demonstrate the concepts of infrared light and sensing to >500 middle school students and their parents.

![Figure 20: National Robotics Week outreach event.](image)

4. Other Outcomes that Relate to Educational Improvement or Workforce Development

a. Two PhD graduate students in electrical engineering are progressing towards graduation and are supported by this project. This includes David Benirschke, a domestic PhD student specifically recruited for this project.

B. Peer Reviewed Journal Articles

Pending-


C. Other Publications


D. Other Presentations

1. Briefings

E. New and Existing Courses Developed and Student Enrollment

<table>
<thead>
<tr>
<th>New or Existing</th>
<th>Course/Module/ Degree/Cert.</th>
<th>Title</th>
<th>Description</th>
<th>Student Enrollment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Existing Course</td>
<td>Fundamentals of Photonics</td>
<td>Graduate course in photonics, including the fundamentals of absorption spectroscopy, reflection based on imaging, and polarimetric imaging</td>
<td>15</td>
<td></td>
</tr>
</tbody>
</table>

F. Software Developed

1. Other
   a. MATLAB Chemometric Analysis Tool: A graphical tool for visualizing hyperspectral data collected by the low-cost microbolometer array. This is currently still under development, but will be available on github following publication.

V. REFERENCES


NPHOTON.2012.307, Available at http://dx.doi.org/10.1038/nphoton.2012.307


