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

Abstract—The mid-infrared (MIR) region of the electromagnetic spectrum contains unique absorption “fingerprints” corresponding to vibrational modes of molecules. ALERT projects, led by Prof. Samuel P. Hernandez-Rivera (University of Puerto Rico) and Prof. Anthony Hoffman (University of Notre Dame), and ALERT industrial partner EOS Photonics are using mid-infrared 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 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 through MIR spectroscopy is limited by the availability of high-performance MIR laser sources and imaging platforms. This project develops technology to heterogeneously integrate multiple laser systems; each uniquely designed for a certain wavelength (i.e., range of residual “fingerprints”) and integrated into a single module employing inter-chip micro-electromechanical systems (MEMS) fabrication techniques. This “Optical Quilt Packaging” technique is optimized for aligning arrays of waveguides on chips, such as the products developed by EOS Photonics. These modules will then be integrated into imaging and detection systems. Over the past year, we fabricated MIR waveguide structures and demonstrated the MEMS coupling technique with sub-wavelength and submicron lateral and axial alignment accuracy between the waveguides of separate chips that have been combined into a single “quasi-monolithic” heterogenous chip. Data from the first year has been used to improve our designs, to increase yield and further decrease inter-chip spacing; the next generation of chips are currently being fabricated. Additionally, numerical calculations have been performed to model the expected performance of our devices to optimize device design and confirm feasibility. Simulations predict < 3 dB insertion loss between waveguides, which would be suitable for extreme-wideband MIR explosive imaging and detection sources at significantly lower cost than monolithic growth of wideband sources. Over the first year, we have also successfully recruited a new US citizen graduate student to take over the primary responsibility of the project starting 7/1/2014.

I. PARTICIPANTS

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II. PROJECT OVERVIEW AND SIGNIFICANCE

The overall goal of the project is to develop technology to enhance ongoing work of ALERT by providing lower cost, wide-bandwidth MIR laser sources and to develop MIR laser-based imaging technology. 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: (1) how do you combine several high-cost laser chips into a single module for sensitive imaging and detection, and (2) how do you perform sensitive spectroscopic imaging in a wavelength range that lacks robust and widely available focal plan arrays and optical components? 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, provide a technology to enhance the commercial offerings of ALERT industrial partners and provide 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.

III. RESEARCH ACTIVITY

A. State-of-the-Art and Technical Approach

The 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.

A.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 cover large ranges over the entire absorption bands of explosive residue 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 explosive 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 ALERT partner EOS Photonics. 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 (Fig. 1).

The proposed OQP leverages advances in electronic quilt packaging, a novel technique developed at the University of Notre Dame (UND) for high speed electronic interconnects. Electronic quilt packaging integrates diverse electronic device technolo-
gies into a quasi-monolithic module by connecting separate dies with solid metallic contacts along the vertical faces for both mechanical and electrical connection (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.

A.1.1 Fabrication process

This year, we have established a fabrication process for MIR OQP; a simplified wafer-scale fabrication flow for alignment only is presented in Figure 3. Deep wells formed at the die boundaries are filled with electroplated copper (Fig. 3a-b). The copper overburden is removed via chemical mechanical polishing (CMP) (Fig. 3c). Ridge or rib waveguides are lithographically defined and etched (Fig. 3d), and then die boundaries are defined using deep reactive ion etching (DRIE) (Fig. 3e), exposing metallized contacts protruding from the edge facets (Fig. 3f). A second deep etch pattern forms narrow perforations along which subsequent die cleaving will occur, forming optically flat waveguide facets (Fig. 3g). (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 [8], and has been done successfully at UND.) The cleave line is positioned such that the nodules extend past the optical flats, enabling a nearly perfect coupling of the waveguides between sensor components. This is the central innovation of this proposal, and to our knowledge is unique to the UND process.

Sensor die components can then be mated to each other for optical coupling, and soldered for mechanical stability (Fig. 3h). All processing steps are compatible with conventional semiconductor processing technologies that are already available at the Notre Dame Nanofabrication Facility (NDNF).
 (> 50 micron) etched facets (Alcatel 601E inductively coupled plasma reactive ion etch (ICP-RIE)) have been demonstrated, as shown in Figures 4a and b.

**Figure 4: Example proof of concepts microfabricated OQP structures fabricated at UND.**
(a) Two separate OQP waveguide modules combined into a single quasi monolithic integrated device (see Fig. 3h for reference).
(b) Front facet of a Si-on-Ge waveguide structure.
(c) Demonstration of Si wafer surface (dark) and DRIE etched facets (light) with surface roughness << λ.
(d) Edge of fabricated structures showing nodules (left) and waveguides (right).

**A.1.2 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 finite-difference time-domain (FDTD) method [9]. This was achieved using MEEP, a freely available software package [10]. The results of these calculations are presented in [11] and summarized below.

- **Dependence of waveguide coupling efficiency on axial gap distance:**

  Transmission between a typical QCL ridge waveguide [12] and single mode, Ge-on-Si rib waveguide [13] was simulated for λ = 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 5. 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 [14].

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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 [15]) is a popular optical material in the MIR [16]–[21], 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 high-efficiency, direct coupling between two different waveguides on separate die.

- 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 6 shows simulations of a $\lambda = 8$ μm QCL waveguide coupled to a Si-on-N 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.

A.2 MIR imaging of trace explosives

Thus far, we have explored OQP to fabricated sources to enable MIR imaging of trace explosives; we also plan on employing coded aperture technology with our laser modules 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 explosive imaging systems typically employ bolometer (i.e., thermal) or semiconductor detector (i.e., photonic) 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 where each point in the line is modulated at a distinct modulation 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; we created a free-space optical chopper [22] (Fig. 7, top dashed box) 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 (Fig. 7, right). Each horizontal line on the photolithography mask has a different spatial frequency. The reflected light is then descanned by the same scan mirror, and is imaged onto the sample by the line scanning microscope. Examples of raw and processed data from [22] is presented in Figure 8. This technology would allow for mid-IR spectroscopic imaging without needing mid-IR detector arrays. Trace explosive 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.

**Figure 7: Coded aperture mid-IR illumination scheme**
- CL: cylindrical lens
- BS: beam splitter
- SM: scan mirror
- PD: photodiode
- PMT: photo-multiplier tube
- OL: objective lens

**Inset:** Illustration of the spatial light modulator.

**Figure 8: Coded aperture data processing and image reconstruction.**
- Original (a-top) and processed (b-bottom) data of a reflection image of a 1951 Air Force test target. The smallest features are 2.2 μm x 11.0 μm. The inset of (a): raw data corresponding to three lines in the image. The sample was illuminated with a 780 nm laser and detected by a single Si photodiode.

**B. Major Contributions**

Year 1:

1. Developed and characterized fabrication process for OQP;
2. Demonstrated subwavelength and submicron lateral and axial alignment without manual microscopic positioning; and
with experimentally verified tolerances.

C. Future Plans

Over the next year, we plan to characterize and evaluate the performance of our module integration technique:

3. Output beam quality (i.e., M2) measurements.

The output of these measurements will determine whether further optimizations are required, such as horn-shaped waveguide coupling or gap index matching material per the descriptions above.

IV. EDUCATION & WORKFORCE DEVELOPMENT ACTIVITY

As part of the “National Robotics Week” event at the University of Notre Dame, our group organized and ran an exhibit on infrared remote sensing entitled “Robots See, Speak, Listen, and Show!” (See Fig. 9). There we made various musical instruments out of infrared range finders to demonstrate the concepts of infrared light and sensing to over 500 middle school students and their parents.

V. RELEVANCE AND TRANSITION

A. Relevance of your research to the DHS enterprise

This project will directly aid the DHS enterprise by providing technologies to improve the sensitivity of residual explosive imaging and detection.

B. Anticipated end-user technology transfer

This technology has applications throughout the defense industry, as well as medical, industrial and environmental fields. Tech transfer will occur through technology commercialization via Indiana Integrated Circuits, LLC, the current licensee of OQP. Additionally, future technology may be developed in collaboration with EOS Photonics. This technology can be adapted for tissue imaging and diagnostics in the medical field, industrial process analytical technology for improved manufacturing – especially in pharmaceutical industry which
current employs contact MIR spectroscopy for quality control and environmental monitoring where the imaging of greenhouse gasses and pollutants is important for regulation enforcement (e.g., DOE, EPA).

VI. LEVERAGING OF RESOURCES

The technology is patented and licensed to Indiana Integrated Circuits, who is collaborating in further improving and charactering the technology to ensure further improvements are commercially viable. Further commercial applications include incorporating EOS Photonics laser arrays with OQP. The MIR imaging system could additionally have commercial value, but is at a lower TRL.

VII. PROJECT DOCUMENTATION AND DELIVERABLES

A. Peer reviewed conference proceedings


VIII. REFERENCES


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