Methane Trace-Gas Sensing Enabled by Silicon Photonic Integration

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Acknowledgement

Partial funding provided by
ARPA-E MONITOR Program

The information, data, or work presented herein was funded in part by the Advanced Research Projects Agency-Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR0000540. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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Outline

- **Oil and Gas Industry use case for innovative trace gas sensors and sensor networks**
- **Evanescent field waveguide sensor design**
- **Spectral extraction, noise analysis, and long-term stability**
- **Integration of an on-chip reference cell and III-V / Si hybrid laser**
- **Summary**

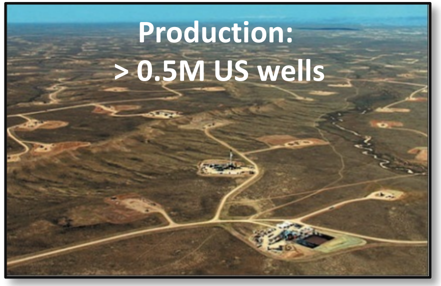
Why Manage Methane Emissions?

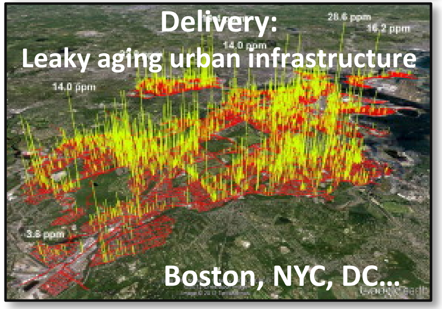
Natural gas is considered as a source of clean energy:

- Compared with coal, burning natural gas produces ½ as much CO_2 per unit of energy generated
- "Bridge fuel" for lowering emissions while transitioning from fossil fuels to renewable energy sources
- ***But….***

Leaking more than ~2-3% of natural gas produced, processed, stored, and delivered would negate its global warming advantage:

- ***Various estimates place leakage rate at 1.6%-10% of total production! (depending upon location/study)***
  - *D.T. Allen et al., PNAS 2013; A. R. Brandt et al., Science 2014; Inventory of U.S. Greenhouse Gas Emissions and Sinks, U.S. EPA.*





N. Phillips et al., Env. Pol. 2013

Fugitive emissions can eliminate advantage over burning coal

Urban safety implications

http://www.huffingtonpost.com/2015/03/26/east-village-explosion_n_6950116.html
http://edition.cnn.com/2014/03/15/us/aging-gas-infrastructure/

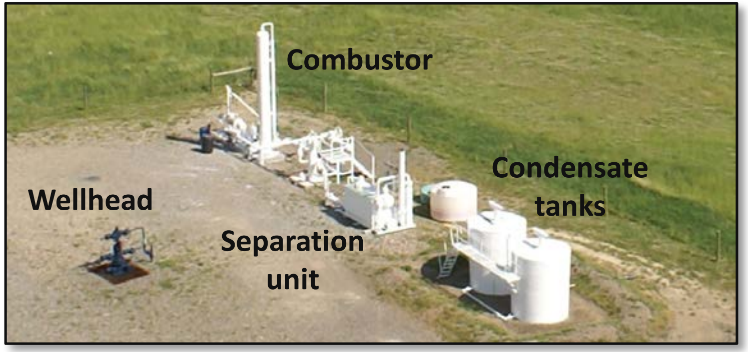
Fugitive Methane Emissions in Natural Gas Processing

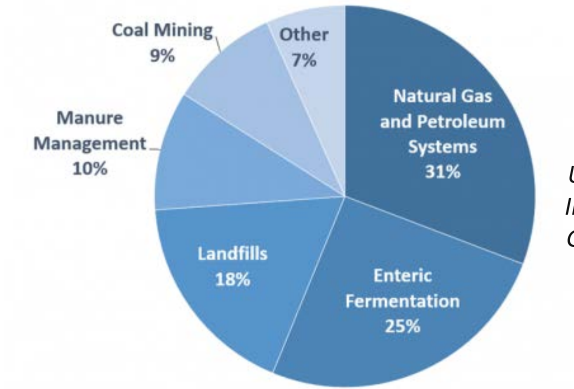
Methane (CH_4) is the second largest contributor to global warming after CO_2:

- Global warming potential of CH_4 is ~37 × greater than CO_2
  - *Alvarez et. al., Proc. Nat. Acad. Sci., 109 (17), pp. 6435-6440, (2012).*
- 10%-30% of global warming impact from human activity

> 0.5 Million active oil and gas wells in the U.S.:

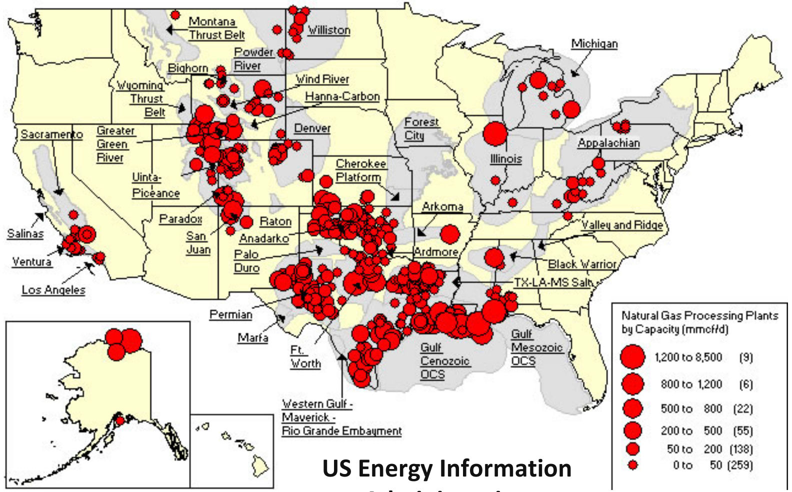
- ~30% of U.S. anthropogenic methane emissions





U.S. Methane Emissions By Source

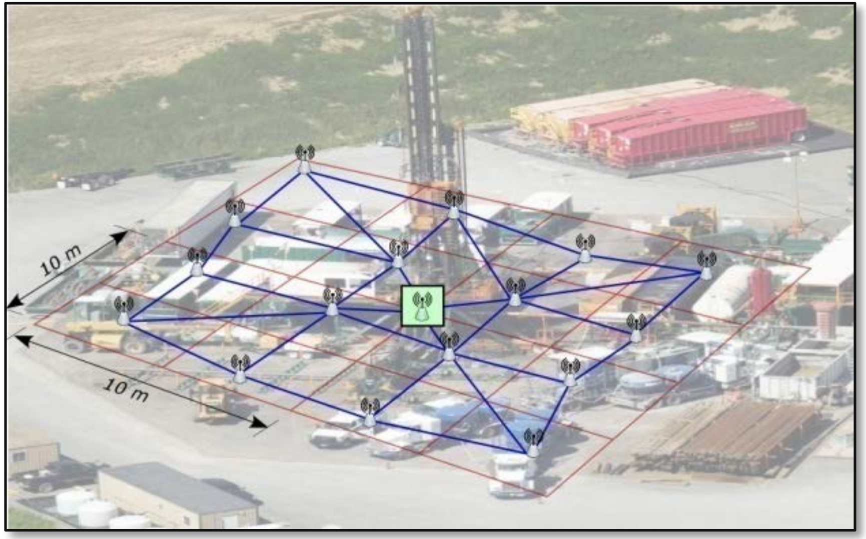
U.S. EPA (2017). Inventory of U.S. Greenhouse Gas Emissions and Sinks: 1990-2015.



US Energy Information Administration

Use Case for Innovative Sensor Networks

An Intelligent Multi-Modal Methane Measurement System (AIMS)



Technological driver: ARPA-E MONITOR Program

- **Cost-effective sensor network enabling continuous monitoring for CH_4 leak detection, localization, and repair**
- ***No viable technology today: Alignment of performance with required cost point is very challenging with today's technology***

Opportunity – Apply Physical Analytics / IoT Solutions to:

- **Significantly reduce fugitive CH_4 emissions across the oil and gas industry**
- **Improve production efficiency and safety, reduce cost**
- **Comply with emissions regulations**
- ***Harness the full potential of natural gas as a clean fuel***

Silicon Photonic Optical Trace Gas Sensor: Key Technical Innovations

Solution for deployment of economical, low-power, continuously monitoring sensor networks

IBM technology value proposition:

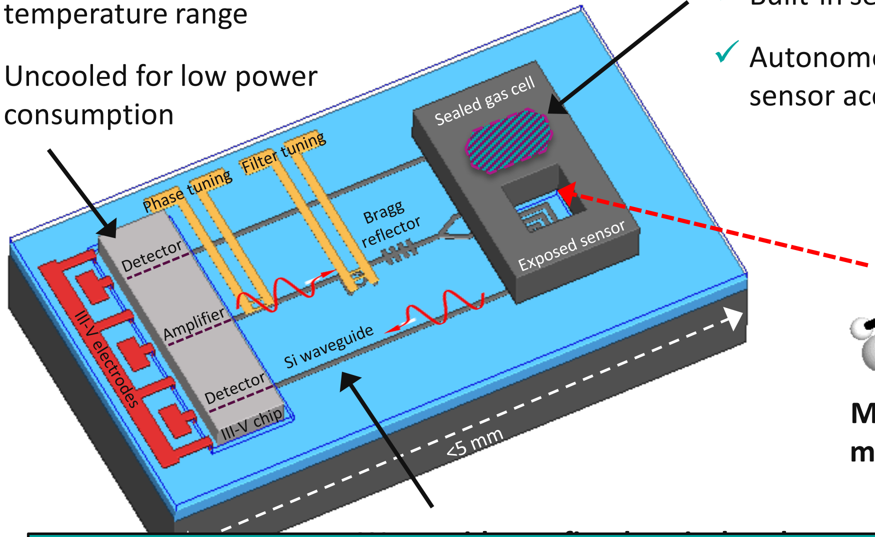
- **Selectivity to molecule of choice**
- **Orders of magnitude lower cost**
  - < $250/sensor (in volume)
- **Low power consumption**
  - < 1 Watt
- **Leverages volume manufacturing**
  - Same infrastructure used to print billions of transistors on a single microprocessor

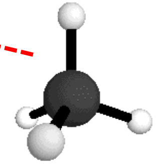
Integrated tunable laser and detector:

- ✓ Operation across wide ambient temperature range
- ✓ Uncooled for low power consumption

On-chip gas reference cell:

- ✓ Built-in self-calibration
- ✓ Autonomous long-term sensor accuracy



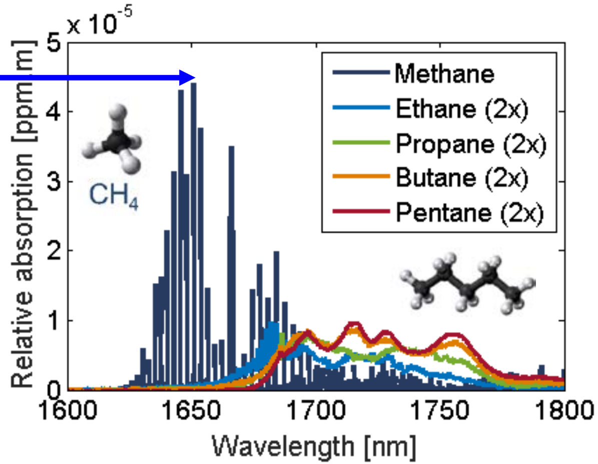


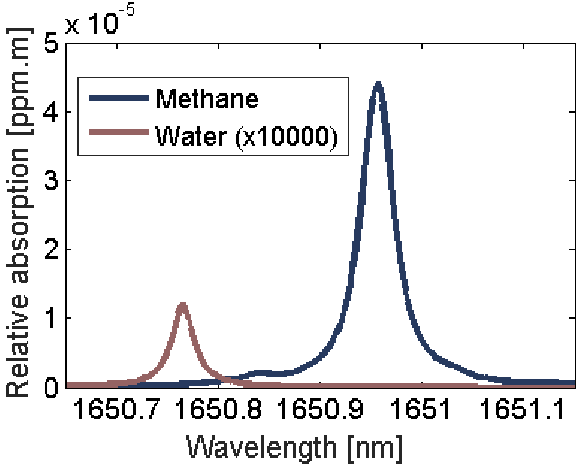
Methane molecule

Sensor sensitivity target: ~10 ppmv CH_4

Achieving Molecular Selectivity with Optical Spectroscopy

CH_4 R(4) line in the in the $2\nu_3$ overtone band





Typical composition of natural gas

Methane	CH_4	70-90%
Ethane	C_2H_6	0-20%
Propane	C_3H_8	
Butane	C_4H_{10}	
Carbon Dioxide	CO_2	0-8%
Oxygen	O_2	0-0.2%
Nitrogen	N_2	0-5%
Hydrogen sulphide	H_2S	0-5%
Rare gases	A, He, Ne, Xe	trace

naturalgas.org

Chemi-resistive VOC sensors offer sensitivity, low cost, low power, *but*:

- Not selective to only CH_4 - other VOCs, humidity, etc.
- Can produce false positives

Optical spectroscopy near 1651 nm *uniquely* identifies CH_4:

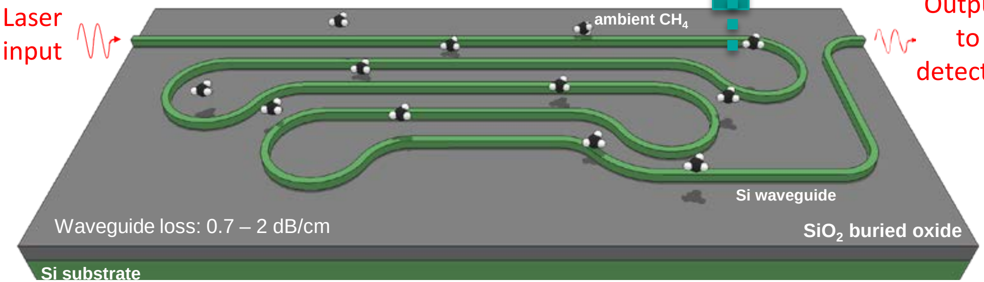
- Low overlap with constituents of natural gas
- Virtually no cross sensitivity to water

Evanescent Field Trace Gas Sensing

Up to 30 cm-long sensor waveguide

Methane molecules within the waveguide mode reduce optical transmission via the Beer-Lambert law

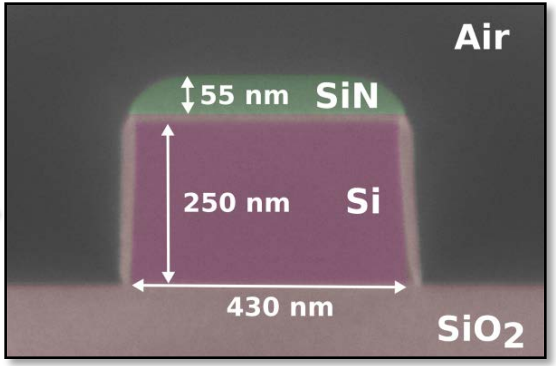
Laser input



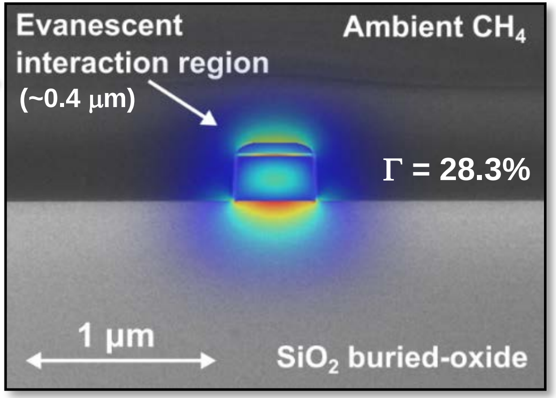
Output to detector

Cross-section

Mode simulation



Waveguide cross-section



TM_{00} electric field profile (E_y)

Direct laser absorption spectroscopy via Beer-Lambert Law

$$I_t = I_0 \exp\left[-\mathrm{L}\cdot\frac{T_R}{T}\cdot p\cdot S\cdot\chi(\nu-\nu_0)\cdot C_r\cdot\Gamma\cdot L_p\right]$$

Concentration: C_r

Absorption coefficient: $-\mathrm{L}\cdot\frac{T_R}{T}\cdot p\cdot S\cdot\chi(\nu-\nu_0)\cdot C_r$

Effective path length: $\Gamma\cdot L_p$

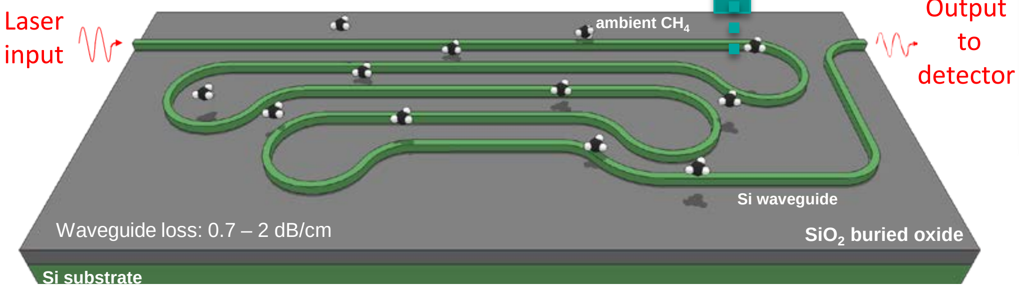
- L - Loschmidt constant
- T_R – reference temperature
- p – partial pressure
- S – integrated linestrength
- χ – lineshape function
- C_r – relative concentration
- Γ – overlap factor
- L_p – physical path length

E. Zhang, L. Tombez, J. S. Orcutt, S. Kamlapurkar, G. Wysocki, W. M. J. Green, CLEO 2016.

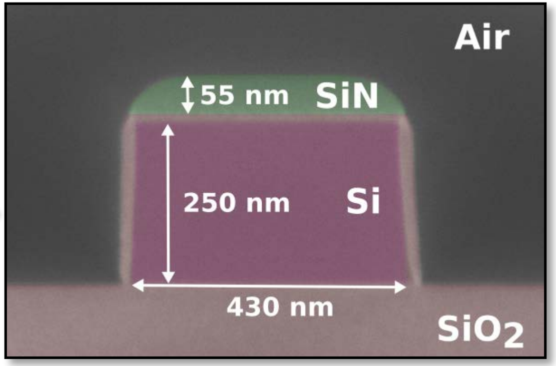
Evanescent Field Trace Gas Sensing

Up to 30 cm-long sensor waveguide

Methane molecules within the waveguide mode reduce optical transmission via the Beer-Lambert law

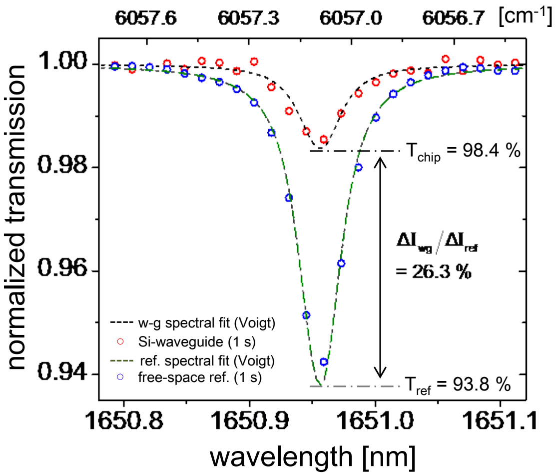


Cross-section



Waveguide cross-section

Experimental data



Methane absorption spectrum

Direct laser absorption spectroscopy via Beer-Lambert Law

Concentration

$$I_t = I_0 \exp\left[-\mathrm{L} \cdot \frac{T_R}{T} \cdot p \cdot S \cdot \chi(\nu - \nu_0) \cdot C_r \cdot \Gamma \cdot L_p\right]$$

Absorption coefficient — **Effective path length**

- L - Loschmidt constant
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- p – partial pressure
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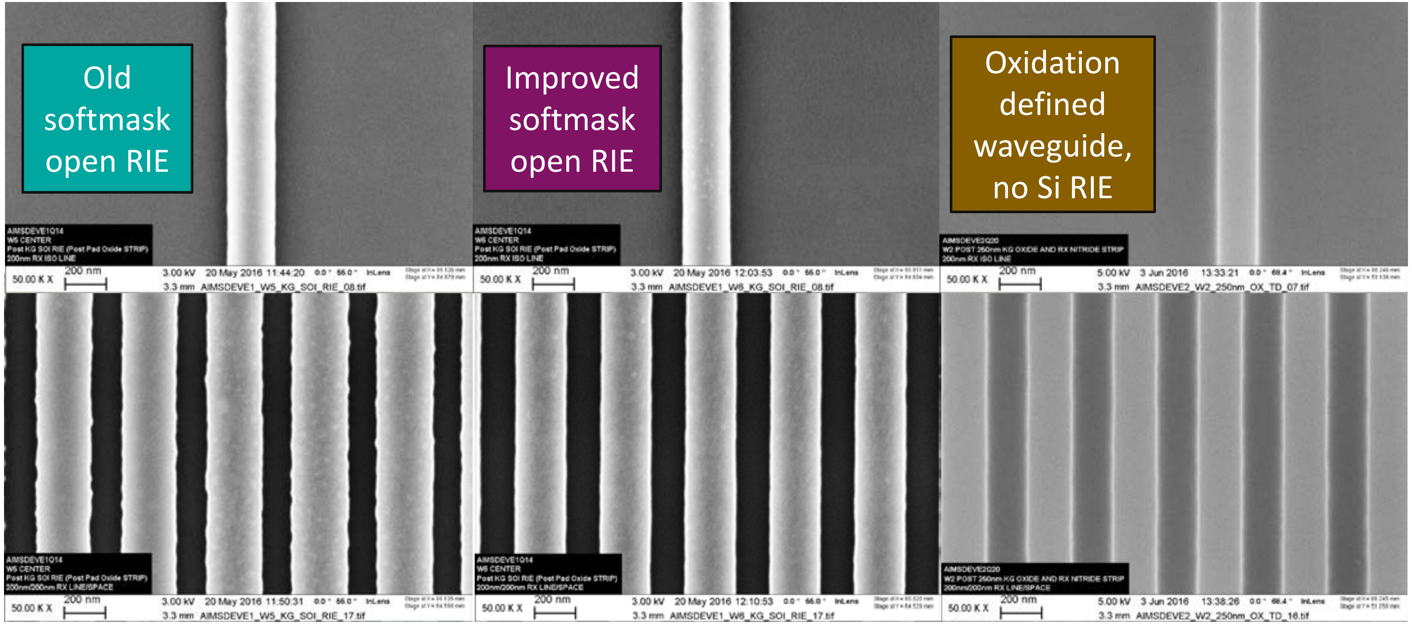
E. Zhang, L. Tombez, J. S. Orcutt, S. Kamlapurkar, G. Wysocki, W. M. J. Green, CLEO 2016.

Line Edge Roughness Generates Internal Etalons



	Old SM Open RIE	Improved SM Open RIE	Oxidation defined waveguide
LER – Isolated (nm)	**3.32 ± 0.20**	**2.45 ± 0.39**	**2.89 ± 0.20**
LER – Array (nm)	7.71 ± 0.45	3.41 ± 0.26	3.30 ± 0.10

Initial positive tone litho process had 5.7 nm LER

New softmask open etch has notable improvement compared to POR:
- Optical measurements to corroborate

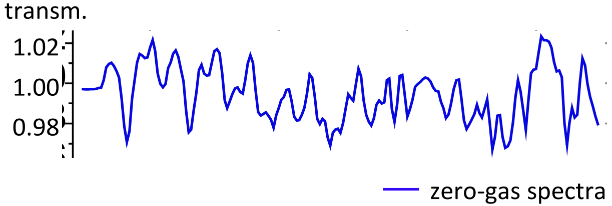
Oxidiation defined waveguides have LER comparable to new process:
- 250nm of SiO_2 grown with SiN mask to recess Si

Internal etalon amplitude depends strongly on polarization:
- Reduced significantly for TM mode compared to TE mode

Consequences of Miniaturization and Internal Etalon Mitigation

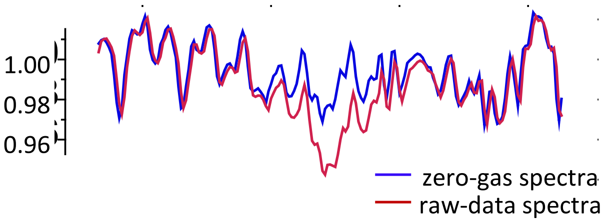
Conventional etalon subtraction

SiPh waveguide etalon background



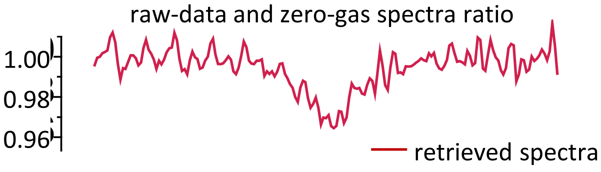
- *High index contrast of Si generates distributed reflections, multi-path interference*

With 2.87% CH_4

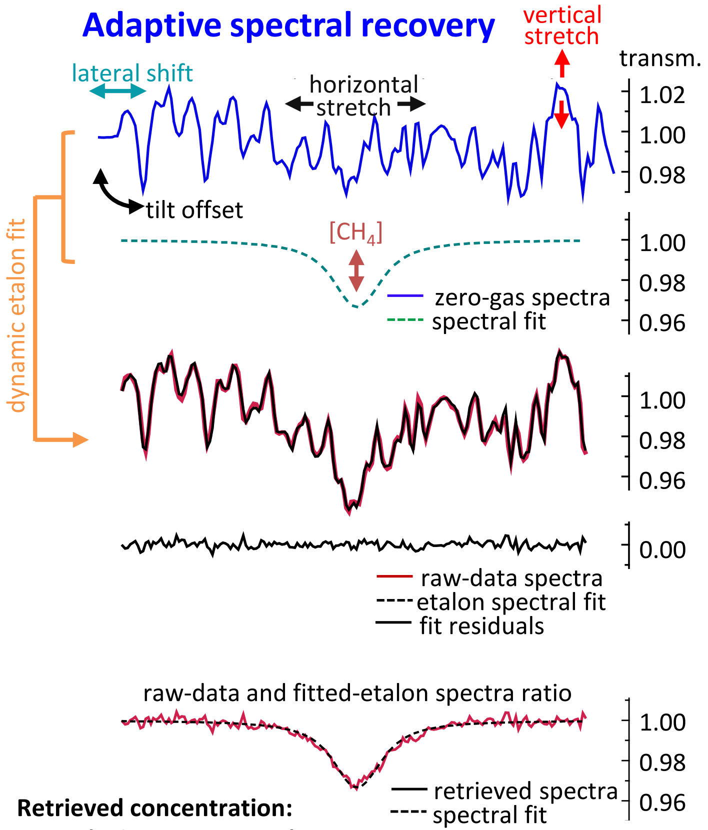


- *Drifting etalon spectrum can mask and cross-talk with the weak absorption signal*

Retrieved CH_4 spectra



Dynamic etalon fitting: Adaptive spectral recovery



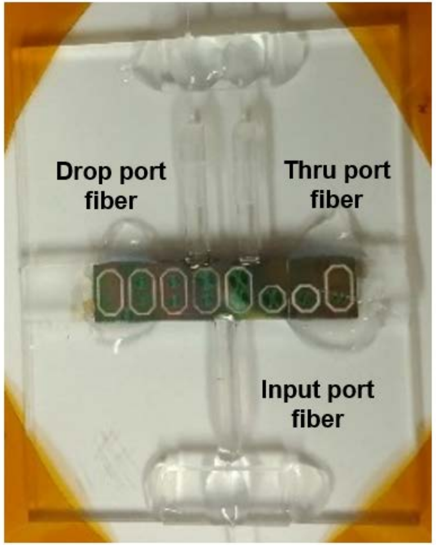
Retrieved concentration: 2.87% (reference CH_4 cell)

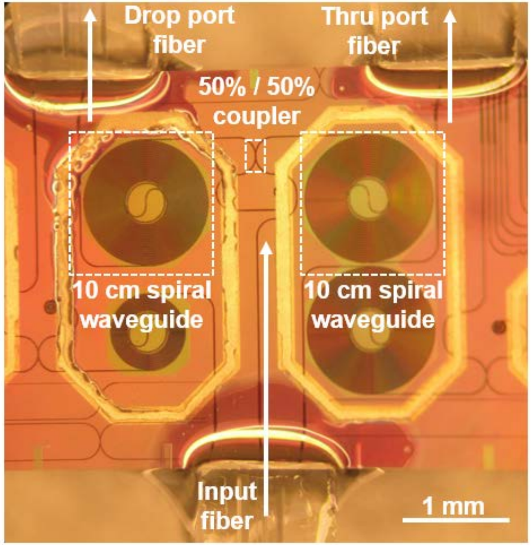
E. Zhang, L. Tombez, J. S. Orcutt, S. Kamlapurkar, G. Wysocki, W. M. J. Green, CLEO 2016.

Methane Minimum Detection Limit

Packaging, fabrication, and design:

- Mechanical stability via fiber pigtailing
- Sample both thru port and drop ports simultaneously
- Improved sensitivity expected with next-generation samples:
  - Larger mode overlap, lower propagation/coupling losses

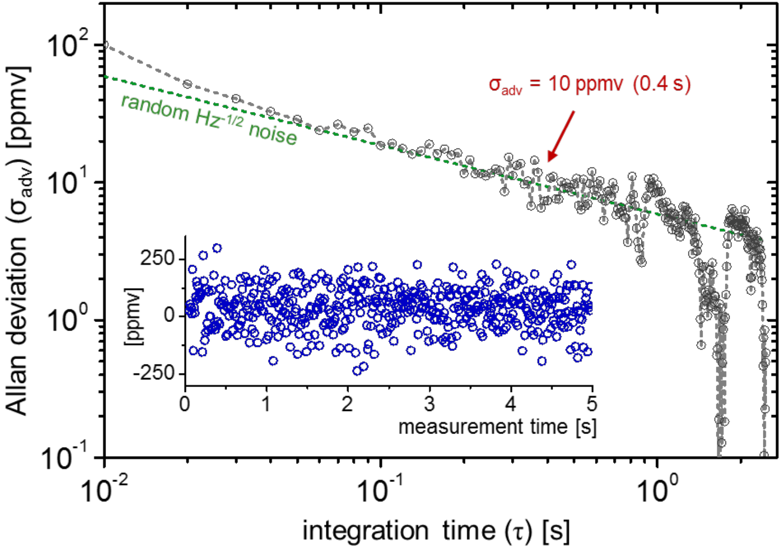




Minimum detection limit

30 cm waveguide, $\Gamma = 25\%$

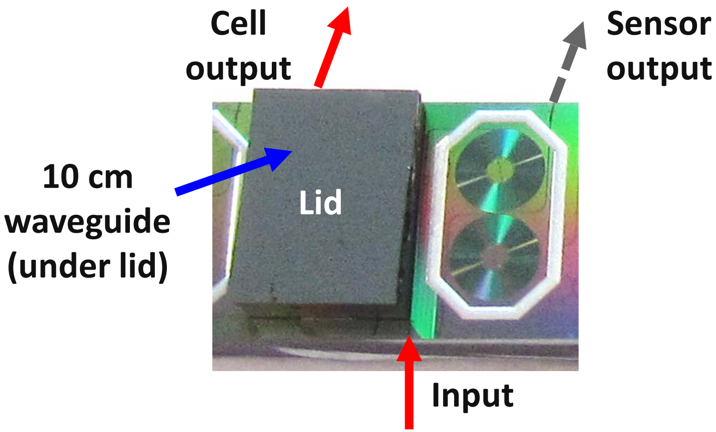
→ 7.5 cm effective path length



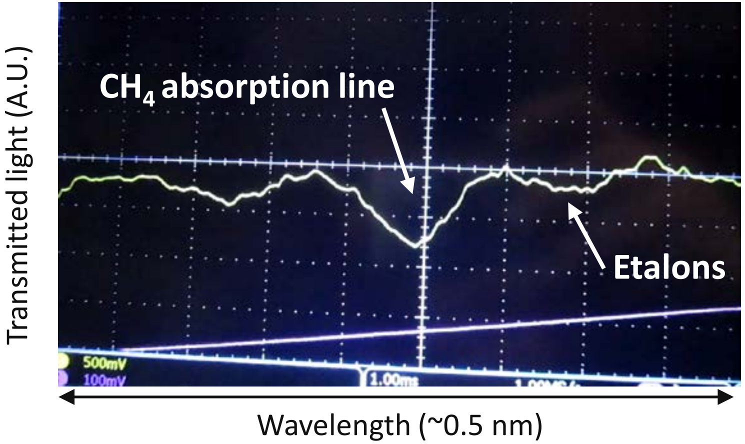
C. C. Teng, C. Xiong, E. J. Zhang, Y. Martin, M. Khater, J. Orcutt, W. M. J. Green, Gerard Wysocki, CLEO 2017.
E. J. Zhang et al., unpublished.

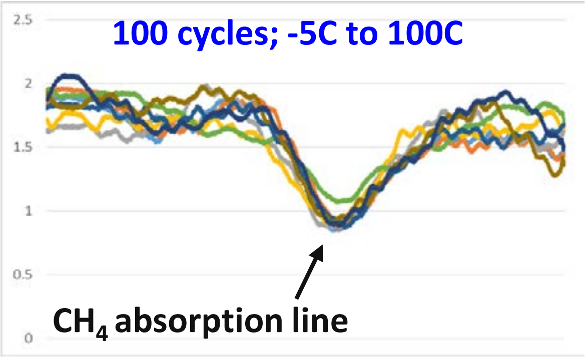
On-Chip Integrated CH_4 Reference Cell

Test configuration



Line scanning spectroscopy while heating chip



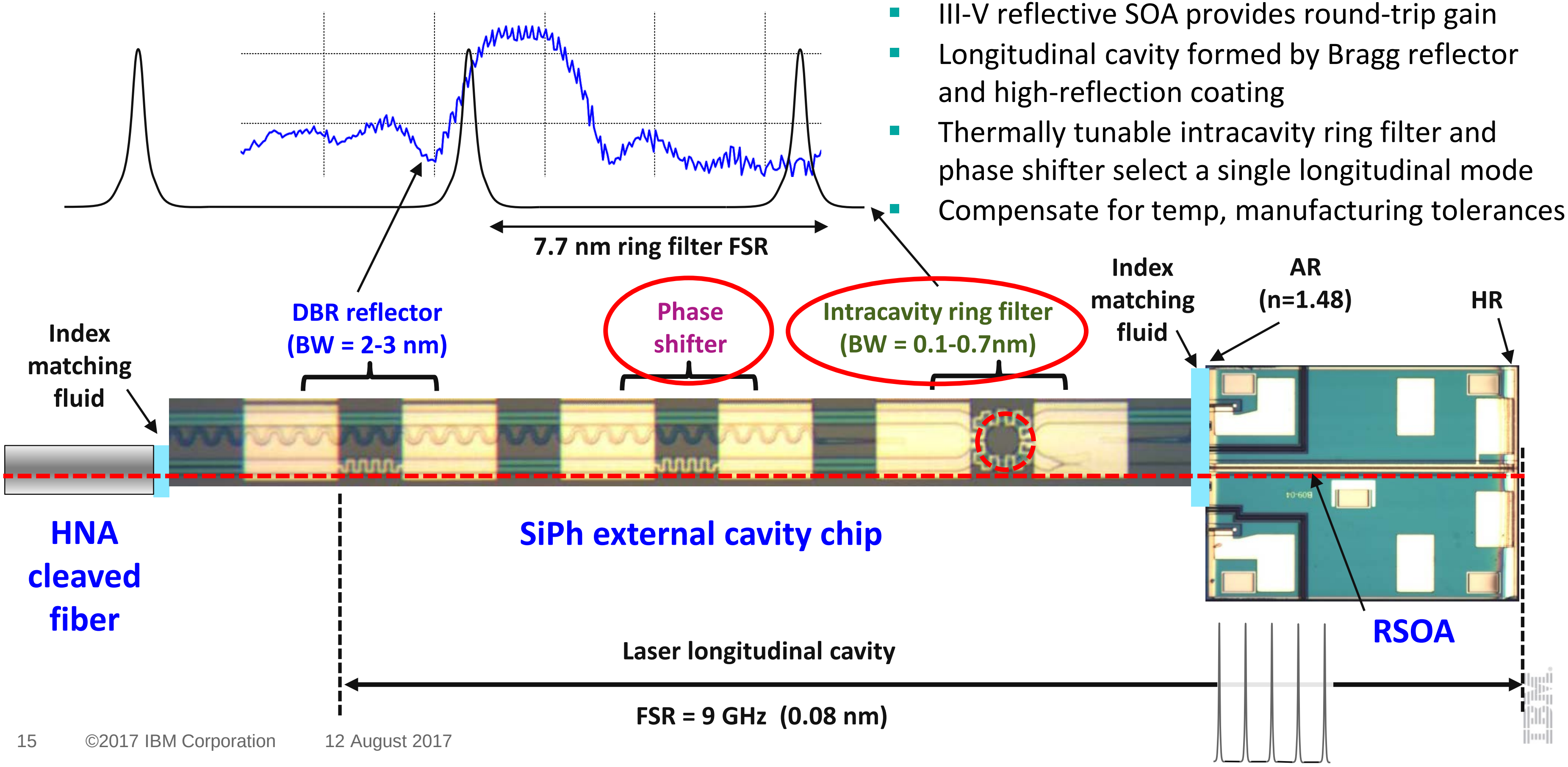


Sequence of line scans for chip ΔT ~2-5 C.

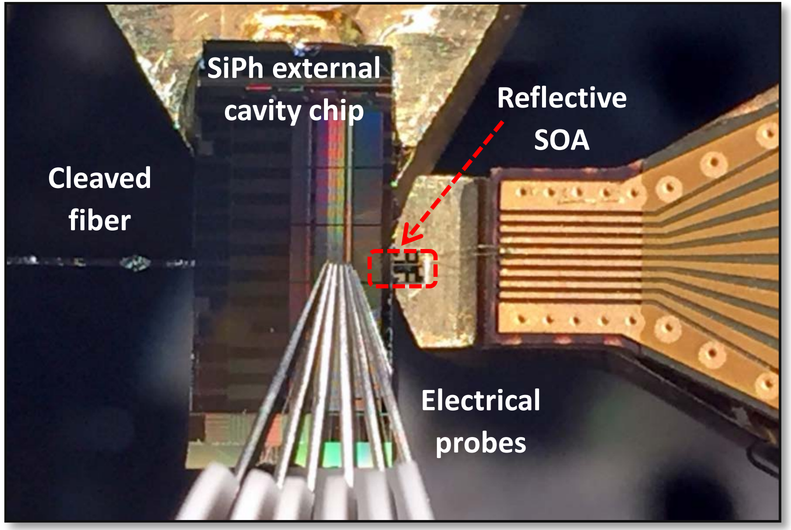
- **Etalons shift with temperature:**
  - Methane absorption line does not
- **Stress testing - cell remains sealed after:**
  - 2 months in ambient lab conditions
  - Thermal cycling; -5C to 100C
  - 20 hours at 107C

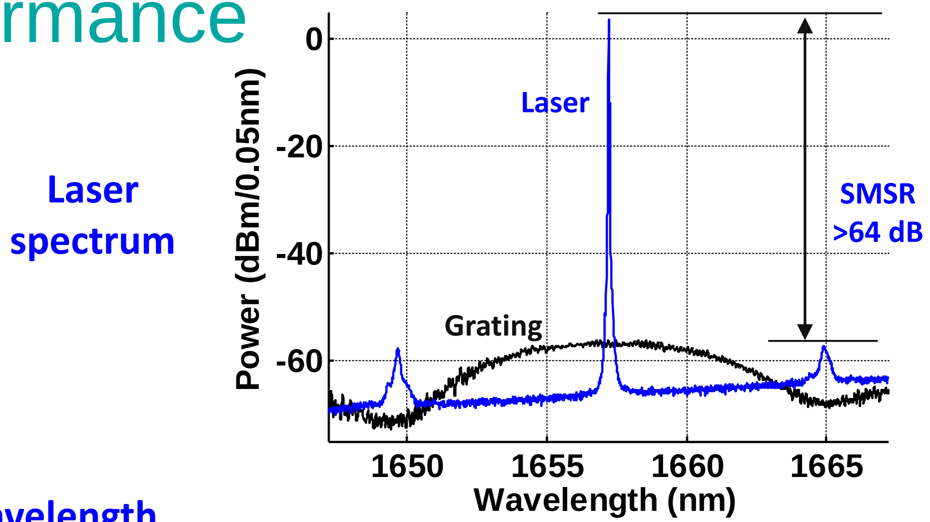
External Cavity Laser Design and Test

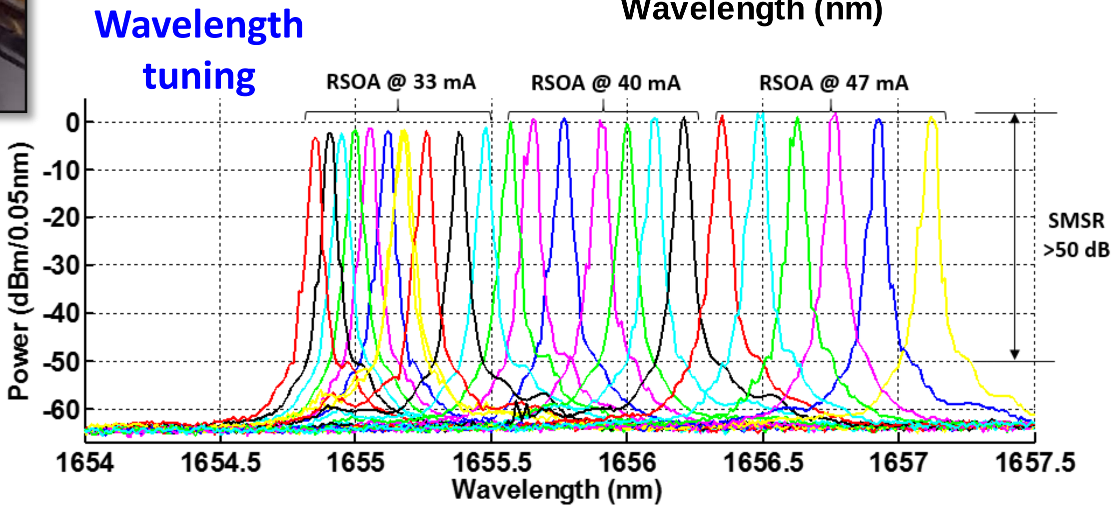
- III-V reflective SOA provides round-trip gain
- Longitudinal cavity formed by Bragg reflector and high-reflection coating
- Thermally tunable intracavity ring filter and phase shifter select a single longitudinal mode
- Compensate for temp, manufacturing tolerances



Hybrid III-V/Si Laser Performance



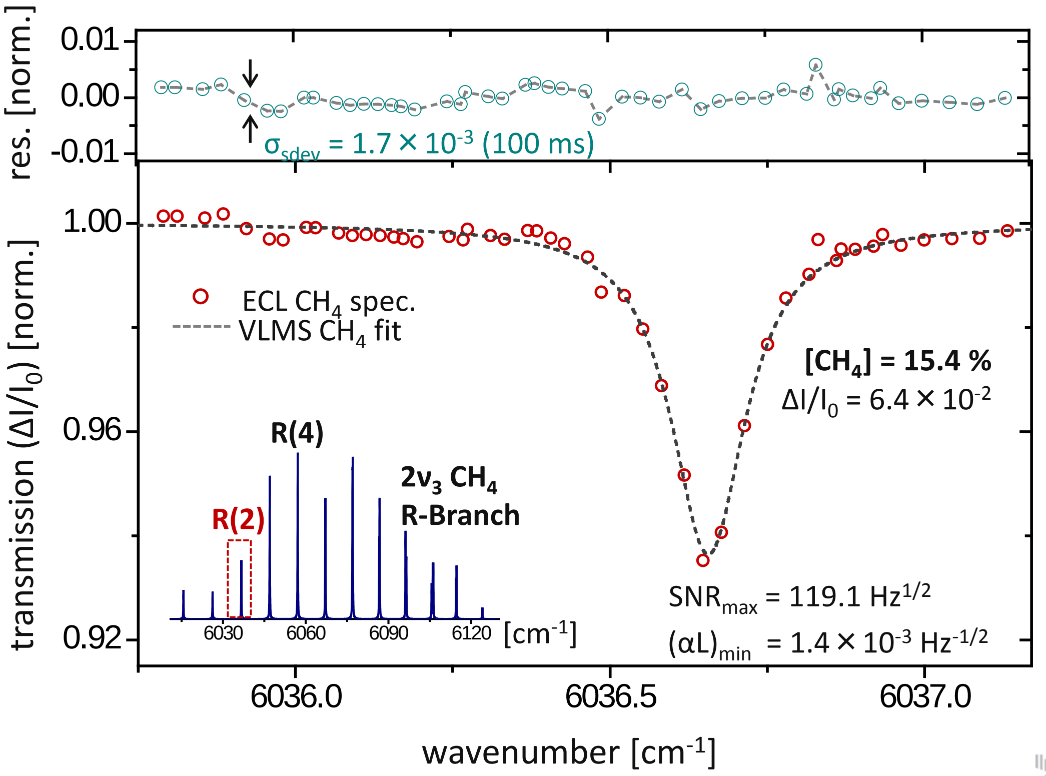




- Single-mode operation from 1650 - 1670 nm
- > 45 dB side-mode suppression ratio
- 2 - 8 nm mode-hop free tuning (depending upon DBR bandwidth)
- 0.5 mW output power (fiber-coupled)
- > 1 mW output power (on-chip)

Methane R(2) Spectral Acquisition

- CH_4 spectroscopy performed on R(2) line (weak, λ = 1656.5 nm) using hybrid III-V/Si laser and a fiber-coupled CH_4 reference cell
- Line fit accurately reproduces the concentration extracted with a commercial DFB laser
- Minor lithographic tweak to DBR grating required to target R(4) line



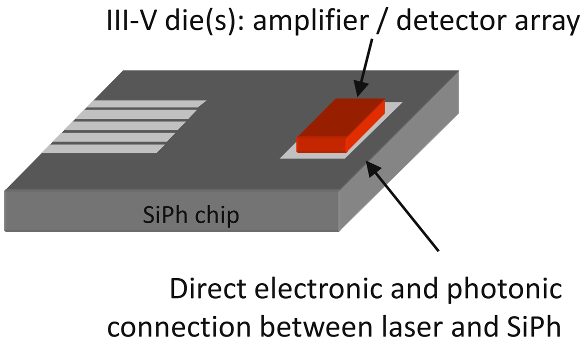
III-V Gain / Detector Chip Attach

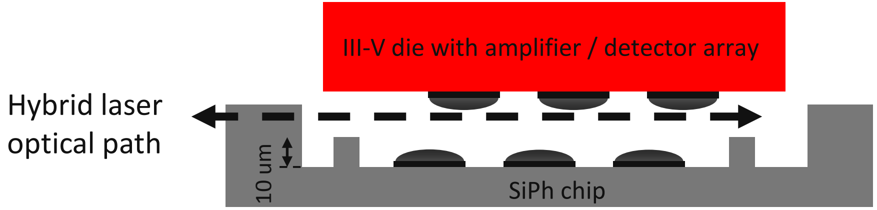
IBM differential:

- Full automation in standard CMOS assembly tooling
- Single or multiple III-V die flip-chipped to SiPh
- Disruptive scalability in volume and cost

Innovation:

- Mode shape engineering to relax tolerance
- Solder surface tension re-aligns III-V chip
- Superior thermal characteristics

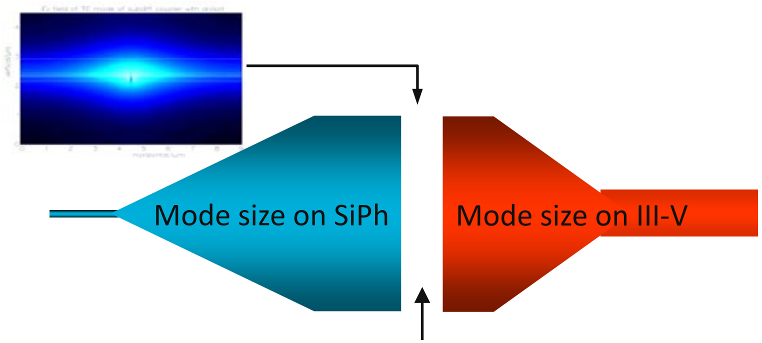




Pick and place, then anneal to reflow

Key challenge:

- Sub-micron tolerances for passive alignment



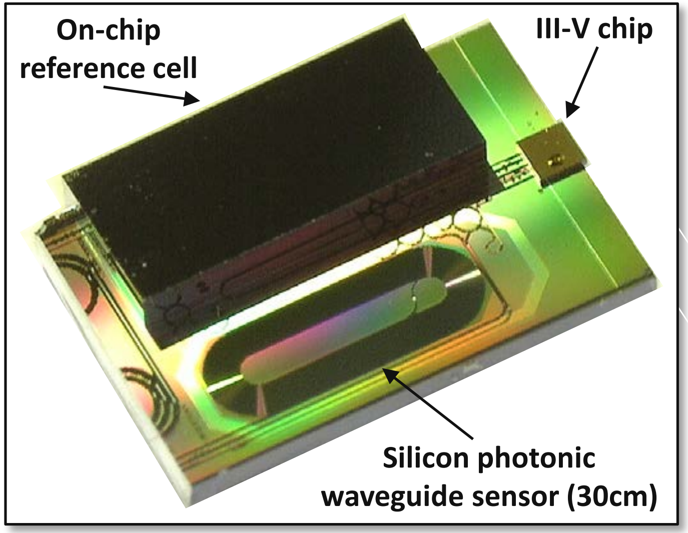
Connection at maximal delocalization

T. Barwicz, et al., GFP 2015; J.-W. Nah et al., ECTC 2015; Y. Martin et al., ECTC 2016.

Key Milestones for 2017

- **Demonstrate hybrid III-V / Si laser assembly:**
  - Single mode tunable laser required for 1650nm methane line scanning
  - ***Facilitates economical, large-scale deployment of continuously monitoring sensor networks***

Mechanical prototype of full sensor assembly



- **Field testing of a fully integrated methane leak detection system:**
  - Deploy a functional sensor network and demonstrate leak detection / localization
  - Taking place at a "mock" testsite, as well as at operating industry partner wellpads

Sensor deployed at industry partner's wellpad

Compelling Technological Advantages

	Commercially Available Optical CH_4 Sensors	Integrated SiPh Chip Sensor
Sensitivity	0.1-1 ppmv	**5 ppmv**
Power	2-10 W	**~0.6 W**
Size	~50 cm	**~5 cm**
Weight	3-10 kg	**~200 g**
Cost	$10k-$25k USD	**$0.25k USD**
Figure of Merit **Sens-power-$-size** **($ppm^{-1}$/(W.k$.m))**	**~0.5**	**22**

> 40x improvement in Figure of Merit

SiPh technology value proposition:

- Orders of magnitude lower cost
- Low power consumption
- Compactness
- Leverages volume manufacturing
- Extensible to a broad range of applications
- ***Facilitates economical, large-scale deployment of continuously monitoring sensor networks***

References:
[1] http://www.axetris.com/en-us/lgd/products/lgd-f200/lgd-f200-a-ch4
[2] http://www.tdlsensors.co.uk/products.html
[3] http://www.geotechuk.com/products/landfill-and-biogas/portable-gas-analysers/tdl-500.aspx

Thank You!

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