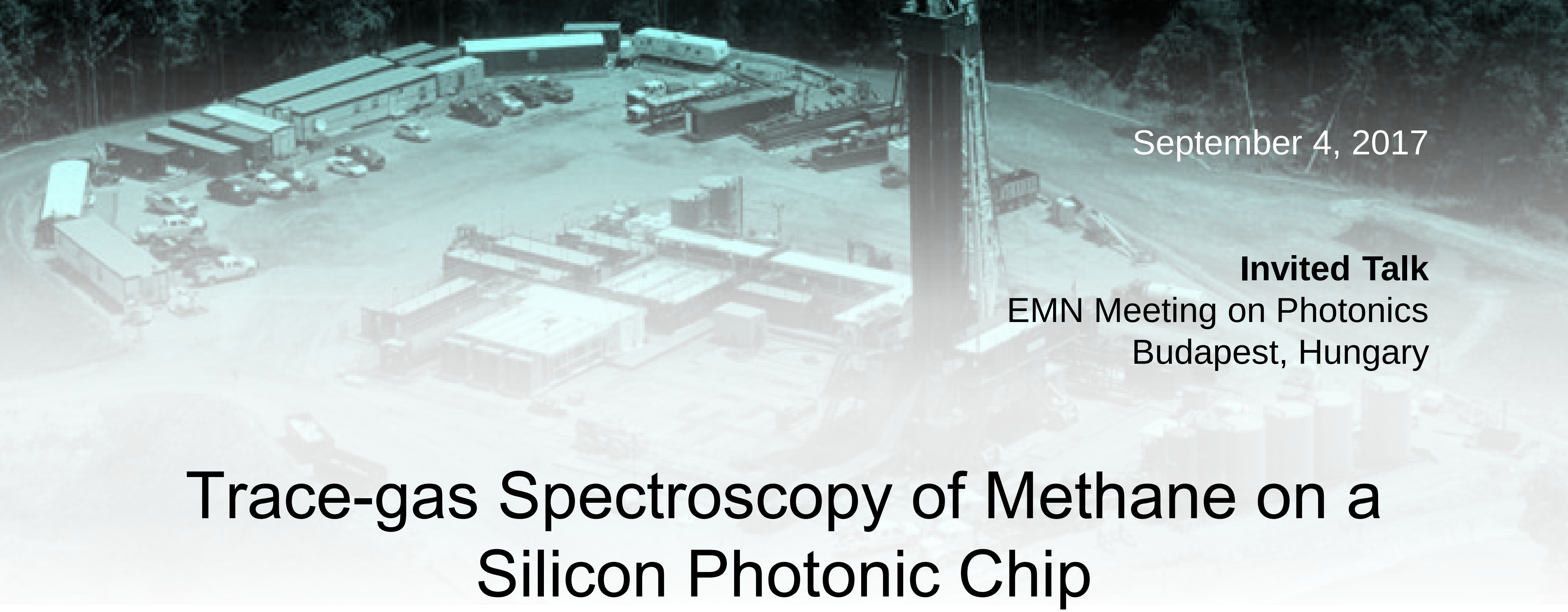

September 4, 2017

Invited Talk
EMN Meeting on Photonics
Budapest, Hungary

Trace-gas Spectroscopy of Methane on a Silicon Photonic Chip

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arpa·e awardee

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IBM

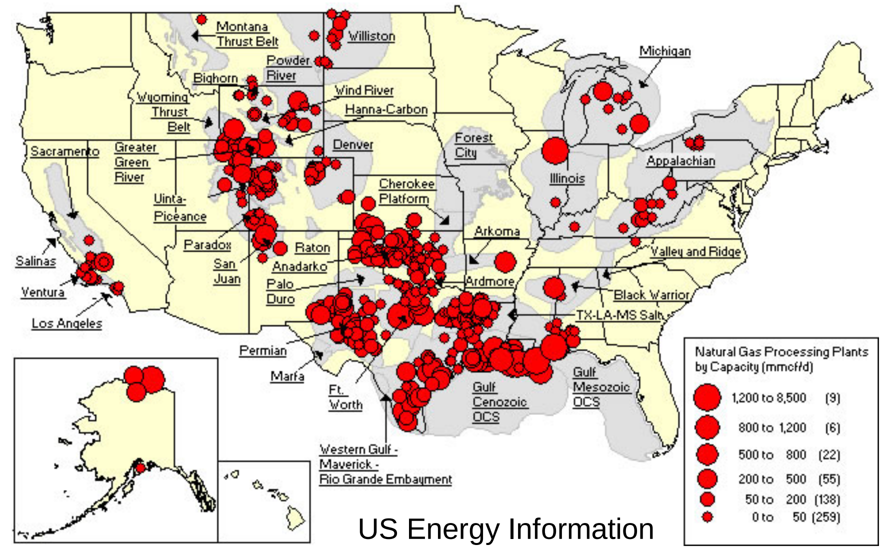
Presentation Outline

- Introduction
  - Motivation: CH_4 fugitive emissions monitoring
- Silicon-photonic waveguide absorption sensor (SPWAS)
  - Silicon-photonic chip sensor design
  - Diagnostic test-bench and CH_4 spectra
- Spectral extraction and noise analysis
  - SPWAS short-term precision and stability
  - CH_4 spectral extraction in the presence of optical etalons
- Towards an external-cavity (EC) III-V / Si hybrid laser
  - ECL noise performance and broadband tunability
  - Preliminary demonstration of TDLAS
- Concluding remarks

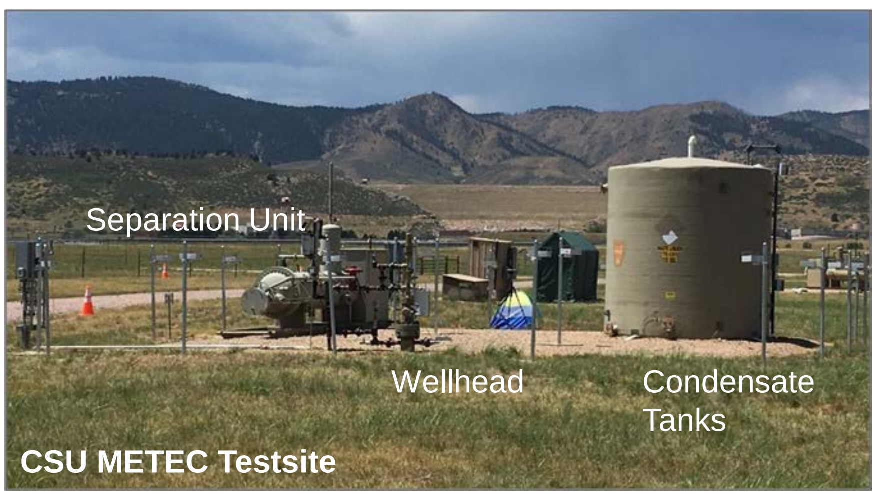
Motivation: CH_4 fugitive emissions monitoring

- > 500,000 active oil/gas wells in USA
- 570 × 10^9 ft^3 of CH_4 leakage in 2009, (59 % leaks during production phase)
- ~ 30% anthropogenic CH_4 emissions
- Radiative forcing of CH_4 is 37× greater than CO_2

Alvarez et. al., "Greater focus needed on methane leakage from natural gas infrastructure," Proc. Nat. Acad. Sci., 109 (17), pp. 6435-6440, (2012).



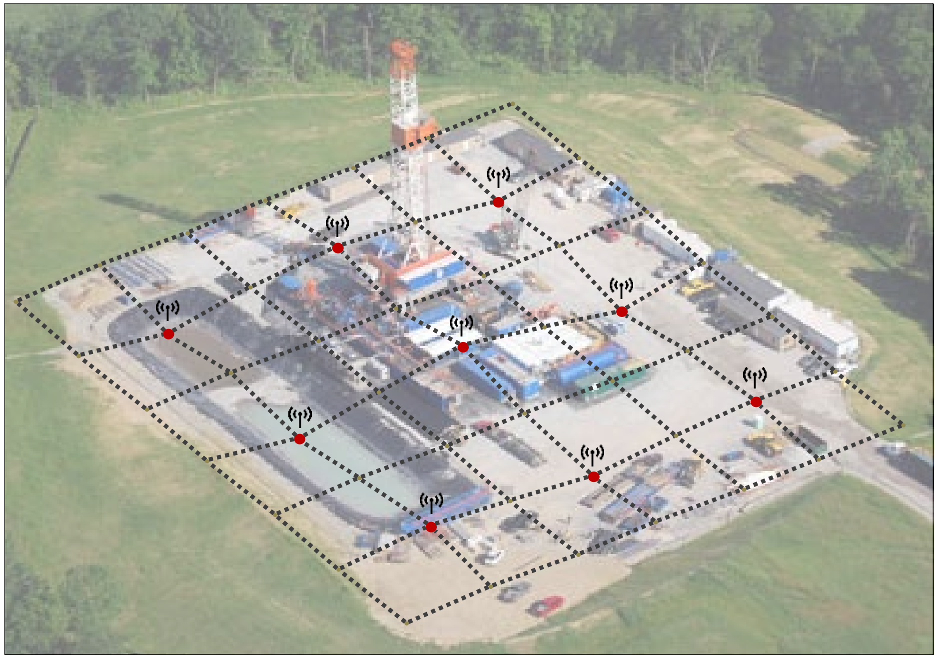
US Energy Information Administration



- CH_4 leakage rate on oil/gas well pad is 2-10% of total production!

Cost-effective sensor network for localization and precise quantification (ppmv-level) of CH_4 on oil and gas production well-pads

Use-case for innovative sensor networks



An Intelligent Multi-Modal Methane Measurement System (AIMS)

Technological driver: ARPA-E MONITOR

- Cost-effective sensor network for continuous CH_4 leak quantification, localization, and repair
- No viable technology today: Alignment of performance with required cost point poses significant challenge

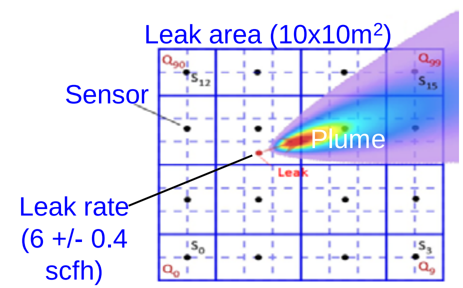
Opportunity driver: Application of physical analytics/IoT solutions to

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

Real-time sensor mesh network (IBM MMT System)

→ **Aggregate/push to Bluemix cloud (MQTT protocol)**

→ **Physical analytics:**
- source inference via inversion
- plume dispersion models
- machine-learned model blending

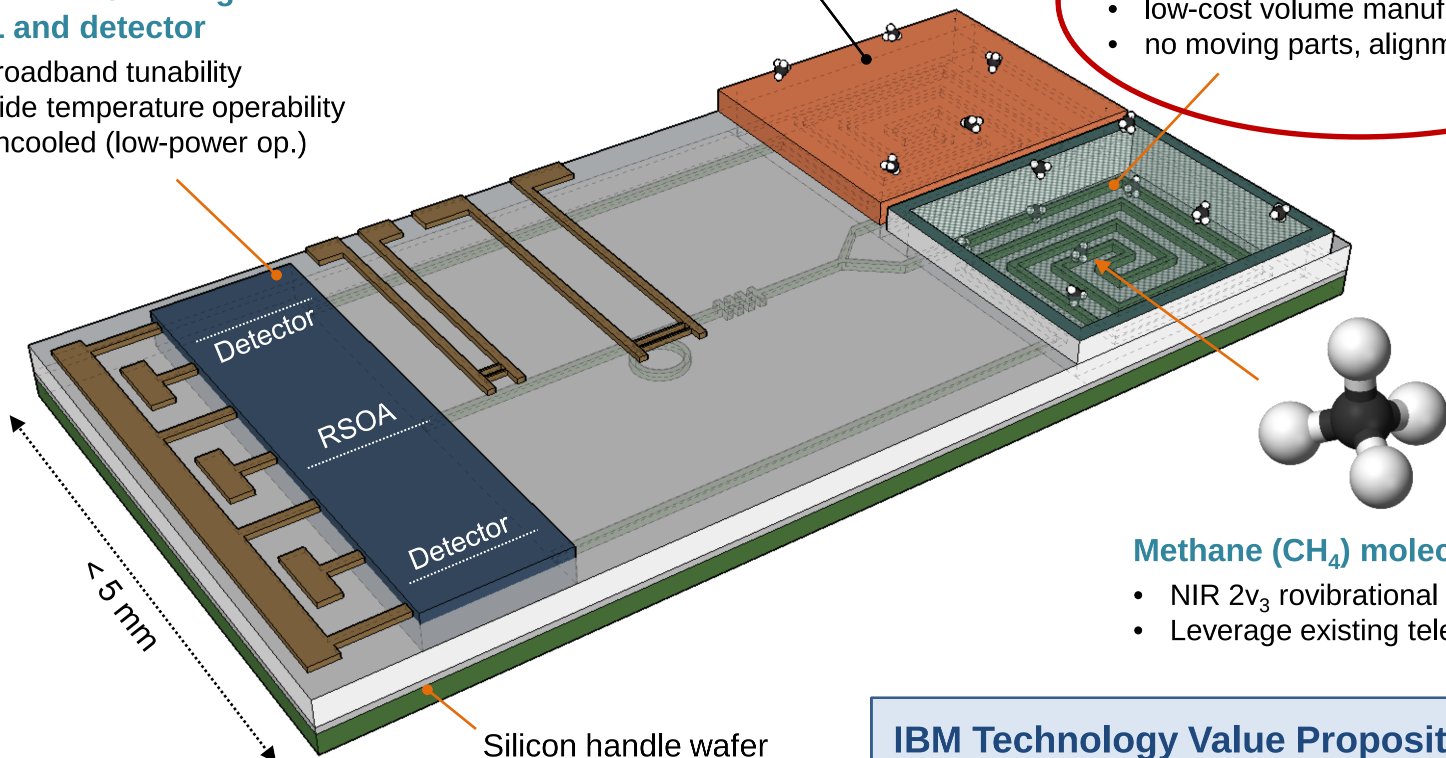


Integrated silicon photonic chip sensor

Hybrid III-V/Si Integrated ECL and detector
- broadband tunability
- wide temperature operability
- uncooled (low-power op.)

On-chip reference CH_4 cell
- on-chip self-calibration
- autonomous long-term accuracy

Waveguide confined optical path
- low-cost volume manufacturing
- no moving parts, alignment-robust



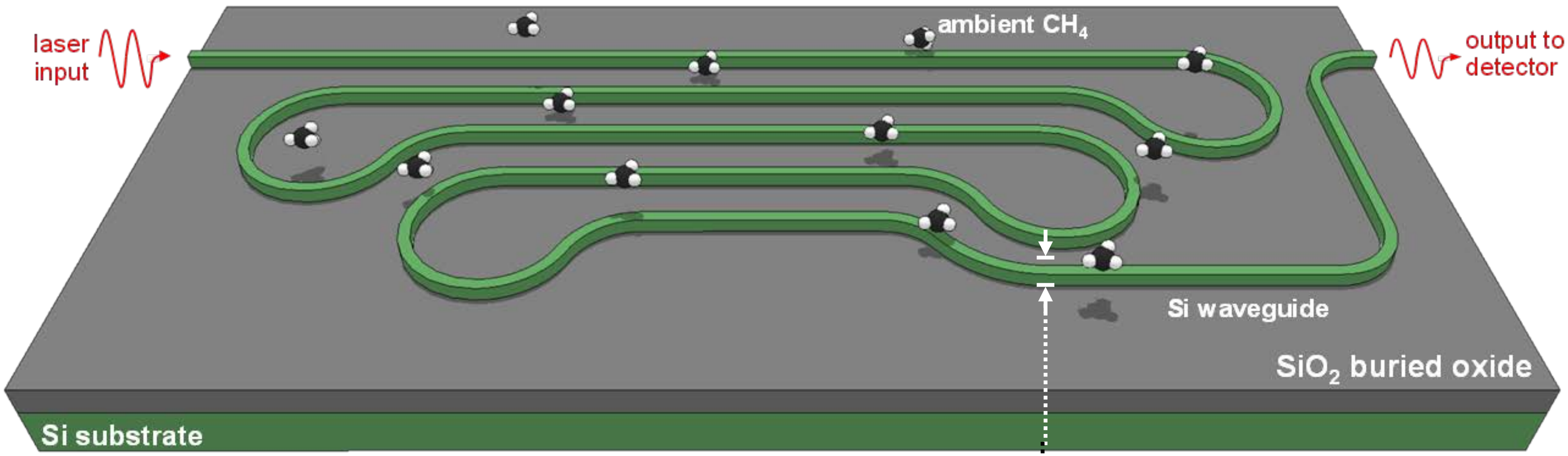
Methane (CH_4) molecule
- NIR $2v_3$ rovibrational band (1651 nm)
- Leverage existing telecom technology

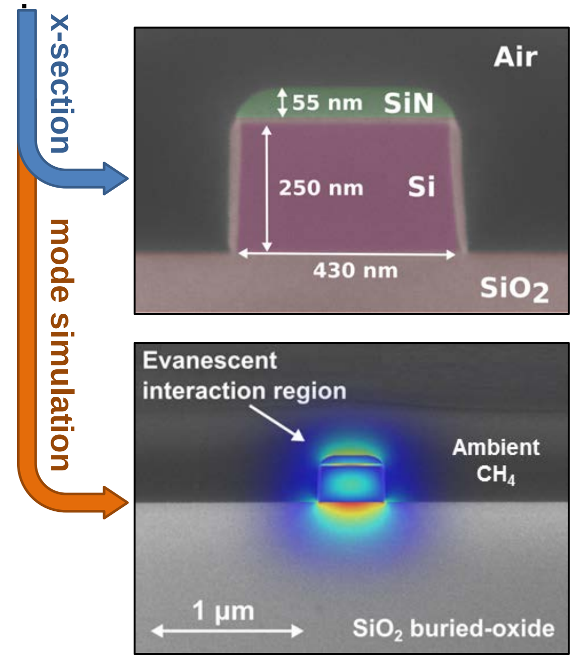
ARPA-E Design Target: 6 scfh CH_4 leak on 100 m^2 well pad within 18.25 days (90 % confidence level) with 1 m^2 spatial resolution

→ **Sensitivity Target: 10 ppmv · $Hz^{-1/2}$**

IBM Technology Value Proposition:
- Broadband TDLAS with molecular specificity
- Low volume cost (< 250 USD / sensor)
- Low power consumption
- Leverages CMOS compatible volume manufacturing

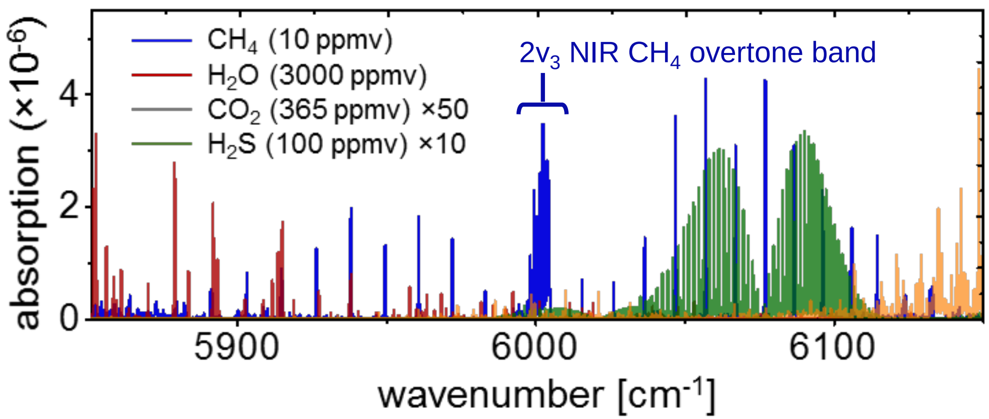
Silicon photonic chip sensor design



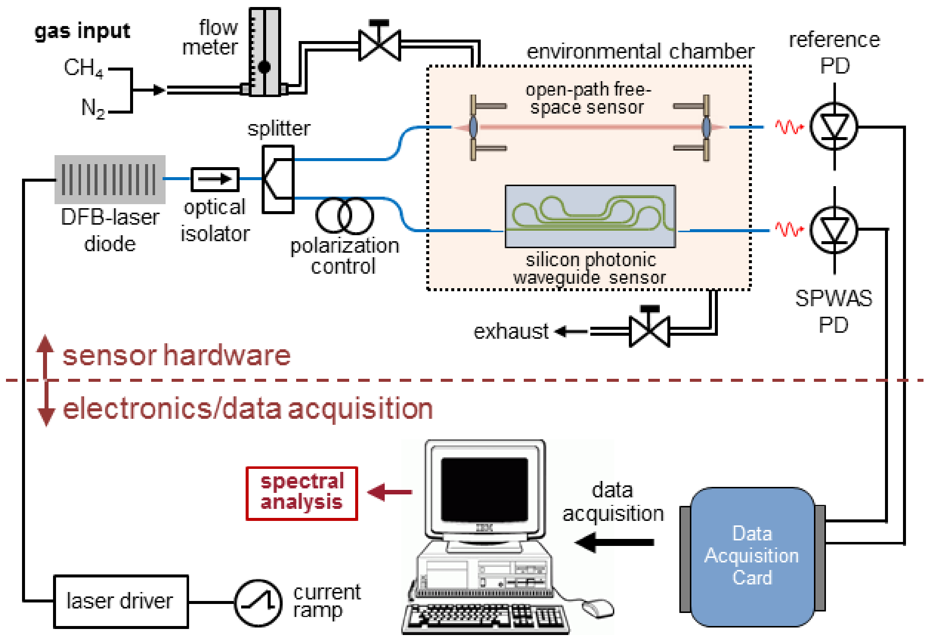


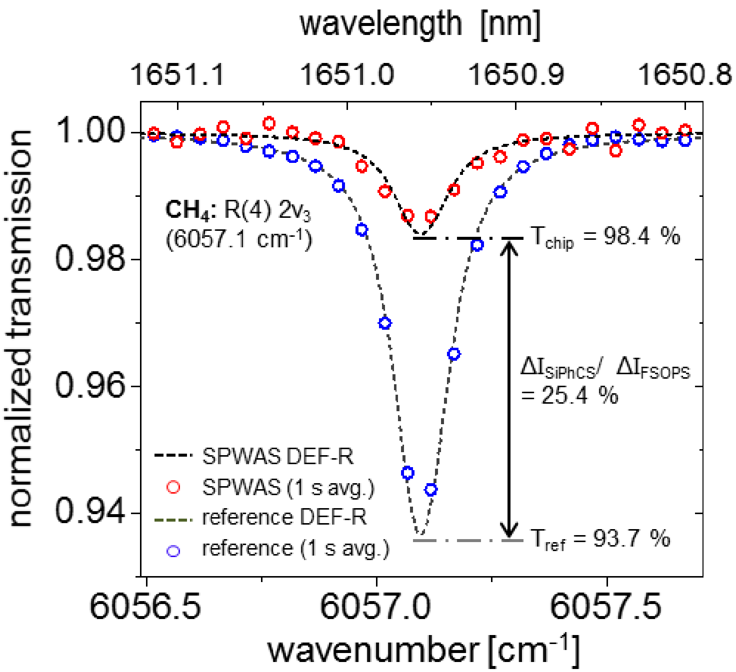
TDLAS via Beer Lambert Law:

- Molecule-specific transition wavelengths (cross-talk free)
- Extensively documented transition parameters for common species (e.g. natural gas constituents)



Diagnostic test-bench and CH_4 spectra





SPWAS acquisition bench-top for TDLAS:

- Simultaneous data acquisition of free-space reference/SPWAS for accuracy benchmarking
- Identical sensor physical path lengths (10 cm)
- 100 Hz current ramp of U-band DFB laser diode
- Uncooled InGaAs amplified photodiodes
- 50 kSa/s, 16 bit resolution NI-DAQ (USB-6001)

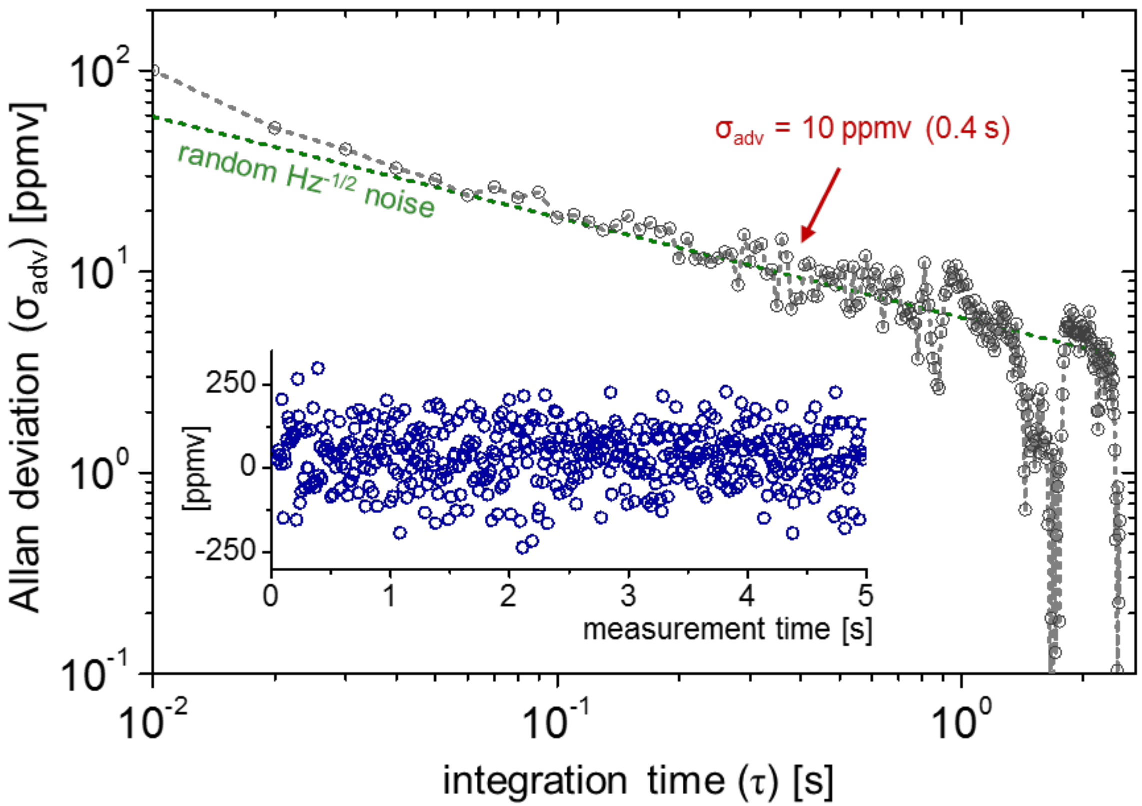
SPWAS/reference spectral comparison:

- Target CH_4 using $2\nu_3$ overtone band at 6057 cm^{-1} (1.65 µm)
- Peak absorption ratio for CH_4 release:

Simulated: Γ = 28.5 %

Measured: Γ = 25.4 %

SPWAS state-of-art short-term precision



Detection sensitivity:

σ_{adv} **= 6.3 ppmv · Hz$^{-1/2}$**

Min. fractional absorption:

$(\alpha L)_{min}$ **= 3.3×10^{-5} Hz$^{-1/2}$**

→ 10 ppmv (0.4 s)

Measurement parameters:

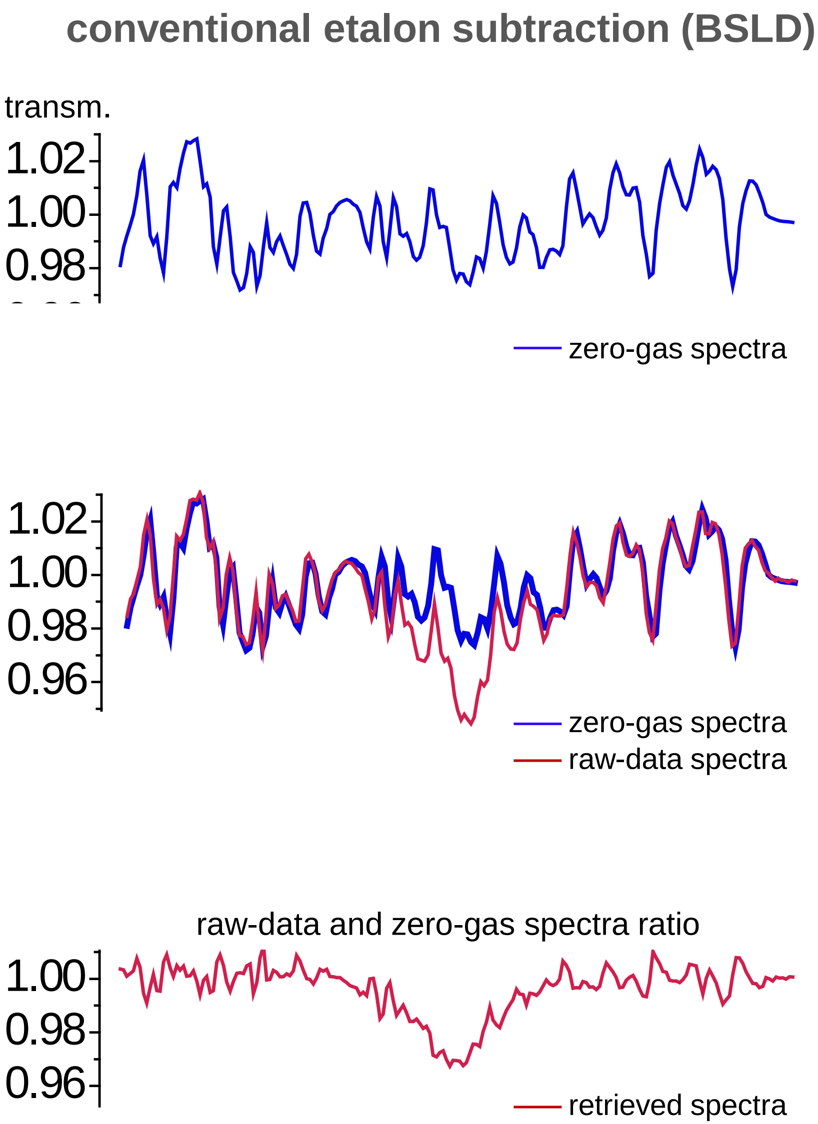
- 30 cm waveguide, TM_{00} mode (Γ = 25 %) → L_{eff} = 7.5 cm
- Voigt LMS spectral extraction (2nd order quadratic baseline)
- 500 kSa/s, 16-bit NI-DAQ

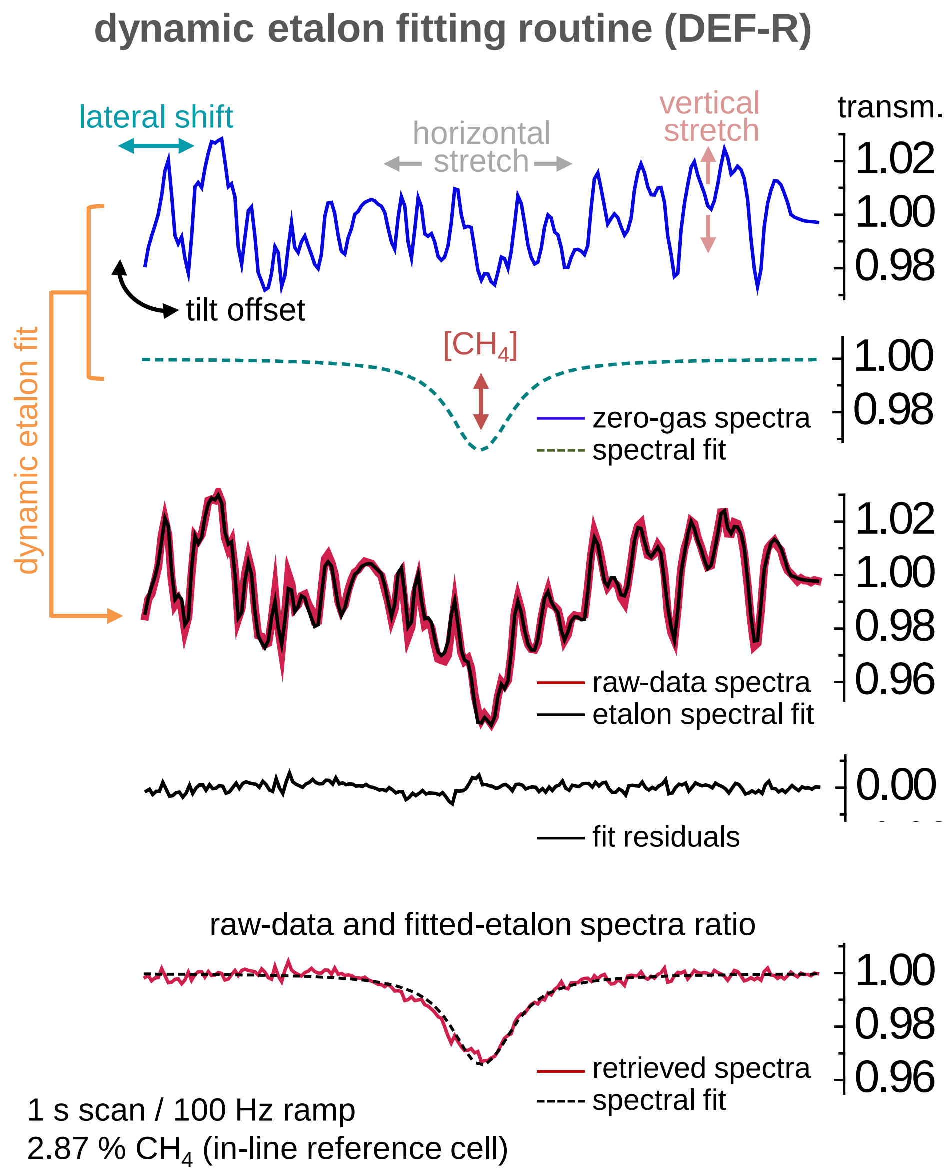
Allan (two-sample) variance stability analysis:

- Short-term measurements to probe SPWAS fundamental sensitivity (500 Hz ramps measured over 5 sec.)
- Data acquisition rates faster than external drift conditions (e.g. mechanical vibrations, thermal swings, etc.)

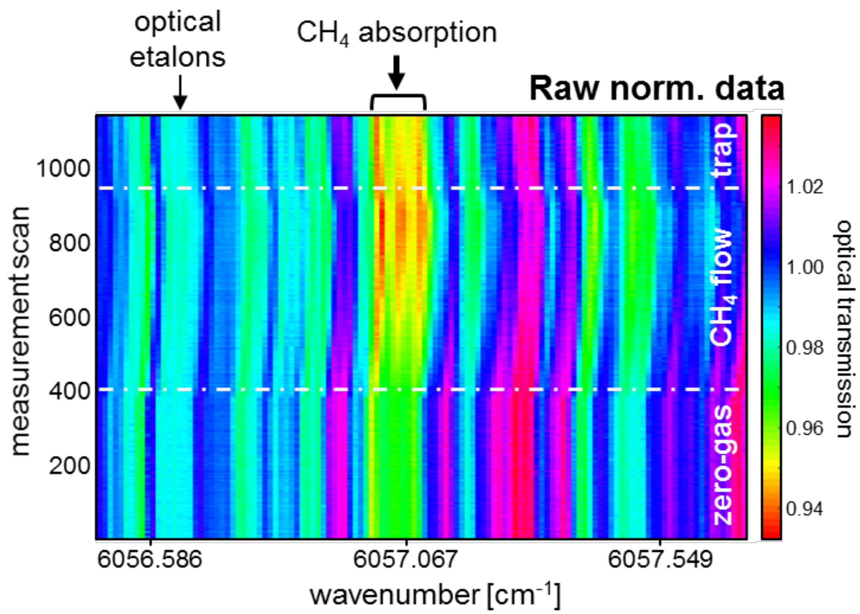
SPWAS performance comparable to conventional free-space TDLAS systems

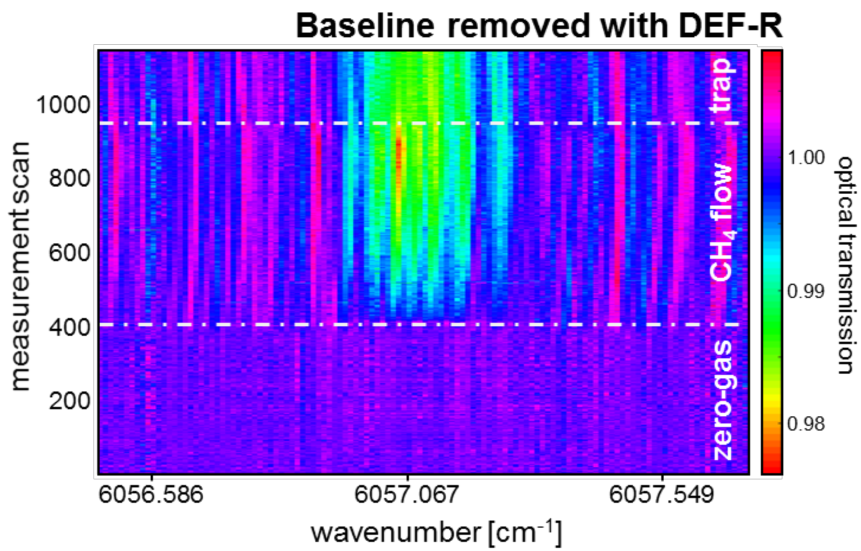
Adaptive spectral retrieval for etalon mitigation





Spectral retrieval during CH_4 flow measurement





Controlled CH_4 release:

- Three stage flow procedure for real-time CH_4 concentration variation:
  1. Zero-gas / ambient laboratory (seal chamber)
  2. Controlled CH_4 release (2.5 vol. % cylinder)
  3. Arrest flow, seal chamber for gas trap
- Significant etalon drift during gas switching

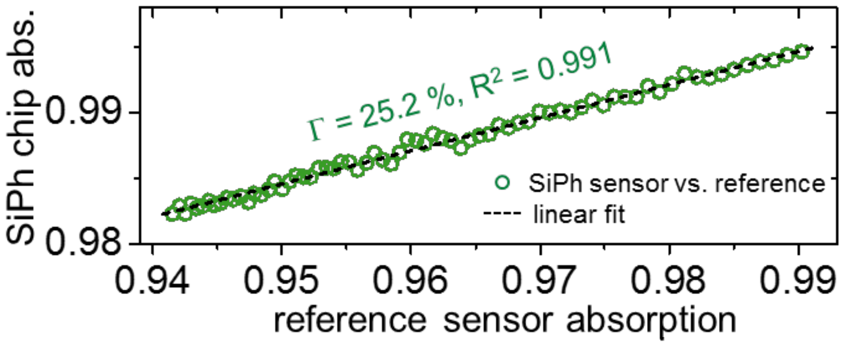
The impact of Dynamic Etalon Fitting:

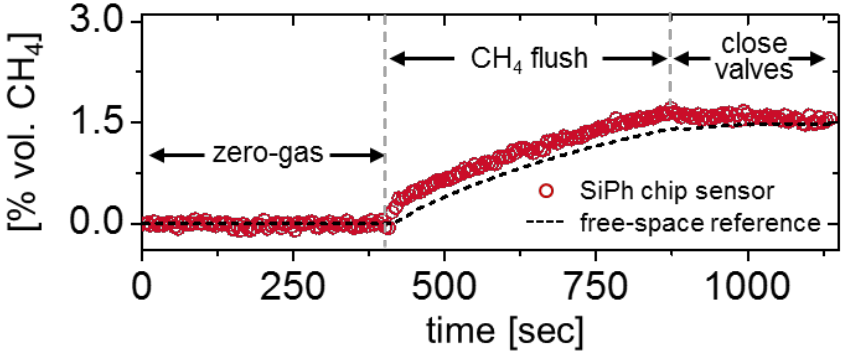
- Initial zero-gas spectral acquisition to provide a nominal baseline for adaptive etalon removal
- Visible spectral enhancement of CH_4 R(4) transition (at 6057.1 cm^{-1}) with DEF-R
- Significantly enhanced visibility of CH_4 flow stages, and corresponding improvement of CH_4 concentration retrieval

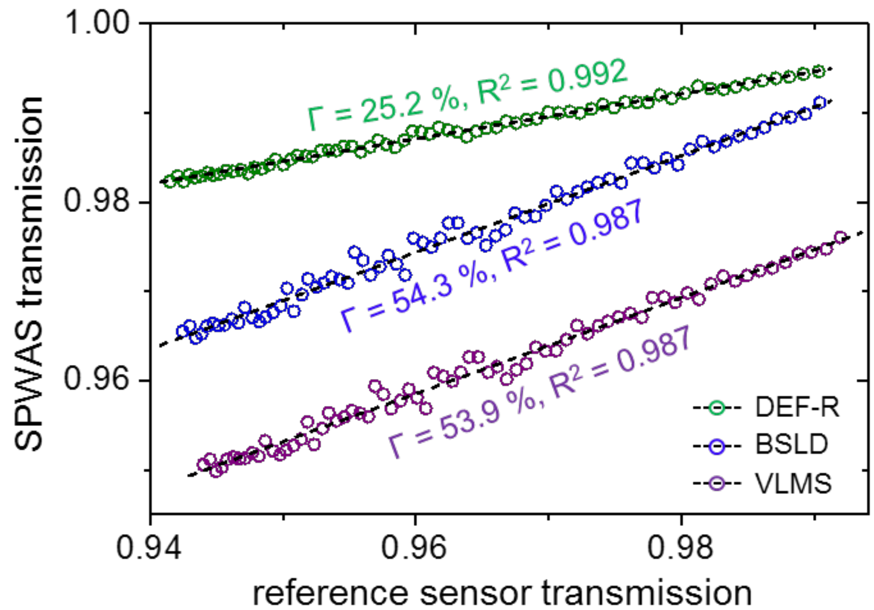
SPWAS accuracy validation using DEF-R

CH_4 concentration retrieval via DEF-R:

- CH_4 retrieval from 3-stage flow measurement
- Good agreement with free-space reference; minor deviations due to spatial nonuniformity of gas flow within environmental chamber
- Concentration correlation during CH_4 flush provides experimental confinement Γ = 25.2 %



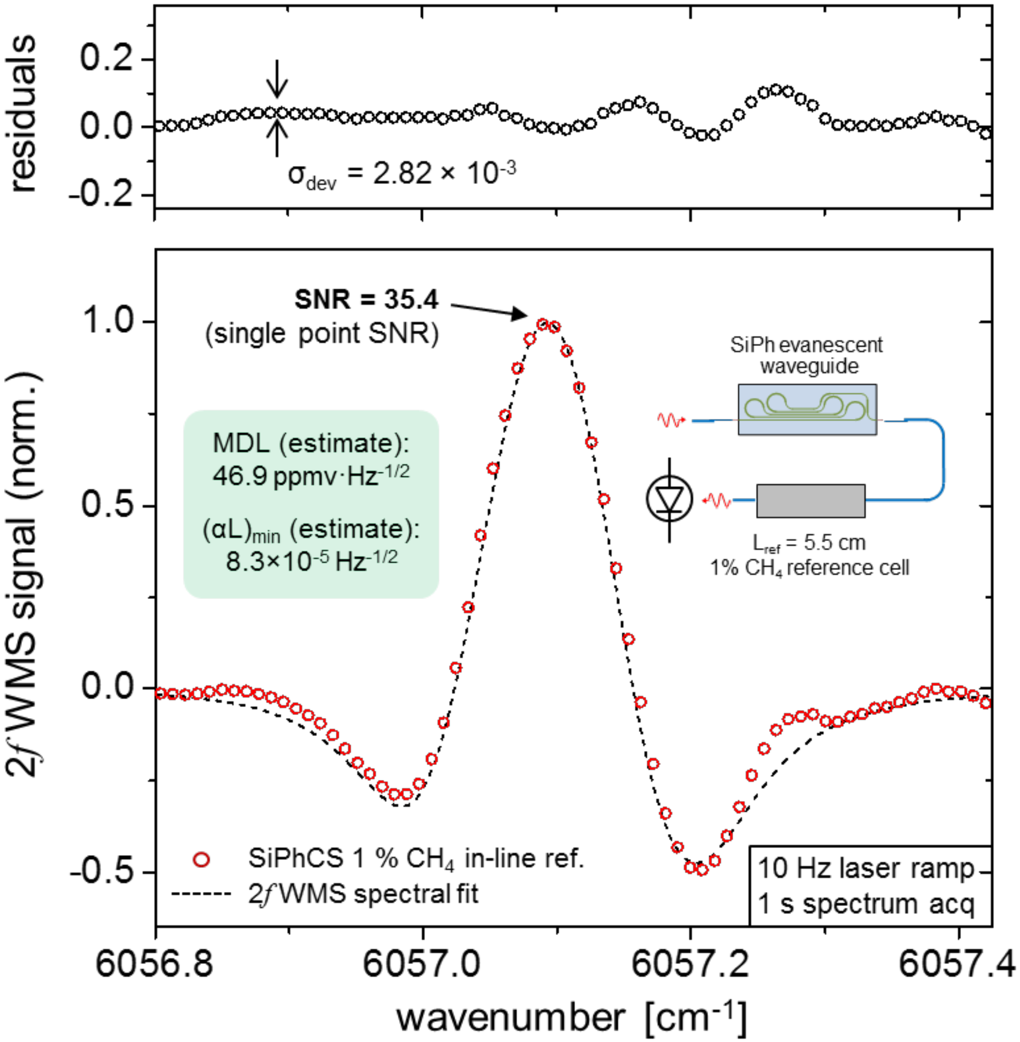




Necessity of adaptive fringe removal:

- Concentration correlation of SPWAS to free-space reference shows true confinement factor only for DEF-R
- VLMS and BSLD susceptible to etalon drifts and accuracy offsets
- Necessary for TDLAS on a silicon platform due to high thermo-optic coefficient (1.8×10^{-4} K^{-1})

Preliminary demonstration of on-chip WMS



Initial demonstration of Wavelength Modulation Spectroscopy (WMS):

- In-line reference cell (5.5 cm, 1 vol. % CH_4)
- 10 cm waveguide length (Γ = 25 %) $\rightarrow$ L_{eff} = 2.5 cm
- $2f_L$ demodulation with f_L = 10.2 kHz laser modulation frequency (near opt. $\Delta\nu_{mod}$)
- 10 Hz laser ramp for line-scanning
- $2f_L$ WMS LMS fit + residual noise analysis

Min. fractional absorption:

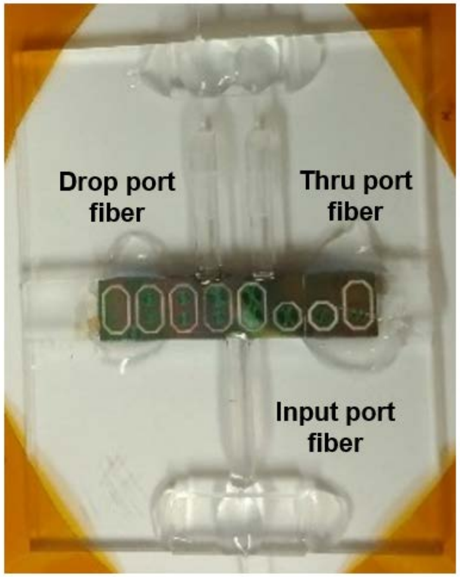
$(\alpha L)_{min}$ = 8.3×10^{-5} $Hz^{-1/2}$

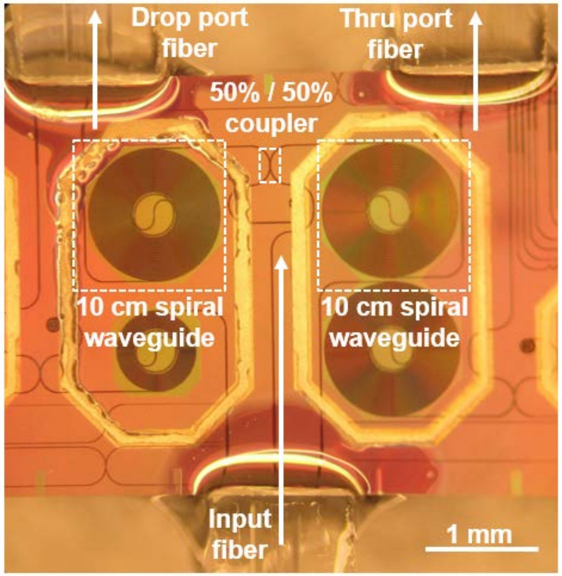
- Sensitivity estimate limited by fringe drifts during gas handling procedures
- optimize modulation depth / fringe dither for rejection of dominant fringe component(s)

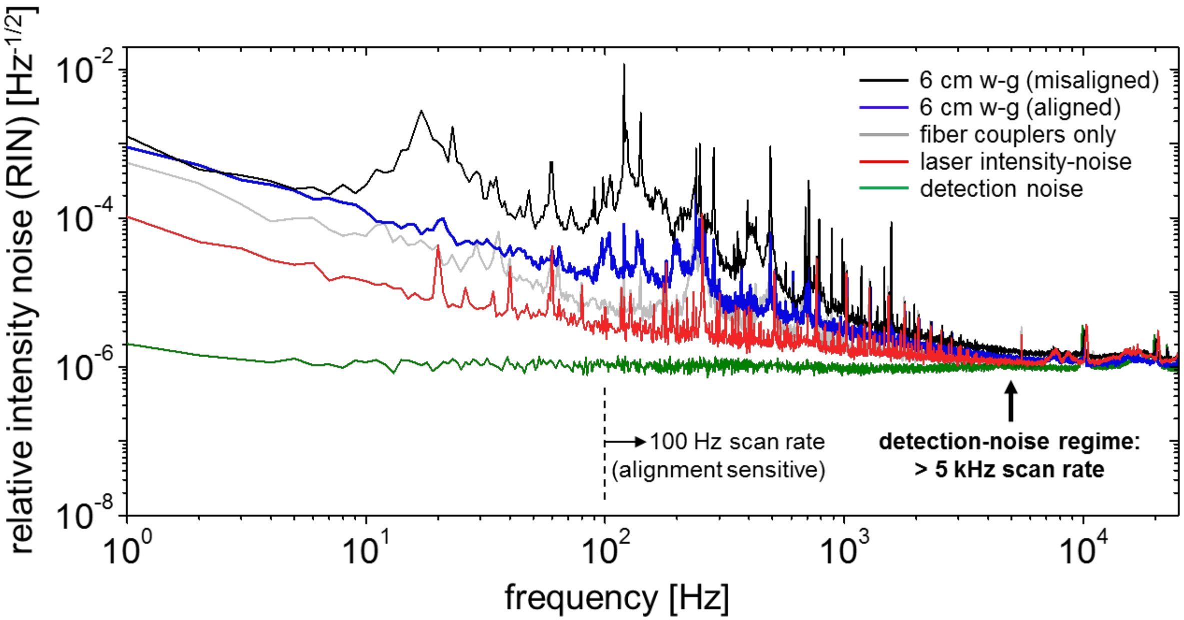
Packaging and improved detection sensitivity

SPWAS packaging and design:

- First-generation optical packaging using fiber-pigtailed waveguide attachments
- Compact SPWAS form factor for outdoor field testing
- Simultaneous measurement of through (sample) and drop (reference) ports
- Longer path length for next generation samples: waveguides up to 60 cm







Mechanical considerations:

- Bench-top mechanical alignment via lensed fibers introduce significant low-frequency noise
- Imposes stringent data sampling requirements due to high ramp rate

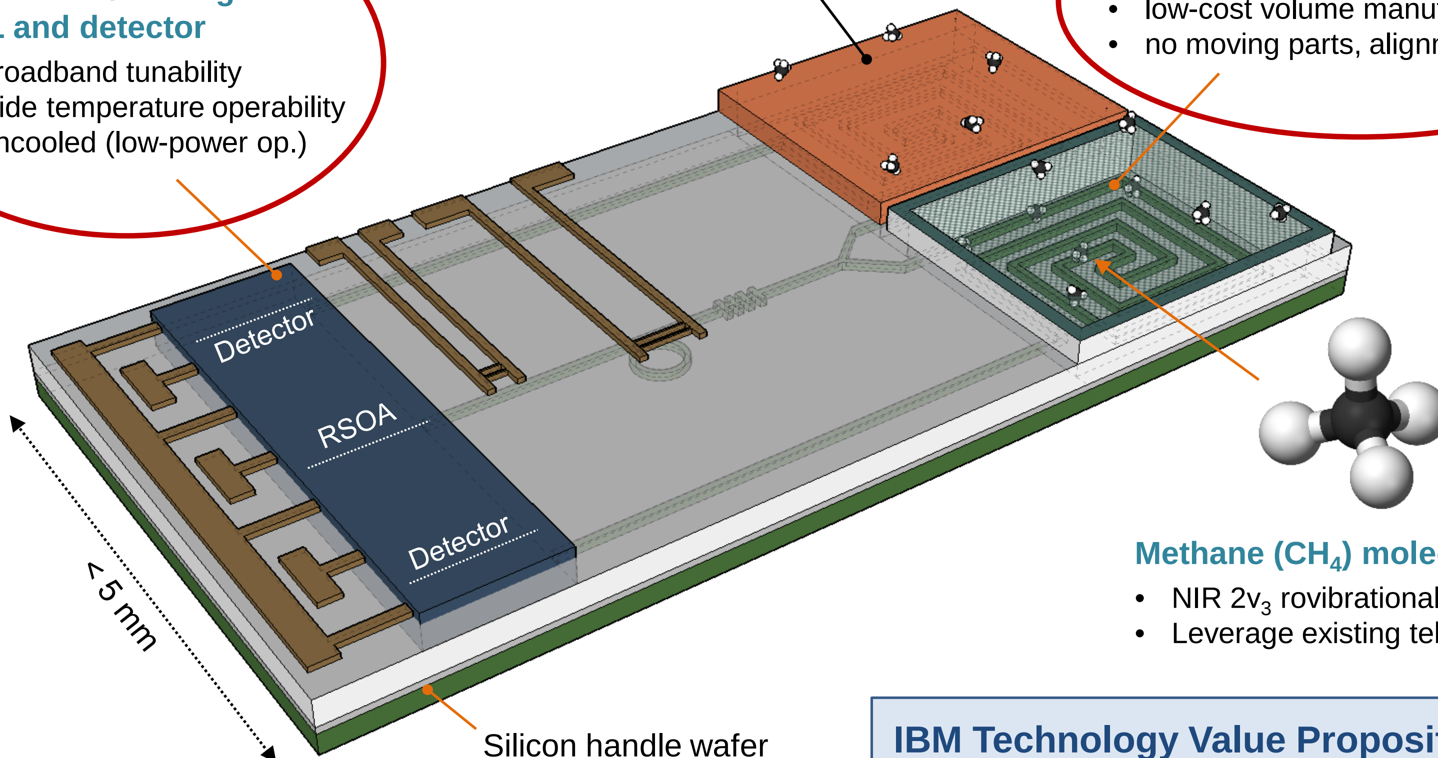
Optical fiber-attach for compact form factor and improved sensitivity

Integrated silicon photonic chip sensor

Hybrid III-V/Si Integrated ECL and detector
- broadband tunability
- wide temperature operability
- uncooled (low-power op.)

On-chip reference CH_4 cell
- on-chip self-calibration
- autonomous long-term accuracy

Waveguide confined optical path
- low-cost volume manufacturing
- no moving parts, alignment-robust



Methane (CH_4) molecule
- NIR $2\nu_3$ rovibrational band (1651 nm)
- Leverage existing telecom technology

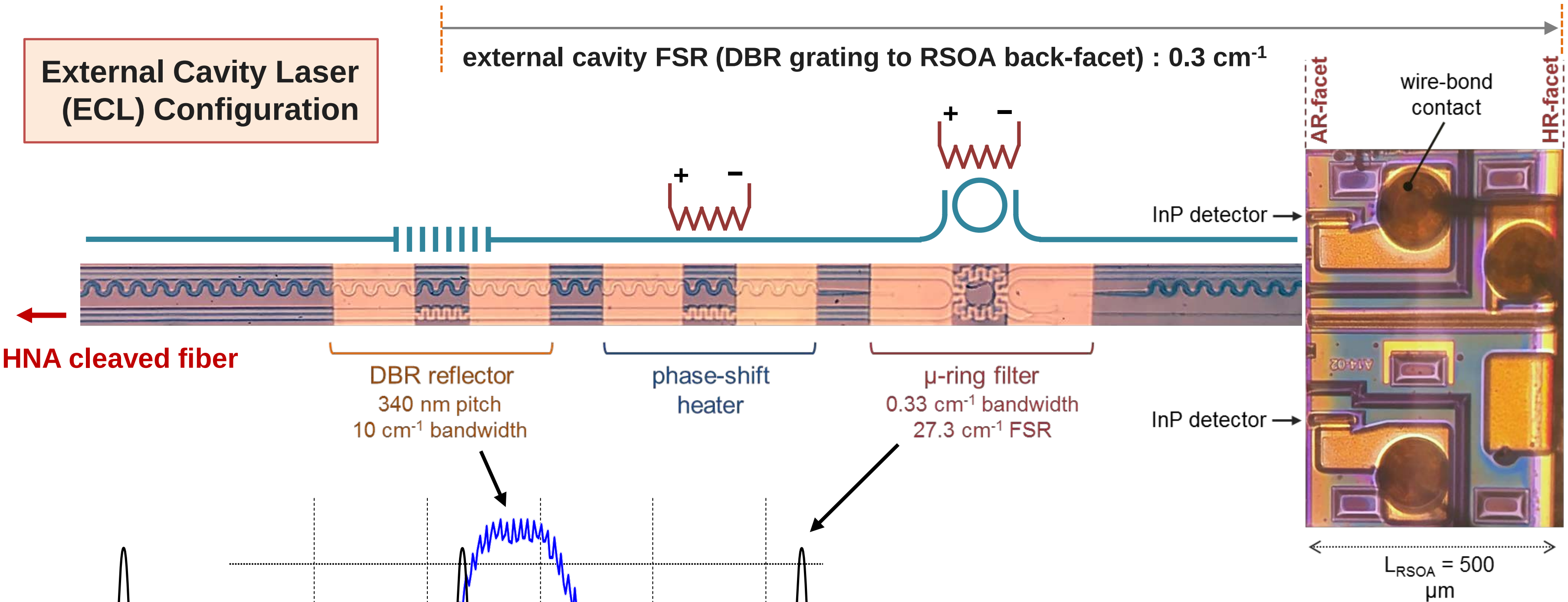
ARPA-E Design Target: 6 scfh CH_4 leak on 100 m^2 well pad within 18.25 days (90 % confidence level) with 1 m^2 spatial resolution

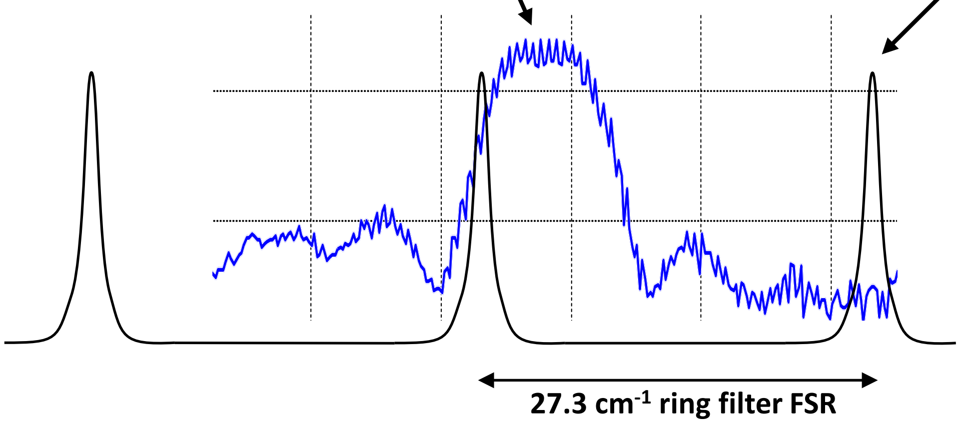
→ **Sensitivity Target: 10 ppmv · $Hz^{-1/2}$**

IBM Technology Value Proposition:
- Broadband TDLAS with molecular specificity
- Low volume cost (< 250 USD / sensor)
- Low power consumption
- Leverages CMOS compatible volume manufacturing

Hybrid III-V/Si broadband ECL development

External Cavity Laser (ECL) Configuration





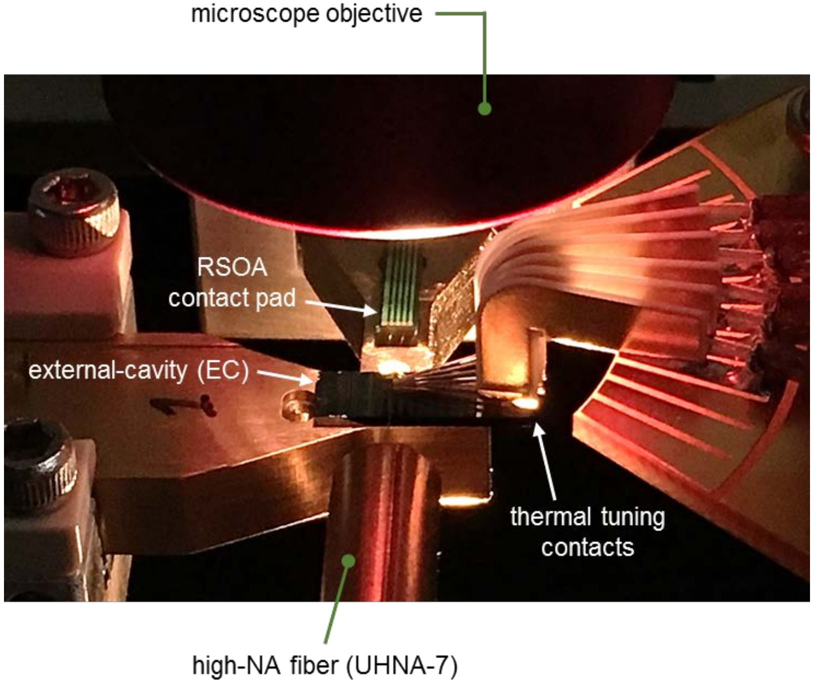
Lasing requires spectral alignment of one ring resonance with a longitudinal cavity mode within the DBR pass-band

- **Demonstrate single mode operation near 1650 nm**

Benchtop ECL demonstration:

- III-V reflective SOA (RSOA) provides round-trip gain
- Laser feedback cavity: DBR reflector to HR-coated RSOA back-facet
- Compensation for manufacturing tolerances and ambient temperature drift

Hybrid III-V/Si broadband ECL development

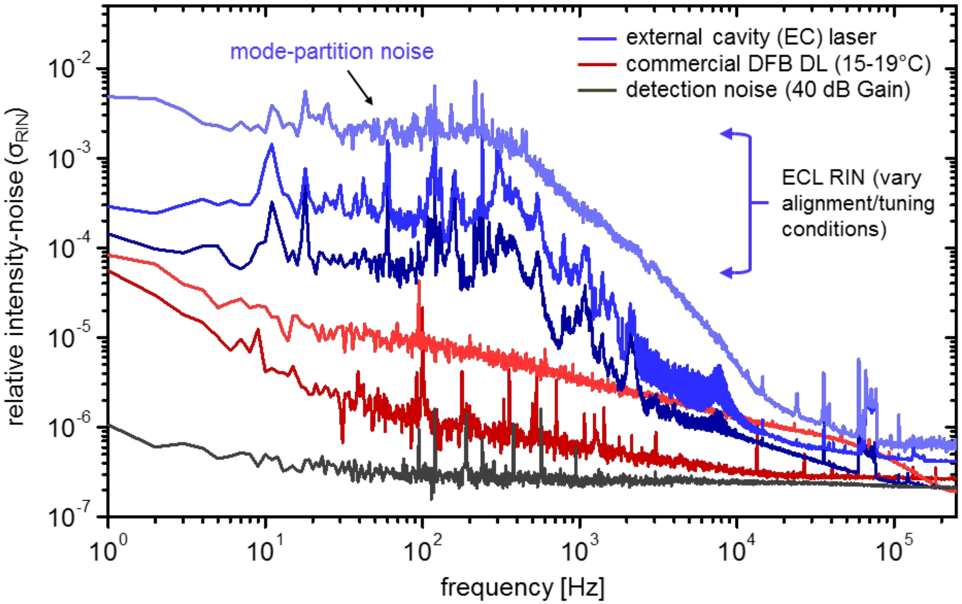


Benchtop ECL configuration:

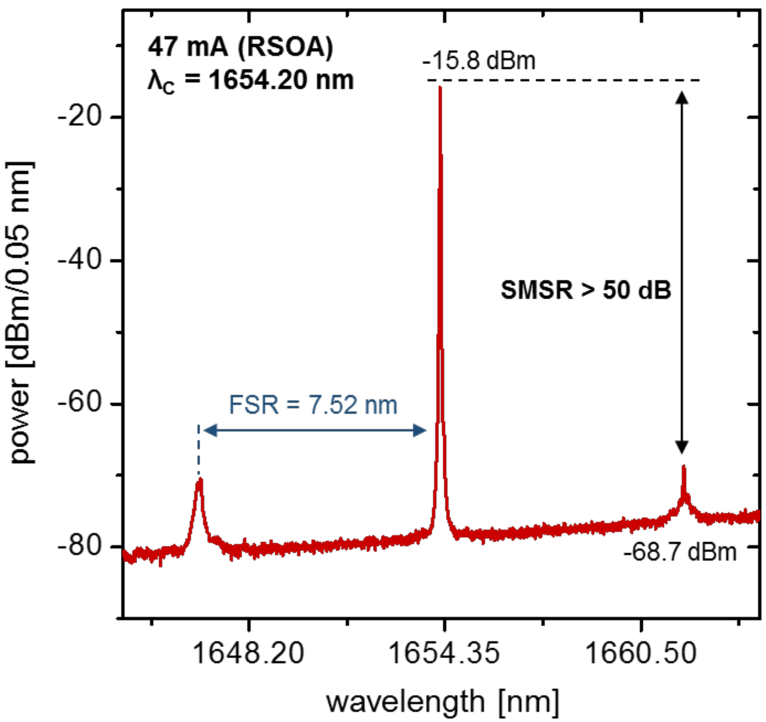
- RSOA facets AR coated for n = 1.48 (front) and HR-coated (back)
- Index matching gel between EC and RSOA interface
- Optical amplification at 1660 nm ± 20 nm
- Silicon external cavity (EC) with internal DBR (~ 2 nm)
- RSOA and HNA fiber mounted on piezo-actuated 6-axis stages for optical alignment

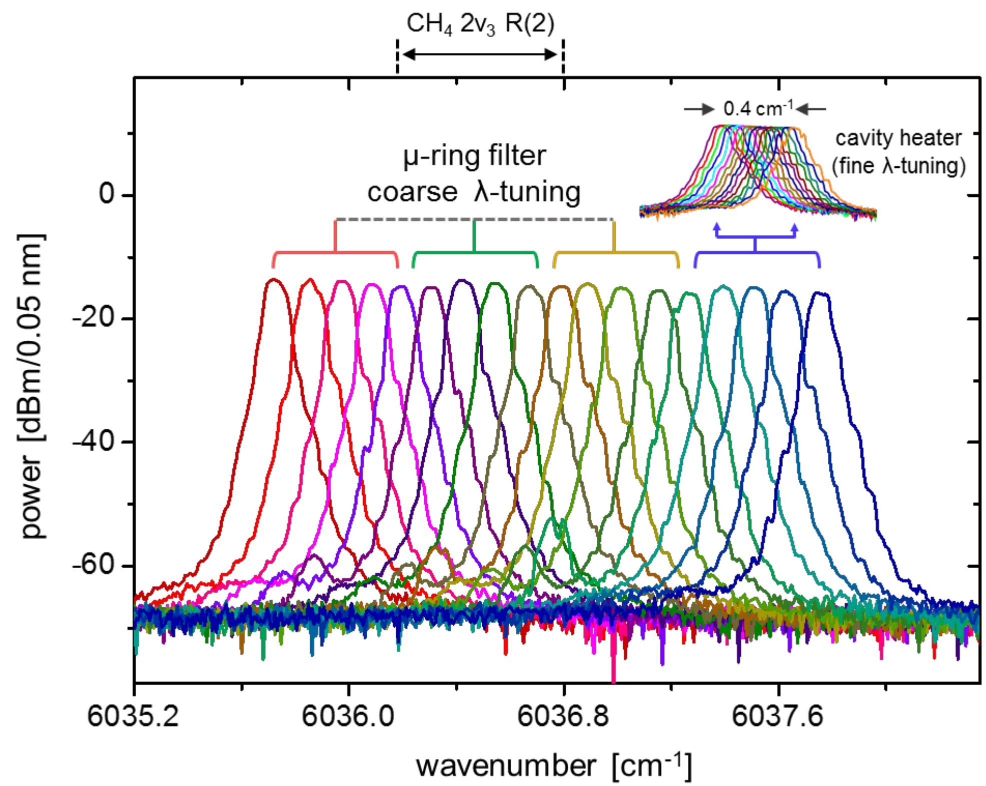
ECL RIN at TDLAS ramp frequencies:

- ECL relative intensity noise (RIN) measured at varying levels above lasing threshold
- Comparison with a commercial U-band telecom diode laser: comparable performance > 10 kHz
- Low frequency noise – primarily mechanical alignment instabilities
- Q4 2017 – anticipate integrated ECL on a chip



Single-mode broadband ECL tunability



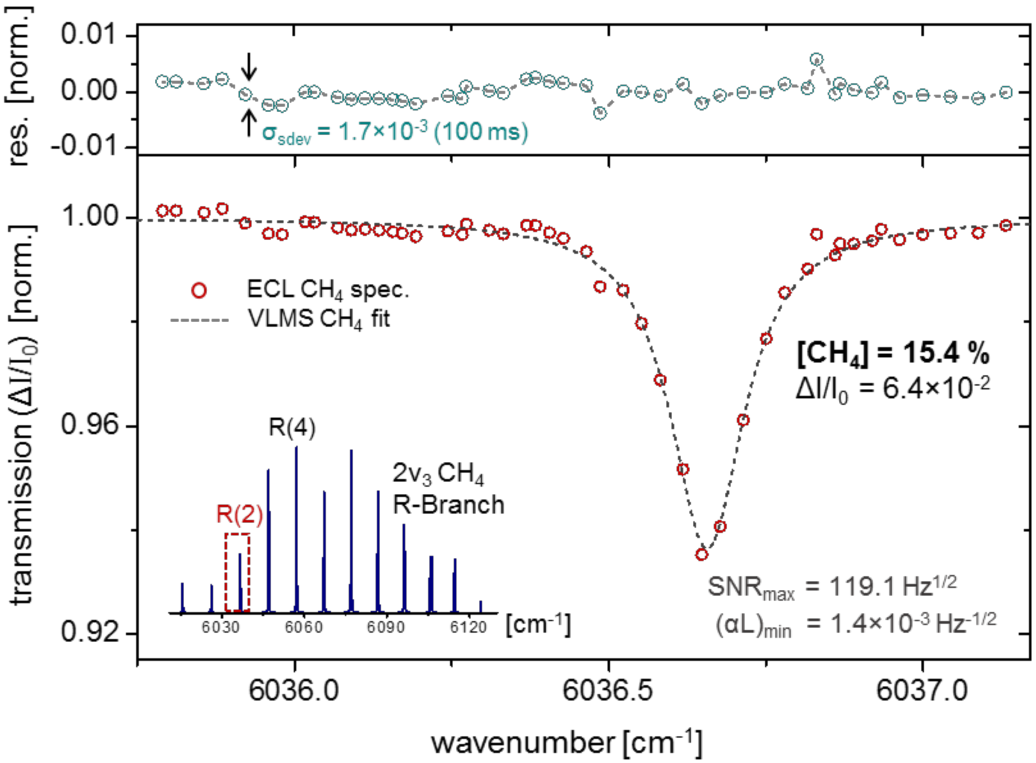


- Thermally tunable intracavity μ-ring and cavity phase shifter select longitudinal mode
- Single-mode operation ~ 1650 nm, with over 50 dB side-mode suppression ratio (SMSR)
- Other λ accessible via DBR pitch variation
- Up to 1 mW ECL output power (output fiber)

Validating broadband ECL tunability:

- Performed > 2 nm mode-hop free tuning (manual)
- Coarse tuning steps using intracavity μ-ring filter, and fine-tuning via thermal cavity phase shifter
- Wavelength suitable for targeting CH_4 $2v_3$ R(2) line at 1656.5 nm (6057 cm^{-1})

ECL spectroscopy of CH_4



ECL for CH_4 spectroscopy:

- Manual tuning of intracavity μ-ring and thermal phase shifter across CH_4 R(2) line at 6036.7 cm^{-1} (1656.5 nm)
- In-line CH_4 reference cell L = 3.0 cm with parallel path for baseline power normalization
- R(2) line below 50 % R(4) transition line-strength

Preliminary sensitivity analysis:

- VLMS: Extract 15.4 % CH_4, consistent with results with commercial DFB laser
- 100 ms acquisition time per spectral point: → sub-Hz effective ramp rate
- Susceptible to low-frequency noise contribution from mechanical instability

Min. fractional absorption:

$$(\alpha L)_{min} = 1.4\times10^{-3}\ Hz^{-1/2}$$

Near-term developments:

1. **Initial demonstration of custom DAC/ADC for high-frequency ECL ramping**
2. **Hybrid III-V/Si integration on a single chip for mitigation of low-frequency RIN**

Integrated silicon photonic chip sensor

Hybrid III-V/Si Integrated ECL and detector
- broadband tunability
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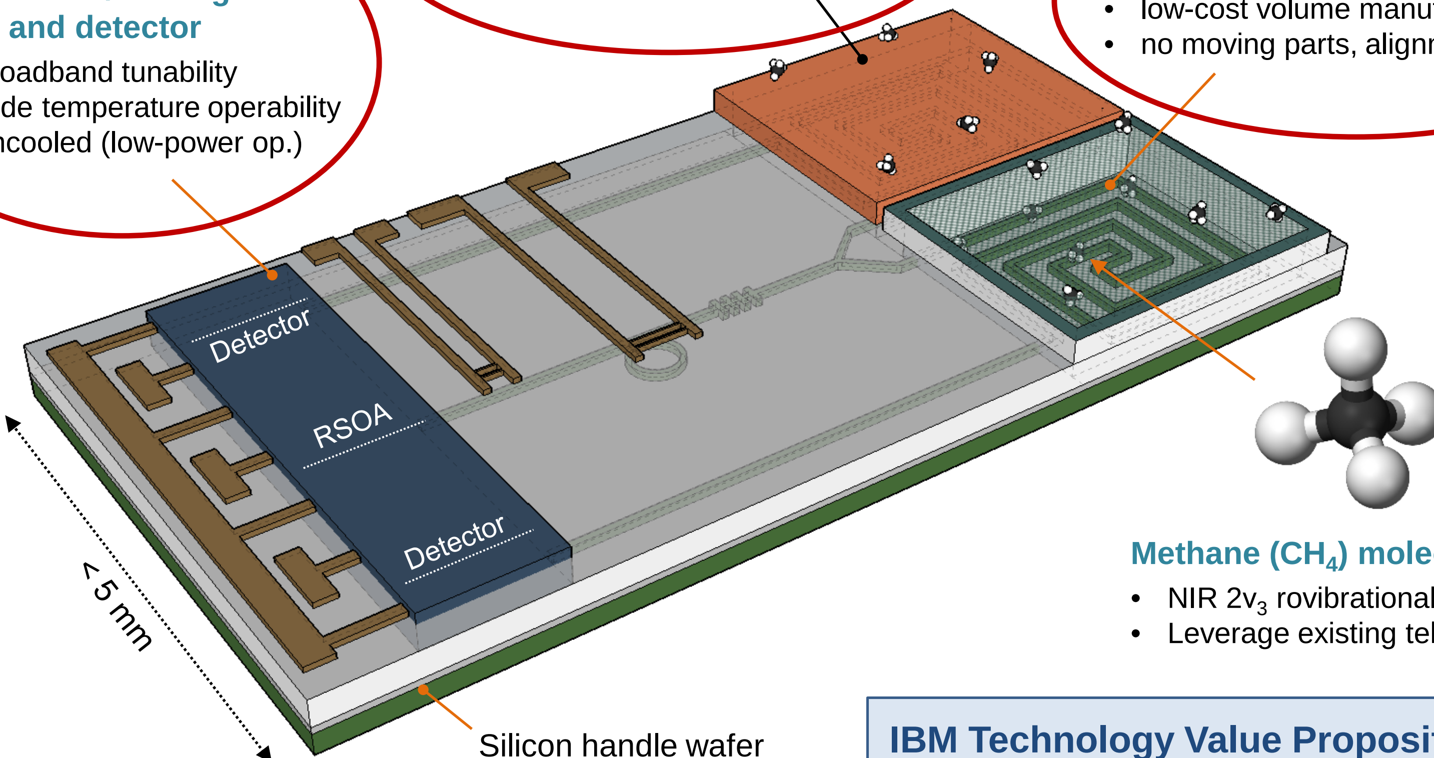

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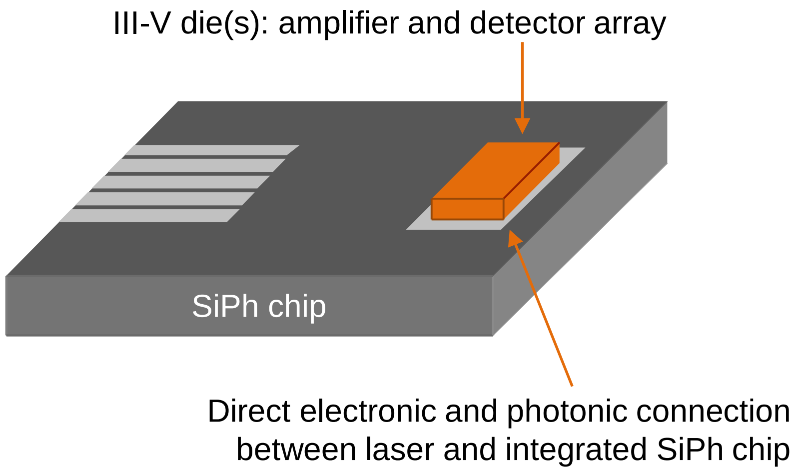
III-V gain / detector chip and reference lid attach

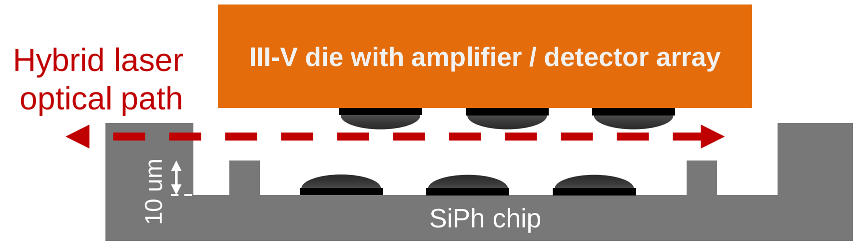
IBM differential:

- Full automation in 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 reflow surface tension aligns III-V chip
- Superior thermal characteristics

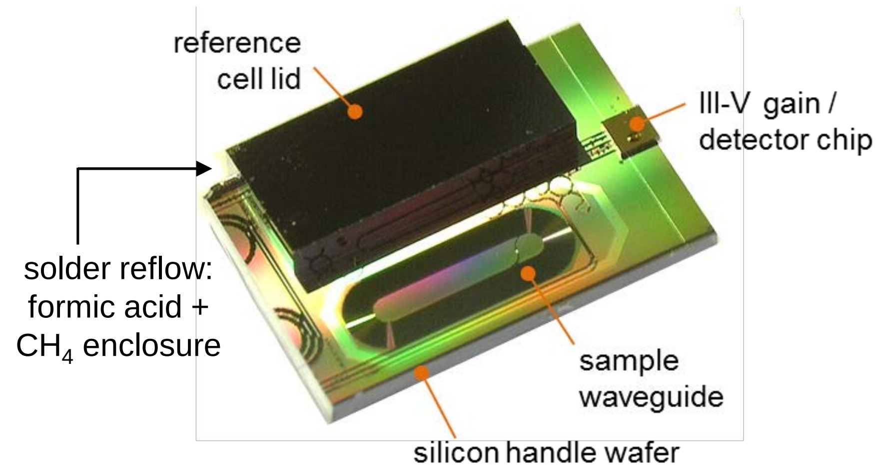




Pick and place, then anneal to reflow

Key Challenge: sub-micron tolerances for passive alignment

Functional Prototype: End of 2017



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

Concluding remarks

On-chip SPWAS for CH_4 spectroscopy:

- Functional demonstration of benchtop Silicon-photonic waveguide absorption sensor (SPWAS) for ambient CH_4 sensing
- $(\alpha L)_{min} = 3.3 \times 10^{-5}\ \mathrm{Hz}^{-1/2}$, consistent with conventional TDLAS systems
- Adaptive dynamic etalon fitting-routine (DEF-R) for reduction of fringe noise and improved long-term accuracy
- Pathway to SPWAS integration for mechanical noise reduction

Demonstration of a broadband tunable actively aligned ECL:

- ~ 1 mW output power, 2 nm tuning range, > 50 dB SMSR
- Preliminary spectroscopy of CH_4 R(2) transition at 1656.5 nm
- Partially integrated prototype expected at the end of 2017

Pathway towards compact, low-power, low-cost sensor nodes to facilitate large-scale deployment of continuously monitoring sensor networks

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