Multi-Gas Sensors for Enhanced Reliability of SOFC Operation

DOE/NETL Cooperative Agreement: DE-FE0031653

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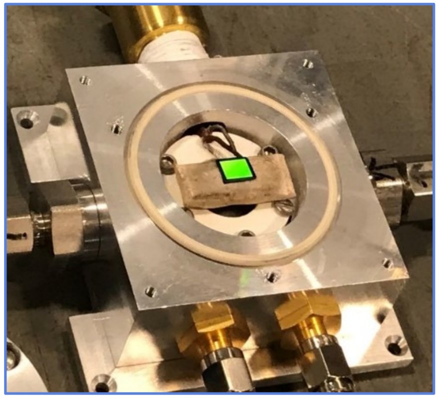


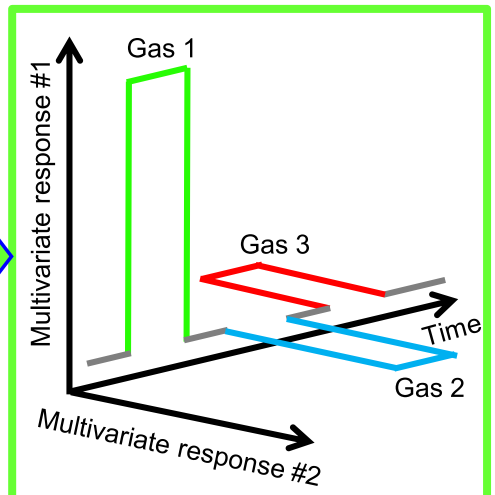
Background

Real-time knowledge of several anode tail gases:

- will allow control of efficiency of reforming process in the SOFC system
- will deliver a lower operating cost for SOFC customers

Status quo:
Mature traditional analytical concepts

Performance need:
Multi-gas discrimination



Example of benchmark instrument for pilot-scale optimizations:

State-of-the-art system (Rosemount Analytical, Model X-STREAM) with multiple detectors:

- non-dispersive infrared detectors for CO, CO_2, and CH_4 gases and high levels of H_2O vapor,
- thermal conductivity detector for H_2,
- capacitance detector for low levels of H_2O vapor

Required periodic recalibration to correct for drift: 2% per week (~100% drift per year)

Unmet need for real-time monitoring of several gases with affordable unobtrusive, cost-effective solution

Project goal and objectives

The project goal is:
to build gas sensors for in situ monitoring of several gases of SOFC systems and to perform their long-term field validation tests.

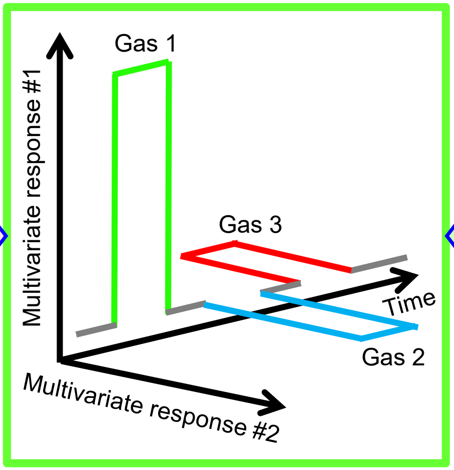
The project objectives are:
(a) to achieve multi-gas monitoring capability with a single multivariable sensor,
(b) to sustain this performance between the maintenance cycles of the SOFC system.

Project period of performance: 08/17/2018 through 08/16/2020

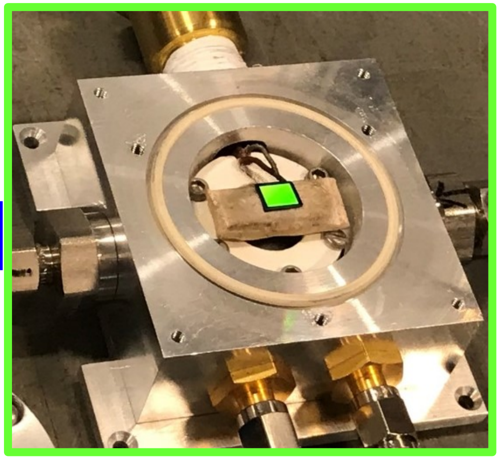
Focus on achieving multi-gas monitoring with a single multivariable sensor

Status quo:
Mature traditional instrumentation concepts

Performance need:
Multi-gas discrimination



Our approach:
Multivariable gas sensors

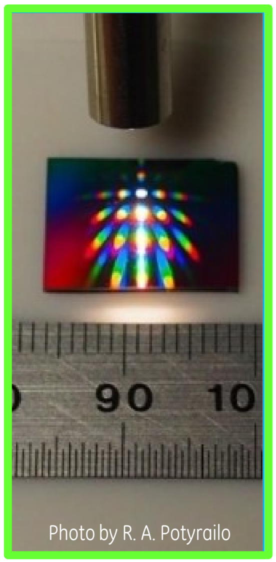


Solving existing need for real-time monitoring of several gases with affordable unobtrusive, cost-effective solution

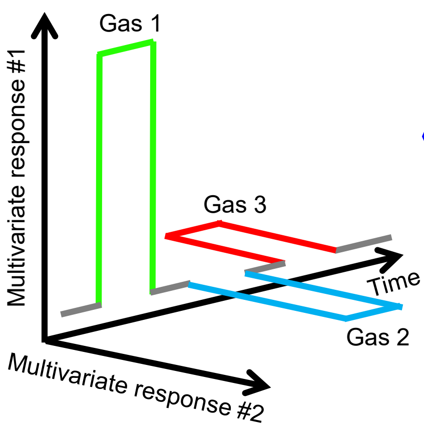
Technical approach

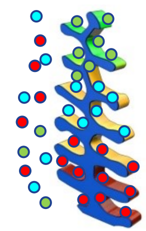
Multi-gas detection in SOFC anode tail gases using bio-inspired multivariable photonic sensors

Our approach:
Multivariable gas sensors



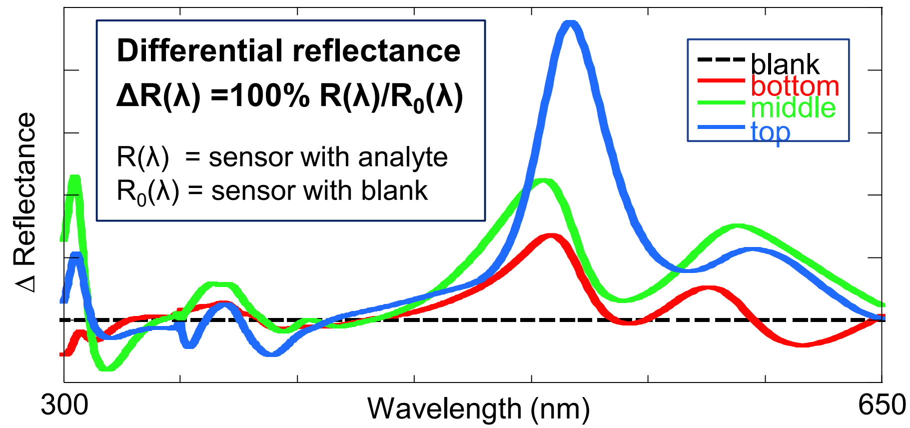
Performance need:
Multi-gas discrimination





Design rules for gas-selectivity control

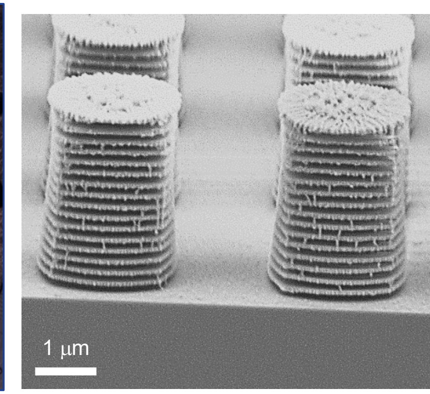
- Spatial orientation of surface functionalization
- Chemistry of surface functionalization
- Extinction and scattering of nanostructure



- Implement bio-inspired multivariable gas sensors for multi-gas quantitation at high temperatures
- Perform laboratory optimization followed by field validation

Potyrailo et al. *Nature Photonics* **2007**
Potyrailo et al., *Proc. Natl. Acad. Sci. U.S.A.* **2013**
Potyrailo et al. *Nature Communications* **2015**
Potyrailo, Carpenter, et al., *J. Opt.*, **2018**

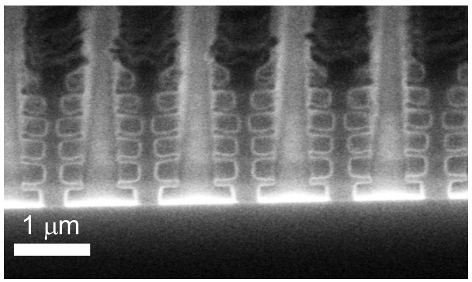
Learning from Nature

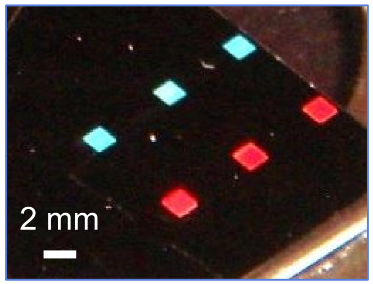


Bioinspiration –
new functionality, beyond Nature

High temperature

Potyrailo, Carpenter, et al., *J. Opt.*, **2018**

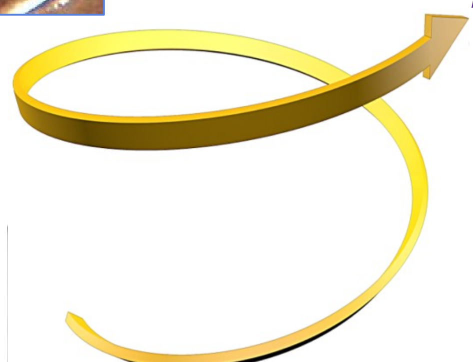


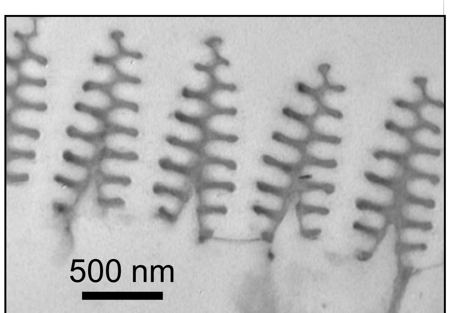


Biomimetics –
recreation of observed functionality

Room temperature

Potyrailo et al., *Nature Communications* **2015**



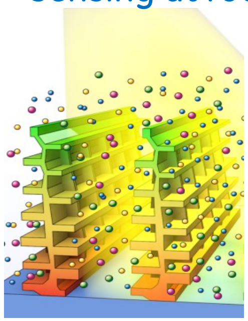


Biomimicry –
imitation of biological systems

Potyrailo et al. *Nature Photonics* **2007**
Potyrailo et al., *Proc. Natl. Acad. Sci. U.S.A.* **2013**

Advancing design rules of nanostructures for high temperature gas-sensing applications

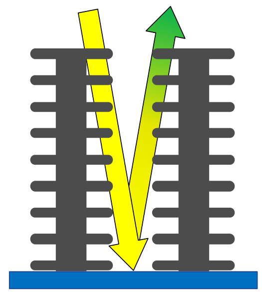
Prior learnings :
Sensing at room temperature



Polymeric nanostructure

Absorption and adsorption of vapors

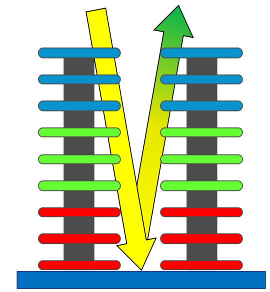
Prior learnings:
Sensing at high temperatures



Inorganic nanostructure

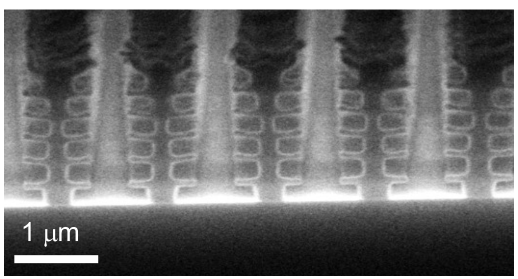
Catalytic surface reactions of gases

Focus of proposed project:
Selective H_2 and CO sensing

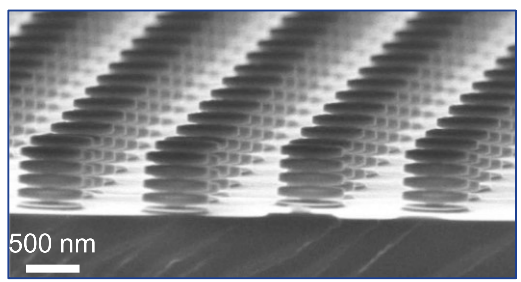


Multi-material inorganic nanostructure

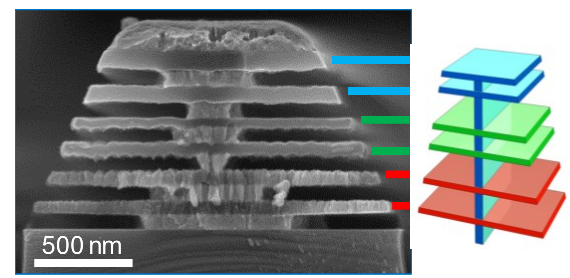
Catalytic surface reactions of gases



Potyrailo et al., *Nat. Commun.* **2015**

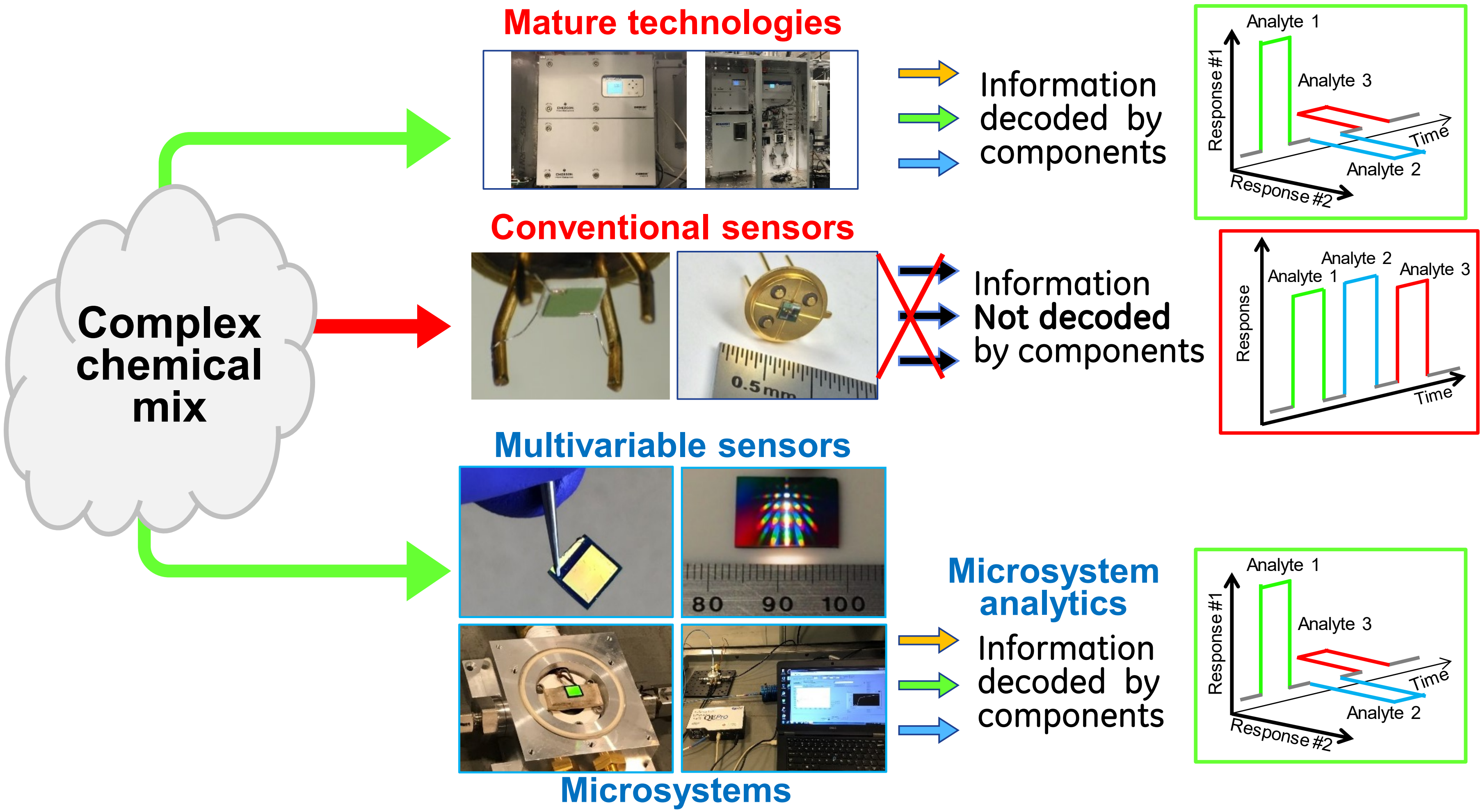


Potyrailo, Karker, Carpenter, Minnick, *J. Opt.*, **2018**



Potyrailo, *Chem. Rev.* **2016**

Sensors, microsystems, and microsystems analytics



Multivariable sensor: sensor with several outputs to detect diverse properties of ambient environment

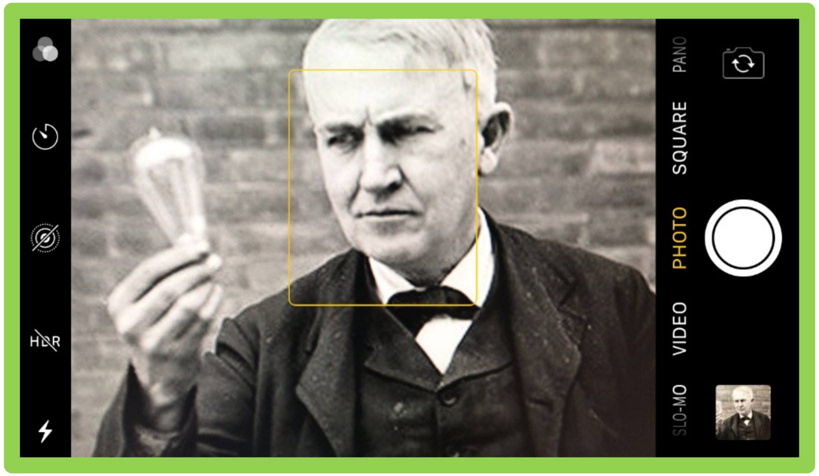
Microsystem: multivariable sensor with sensor-excitation and signal-processing units

Microsystem analytics: data-processing algorithms with feedback to sensor-excitation and signal-processing units

Software-driven boost of system performance in consumer products

Smart phones: digital zoom, brightness control

Smart phones: face recognition



Car driving modes

Tools for data analysis of multivariable sensors: machine learning, multivariate statistics

Supervised learning
Artificial neural network
Bayesian statistics
Case-based reasoning
Gaussian process regression
Gene expression programming
Group method of data handling
Inductive logic programming
Instance-based learning
Lazy learning
Learning Automata
Learning Vector Quantization
Logistic Model Tree
Minimum message length
Probably approximately correct learning
Random Forests
Support vector machines
Symbolic machine learning

Unsupervised learning
Expectation-maximization algorithm
Vector Quantization
Generative topographic map
Information bottleneck method
Self-organizing map
Association rule learning
Hierarchical clustering
Single-linkage clustering
Conceptual clustering
Cluster analysis
K-means algorithm
Fuzzy clustering

Semi-supervised learning
Generative models
Low-density separation
Graph-based methods
Co-training

Reinforcement learning
Temporal difference learning
Q-learning
Learning Automata

Deep learning
Deep belief networks
Deep Boltzmann machines
Deep Convolutional neural networks
Deep Recurrent neural networks
Hierarchical temporal memory

Wikipedia.org

Our machine learning tools

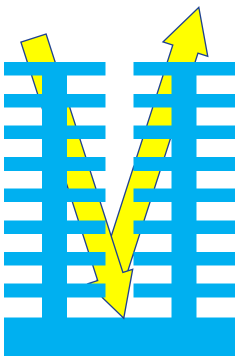
- Principal component analysis (PCA)
- Discriminant Analysis (DA)
- Artificial Neural Network (ANN)
- Hierarchical cluster analysis (HCA)
- Support Vector Machines (SVM)
- Independent Component Analysis (ICA)
- Partial least squares (PLS) regression
- Principal Component Regression (PCR)

Potyrailo *Chem. Rev.* **2016**

Increasing role of data analytics in high performance sensing

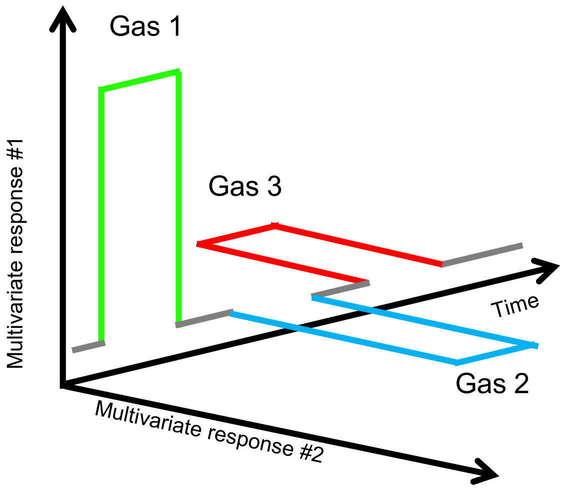
Project technical tasks

Fabrication of optical transducer



Task 2

Lab validation with analytes and interferences



Task 3

Field validation and benchmarking with analytes and interferences

Task 4

Discussion

Q & A