Water Resource Protection with *in-situ*, Raman Sensors for Real-Time Assessment of Emergent and Emerging Contaminant Mixtures

Mark A. Nanny[1,2] , Binbin Weng[3]
Joseph M. Suflita[2,4], Rouzbeh Moghanloo[5]

The University of Oklahoma

[1]School of Civil Engineering and Environmental Science
[2]Institute for Energy and the Environment
[3]School of Electrical and Computer Engineering
[4]Dept. of Microbiology and Plant Biology
[5]School of Petroleum and Geological Engineering

Protecting Water Resources from Regulated and Emerging Chemical Contaminants:

Current Challenges, Infrastructure Needs, and Desired Outcomes

Current Challenges:

- **Managing Regulated Chemical Contaminants**
  - Lack of efficient and economic analytical methodology
  - Need for real-time monitoring response
  - Need for spatial and temporal sampling flexibility
    - Point source vs. non-point source
    - Continual monitoring over large spatial scale
  - Data quantity and quality
    - Rapid assessment, accurate modeling and prediction
- **Identifying / Characterizing Emerging Chemical Contaminants**
  - Need for new analytical methodology
    - Robust, *in-situ*, remote, sensitivity, simple, networked
  - Threats posed by contaminant degradation products and chemical mixtures
  - Impacts on biological activity and public health

Infrastructure Needs:

1. DETECTION / MONITORING

- **Microchip Raman Sensors**
  - *In-situ* and remote
  - Real-time response
  - Quantitative and analyte specific / selective
  - Adaptable as a sensor network over large spatial scales
    - Point source to water shed scale
  - Operate in diverse aquatic environments

2. IMPACT CHARACTERIZATION / ASSESSMENT

- **Validation, Standardization and Quantification of Sensor**
  - Optimize sensor sensitivity and resolution for contaminant characterization in complex mixtures
  - Detect abiotic and microbial transformations
- **Sensor Environmental Baseline Response**
  - Determine a definition of "safe" vs. "unsafe" contaminant levels
- **Calibration Sensor Response to Biological Activity**
  - Microbial respiration for identifying contaminants amenable to biodegradation
- **Sensor as a remote, *in-situ* "Real-Time" Hazard Assessment Monitor**

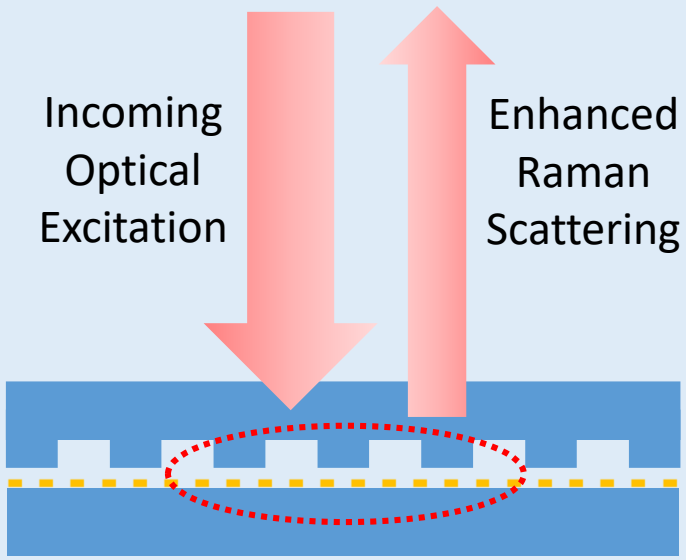
3. MODELING / PREDICTION

- **Real-time coupling with sensor network**
  - Continual updating of monitoring data
- **Real-time modeling of contaminant transport and fate**
  - Concentration and mass flux
  - Degradation rates
- **Simulation / Prediction Capability**
  - "What if" scenarios
  - Evaluate remediation responses
  - Prediction of end of threat
- **Adaptive, Intuitive Interface for Resource Managers, Emergency Responders, and Practitioners**

Desired Outcomes:

- **Informed Response to Contamination Threat**
  - Informed and based upon real-time data
- **Stakeholder Ease of Use and Interpretation**
  - Individuals – private wells
  - Industry – monitor discharges
  - Municipal – drinking water treatment and waste water reclamation
- **Effective analytical tool to develop regulatory assessments**
- **Applications of Technology for Water Resource Management**
  - Monitor contaminant plumes
  - Sentinel systems for protecting water quality
  - System for detecting spillage or release of regulated compounds
  - Evaluation of contaminant remediation effectiveness

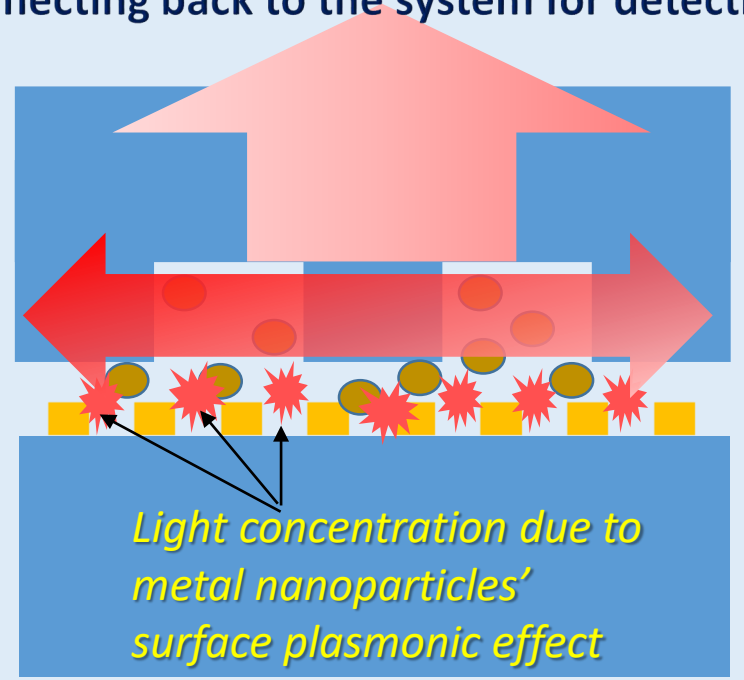
Schematic of the proposed sampling/sensing integrated micro-chip Raman sensor



Innovative chip-scale analyte sampling and Raman signal enhancing vessel device

Mechanism Explanation in Zoom-In Figure

Enhanced Raman Scattering Signal reflecting back to the system for detection



:Dielectric Lateral Grating.

:Gold or Silver Nanoparticles.

:Analyte in water solution.

Mechanism I: Guided Resonant Mode (GRM) Enhanced Raman Scattering by Dielectric Nano-Gratings;

Mechanism II: Surface Enhanced Raman Scattering (SERC) by Metal Nanostructures on the Interface.

Preliminary Results: Sampling/sensing integrated micro-chip Raman sensor

Dr. Binbin Weng

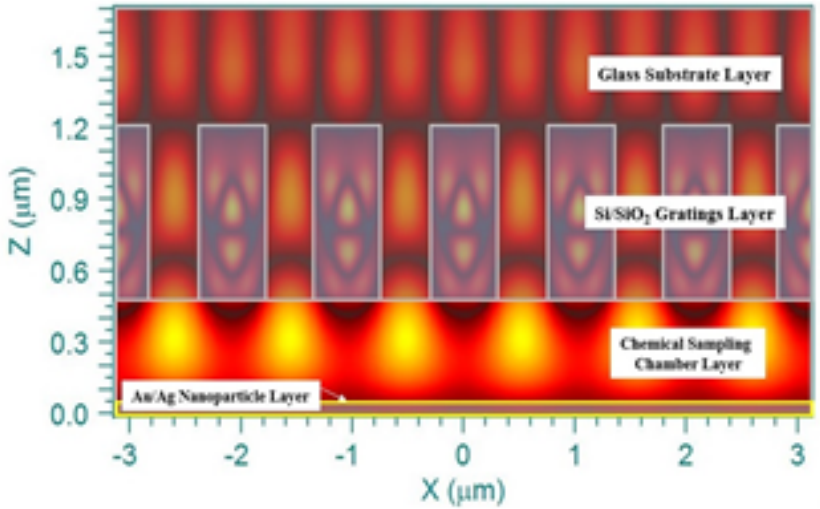


Figure 1. Preliminary simulation results: the spatial distribution of the total electric field of the modulated laser light at 1064 nm within the proposed PCW-SERS structure.

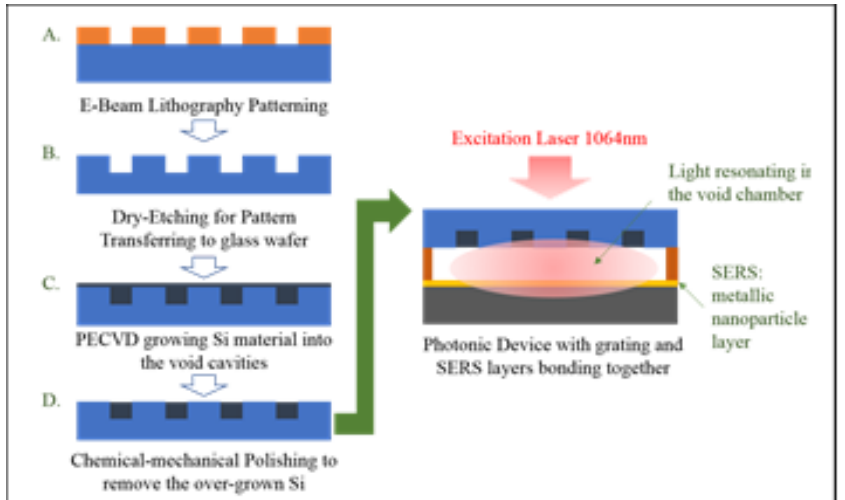


Figure 2. the schematic of the process flow to fabricate the PCW film and form a chamber with the SERS film.

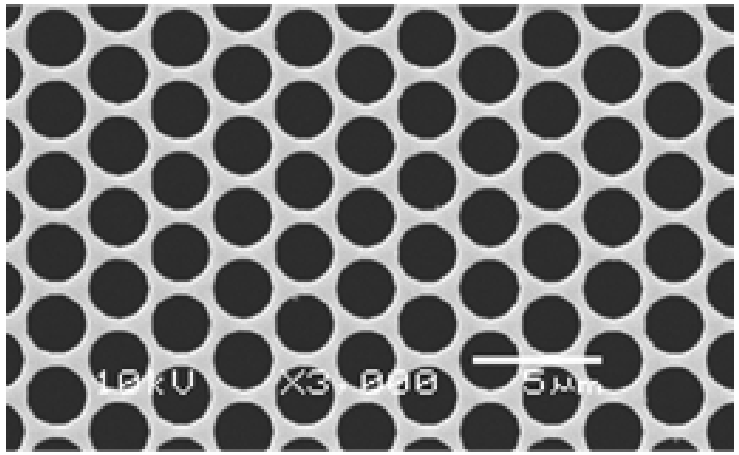
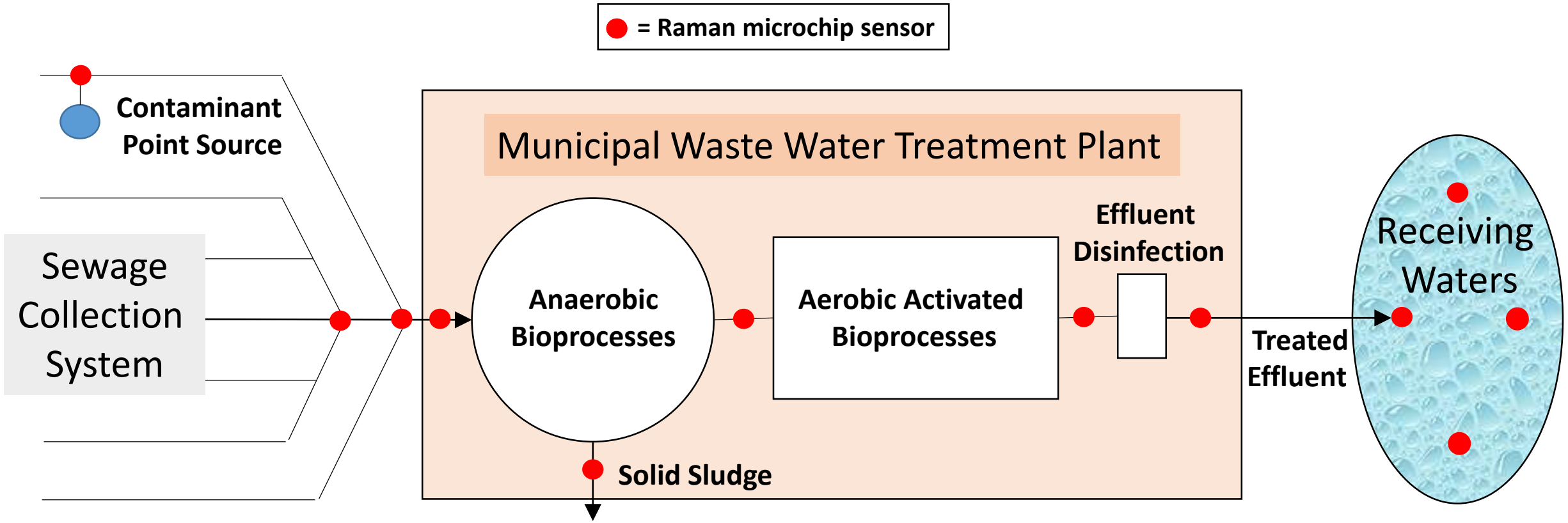


Figure 3. Top-view scanning electron microscopy image of a two-dimensional photonic crystal structure made from Si wafer.

Monitoring the Fate of Regulated Compounds and Contaminants of Emerging Concern in Municipal Waste Water Treatment Systems



- Control point-source releases
- Real-time monitoring for unexpected releases
- Real-time characterization of raw sewage contaminants

- Real-time monitoring of:
  - Contaminants entering / leaving WWTP
  - System performance
  - Formation of contaminant metabolites and disinfection by-products of concern
- Prevention of negative microbial impacts (anaerobic & aerobic) from unexpected contaminant pulses

- Sensor network to monitor contaminant transport & fate in aquatic environ.
- Water reuse management
- Protect public health & water quality

Sensor array deployment & application