



# Sandia National Laboratories

## Hydrogen Fuel and Infrastructure R&D Workshop

### *Fuel Cell & Hydrogen Energy Association*

November 15, 2018

Chris LaFleur

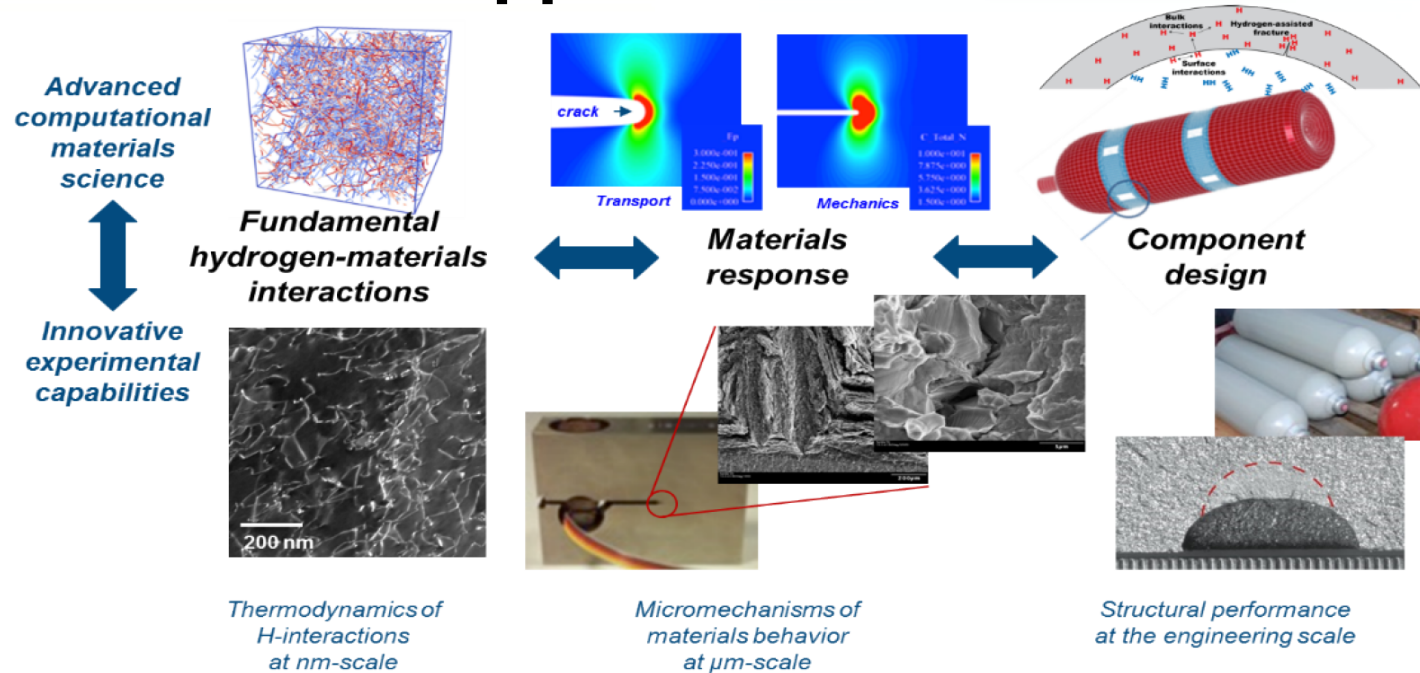
Joe Ronevich

SAND2018-XXXX PE

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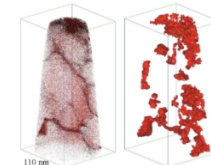
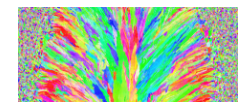
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# Developing a fundamental understanding of materials compatibility with H<sub>2</sub> starts from atoms and extends to applications



Sandia maintains unique capabilities to support research on *Hydrogen Effects on Materials*

- In situ mechanical testing ( $P > 100$  MPa (20 ksi) and  $230\text{K} < T < 400\text{K}$ )
- Long-term, high-pressure H<sub>2</sub> exposure
- Computational materials science expertise
- Full-suite of state-of-the-art materials characterization tools
- Hydrogen Transport and Trapping Laboratory
- Hydrogen-Surface Interactions Laboratory





## Metals



## Polymers

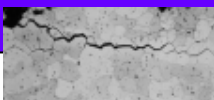
Lead:  **Sandia National Laboratories**

Lead: **Pacific Northwest**  
NATIONAL LABORATORY

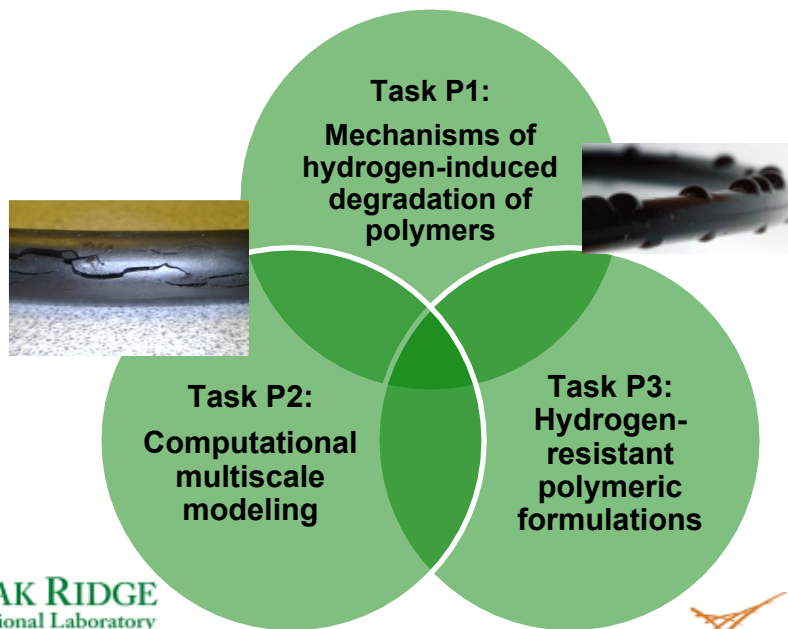
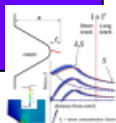
**Task M1: Hydrogen-resistant, high-strength ferritic steel microstructures**



**Task M2: High-strength aluminum alloys (moisture + H<sub>2</sub>)**



**Task M3: Transferability of damage and crack nucleation in hydrogen environments**



Sandia National Laboratories



Industry and University partnerships are encouraged and welcomed



# International collaborations and partnerships extend the reach and impact of Sandia's programs

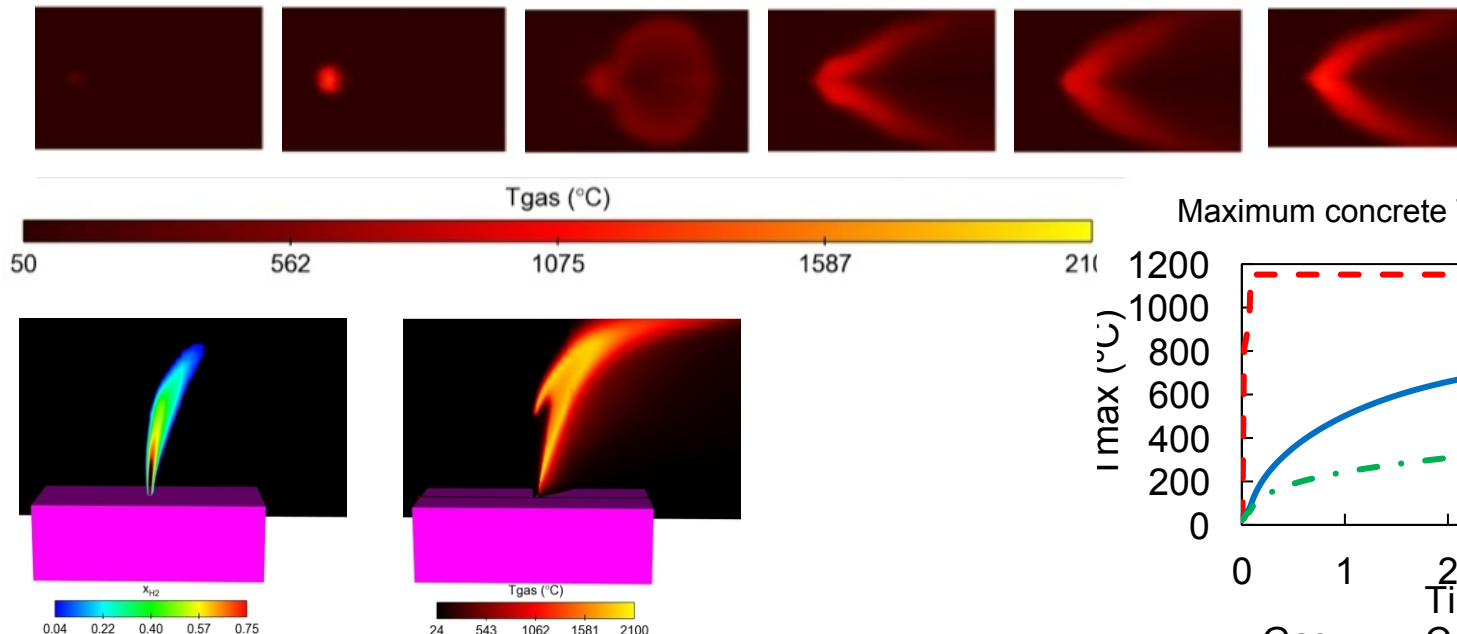
- MOU on high-hardenability steels
  - Materials from JSW (Asia), Tenaris (Europe) and Fibatech (North America)
  - Establish broad consensus on materials performance and platform for communication to code community
- Testing in collaboration with SAE FC Task Force and UN GTR
  - Joint effort to develop testing capabilities and methods for materials acceptance with Kyushu University, MPA Stuttgart and Sandia National Laboratories
  - Remove national barriers to materials selection in core markets
- Advanced pipeline materials and welding technologies
  - Interagency collaboration with NIST, ORNL and SNL
  - Extend results to other US agencies (DOT) and leverage expertise at DOE labs
- Informal collaboration with international manufacturers and universities on damage in polymers
  - Leverage active programs (Kyushu) and established knowledge on polymer materials and environmental effects
  - Develop leadership in hydrogen effects in polymers, demonstrating new unique capability for pressure cycling materials at controlled temperature



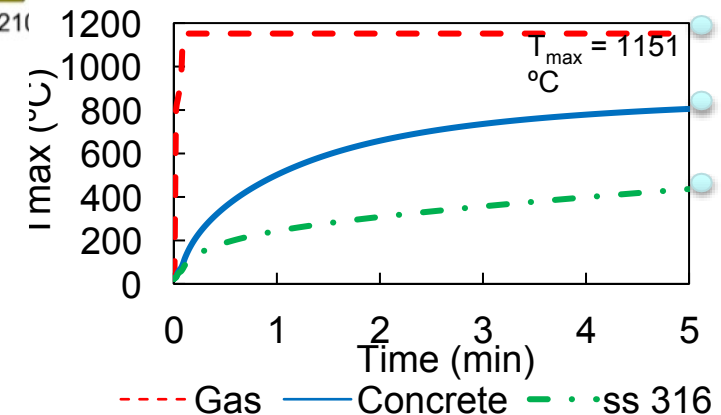


# Risk and Modeling of Fuel Cell Electric Vehicle (FCEV) in Tunnels

- Provide the necessary information to authorities in the Northeast Corridor for their determination if FCEVs will be permitted in tunnels
- Perform comprehensive risk analysis and consequence modeling for specific scenarios

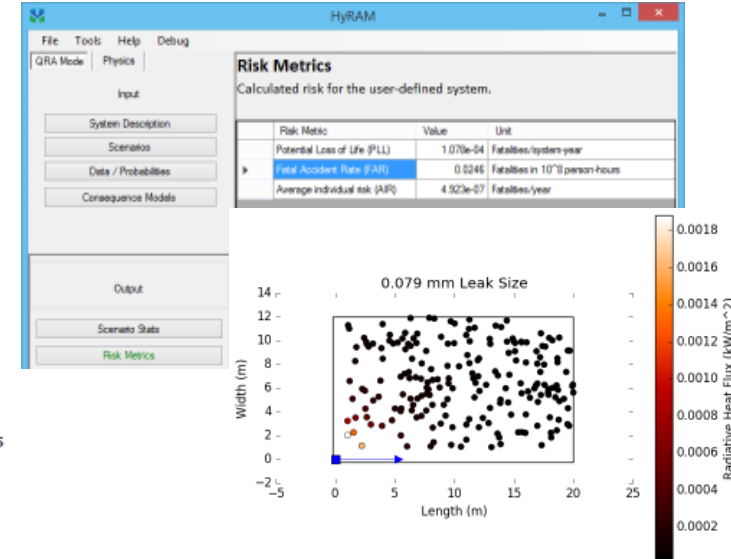
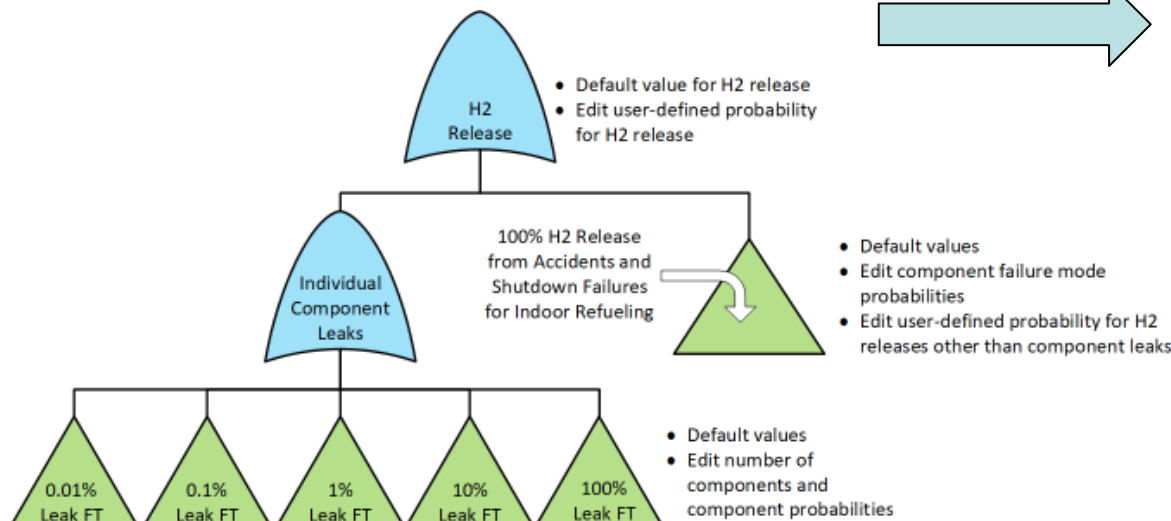


Maximum concrete Temperature vs. Time



# QRA Progress: Expanding HyRAM QRA flexibility beyond hydrogen refueling stations

- Develop additional QRA capability to enable HyRAM to be applied to a larger variety of H<sub>2</sub> applications
  - Users will be able to edit the parameters of the existing fault tree to alter the risk analysis for different applications
  - Underlying physics-based analysis would remain the same
  - Version 2.0 expected to be released once copyright updated



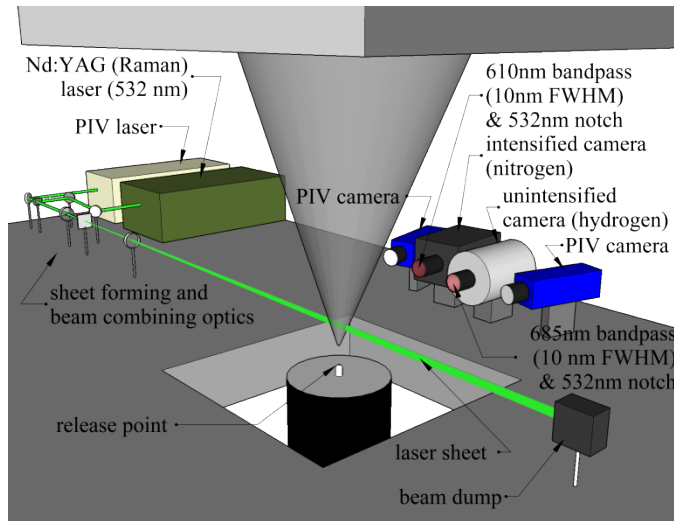
**Version 1.1 download at**  
<http://hyram.sandia.gov>



# Near Term Research Direction: LH2 and Additional Fuels

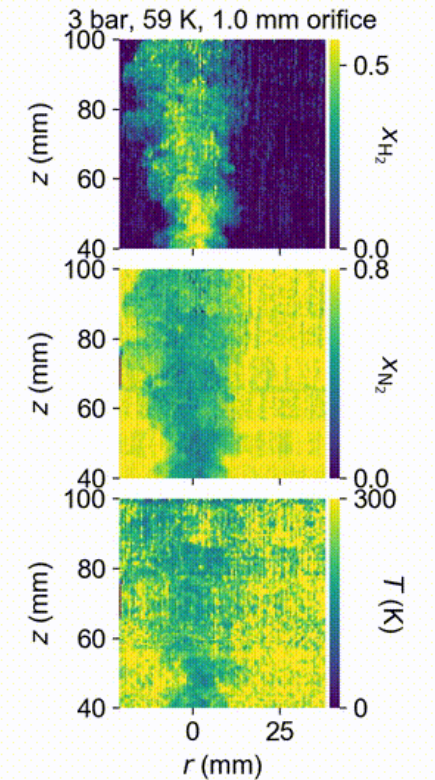
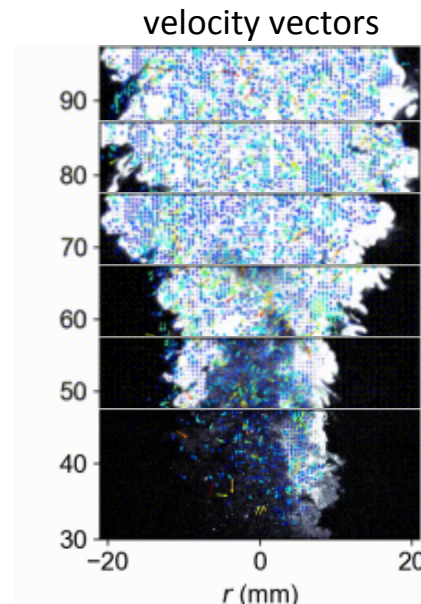
- Publish HyRAM 2.0
  - Updated QRA analysis to allow for customization and fidelity
  - Critical bug fixes which improved and clarified user interface
- Incorporating LH2 models and risk analysis into HyRAM
  - Incorporate **validated liquid/cryogenic H2 release behavior model**
  - **Generate data/probabilities** for liquid hydrogen system component failures, leak frequencies, detection effectiveness, etc. based on operating experience or other information
- Expanding HyRAM to AltRAM (Alternative Fuels Risk Assessment Models)
  - Customization of the components, failure modes and accidents, will allow for the risk analysis of alternative fuels (CNG, LNG, LPG) **with the addition of appropriate physics/behavior models**

# H<sub>2</sub>-N<sub>2</sub> Raman imaging and particle imaging velocimetry are used to measure concentration, temperature, and velocity of cryogenic H<sub>2</sub>



Independent model parameters:

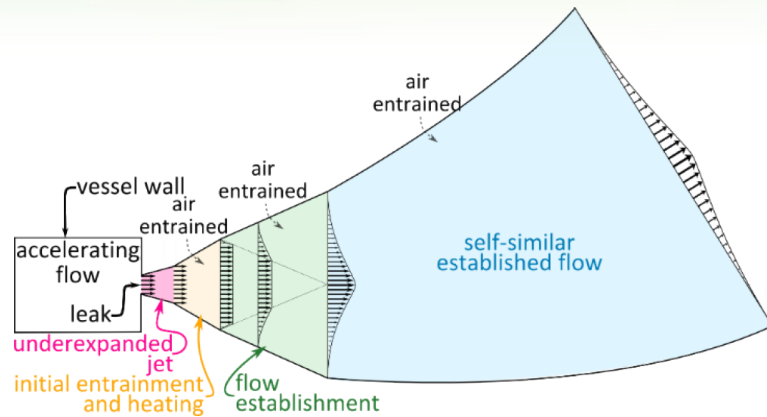
- ✓  $T$  - temperature
- ✓  $x$  - mole fraction
- ✓  $v$  - velocity
- ✓  $B$  - halfwidth (both velocity and concentration)



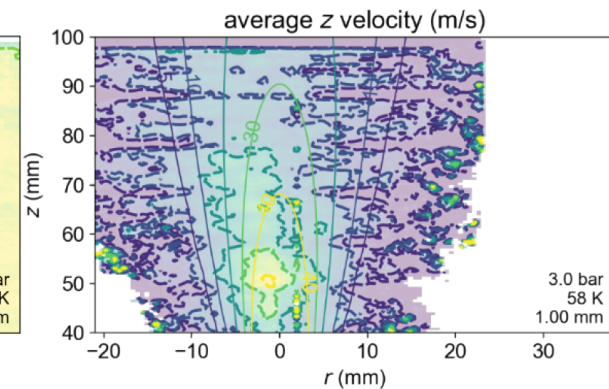
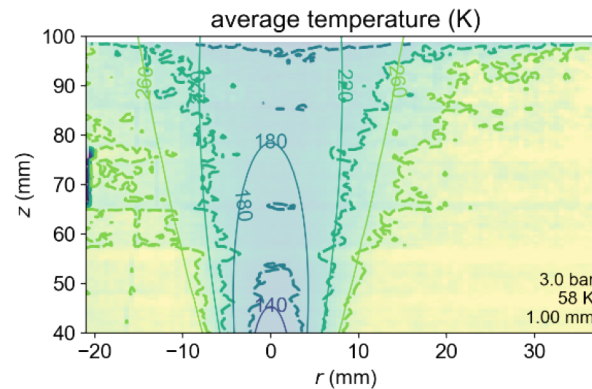
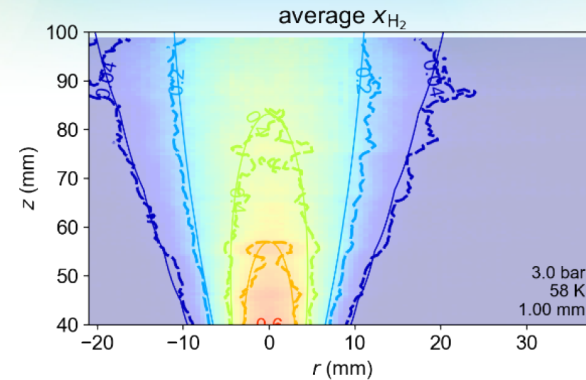
➤ Laboratory facilities provide unique, first of its kind capability to measure hydrogen leaks, concentrations, and ignitibility



# ColdPLUME model shows good agreement with the data



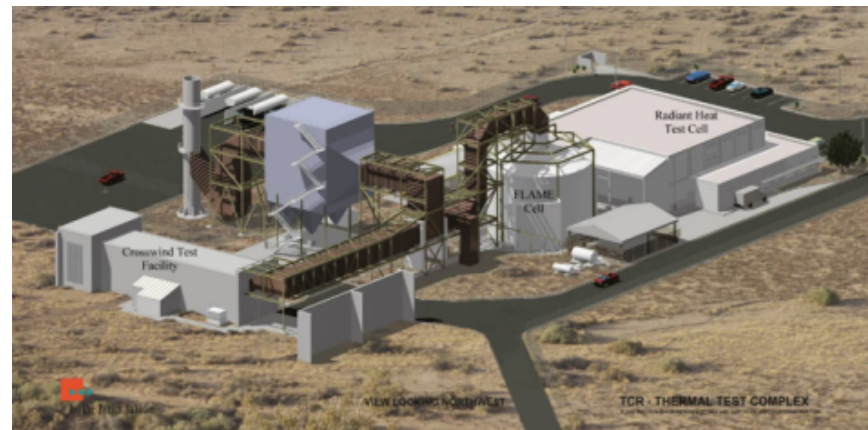
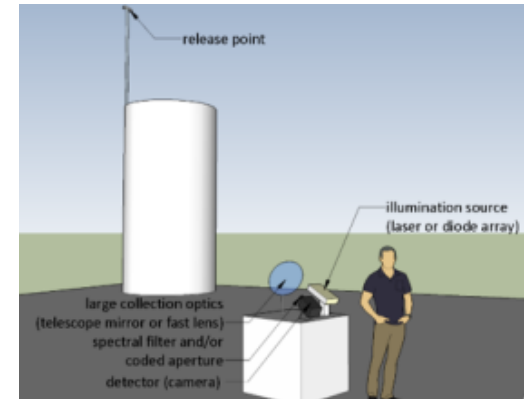
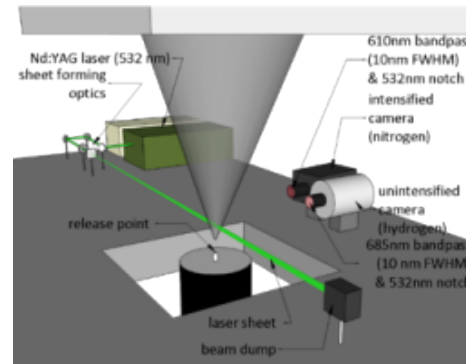
- Experimental results shown by shading and thick, dashed lines
- ColdPLUME model results are thin, solid lines



- Model accurately simulates mole fraction, temperature, and velocity
- Can be used as a predictive tool for a wide variety of scenarios

# Lab scale data is great for model validation but we are working to scale-up our Raman imaging techniques

- **Remaining priorities for  $LH_2$ :**
  - Relate concentration data to ignition distance
  - Study non-circular orifices
  - Characterization and modeling of
    - Interactions with ambient (i.e. wind)
    - Pooling
    - Evaporation from  $LH_2$  pools
- Currently developing an imaging diagnostic for outdoor and large-scale experiments
  - Quantitative concentration measurements
  - 2- or 3-dimensions
  - Video frame rates
  - Portable
- Will apply diagnostic to normally occurring outdoor releases (e.g., venting after  $LH_2$  fill)
- Dedicated validation experiments (pooling, cross-wind) at well-controlled facilities next fiscal year (FY19-20)



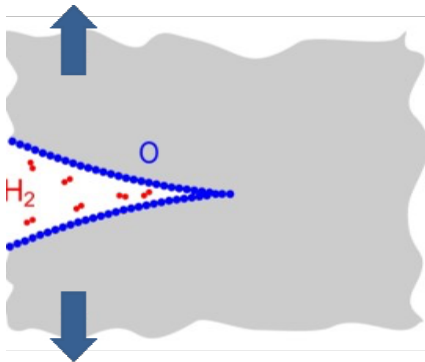


# Questions



# Sandia program(s) take a holistic approach to understanding *Hydrogen Effects on Materials*

- Surface interactions
- Transport and trapping
- Rapid gas decompression



**Environment**

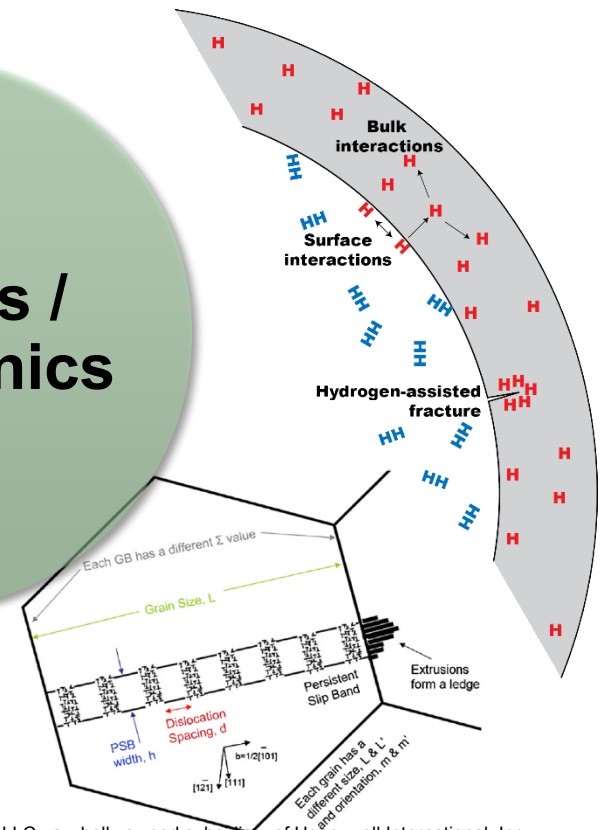
- Hydrogen-assisted fatigue and fracture
- Hydrogen effects on deformation

**Materials**

**Stress / Mechanics**

*Hydrogen embrittlement occurs in **materials** under the influence of **stress** in hydrogen **environments***

- Mechanisms of fatigue and fracture
- Evolution of damage





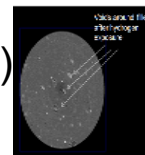


# Sandia maintains unique capabilities to support research on *Hydrogen Effects on Materials*



## Hydrogen Effects on Materials Laboratory

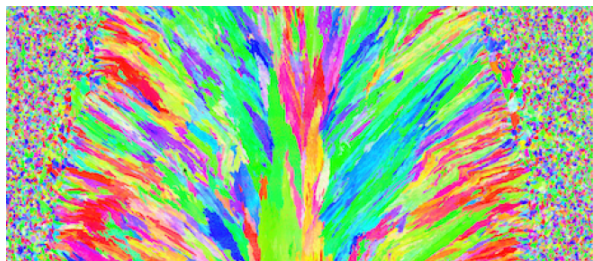
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- Long-term, high-pressure H<sub>2</sub> exposure
- Pressure cycling at controlled temperature



Environment

Materials

Stress / Mechanics

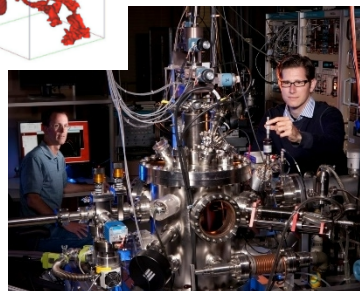
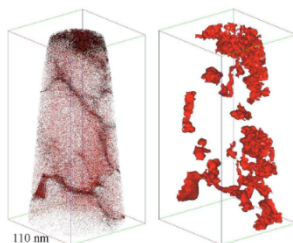


## Active materials science community

- Computational materials science expertise
- Full-suite of state-of-the-art materials characterization tools
- Joining laboratory (austenitic steels, non-ferrous materials)

## Hydrogen Transport and Trapping Laboratory

- Diffusion and permeation
- Thermal desorption spectroscopy
- Local-electrode atom probe tomography



## Hydrogen-Surface Interactions Laboratory

- Low-energy ion spectroscopy
- Ambient pressure x-ray photoelectron spectroscopy
- Kelvin probe atomic force microscopy