SAND2019-12732PE

Hydrogen Economy:

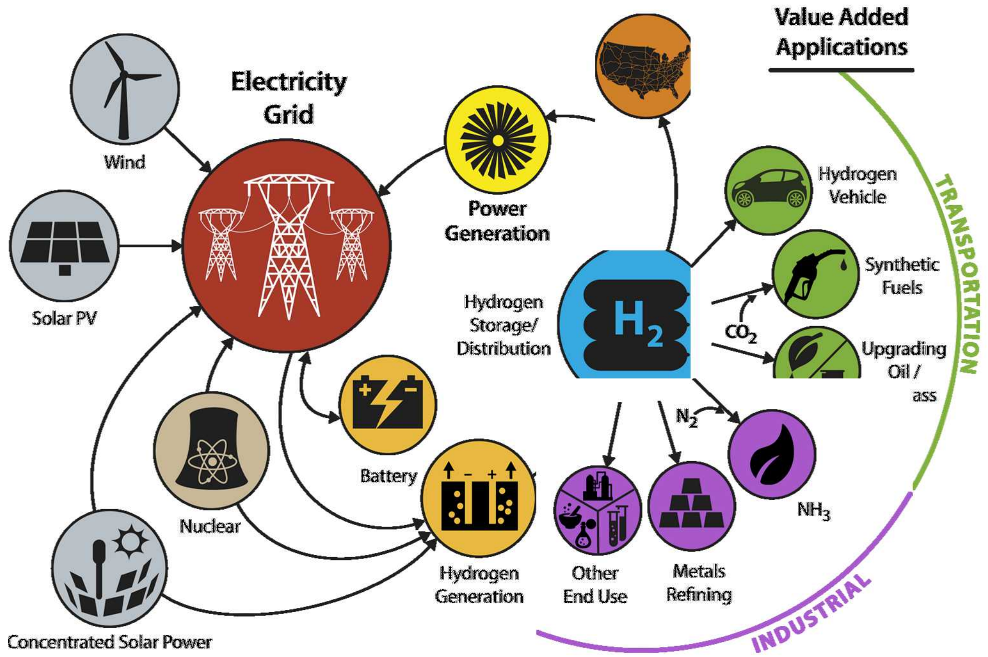
US DOE Initiatives

T. A. Venkatesh and D. Mahajan
Institute of Gas Innovation Technology (I-GIT)
Stony Brook University
New York

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

H2@Scale

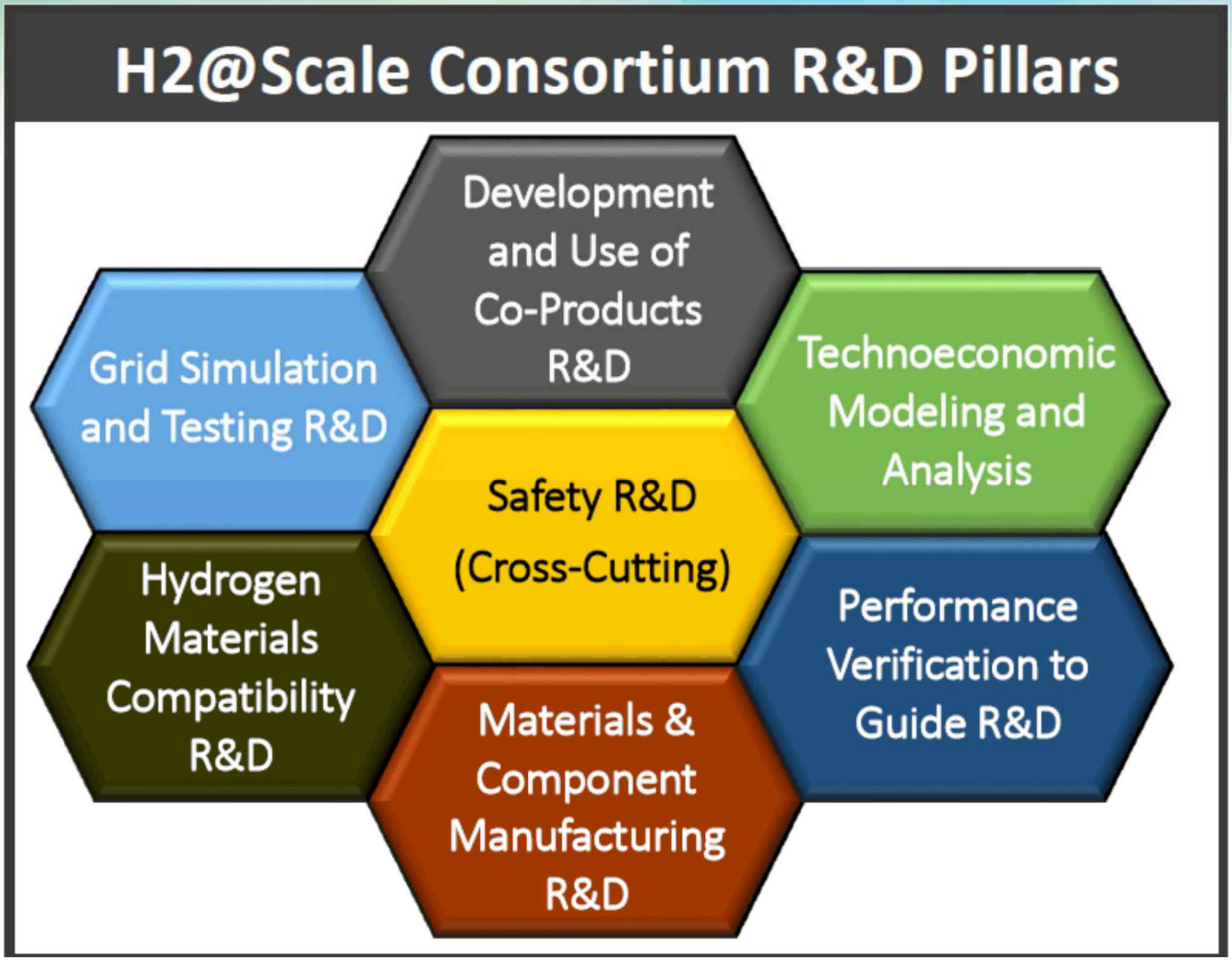
- H2@Scale is a U.S. Department of Energy (DOE) initiative that brings together stakeholders to advance affordable hydrogen production, transport, storage, and utilization to increase revenue opportunities in multiple energy sectors.
- It is a framework in which national laboratories and industry can work together through government co-funded projects to accelerate the early-stage research, development and demonstration of applicable hydrogen technologies.



More than 25 industry projects are currently part of the H2@Scale initiative.

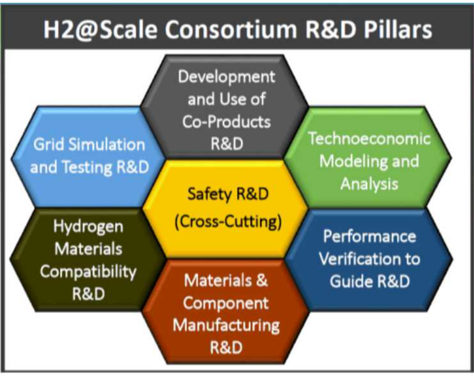
DOE

H2@Scale



H2@Scale Consortium R&D Pillars
Development and Use of Co-Products R&D
Grid Simulation and Testing R&D
Technoeconomic Modeling and Analysis
Safety R&D (Cross-Cutting)
Hydrogen Materials Compatibility R&D
Performance Verification to Guide R&D
Materials & Component Manufacturing R&D

DOE



SAND2019-2740C

H-Mat Overview

Science-based advancement of materials for hydrogen technologies

PI: Chris San Marchi (SNL) and Kevin Simmons (PNNL)

Close to 1,600 miles of pipelines in the US are dedicated to hydrogen conveyance

H-Mat addresses materials-compatibility science questions

Metals

Task M1
High-strength ferritic steel microstructures

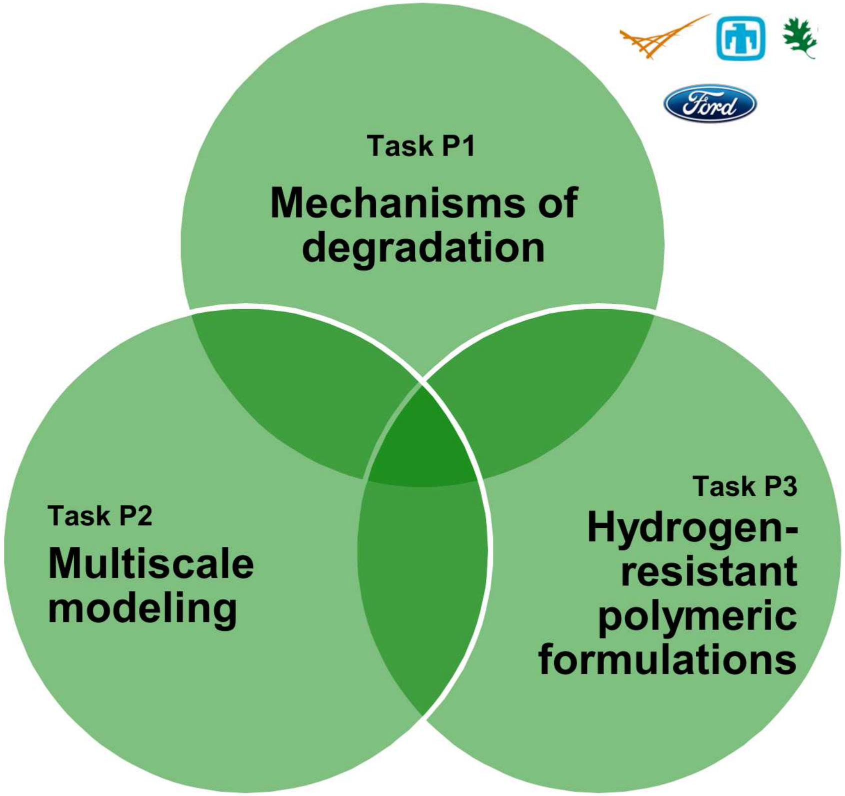
Task M2
High-strength aluminum alloys

Task M3
Transferability of damage and crack nucleation

Task M4
Microstructure of austenitic stainless steels

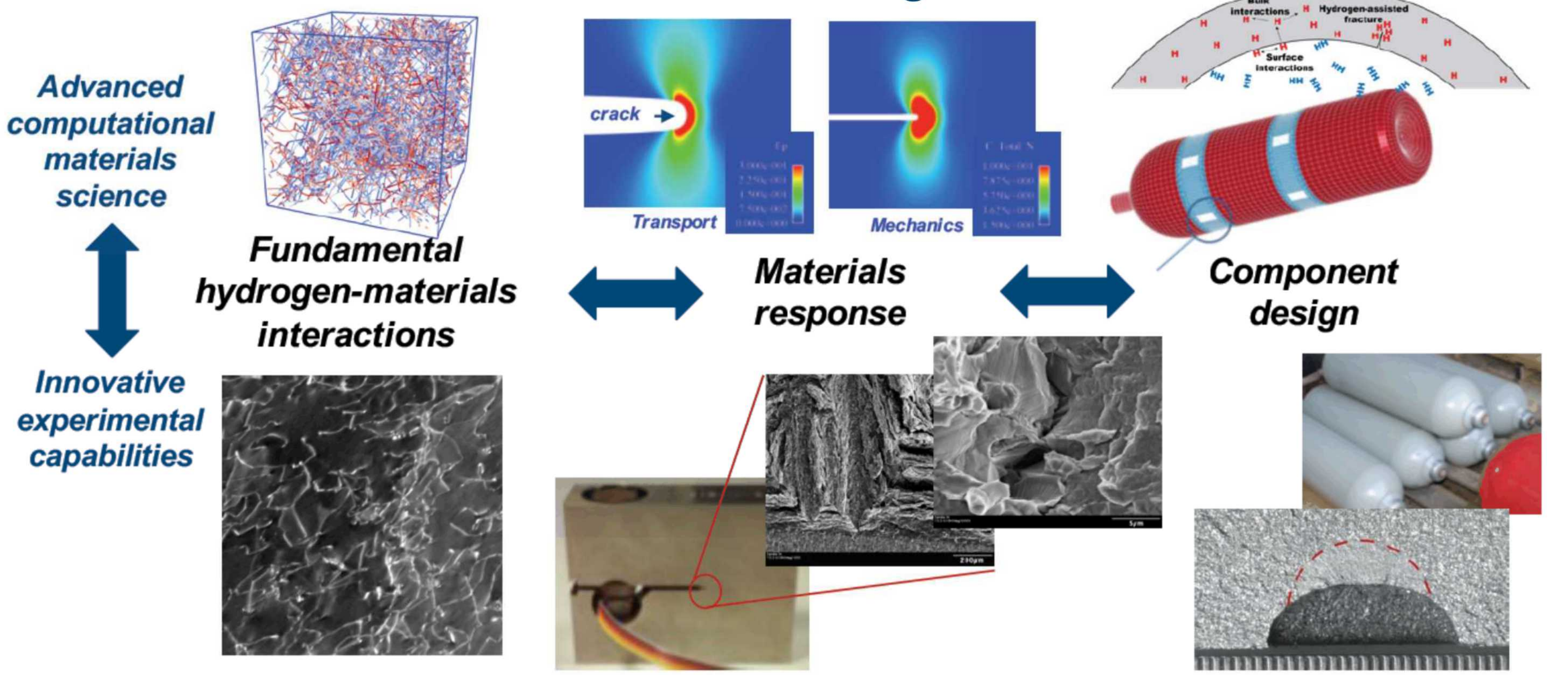
Task C1
Materials for cryogenic hydrogen service

Polymers



Engineering performance depends on mechanisms manifest at nanometer length scales

<u>Approach</u>: Integrate innovative computational & experimental activities across length scales

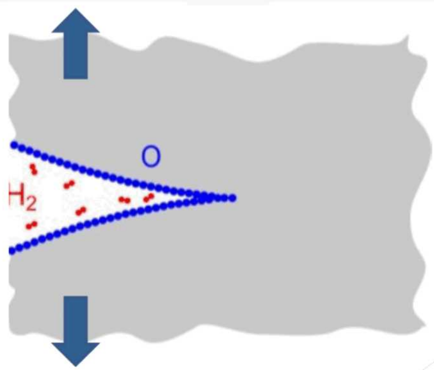


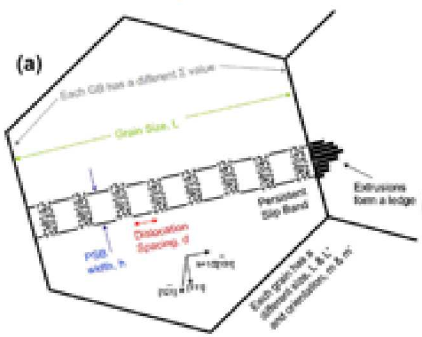
Thermodynamics of H-interactions at nm-scale

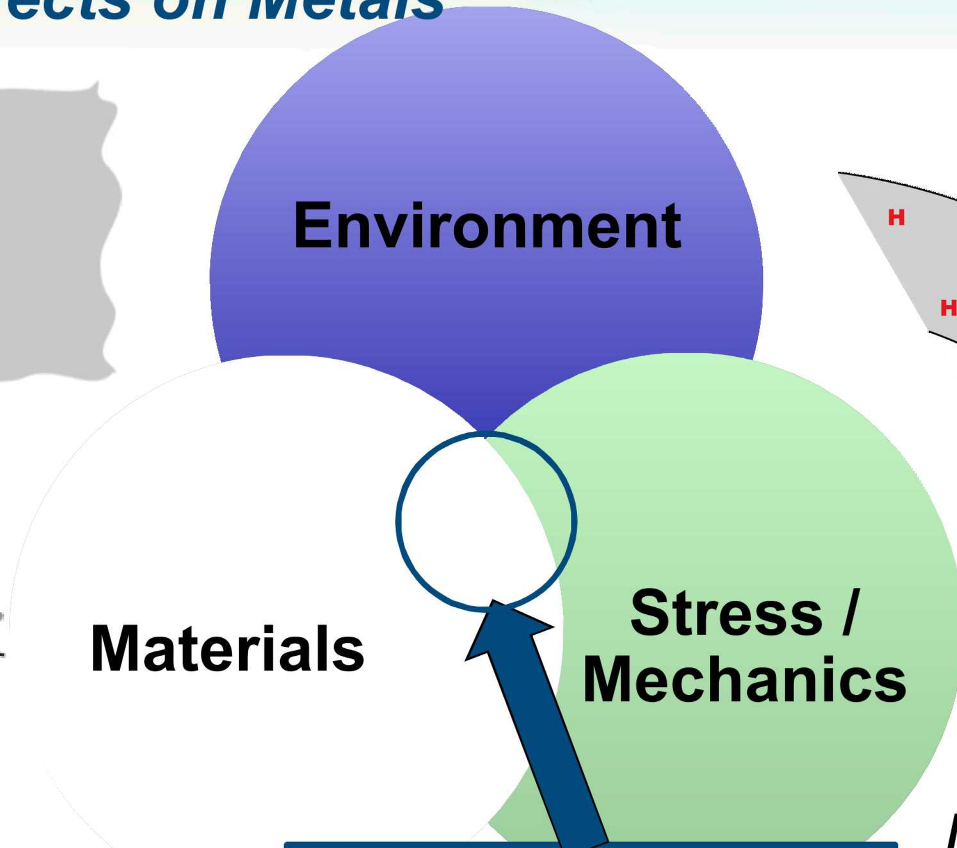
Micromechanisms of materials behavior at μm-scale

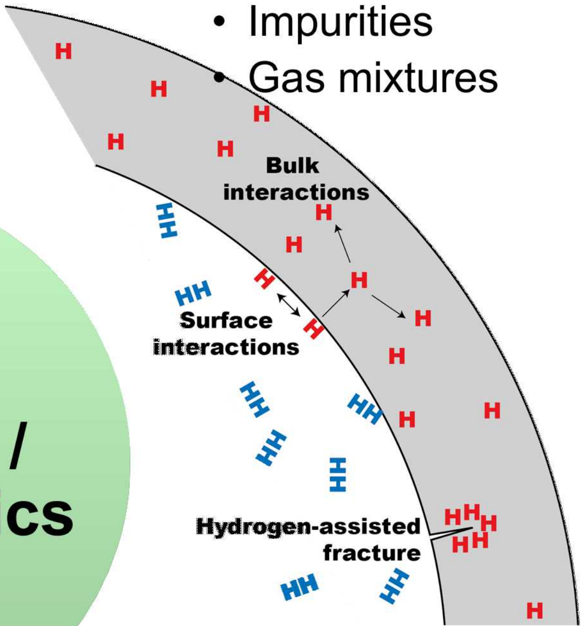
Structural performance at the engineering scale

Consider the intersection of *environmental*, *mechanics* and *materials* variables to understand *Hydrogen Effects on Metals*









Environment

- Low temperature
- High pressure
- Impurities
- Gas mixtures

Materials

- High-strength
- Hydrogen-enhanced plasticity
- Boundary cracking
- Surface passivation

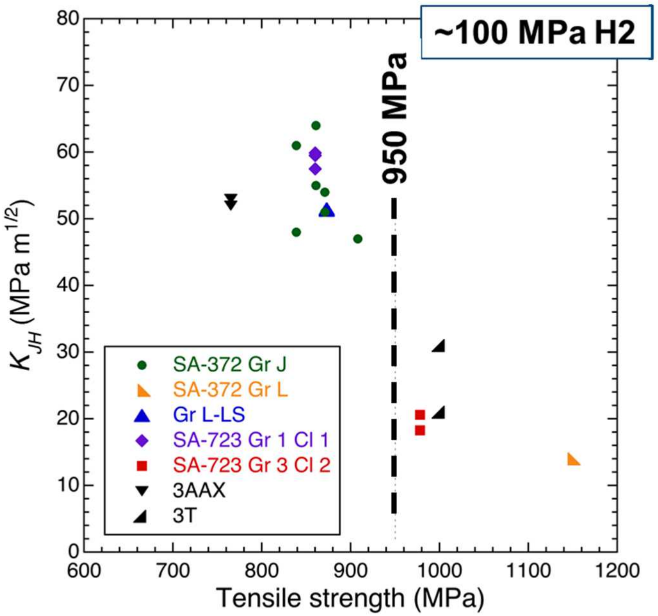
Hydrogen embrittlement occurs in ***materials*** *under the influence of* ***stress*** *in hydrogen* ***environments***

Mechanics

- Autofrettage
- Short crack behavior
- Fatigue crack initiation
- Fracture resistance

Hydrogen-resistant, high-strength ferritic steel microstructures (task M1)

Science question:
Are there high-strength steel microstructures that can be resistant to hydrogen effects?



- Mechanical testing of steels in high pressure H_2
- Development of unique microstructures (e.g., austempering)
- Microstructural and fracture characterization
- Kelvin Probe Force Microscopy to investigate hydrogen distribution in different microstructures
- Modeling of Fe-C-H (DFT and MD) to explore preferential locations for hydrogen in microstructure from physics standpoint

Engineering goals:
- **Achieve K_{JH} > 50 MPa m$^{1/2}$ for steels with UTS > 950 MPa**
- **Ferritic steel microstructures with tensile strength up to 1100 MPa and 50% increase of fracture resistance in high-pressure hydrogen**

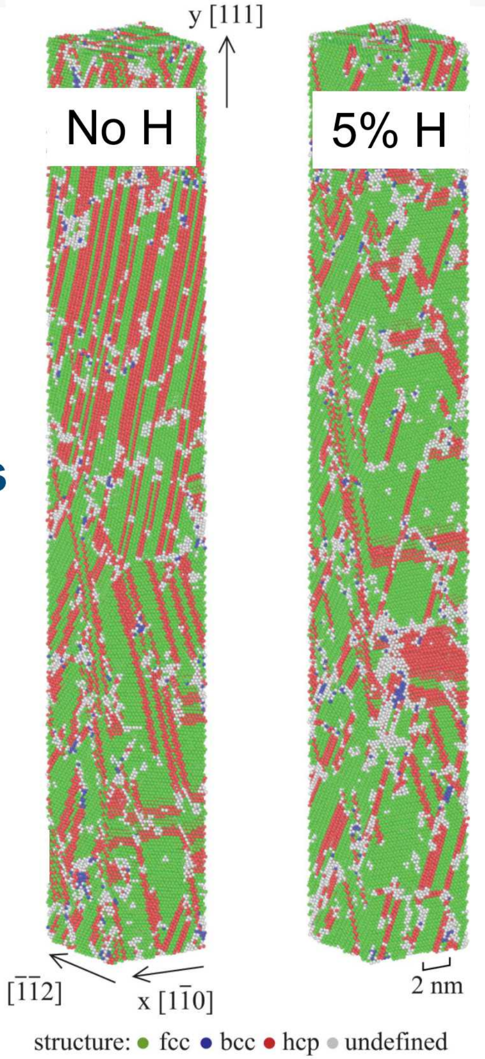
High-strength ferritic steel microstructures (task M1)

Fe-C-H interatomic potential has been implemented into LAMMPS and provides platform for microstructural studies

- Comparison of predicted deformation structures with/without hydrogen identifies potential sites of damage accumulation and fracture initiation
- Novel microstructures identified in collaboration with partners (future iterations planned)

In progress

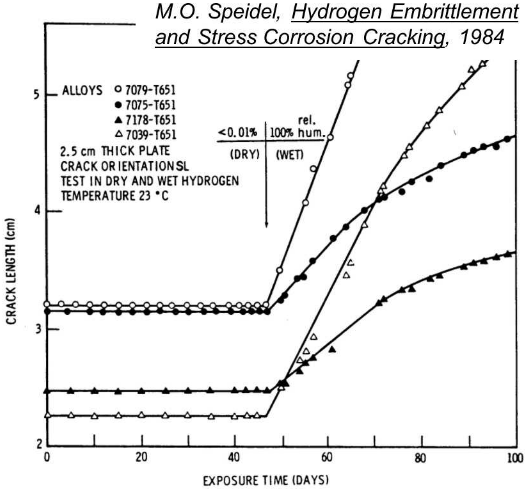
- MD simulations will evaluate hydrogen interactions with different ferritic steels microstructure
  - provide insights to interactions of hydrogen with microstructure
- Kelvin probe force microscopy (KPFM) techniques
  - measure local hydrogen relative to microstructure
- Fatigue and fracture tests in high-pressure H2
  - demonstrate resistance to hydrogen-induced fracture



High-strength aluminum alloys (task M2)

Science question:
What are the mechanisms of environmental embrittlement of high-strength aluminum alloys in high-pressure hydrogen?
(in particular, what is role of moisture?)

M.O. Speidel, Hydrogen Embrittlement and Stress Corrosion Cracking, 1984



- Mechanical testing of aluminum in mixed gases (H_2 + H_2O) at high pressure
- Kelvin Probe Force Microscopy to investigate moisture on Al surfaces
- Modeling of moisture on Al surfaces to identify and quantify mechanisms of H uptake (DFT) and microstructural interactions of dissolved H (MD)

Engineering goals:
- **Hydrogen-compatible microstructures of aluminum alloys with yield strength >350 MPa that are insensitive to standardized moisture limits for fuel-grade hydrogen (5ppm H_2O)**
- **Specification of environmental conditions under which aluminum is not degraded in gaseous (and liquid) hydrogen environments**

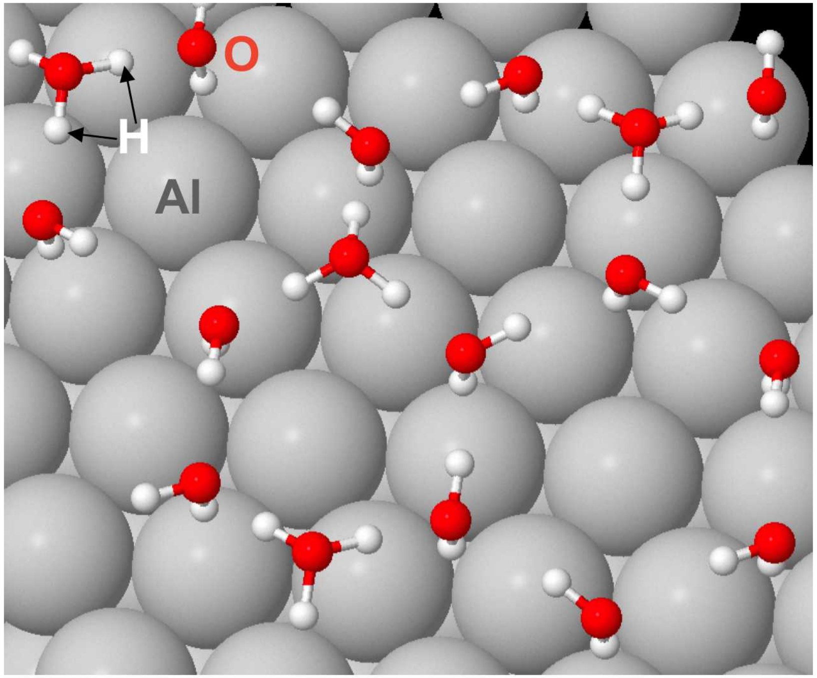
High-strength aluminum alloys (task M2)

First principles calculations are illuminating of the role of moisture in metal-hydrogen interactions

Initial DFT results suggest the presence of water might affect the kinetics of hydrogen absorption

In progress

- MD simulations to evaluate the effect of hydrogen on dislocation mobility
  - hypothesized role on fracture
- Kelvin probe force microscopy (KPFM) techniques
  - measure local hydrogen relative to microstructure
- Fracture tests in hydrogen-water gas mixtures
  - experimental evidence of hydrogen-induced fracture

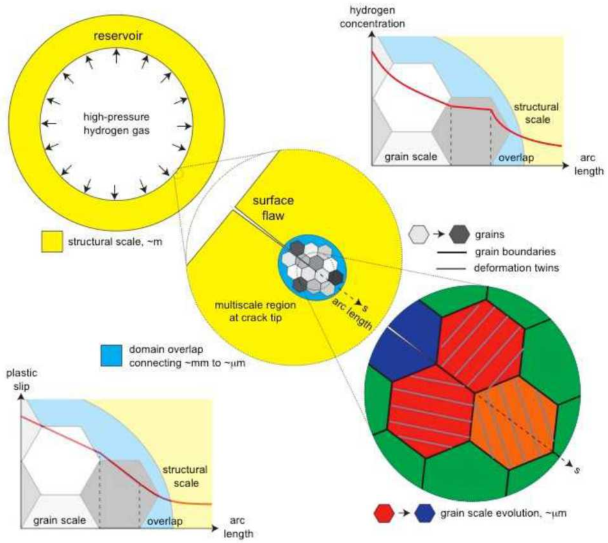


DFT calculations of Al(111) surface show hydrogen is more strongly bound in mixed water-hydrogen layer than in the absence of water.

Mechanisms of hydrogen-deformation interactions in austenitic stainless steels (task M4)

Science question:
How does hydrogen change deformation and fundamental boundary interactions in austenitic stainless steels?

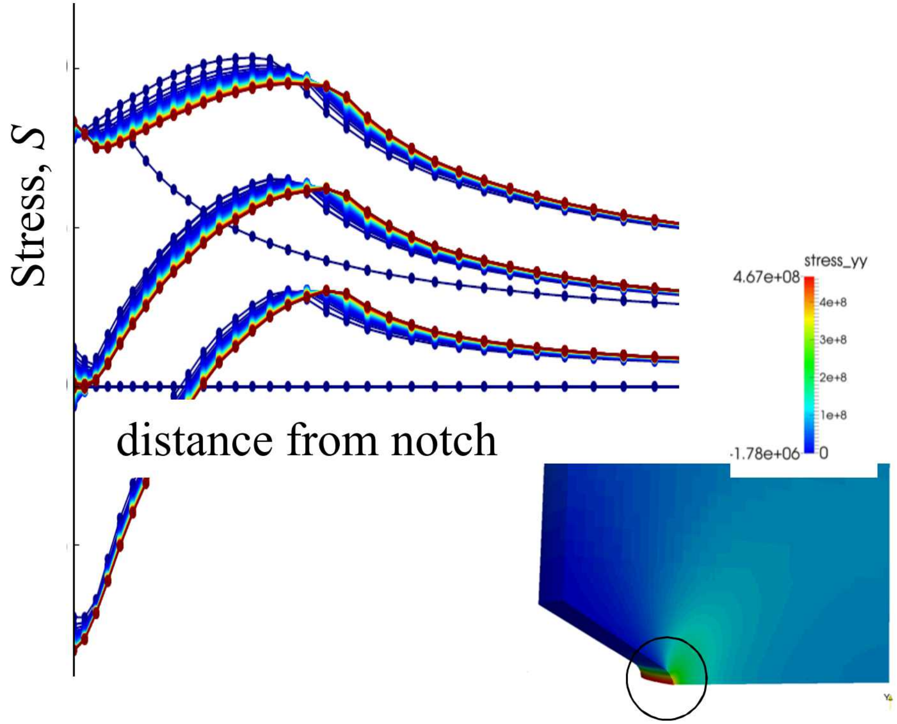
- Develop methods to test and evaluate single crystals (leveraged) and oligocrystals of austenitic stainless steels
- In situ testing and local characterization of strain and damage accumulation
- Micromechanical modeling of oligocrystals with internal hydrogen (CP) to illuminate mechanisms of hydrogen-microstructure interactions



Engineering goals:
- **Microstructural design concepts that improve ductility of austenitic stainless steels in high concentration of hydrogen**
- **Accessible micromechanical modeling tools (CP) sensitive to hydrogen transients, local microstructure, and phase transformations**

Damage and crack nucleation (task M3)

Develop and utilize techniques to identify and monitor crack formation, coupled with mechanics modeling

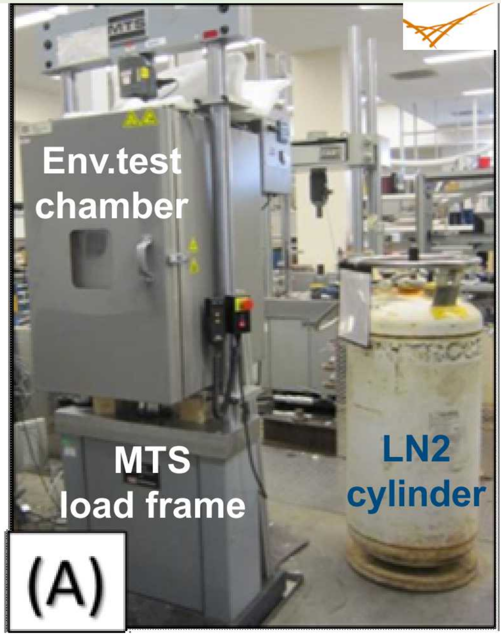


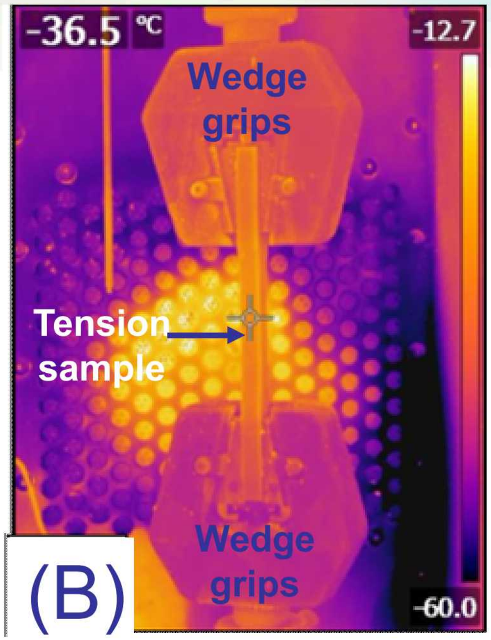
4-point probe provides very sensitive measure of crack initiation and advance

Solid mechanics modeling coupled with measurement of crack initiation provides new strategy to quantify nucleation

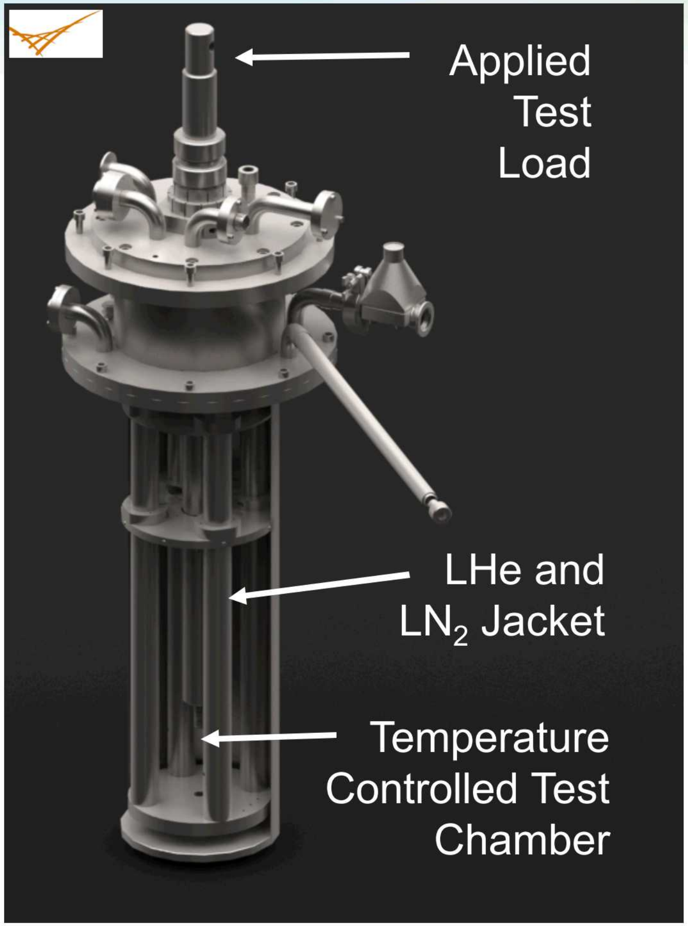
Metals for cryogenic applications in hydrogen service (task C1)

Cold/Cryo-temperature mechanical testing capabilities





- **MTS load frame with environmental chamber for heating or liquid nitrogen: -130 to +315˚C**
- **Strain measurement**
  - **Extensometer capabilities to -253˚C**
  - **Digital image correlation (DIC)**

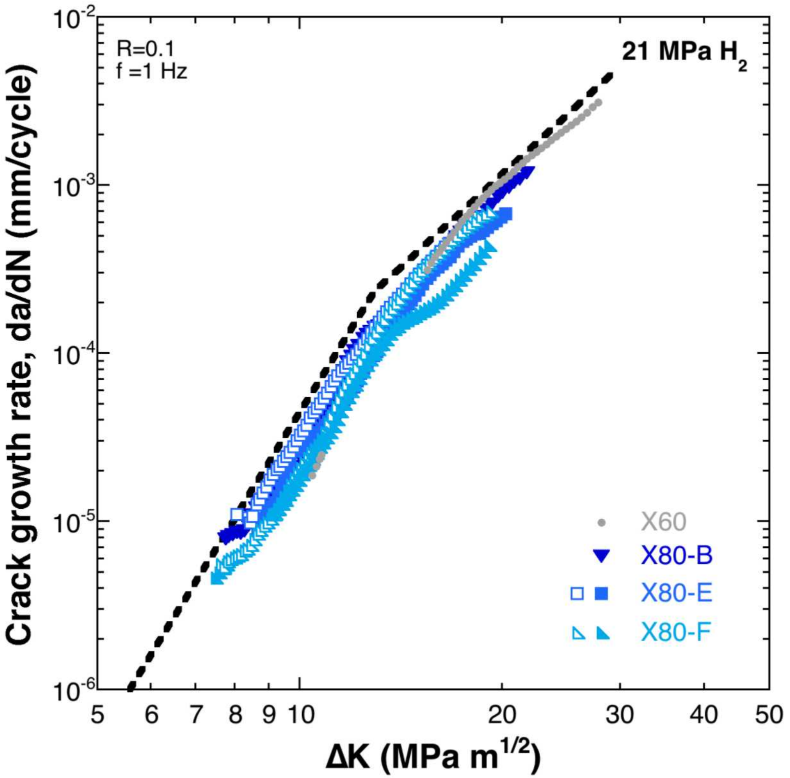


Schematic of liquid helium-cooled Janis Research dewar

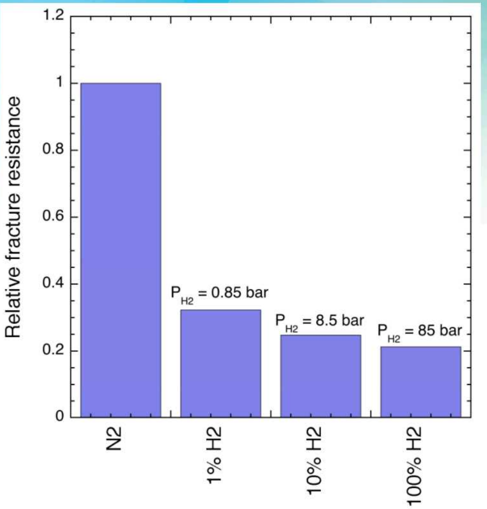
Summary

- ***Hydrogen degrades mechanical properties of most metals***

- **How does gaseous hydrogen affect fatigue and fracture of pipeline steels?**
  - ***Fatigue is accelerated by >10x and fracture resistance is reduced by >50%***

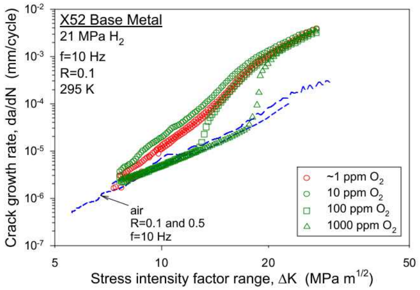


Summary



- **Is there a threshold below which hydrogen effects can be ignored?**
  - ***NO, even small amounts of hydrogen have large effects***

- **Can the effects of hydrogen be masked by other physics?**



  - ***Oxygen can mitigate the effects of hydrogen in some cases, which perhaps can be exploited***

- **What is the implication of hydrogen on life of pipelines?**
  - ***If fatigue cycles are modest, lifetime calculations suggest long life in hydrogen***