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Sandia National Laboratories

H2FC Hydrogen and Fuel Cells Program

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R&D for Hydrogen Compatibility of Materials: Safety, Codes and Standards and H-Mat

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Joint Hydrogen Delivery and Storage (HDSTT) and Codes & Standards (CSTT) Tech Team Meeting

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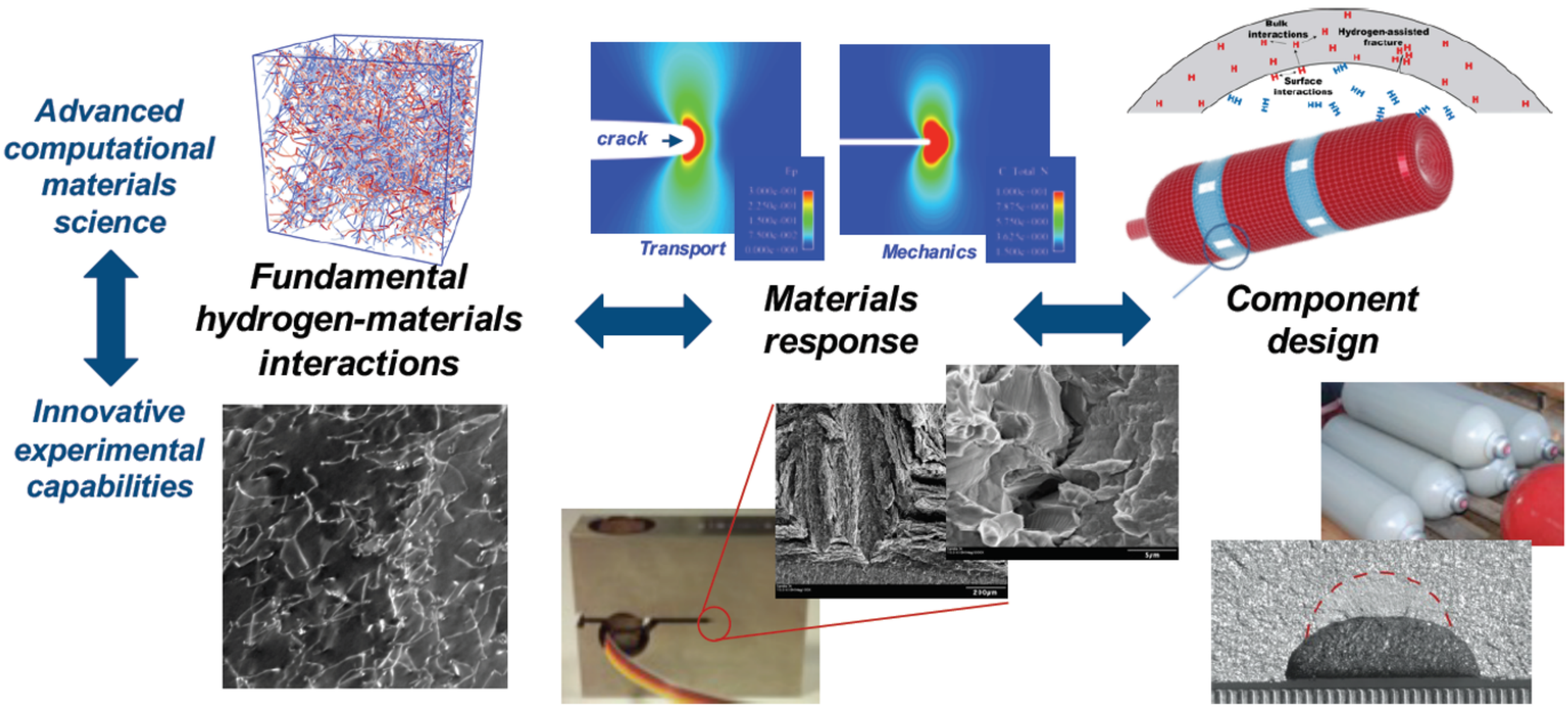
Approach to Hydrogen Compatibility Studies:

Integrate innovative computational & experimental studies across length scales to unravel mechanisms at nanometer length scale and quantify performance at engineering length scale

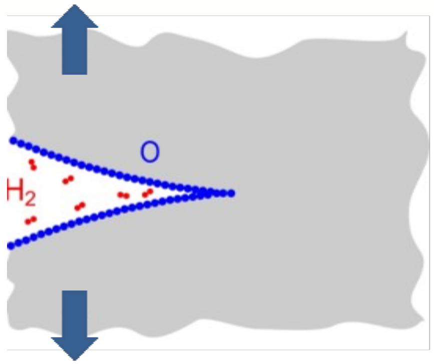


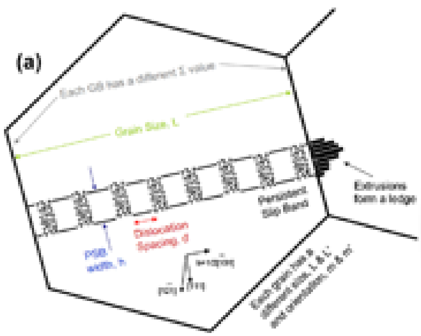
Thermodynamics of H-interactions at nm-scale

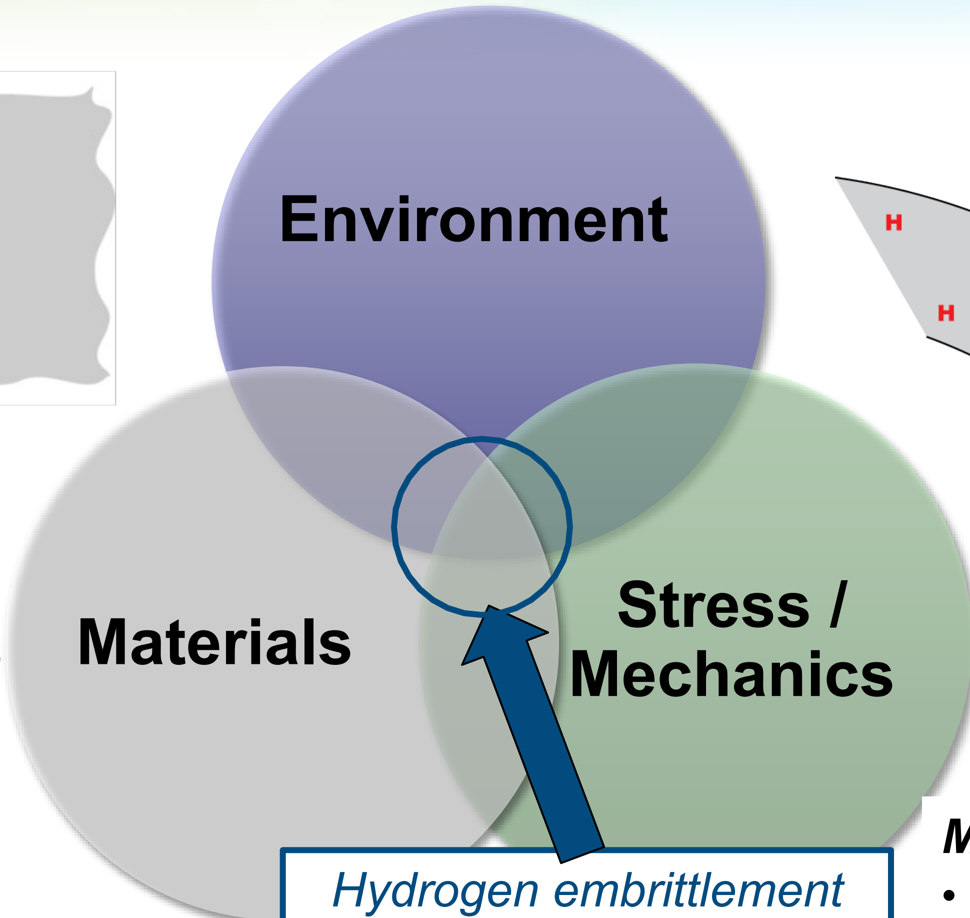
Micromechanisms of materials behavior at μm-scale

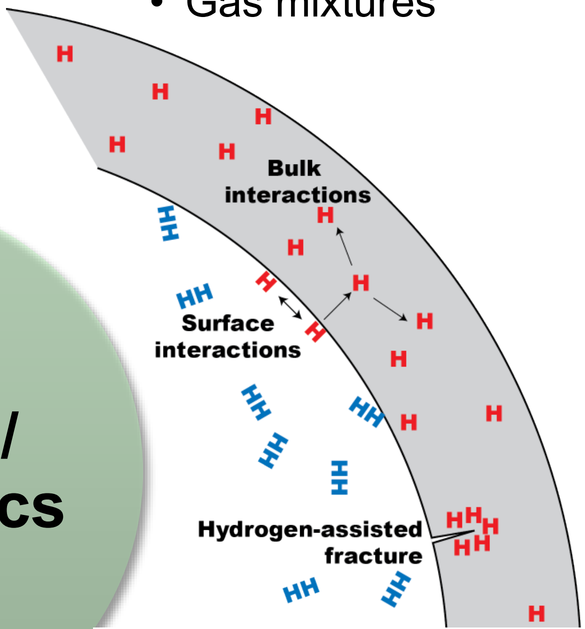
Structural performance at the engineering scale

Framework for deconstructing physics of *Hydrogen Effects on Materials*









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

H-Mat addresses materials-compatibility science questions

Metals

Task M1
Hydrogen-resistant high-strength ferritic steels

Task M2
High-strength aluminum alloys for hydrogen service

Task M3
Hydrogen-assisted crack nucleation in design

Task M4
Microstructural effects on H-deformation interactions

Task C1
Materials for cryogenic hydrogen service

Polymers

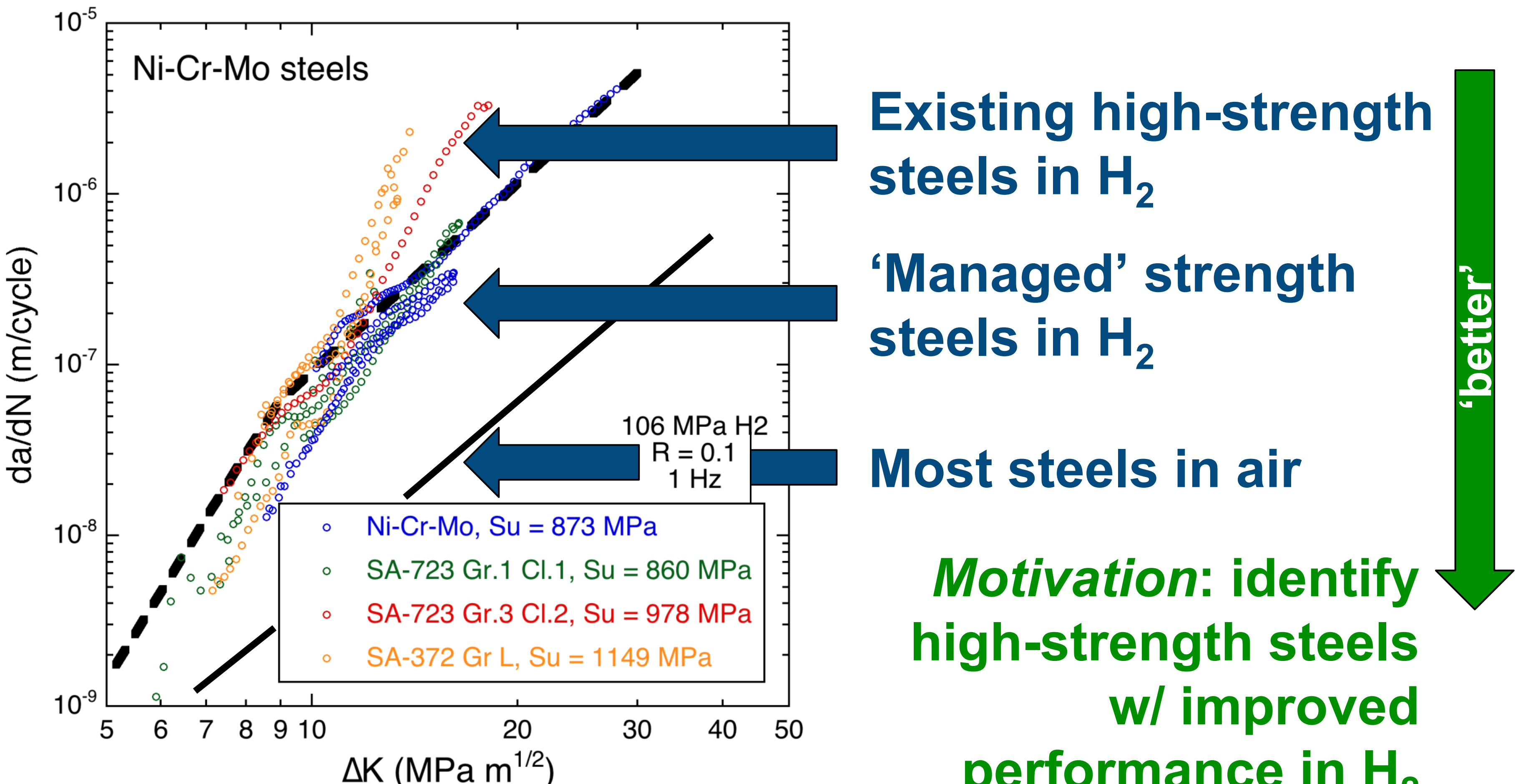
Task P1
Mechanisms of degradation

Task P2
Multiscale modeling

Task P3
Hydrogen-resistant polymeric formulations

Hydrogen-resistant, high-strength ferritic steels

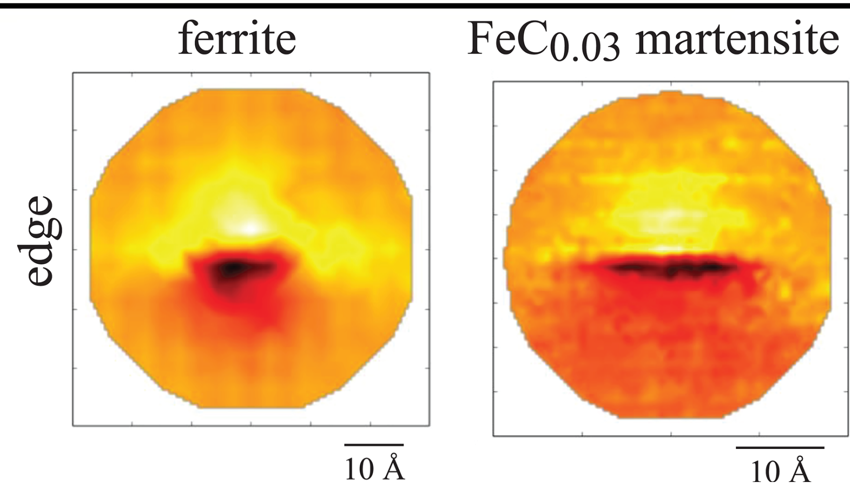
Question: **Are there high-strength steel microstructures with improved resistance to hydrogen effects?**

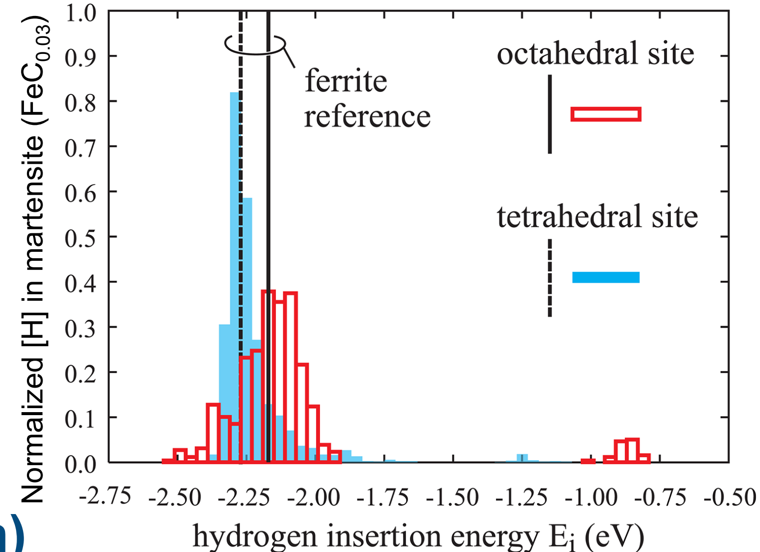


***Motivation*: identify high-strength steels w/ improved performance in H_2**

Hydrogen-resistant, high-strength ferritic steels

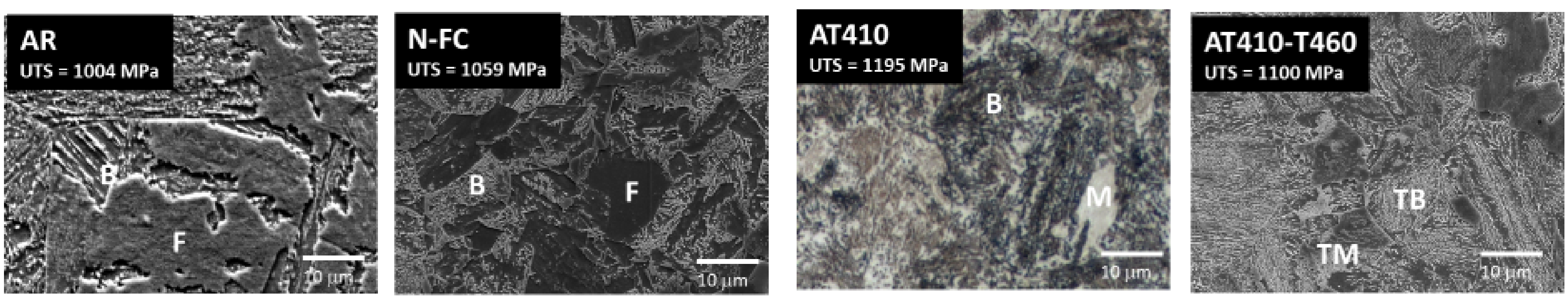
Atomistic simulations inform baseline character of steel phases and inform microstructural design efforts





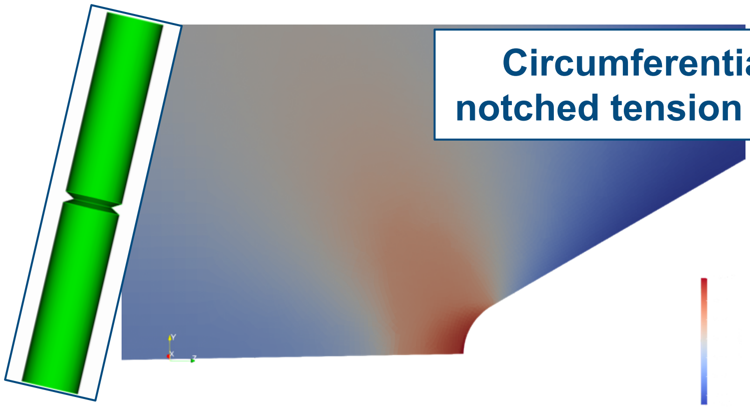
- **How does hydrogen interact with steel microstructure? (Fe-C-H MD simulation)**

- **Can model microstructures enable evaluation of modeling results?**

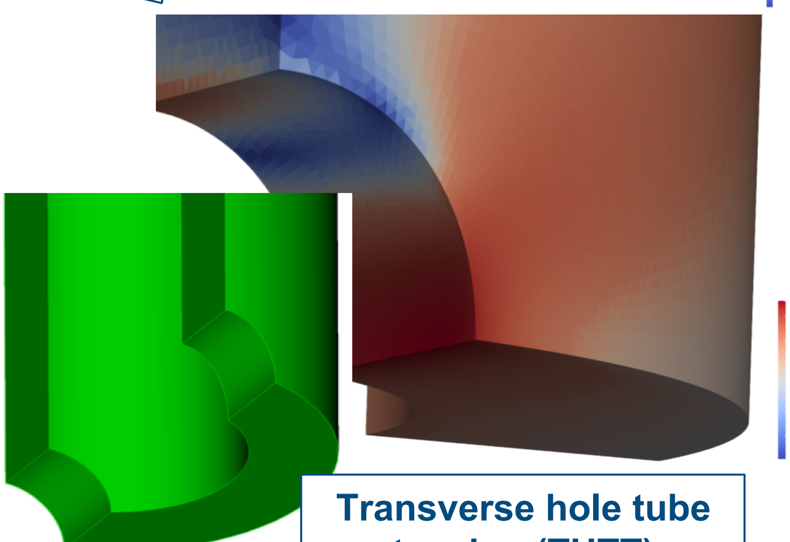


Hydrogen-assisted crack nucleation in design

Question: **Can crack nucleation be predicted and integrated into a design strategy?**



Circumferentially notched tension (CNT)

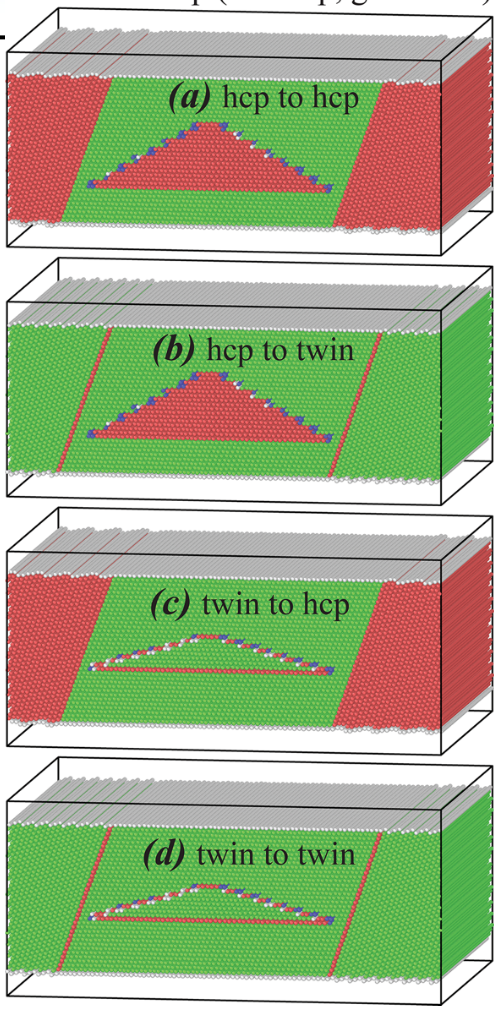


Transverse hole tube tension (THTT)

Engineering-scale models evaluate mechanics of the problem

Atom-scale models inform models of damage evolution

Structure map (red: hcp, green: fcc)



Hydrogen-assisted crack nucleation in design

Deformation / damage observations and modeling advance understanding and inform physics-based models

- **High-resolution microscopy (in other work) shows H promotes deformation-induced martensitic transformations**

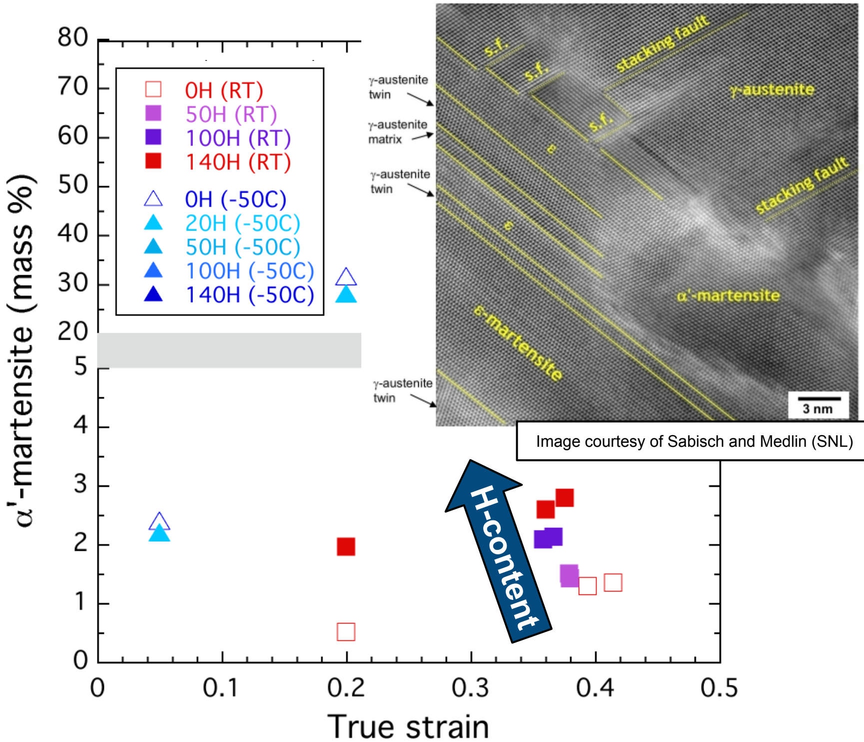
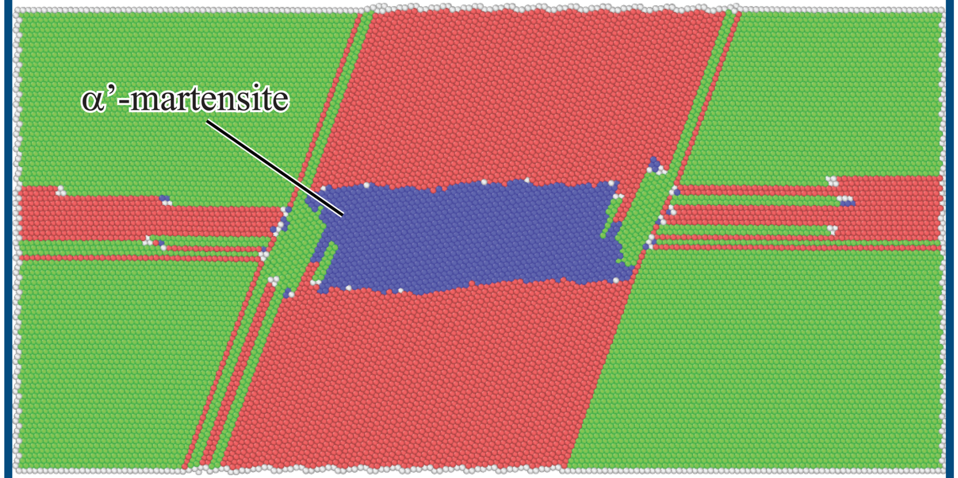


Image courtesy of Sabisch and Medlin (SNL)

collision of an ε-martensite band (screw Burgers vector) with an ε-martensite band at τ = 1.15 GPa



green: fcc, red: hcp, blue: bcc

5 nm

- **Can atomistic simulation predict observed characteristics of deformation structures (i.e., formation of α'-phase)?**
- **Can simulations combined with experiments quantify damage?**

Microstructural effects on hydrogen-deformation interactions in austenitic stainless steels

Question: **How does hydrogen affect deformation and damage accumulation in austenitic stainless steels?**

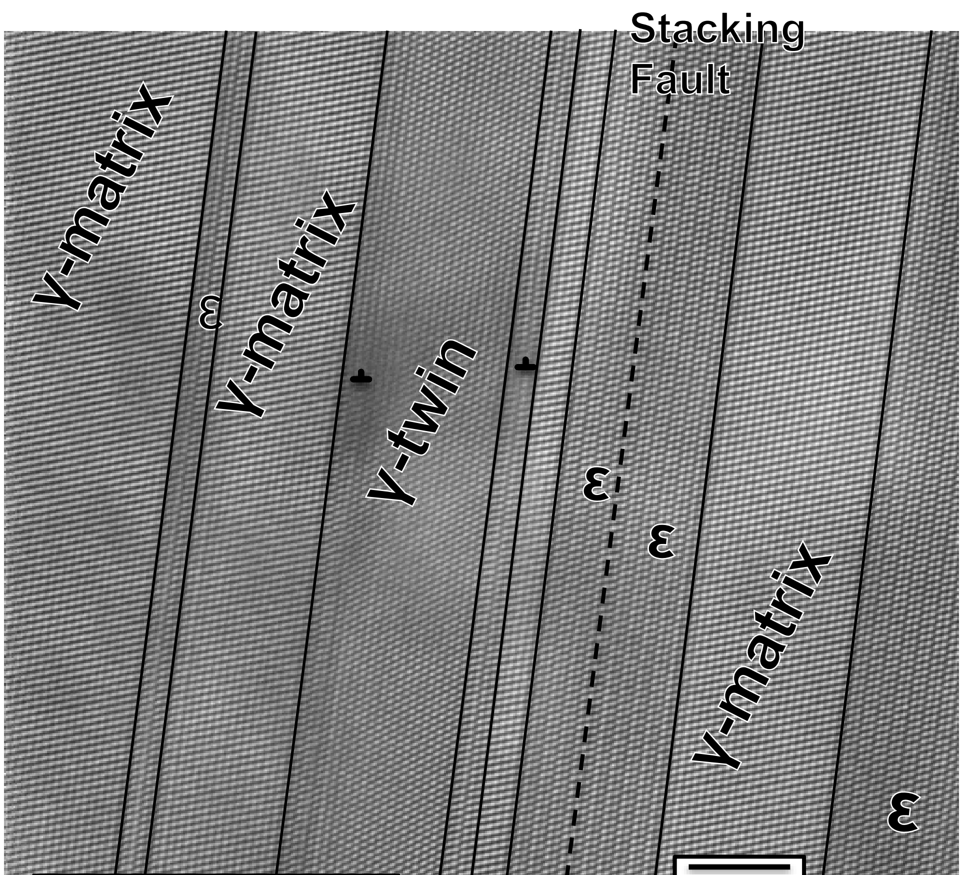


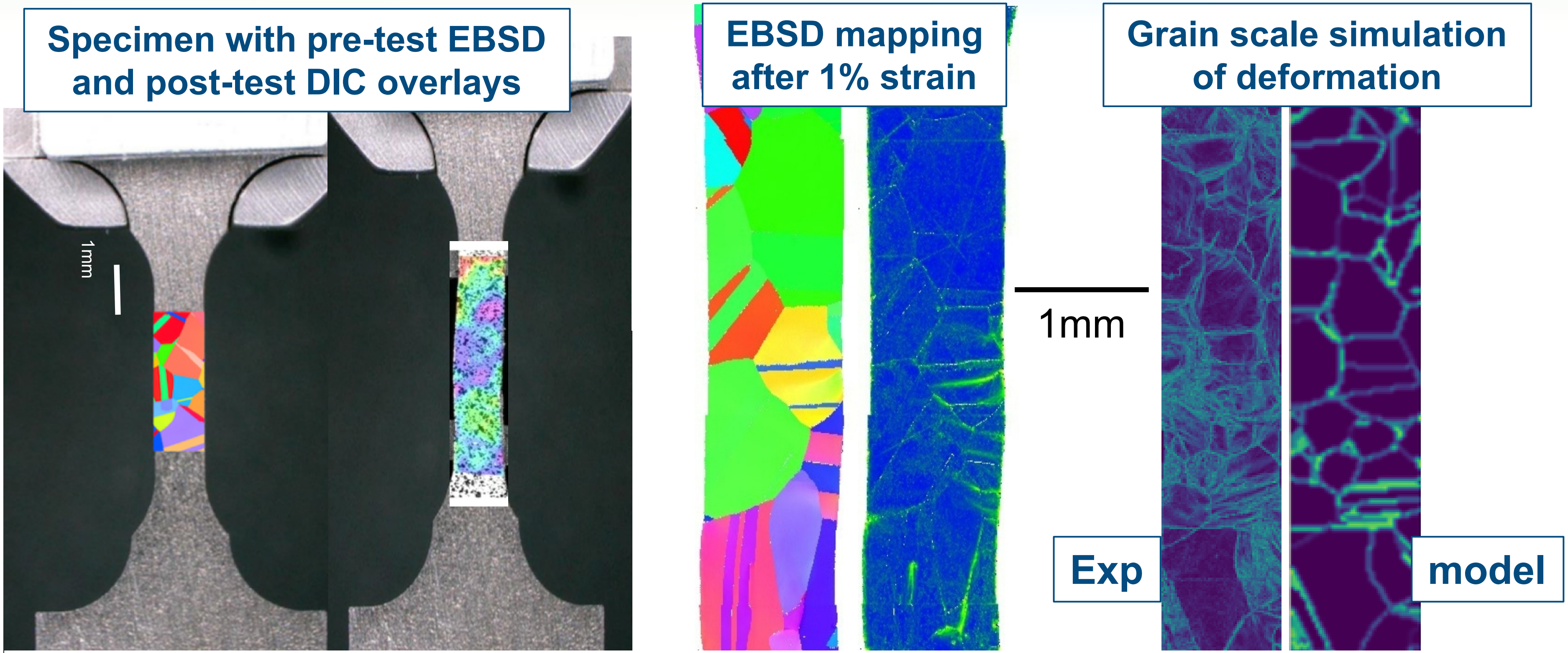
Image courtesy of Sabisch and Medlin (SNL)

Atomic scale observations show that

- **Hydrogen promotes formation of ε-martensite**
- **Hydrogen suppresses deformation twinning**
- **Overall changes in deformed microstructures are relatively subtle (nm-length scale), whereas fracture is substantially affected by hydrogen**

Hydrogen-deformation interactions in austenitic stainless steels

Mesoscale models are needed to understand the macroscopic evolution of the fracture process



- Can state-of-the-art characterization of deformation in small ensembles of grains illuminate mesoscale damage leading to H-assisted fracture?
- Can complementary simulations of grain-level deformation inform microstructural design strategies?

Safety, Codes and Standards activity in *materials mechanics* complements the H-Mat *materials science* approach

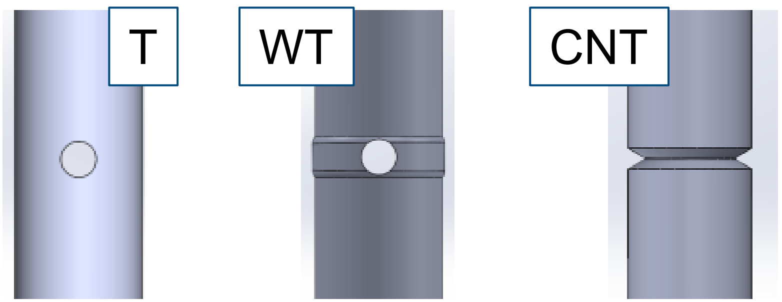
Objective: Enable technology deployment by **applying foundational research toward the development of science-based codes and standards**

- **Subject Matter Expertise (SME)**
  - Develop and maintain material property database and informational resources to aid materials innovation for hydrogen technologies
- **Test method development**
  - Develop science-based materials test methods and guidelines by working with SDOs and the international community to validate and incorporate methods in globally harmonized testing specifications
- **Implementation of critical testing and understanding**
  - Execute materials testing to address *targeted* data gaps and technology deployment
  - Coordinate activities with strategic and international partners

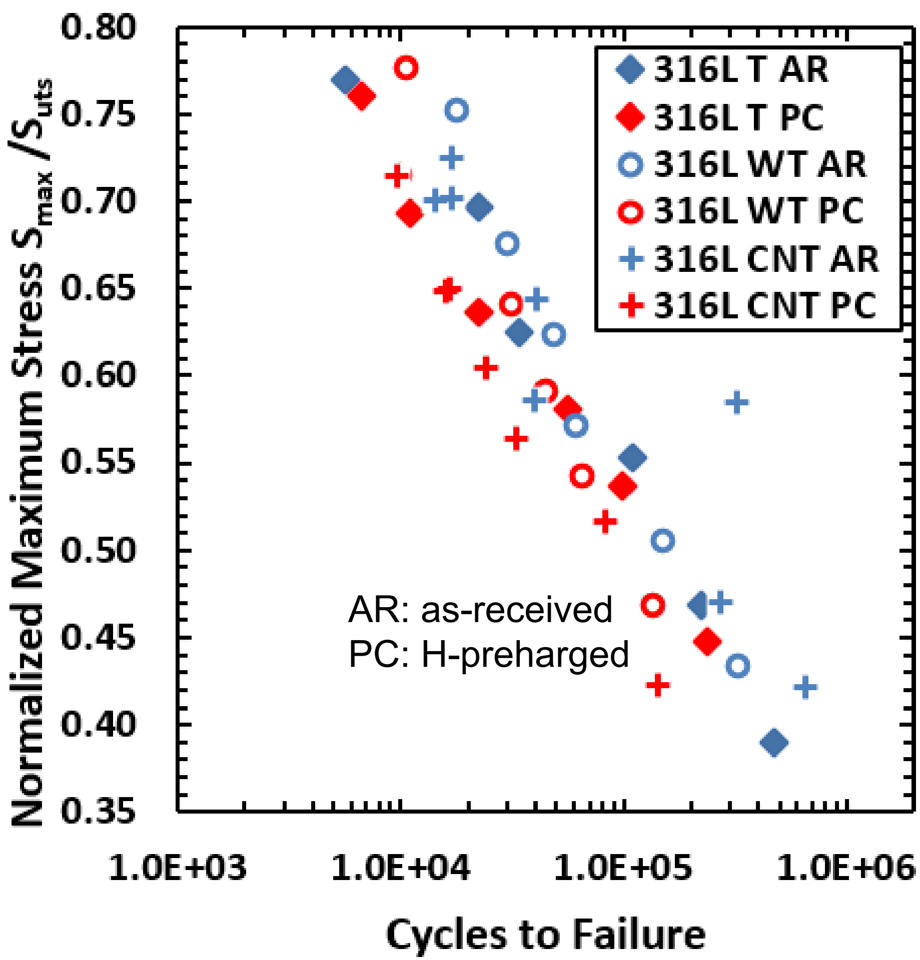
Advancing test methods: Welds

Question: **Can other geometries be implemented to evaluate fatigue of welded configurations?**

T: Tube
WT: Welded Tube (orbital weld)
CNT: Circumferentially Notched Tension



stress concentration factor: K_t = 3



Orbital welded tubing displays fatigue performance consistent with non-welded tubing and bar material

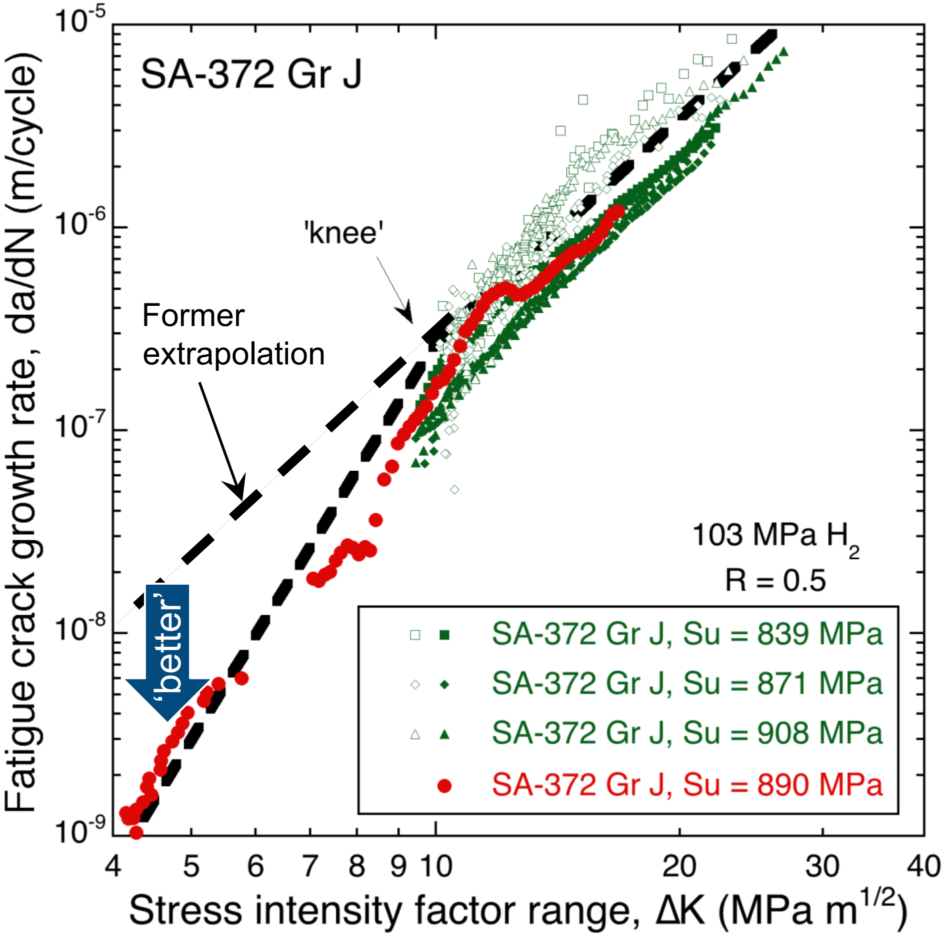
Contributions to ASME codes: Code Case 2938

Question: **Can fatigue trends be captured with simple and 'universal' empirical relationship for design?**

$$\frac{da}{dN} = C\left[\frac{1 + C_H R}{1 - R}\right]\Delta K^m$$

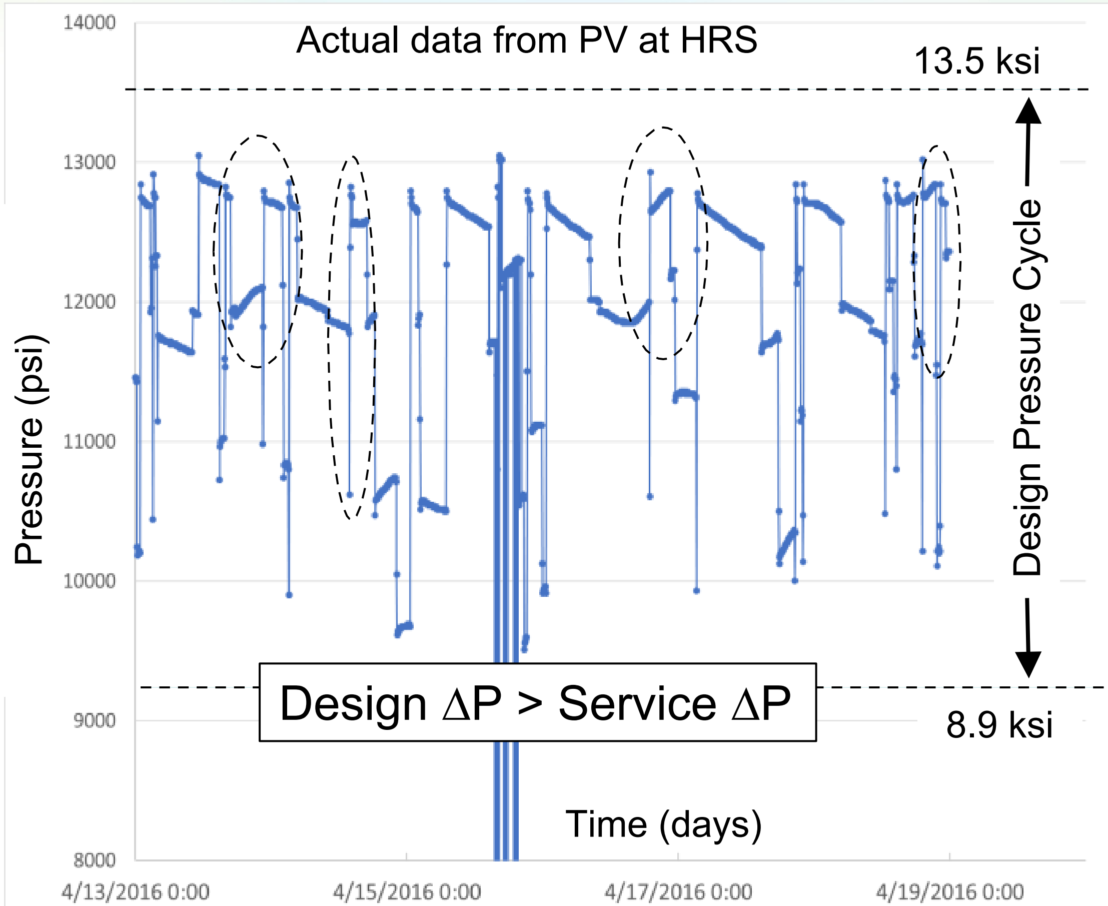
Relatively simple power law relationship implemented in ASME design code for PVs

- **Eliminates need for extensive testing (of common steels)**
- **Extends design life (by analysis) by a factor of 2-5 times for typical designs**



Demonstrating opportunity for 'life extension' through assessment of service environment

- **Evaluation of service data shows actual pressure cycles are significantly less than design cycle**
- **Design calculations using actual pressure cycles suggests significant remaining life**



Life can be extended by analysis after the original design life is reached (presumably) using existing Code

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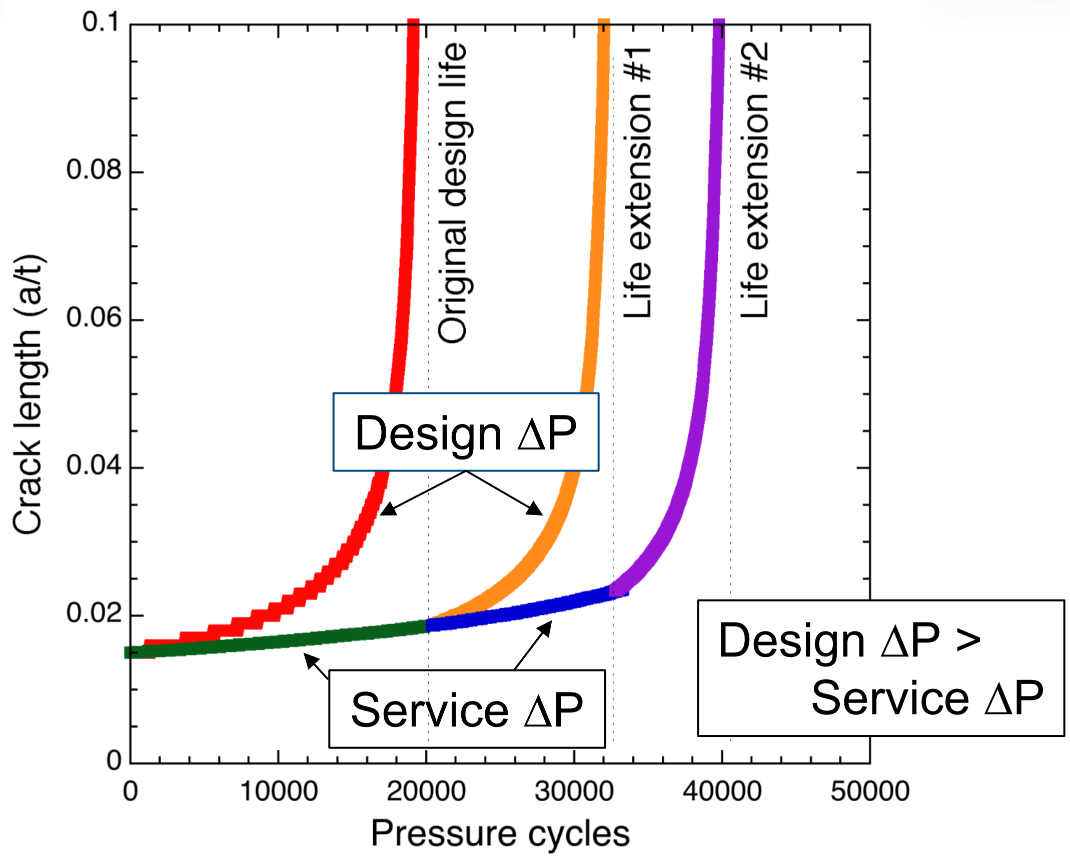

Life can be extended by analysis after the original design life is reached (presumably) using existing Code

Summary

H-Mat Hydrogen Materials Compatibility Consortium

- **H-Mat**
  - Vibrant research activities across length-scales (atoms to engineering) on relevant materials compatibility challenges
  - Focused on foundational understanding and predictive computational materials science to inform materials and microstructural design
- **Test method development**
  - Test method for difficult-to-test welds was developed; other geometries could be considered to accommodate unique manufacturing or welding configurations
  - FCGR design curves for steels in hydrogen included in ASME BPVC
    - Curves extrapolate well over wide range of ΔK (including near threshold)
    - Higher fidelity data suggest longer life of vessels for high-P storage
- ***Standardization***
  - International coordination has resulted in a relatively simple fatigue metric for materials evaluation in vehicle applications: SAE J2579 and UN GTR no. 13
  - Analysis shows that more accurate accounting of actual pressure cycles can extend useable life > 2X
  - Evaluating pressure dependence in fatigue rules for application to low-pressure and blended gas applications

Backup/Extra

Collaborations

- **National Laboratories**
  - Task teams integrated across laboratories, leveraging expertise at individual labs
- **Academic partners**
  - *Colorado School of Mines*: identification and custom heat treatment of high -strength ferritic steels
  - *University of California Davis*: fatigue behavior of austenitic stainless steels
  - *Rutgers University*: atomistic simulation of defects
- **New H-Mat partners**
  - *Colorado School of Mines, Hy-Performance Materials Testing LLC, MIT, Univ Alabama, Univ Illinois (UIUC)*
- **Industry partners**
  - *Swagelok*: letter of support and interest in high-strength microstructure
  - *Luna Innovations:* SBIR on NDE to identify damage prior to cracking
- **International research institutions (informal)**
  - *Kyushu University, University of Stuttgart, Korea Research Institute of Standards and Science*: regular communications on capabilities, data

Collaborations (SCS)

- ***Standards Development Organizations (SDOs)***
  - SAE & UN GTR: Test method for SAE J2579 and proposed method for GTR no. 13 Phase II is based on extensive international discussion with organization stakeholders and automotive OEMs
  - ASME BPVC: Code case adds design guidance to Article KD-10; ASME community and stakeholders are engaged in tank life extension discussion as well as requesting assistance on fatigue life versus fatigue crack growth methodologies
- **Industry partners**
  - Partners communicate materials testing gaps/needs and provide technology-relevant materials (FIBA Technologies, Tenaris-Dalmine, JSW, Swagelok)
  - International MOU: evaluation of Ni-Cr-Mo PV steels, motivation of Code Case for ASME BPVC and future testing plans (threshold fatigue crack growth and $R < 0$)
  - NASA-WSTF and Digital Wave: non-destructive evaluation of metal liner in tanks
  - Becht Engineering and Air Products: comparison of actual service environments and design criteria, evaluation of margin in design and opportunity for life extension
- ***International research institutions***
  - Performance-based fatigue evaluation in the context of SAE is focus of R&D collaboration with international community, including collaborative research activity in Japan (Kyushu Univ) and Germany (MPA Stuttgart)
    - Korea and China have expressed interest to participate as well