SAND2013-4192P

Used Fuel Disposition Campaign

Multi-resolution metal/hydride model for the mechanical behavior and performance of used nuclear fuel Zircaloy cladding

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UNF NCT Loading & Structural Performance
May 22, 2013

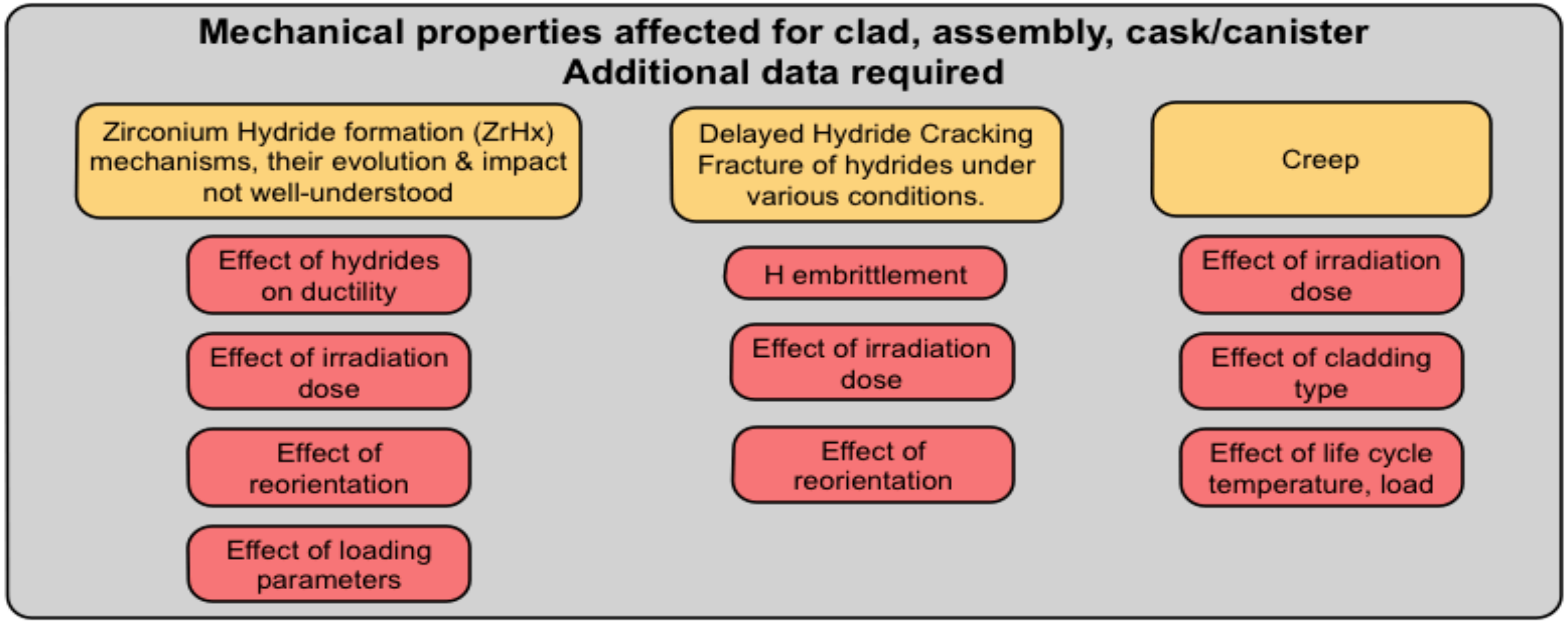
Acknowledgments

- Glen Hansen
- Jake Ostein (Initial mechanical model)
- Qiushi Chen (Initial mechanical model)
- Carl Beyer

Content

- Current state of the art of modeling of cladding behavior modeling:
  - Hydride formation and nucleation
  - Mechanical behavior
- Mechanical behavior of hydrided clad
- Hydride nucleation and growth
- How does it fit within the UFDC campaign?

The UFD gap analysis report identified cladding performance degradation mechanisms and ranked them by importance



Mechanical properties affected for clad, assembly, cask/canister
Additional data required

Zirconium Hydride formation (ZrHx) mechanisms, their evolution & impact not well-understood
- Effect of hydrides on ductility
- Effect of irradiation dose
- Effect of reorientation
- Effect of loading parameters

Delayed Hydride Cracking Fracture of hydrides under various conditions.
- H embrittlement
- Effect of irradiation dose
- Effect of reorientation

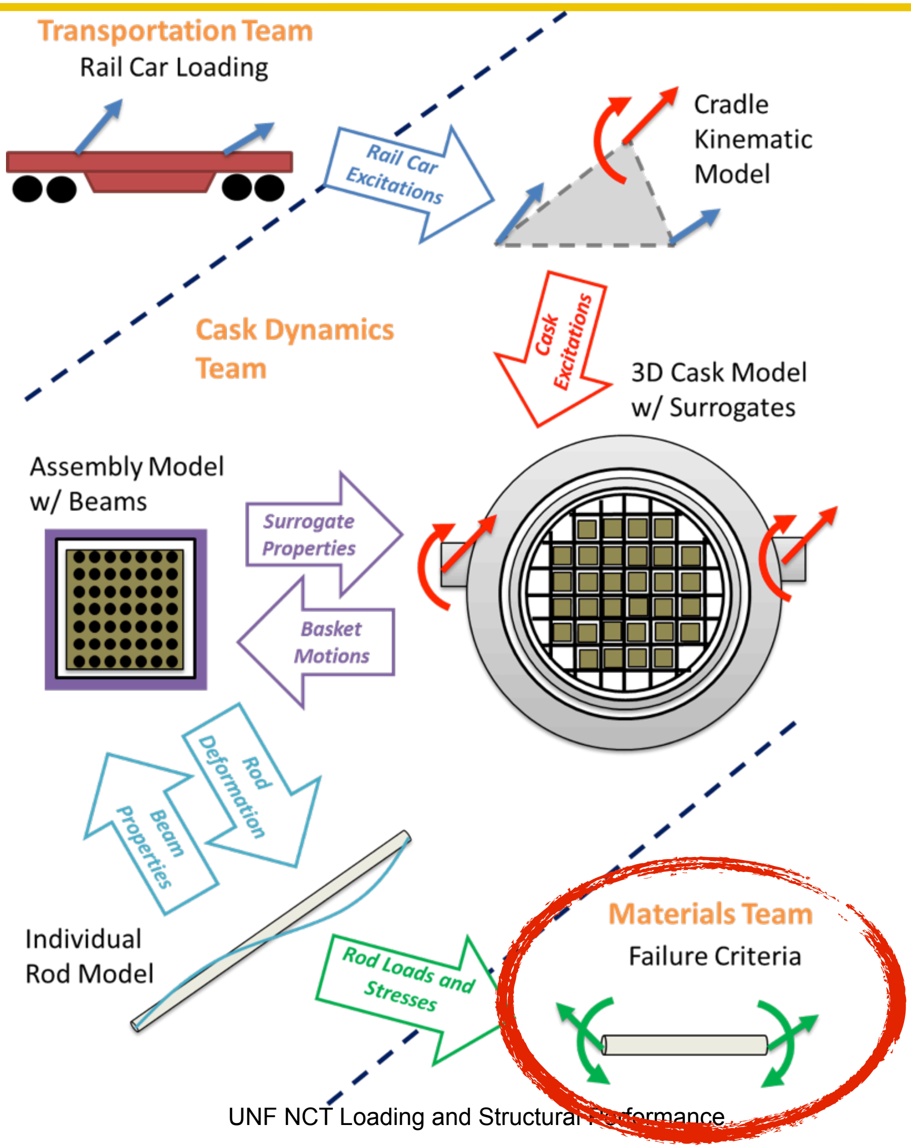
Creep
- Effect of irradiation dose
- Effect of cladding type
- Effect of life cycle temperature, load

[Hanson, B. et al., FCRD-USED-2011-000136, 2011.]

[Maheras, S.J. and S.B. Ross, FCRD-USED-2011-000323, 2011.]

- **These issues impact the dynamic response of fuel assemblies as well as the associated materials properties uncertainties and boundary conditions uncertainties (storage history, loading conditions).**
- **Driving forces: (Peak and time) temperature, cladding stresses, burnup level.**

Modeling and Simulation: from system dynamics to single fuel pin modeling



Modeling of hydride precipitation: thermodynamics and precipitation kinetics theory

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PREPRINT

A DEFORMATION AND THERMODYNAMIC MODEL FOR HYDRIDE
PRECIPITATION KINETICS IN SPENT FUEL CLADDING

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Scientific Basis for Nuclear Was
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Hydride reorientation in Zircaloy-4 cladding

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[a] Department of
[b] Institute

Abstract

The formation of radial hydride
target hydrogen levels from 100 to
hydrides by a hydride reorientation
isothermal treatment. Based on the
ior of hydrides in Zircaloy claddin
precipitates were developed. The t
hydrogen concentration.
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PACS: 28.52.Fa

1. Introduction

The mechanical properties o
be adversely affected by the pre
when they are oriented toward
tubing (i.e. radial hydride) [1–
hydrides in Zircaloy materials i
rication history, texture and str
sufficient ductility to keep its i
vice, Zircaloy fuel cladding tu
well controlled condition to en
tial hydride platelets are to dev
However, radial hydrides can b
process, when a specimen is coo
temperatures at which hydride
the case, Zircaloy fuel cladding
ger internal pressure and to ha

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An elastoplastic phase-field model for the evolution of hydride precipitation in zirconium. Part II: Specimen with flaws

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1. Introduction

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The terminal solid solubility of hydrogen in irradiated Zircaloy-2 and microscopic modeling of hydride behavior

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Modeling of hydride precipitation: thermodynamics and precipitation kinetics theory

- **Rate of ZrHx nucleation in Zr matrix:**

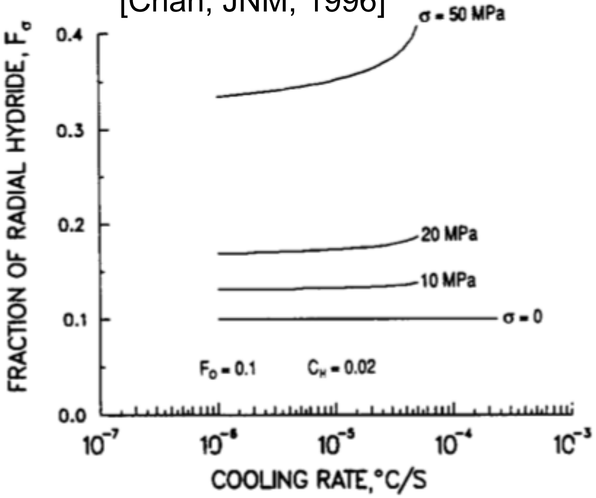
$$J = \frac{D c_H}{\lambda_{\mathrm{Zr}}^2} \left(\frac{\rho_{\mathrm{CW}}}{\lambda_{\mathrm{Zr}}} + N_\phi + N_{\mathrm{GB}} \right) \exp\left(\frac{-\Delta G}{kT} \right)$$

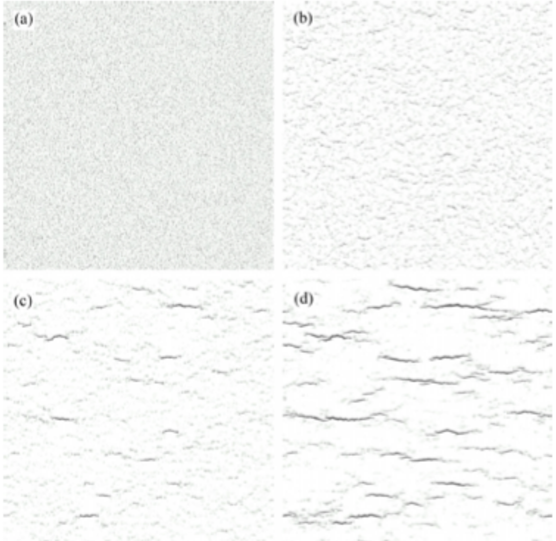
- **Input parameters**
  - Temperature
  - H diffusion
  - H concentration
  - Defect density (irradiation, dislocations, other defects)
  - Critical activation energy for nucleation
  - Stress level
  - Hydride misfit strain
  - TSSP solvus, solution solvus. Solubility limit of the material

- **Modeling methodology**
  - Finite Element
  - Finite Difference
  - Phase Field modeling (grain level)
  - Kinetic Monte Carlo simulations (grain level)

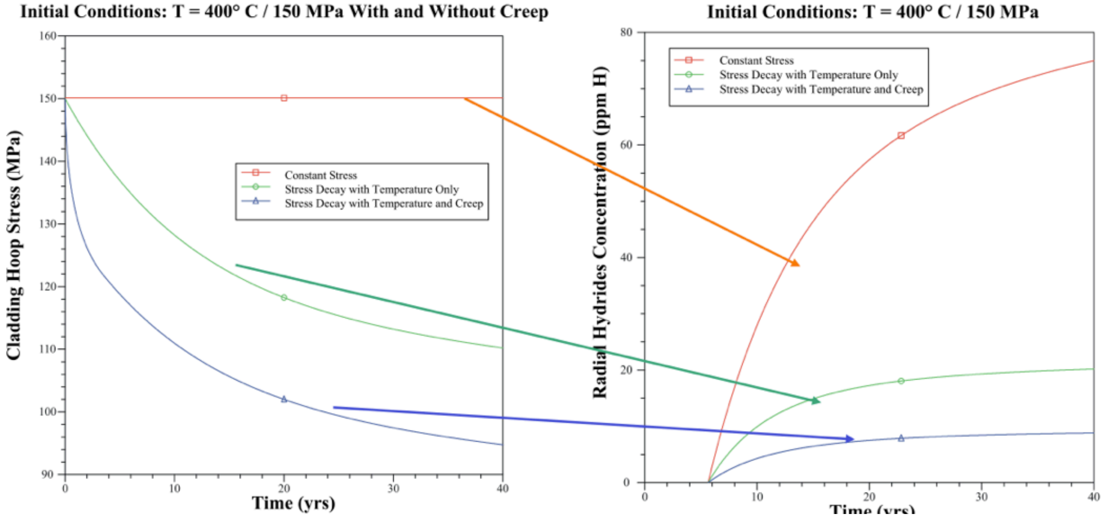
The formation of hydrides can be simulated for various drying scenarios (i.e. what is the state of the material as it is ready to be shipped?)

[Chan, JNM, 1996]

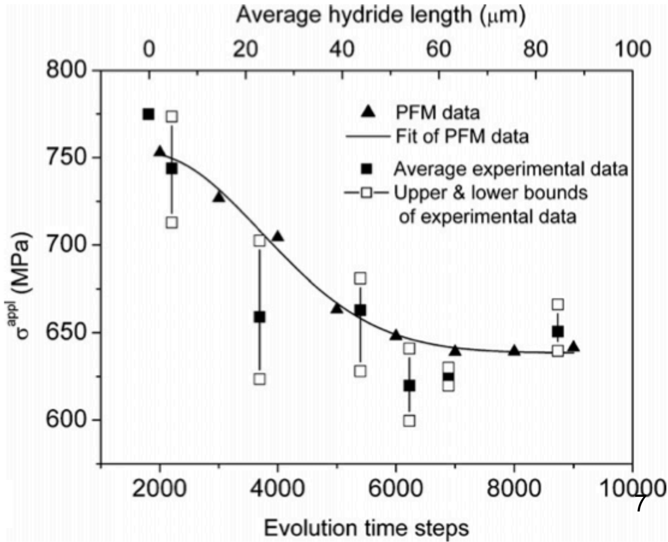




[Guo, JNM, 2008]



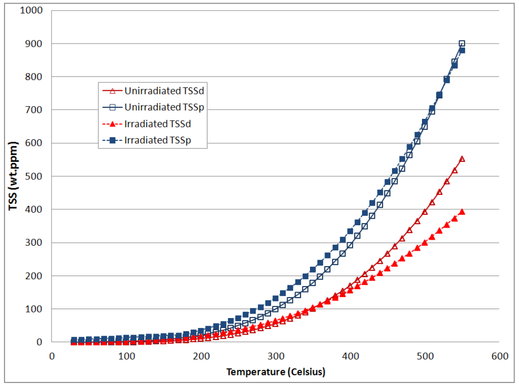
Stress History During Dry Storage

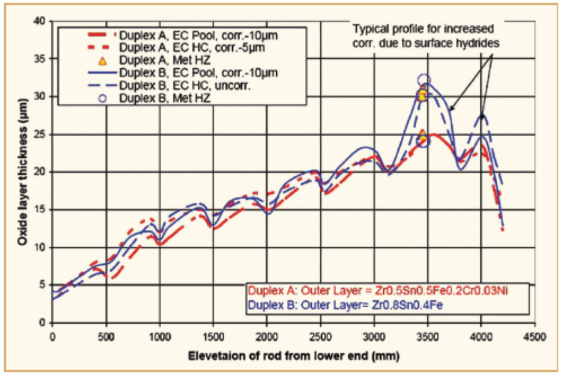


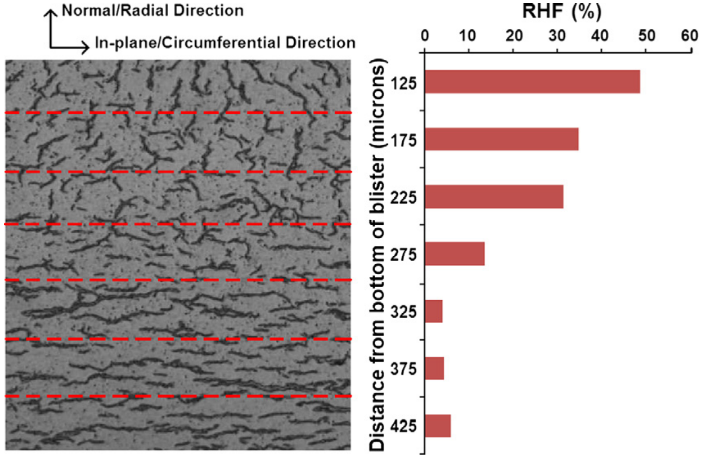
The formation of hydrides can be simulated for various drying scenarios (i.e. what is the state of the material as it is ready to be shipped?)

- **Typical output:**
  - Volume fraction of radial hydride vs. time at different stress levels
  - Volume fraction of radial hydride vs. cooling rate
  - Hydride connectivity and length (PFM)

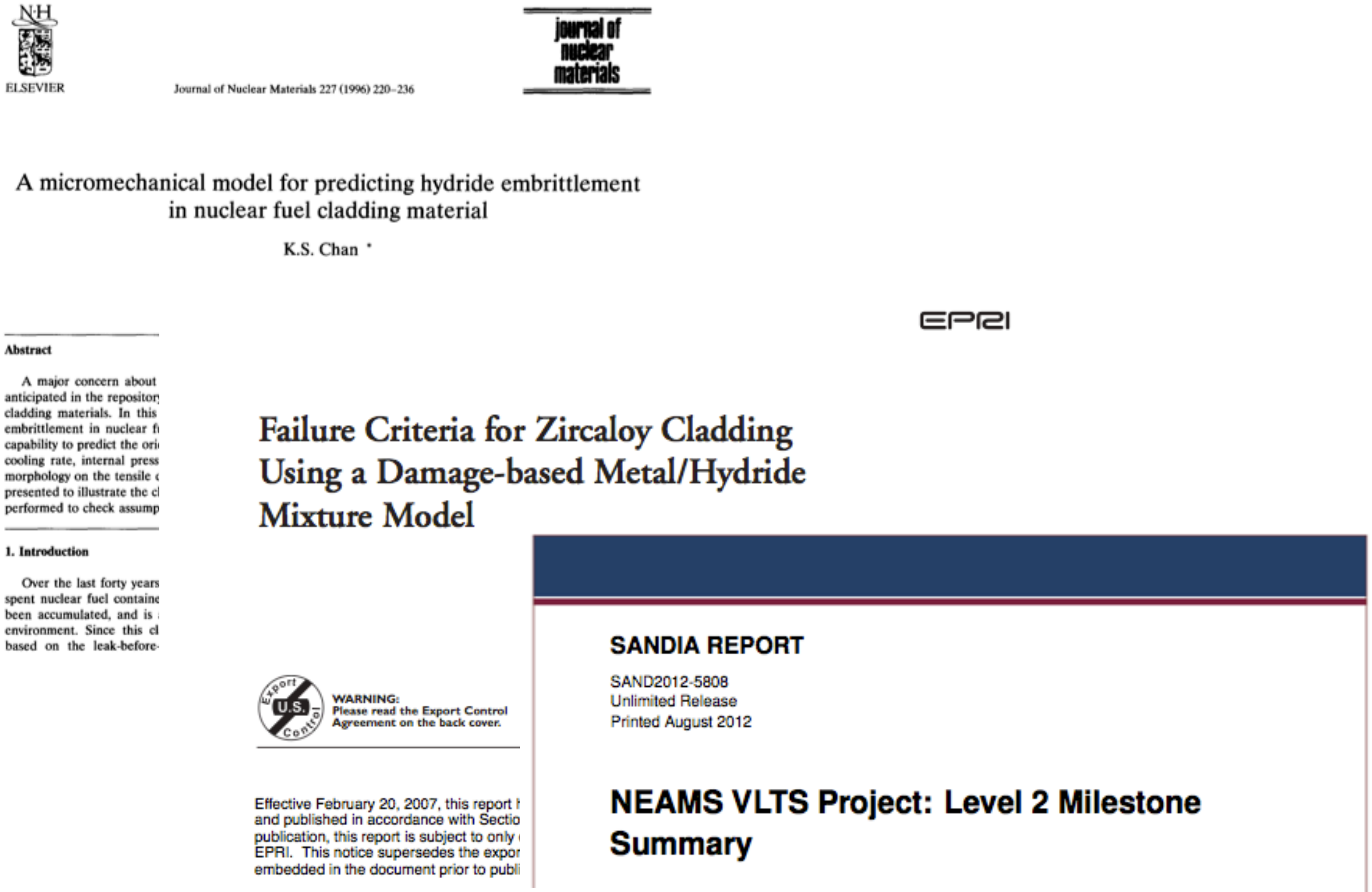
- **Verification and validation:**
  - Terminal Solid Solubility (TSS): Differential scanning calorimetry experiments
  - Microscopy quantification of precipitation morphology (Arborelius, Billone, Chung, Motta) for various configurations
  - In-situ XRD (T + σ) (Motta)
  - Limited by time constants and irradiation







Failure and damage criteria for Zircaloy cladding based on fracture mechanics and micromechanics



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Journal of Nuclear Materials 227 (1996) 220–236

journal of nuclear materials

A micromechanical model for predicting hydride embrittlement in nuclear fuel cladding material

K.S. Chan *

Abstract

A major concern about
anticipated in the repositor
cladding materials. In this
embrittlement in nuclear f
capability to predict the ori
cooling rate, internal press
morphology on the tensile
presented to illustrate the c
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1. Introduction

Over the last forty years
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EPRI

Failure Criteria for Zircaloy Cladding Using a Damage-based Metal/Hydride Mixture Model

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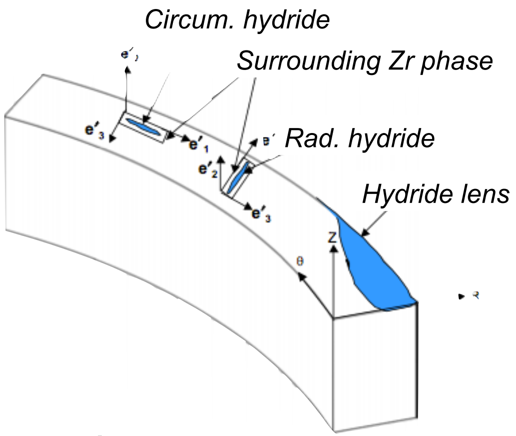
NEAMS VLTS Project: Level 2 Milestone Summary

Failure and damage criteria for Zircaloy cladding based on fracture mechanics and micromechanics

- Ductility of a hydrided material comes from two contributions: (i) **hydrides** (brittle phase) and (ii) the **matrix ligaments** (ductile phase). Distinction between circumferential and radial hydrides.



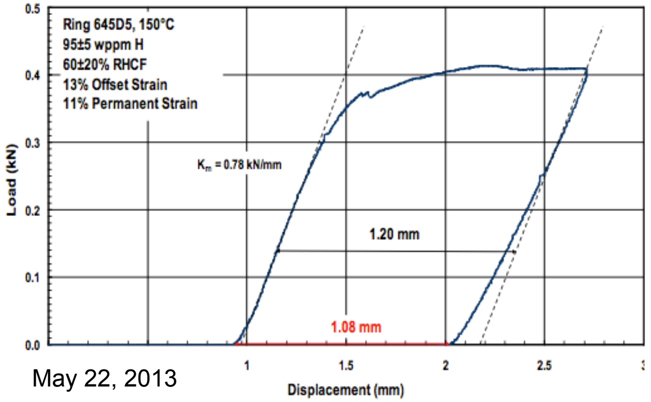
- **Input parameters**
  - Hydride length and connectivity
  - Volume fraction of hydride and their orientation
  - Elasto-plastic properties of Zr matrix and hydrides (E, μ, σ_Y, H_0)
  - Temperature
  - Loading mode
  - Irradiation

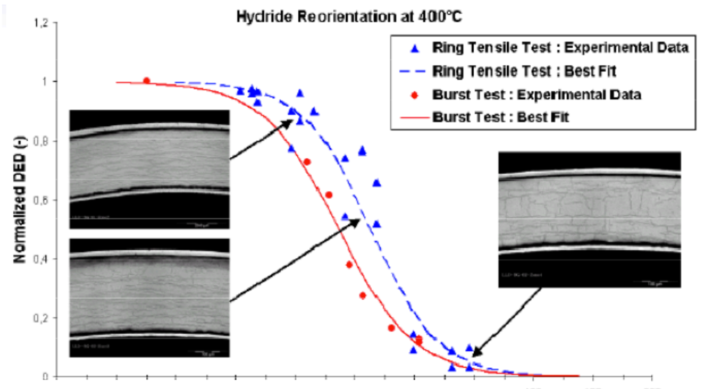
- **Modeling methodology**
  - Finite Element (continuum)
  - Crystal Plasticity Finite Element (i.e. grain level model)

The mechanical behavior of damaged cladding and rupture criteria can be extracted from these types of simulations

- **Typical output:**
  - Constitutive behavior of hydrided cladding
  - Ductile-to-Brittle transition (DBT)
  - Fracture criteria

- **Verification and validation:**
  - Tensile/Bend tests / ring compression tests of hydrided specimen in controlled environments (Billone, Wang)
  - Ring tensile test and burst test
  - H.P. Robinson data with 72 GWD and 63 GWD burnup with a known neutron fluence
  - Verification and validation of the model for cladding with mixed hydride structure is limited by data (irradiation and hydride re-orientation)





Cladding mechanical model incorporating hydride effects

- **J2 fiber damage model**
  - Zr matrix treated as an elasto-plastic material
  - Hydrides modeled as “fibers” with an associated orientation (radial vs. circumf.)

$$\boldsymbol{\sigma} = f_m \boldsymbol{\sigma}_m + \sum_i^n f_i \boldsymbol{\sigma}_i$$

$$\boldsymbol{\sigma}_m = (1 - \xi_m)\boldsymbol{\sigma}^0 = (1 - \xi_m)\boldsymbol{\tau}^0 / J$$

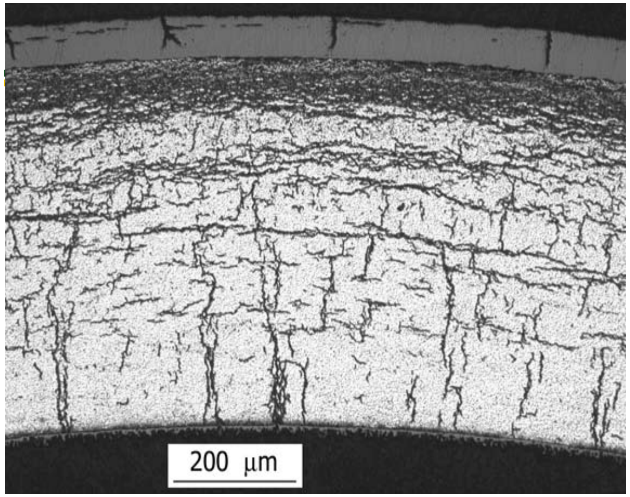
damage parameter

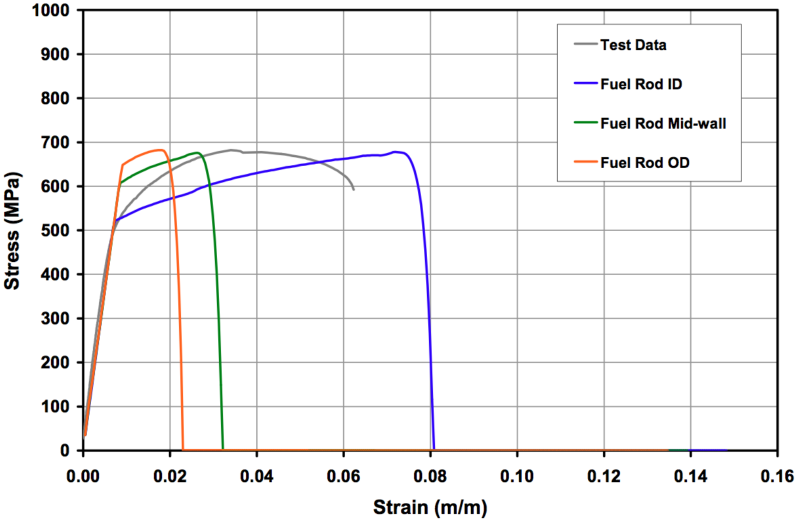
$$\xi(\alpha) = \xi_\infty [1 - \exp(-\alpha/\tau)]$$

maximum thermodynamic force

damage saturation parameter

dimensionless maximum damage

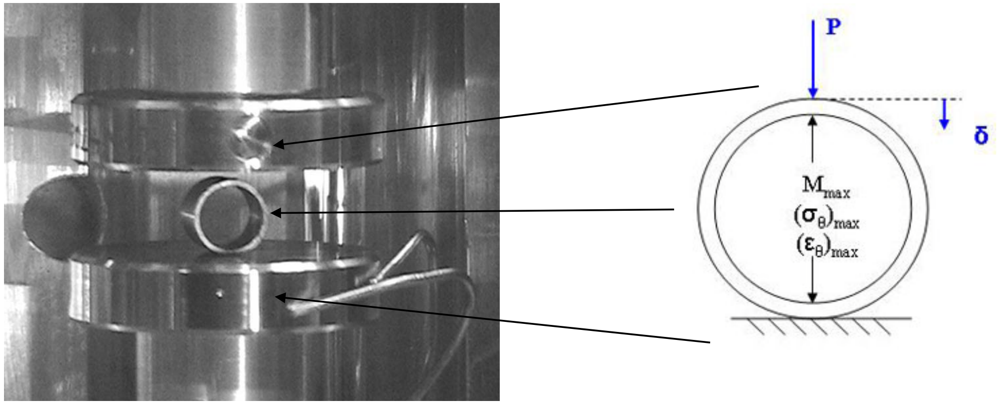


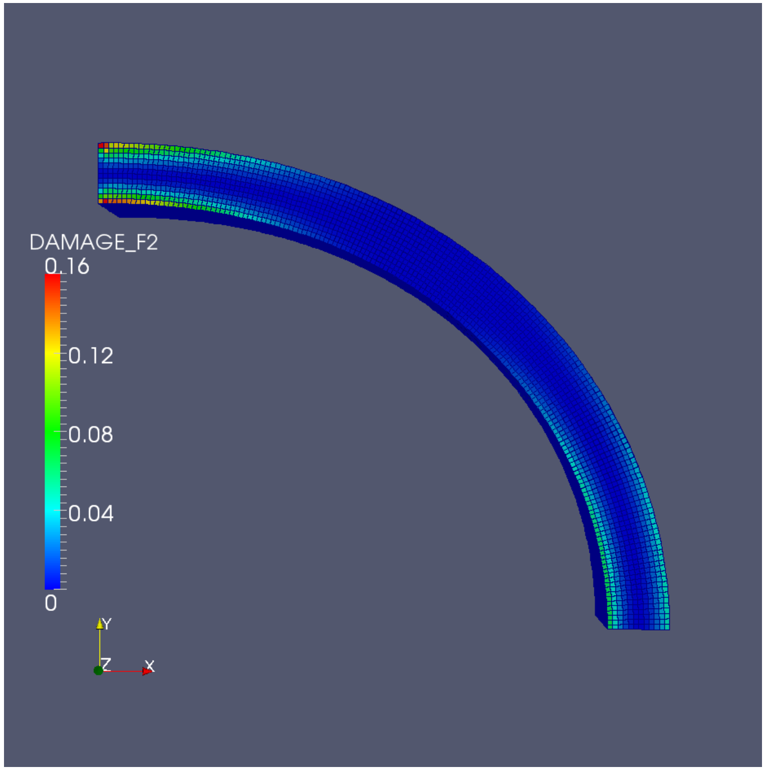


[Stress-strain response at 300 ^{o}C, J. Rashid et.al., EPRI, 2009]

Calibration and validation this material model

- **ANL ring compression test**

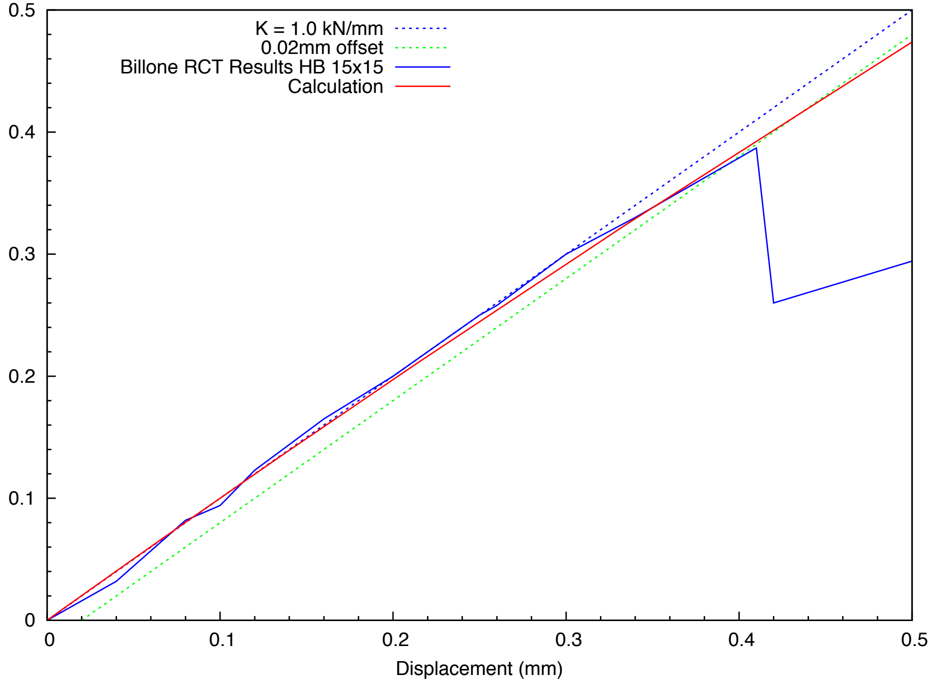


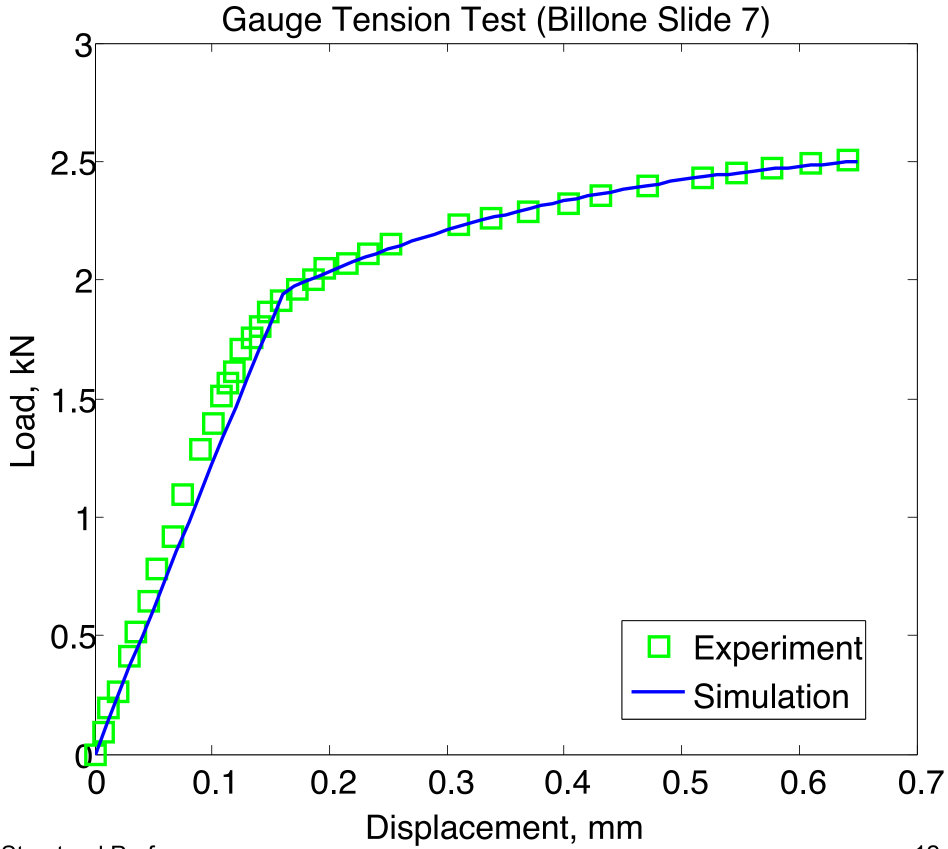


[Stress-strain response at 300 ^{o}C, J. Rashid et.al., EPRI, 2009]

Calibration and validation this material model

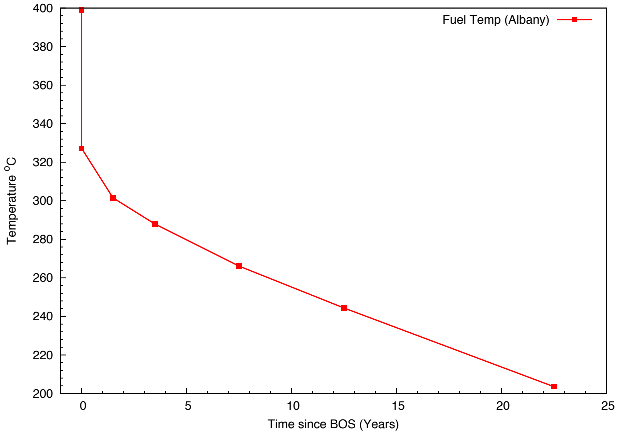
- **The volume fraction of radial hydrides vs. circumferential hydride impact ring load/displacement behavior.**
- **Need for additional non-RCT data for validation.**



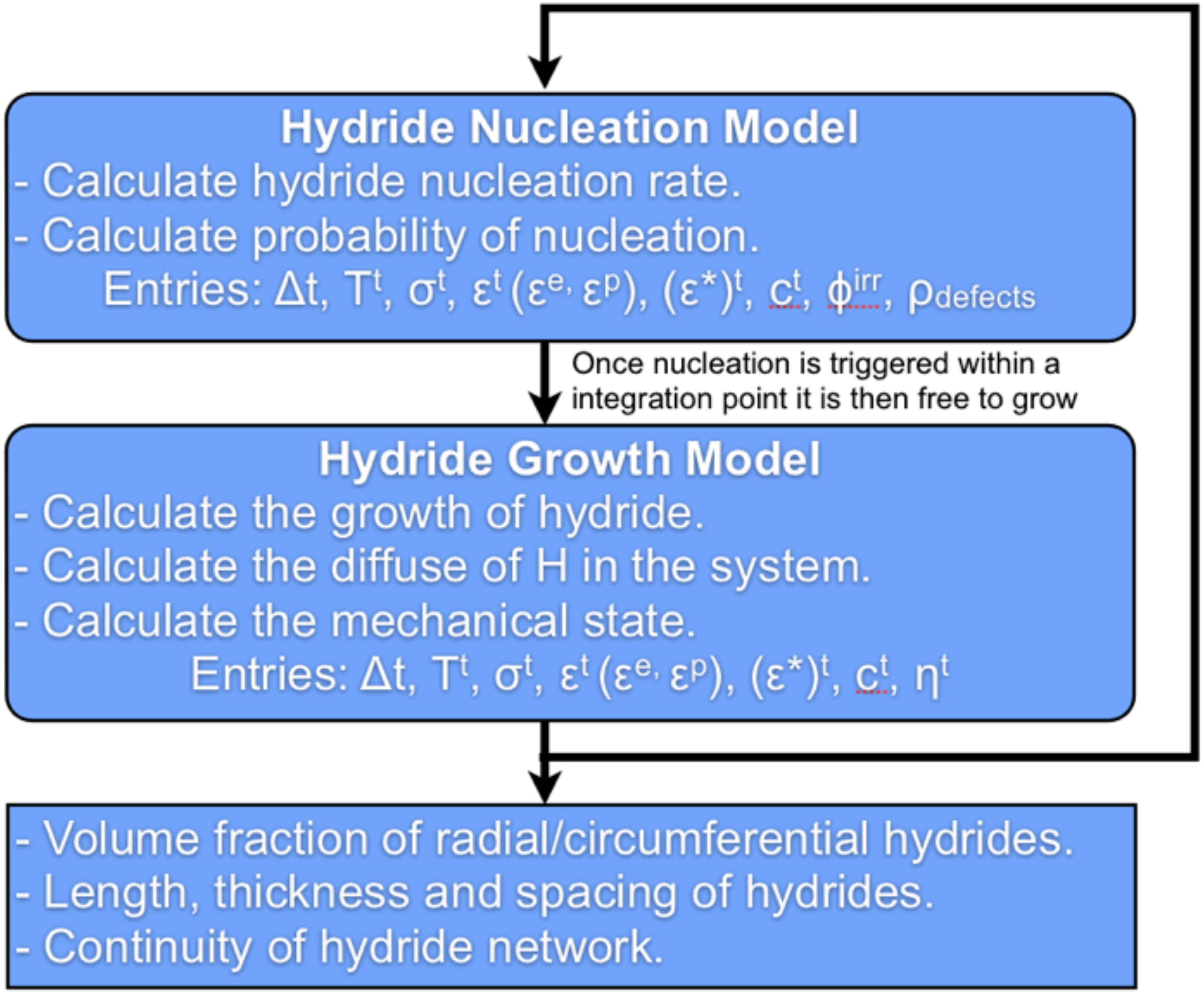

Gauge Tension Test (Billone Slide 7)

What is the state of the clad material as it is ready to be shipped?
Hydride nucleation and growth model

Heat equation →



Temperature driven by decay heat and environmental conditions



Hydride Nucleation Model

- Calculate hydride nucleation rate.
- Calculate probability of nucleation.

Entries: Δt, T^t, σ^t, $\varepsilon^t\,(\varepsilon^{e,}\,\varepsilon^{p})$, $(\varepsilon^*)^t$, c^t, ϕ^{irr}, $\rho_{defects}$

Once nucleation is triggered within a integration point it is then free to grow

Hydride Growth Model

- Calculate the growth of hydride.
- Calculate the diffuse of H in the system.
- Calculate the mechanical state.

Entries: Δt, T^t, σ^t, $\varepsilon^t\,(\varepsilon^{e,}\,\varepsilon^{p})$, $(\varepsilon^*)^t$, c^t, η^t

- Volume fraction of radial/circumferential hydrides.
- Length, thickness and spacing of hydrides.
- Continuity of hydride network.

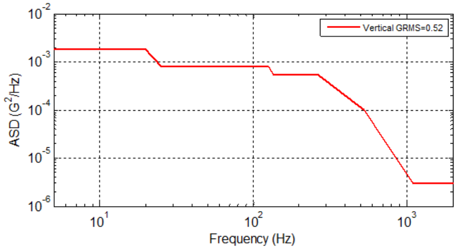
Based on the current state-of-the-art, gaps and limitations for materials behavior have been identified

- **Mechanical properties after extended storage is not clearly known:**
  - Hydride fraction, connectivity, morphology.
  - Extent of cumulative damage due to the combination of hydrides and irradiation.
  - Fundamental physical properties not clearly characterized (activation energy, diffusion coefficients, hydride misfit strain, oxidation rate).
  - Mechanical properties not clearly characterized (fracture toughness, hardening modulus, hydride mechanical properties).
  - Combined effect of hydriding and creep.
  - Effect of cladding annealing (annealing of radiation damage and impact on materials properties).
- **The performance requirements for NCT are not clearly defined**
  - "We want to be X% confident that Y% of the fuel pin will not see a strain exceeding Z "?
  - Definition of performance requirements both at the assembly level and fuel pin level? (NUREG-1567 accepts 1% rod breakage for normal conditions)

How does this integrate within the UFDC experimental efforts?

- **SNL shaker table test (McConnell, SNL)**
  - Measure the structural response directly on a mock fuel rods in an 17 X 17 PWR fuel assembly when subjected to vibration and shock loads simulating those produced during normal transport by truck.
  - Equipped with 18 accelerometers and 46 strain gauges.
  - Provide data to calibrate and validate vibrational and dynamics models of fuel assembly.

Figure 3.0-1: Recommended Random Vibration Test Specification



- **High Burnup UNF bend testing on cladding with fuel in place (Wang, ONRL)**
  - Measure mechanical response of H.B. Robinson WE 15x15 rod segments w/ 63-67 GWd/MTU average burnup.
  - Provide data to calibrate and validate constitutive models for hydrided and irradiated clad.
- **Ring compression test on UNF cladding following simulated drying (Billone, ANL)**
  - Ring compression tests to provide input for pinch or crush loading analysis.
  - Provide data to calibrate and validate constitutive models for DBTT and irradiated clad.
  - Provide data for characterization of hydride length (continuity), orientation and distribution.
- ***In-situ* XRD measurements at Advanced Photon Source (Motta, PSU)**
  ***In-situ* ion irradiation TEM at SNL (Clark, SNL)**
  - Provide microscale data to calibrate and validate constitutive models for hydride re-orientation / hydride embrittlement.

Multiresolution schemes are necessary to appropriately model the mechanical constitutive behavior of clad as it is ready to be shipped

- **Development of a finite element based mechanical model for the constitutive behavior of hydrided clad materials.**
    - Depends on hydride orientation
    - Accounts for damage of hydrided "fibers"
- **Development of a hydride nucleation and growth model for the initial materials conditions prior to transport.**
    - Accounts for irradiation
    - Accounts for cooling history
    - Hydride characterization metrics: orientation, continuity, length
- **Validation and calibration of models with experimental data.**