Hydrogen Embrittlement Fundamentals, Modeling, and Experiment

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Hydrogen Embrittlement Mechanisms

- Several candidate mechanisms have evolved over the years each of which is supported by a set of experimental observations and strong personal views

- Viable mechanisms of embrittlement
  - Stress induced hydride formation and cleavage
    - Metals with stable hydrides (Group Vb metals, Ti, Mg, Zr and their alloys)
    - Supported by experimental observations
  - Hydrogen enhanced localized plasticity (HELP)
    - Increased dislocation mobility, failure by plastic deformation mechanisms
    - Supported by experimental observations
  - Hydrogen induced decohesion
    - Direct evidence is lacking
    - Supported by First Principles Calculations (DFT)

- Degradation is often due to the synergistic action of mechanisms

Embrittlement and Phenomenology

- **Fractographic evidence suggests that low strength steels under static loading fail by**
  - **Hydrogen-assisted transgranular fracture induced by void or microcrack initiation through decohesion at internal interface (precipitate/inclusion or phase boundaries) ahead of a crack or notch accompanied by shear localization (HELP) leading to the linking of the void/microcrack with the tip of the crack**
  - **Fracture is controlled by yield strength level and microstructure**

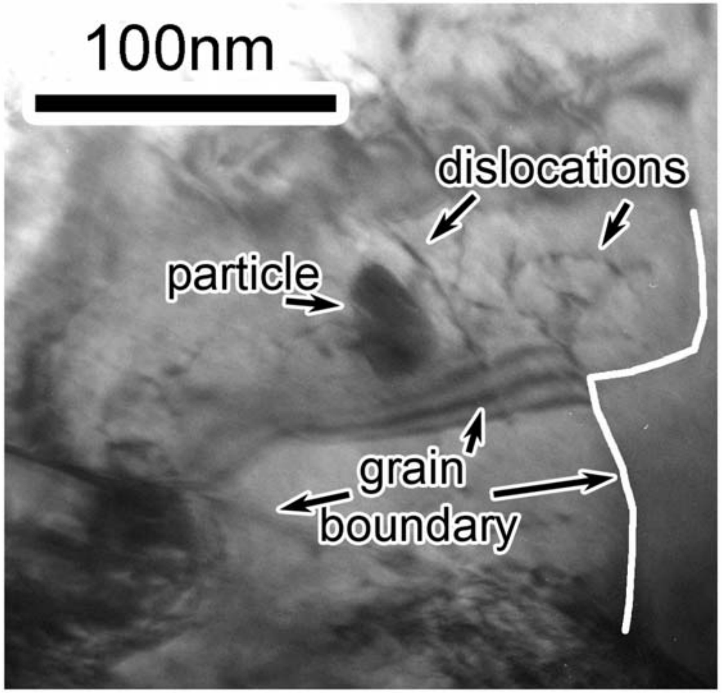
- **Our contention, which needs to be verified through experiment, is that embrittlement**
  - **Under static load is a result of the synergistic action of the HELP and decohesion mechanisms**
  - **Under cyclic load can be intergranular (extremely dangerous mode of failure)**

New Steel Microstructure-Oregon Steel Mills (OSM)

API Grade	C	Mn	Si	Cu	Ni	V	Nb	Cr	Ti
X70/80	0.04	1.61	0.14	0.22	0.12	0.000	0.096	0.42	0.015

acicular ferrite microstructure

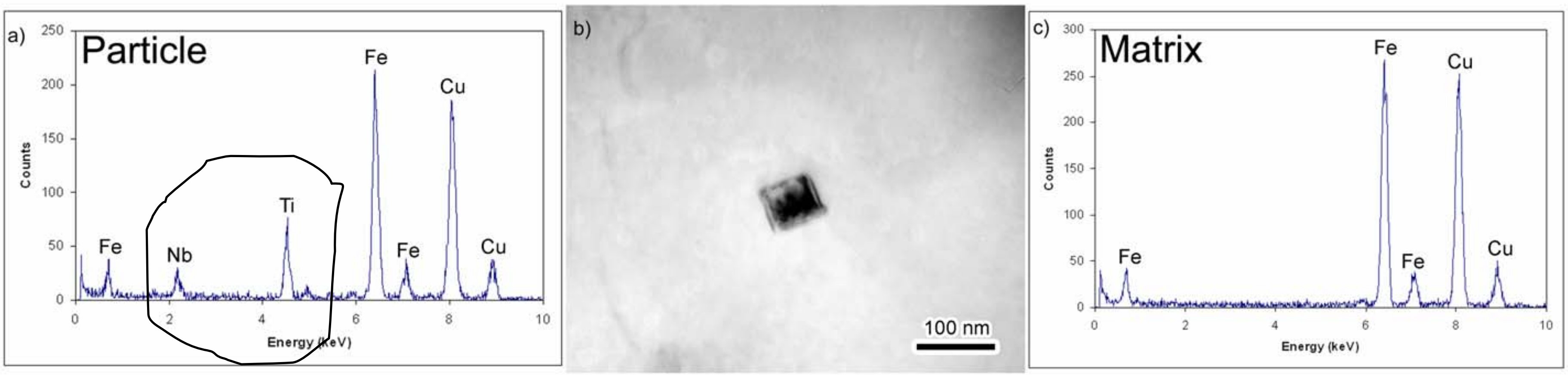
Defects in microstructure, particularly precipitates, act as trap sites for hydrogen



- High dislocation density in some regions
- Irregular grain boundaries and small grains, indicative of microstructure that has not been fully recrystallized and recovered.

Relatively low precipitate density (inside the matrix)

Particle Composition
Energy Dispersive Spectroscopy

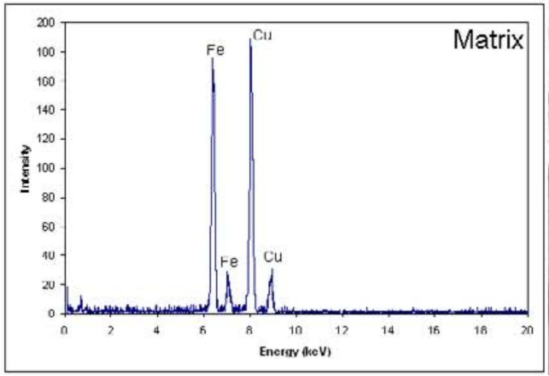


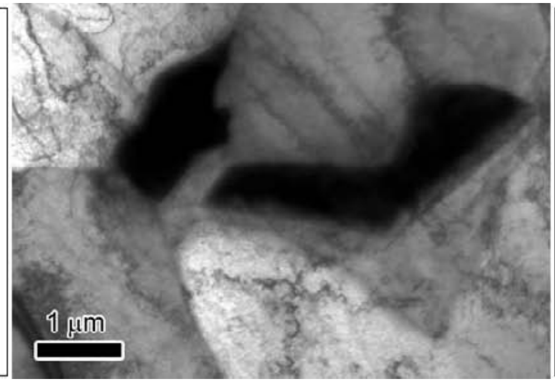
- a) EDS spectrum from particle
- b) Bright field TEM image of typical rectangular particle
- c) EDS spectrum from matrix

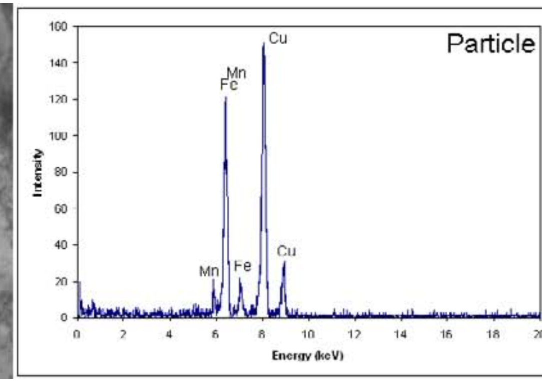
- EDS analysis of fine precipitate inside ferrite grain suggests that precipitate is composed of Ti and Nb

(window detector: C, N, O not detected)

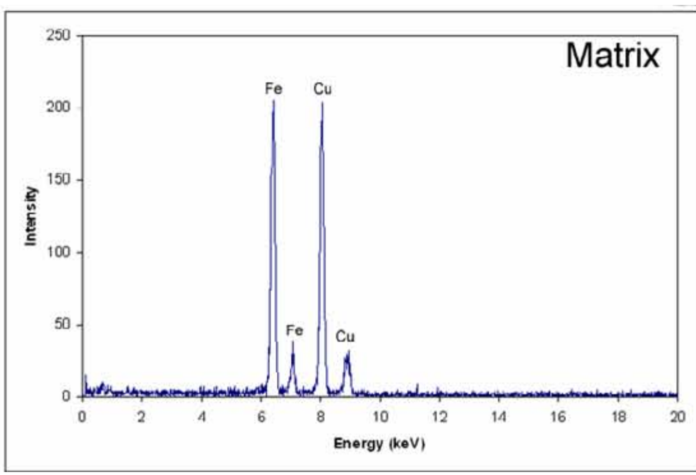
Steel Microstructure-Air Liquide Pipeline

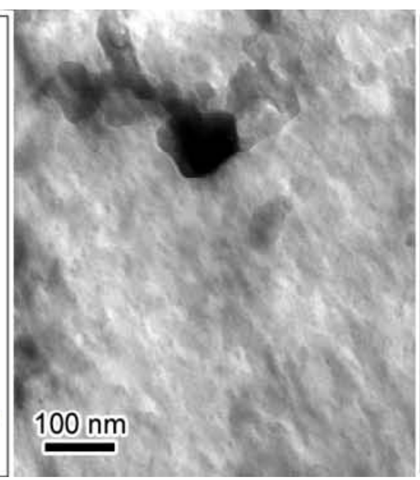


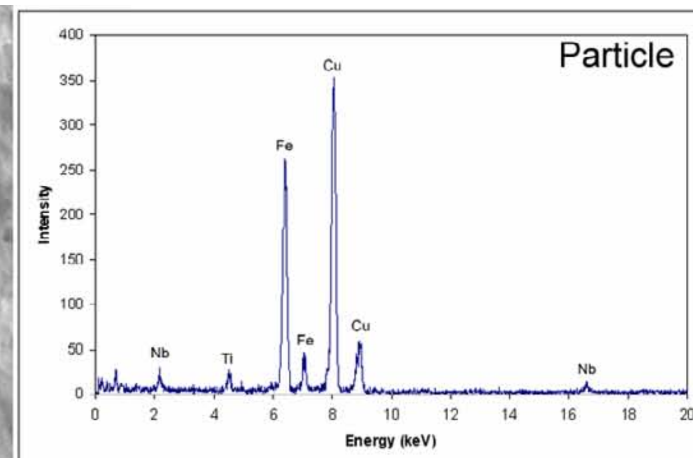




Large intergranular particles (cementite)







Small intragranular particles (carbides with Nb and Ti)

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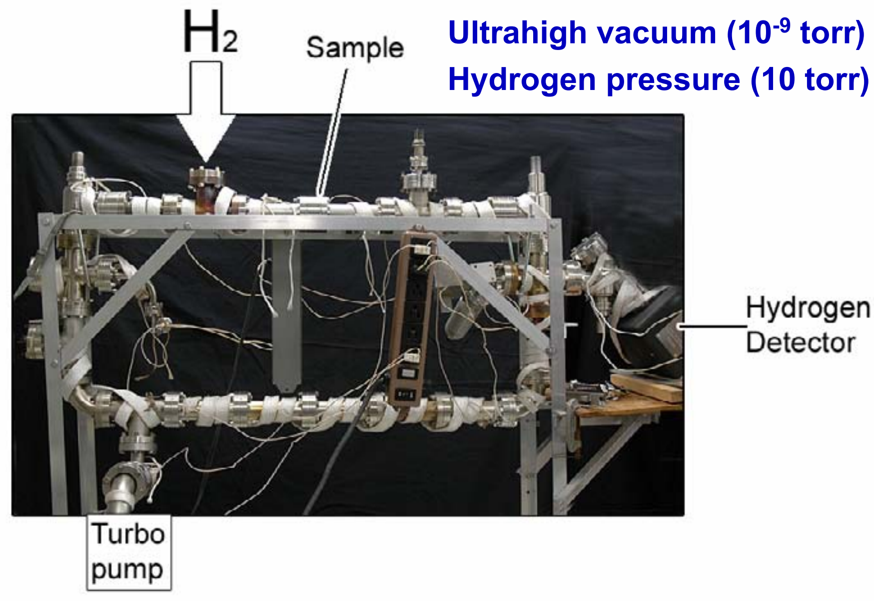
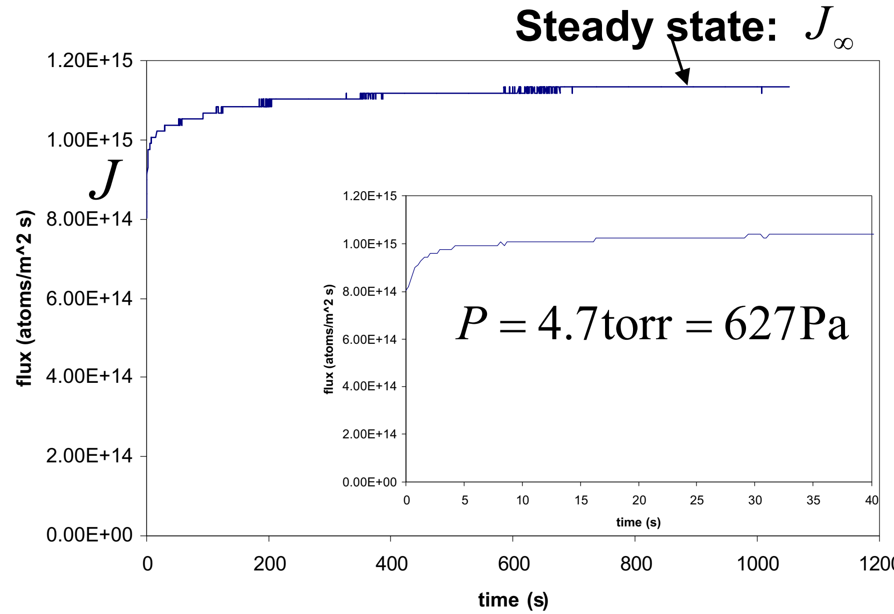
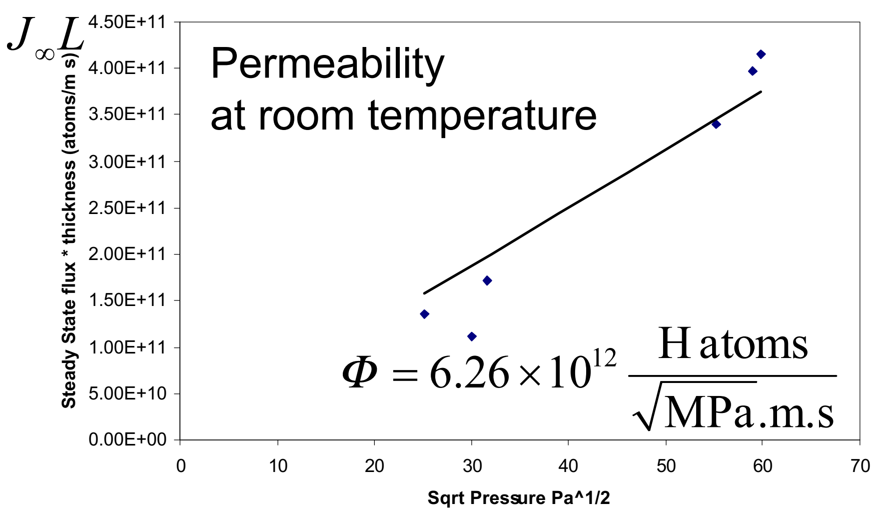
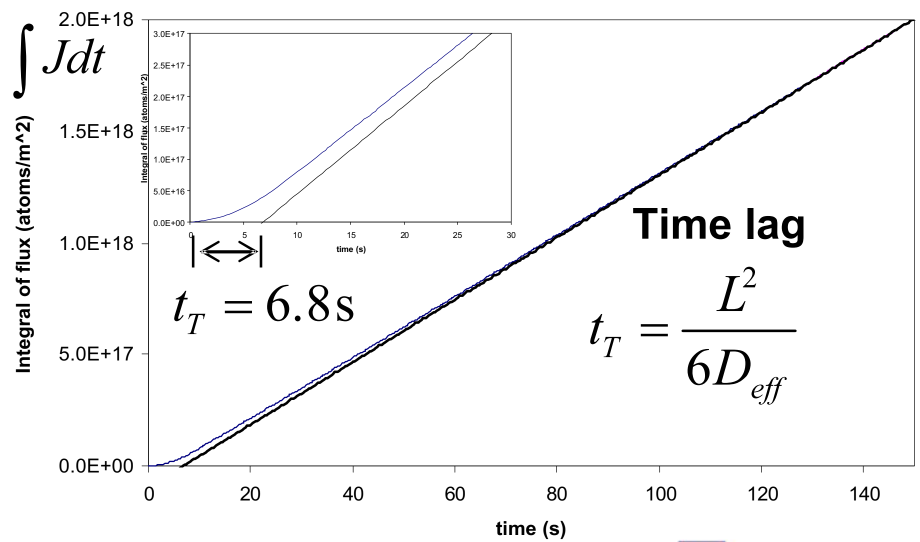
Hydrogen Permeation Measurements

Ultrahigh vacuum (10^{-9} torr)
Hydrogen pressure (10 torr)



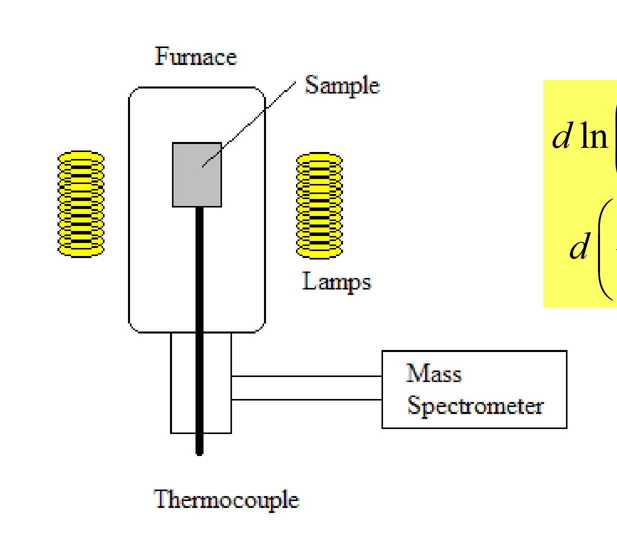




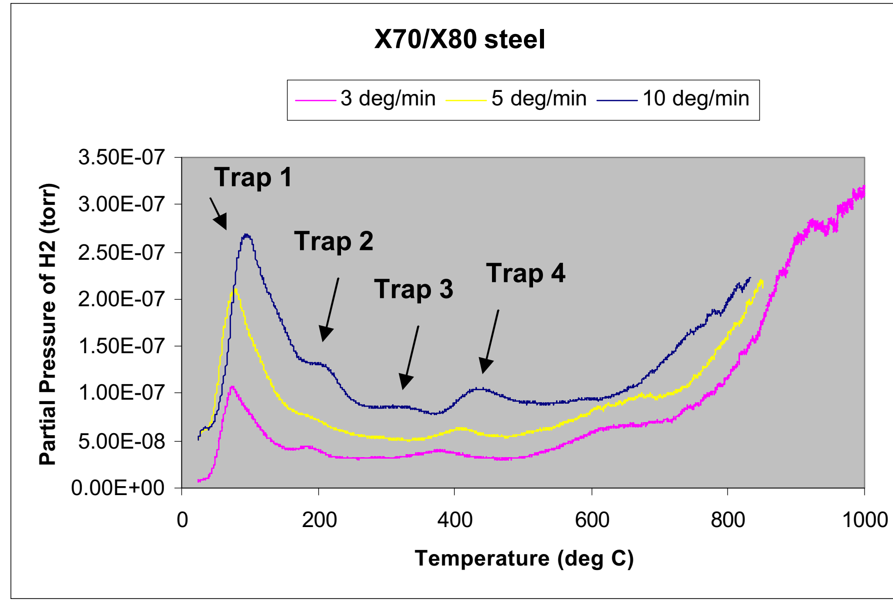


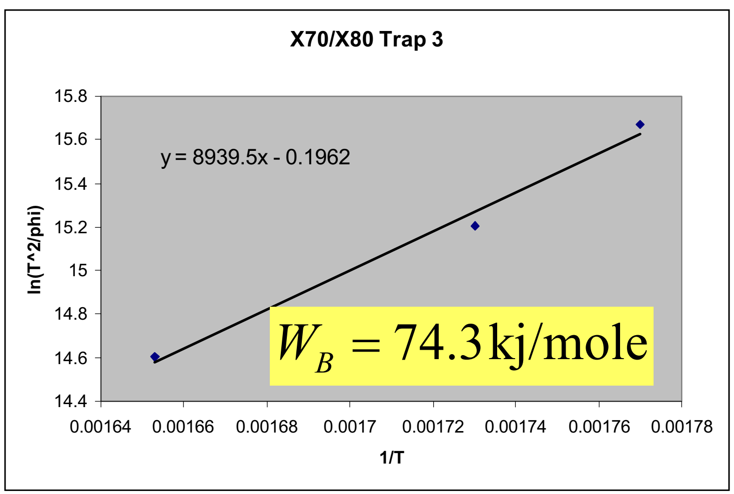
- Oregon Steel Mills sample: thickness $L = 120\,\text{microns}$
- room temperature

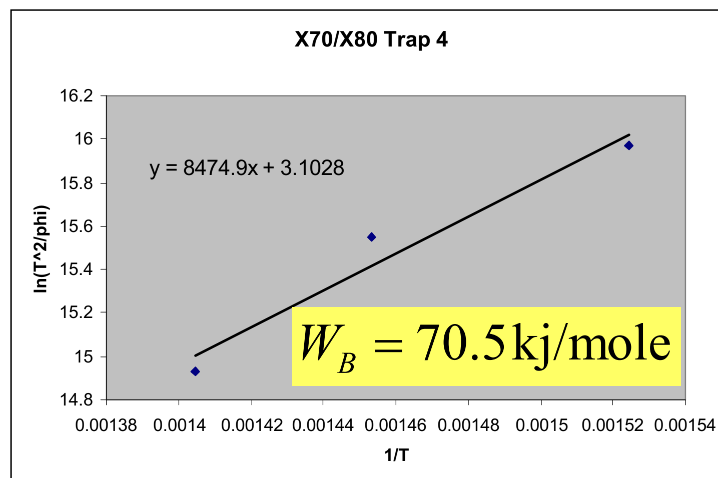
Thermal Desorption Spectroscopy



$$\frac{d\ln\left(\frac{\Phi}{T_{\max}}\right)}{d\left(\frac{1}{T_{\max}}\right)} = \frac{W_B}{R}$$







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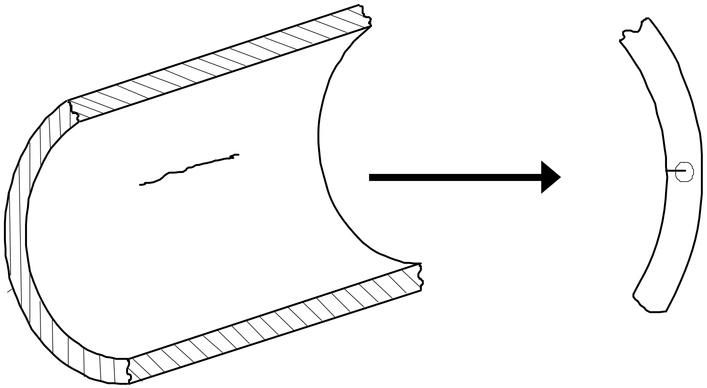
Materials Characterization

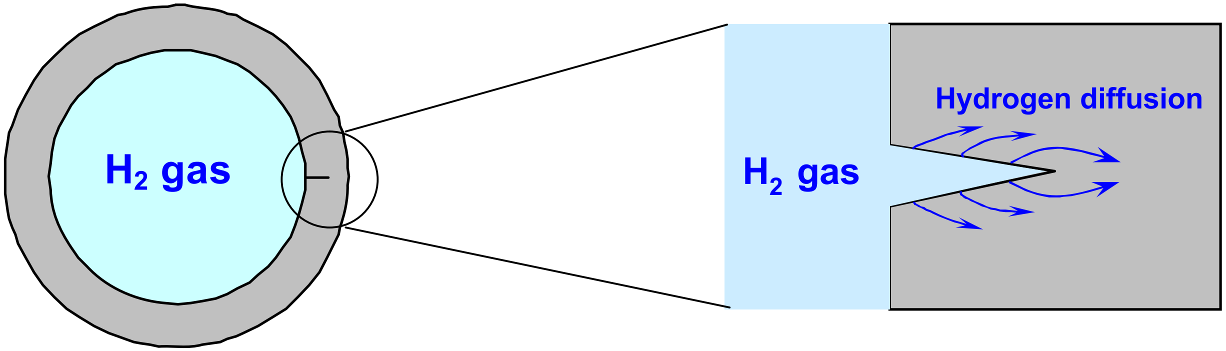
- TEM and TDS
  - will provide the trap binding energy.
- Permeation studies along with numerical simulation of diffusion transients
  - Will validate the trap binding energy determination
  - Will provide the trap density
- Coated samples (SECAT)

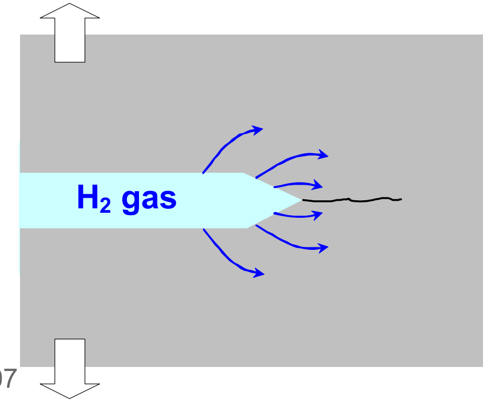
- Similar coordinated approach is needed to identify the fracture mechanisms under all loading scenarios
  - Rising load fracture toughness
  - Subcritical crack growth
  - Fatigue

Fracture Mechanics Approach to Design



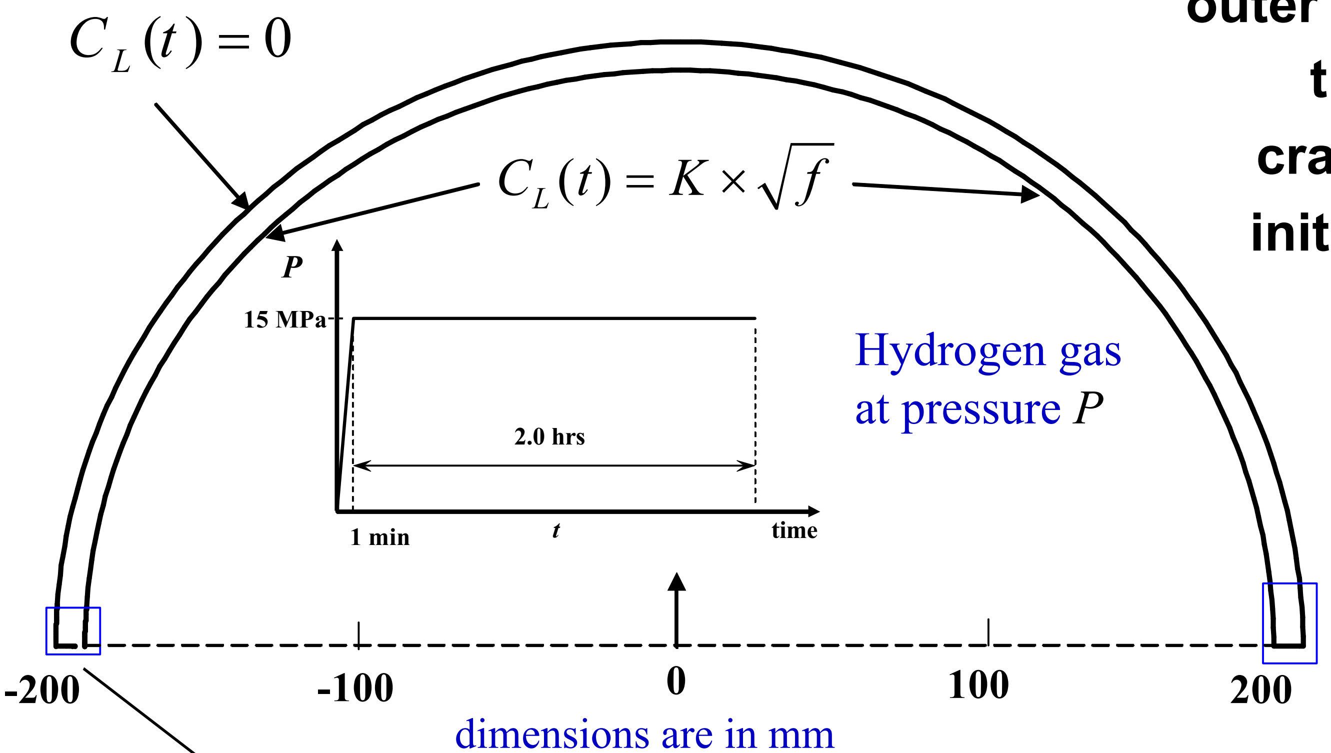
Determine the stress, deformation, and hydrogen concentration fields ahead of an axial crack in a pipeline





Case study related to subcritical crack growth experiments carried out at Sandia

Cracked Pipeline: Problem Statement



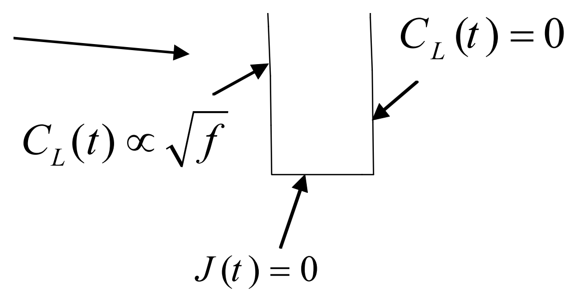
outer diameter: 40.64 cm

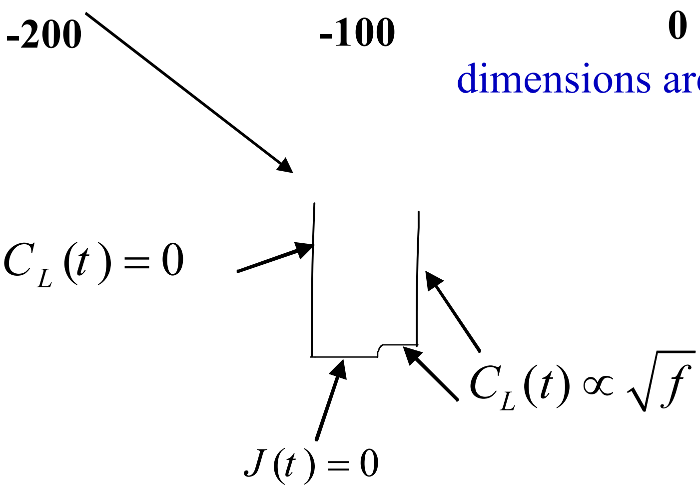
thickness: $h = 9.52$ mm

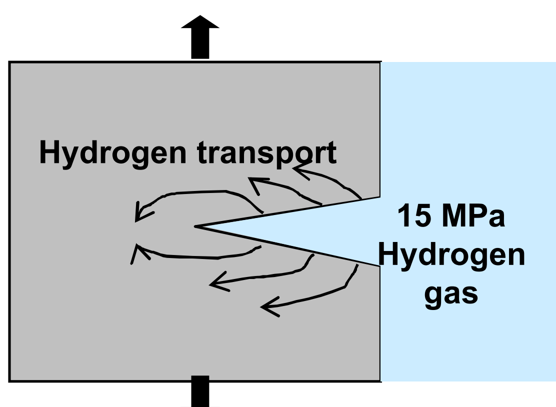
crack depth: $a = 1.9$ mm

initial CTOD: $b_0 = 1.5\ \mu\text{m}$

$a / h = 0.2$







K : **Solubility**

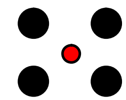
J : **Hydrogen flux**

P : **Pressure**

f : **Fugacity**

Hydrogen Transport Analysis

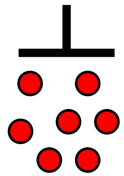
- **Diffusing hydrogen resides at**
  - **Normal Interstitial Lattice Sites (NILS)** $C_L = \beta\theta_L N_L$

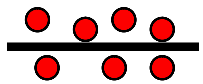


θ_L = NILS occcupancy
β = number of NILS per solvent atom.
N_L =number of solvent atoms/m^3.

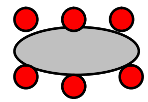
  - **Trapping Sites** $C_T = \alpha\theta_T N_T$
    - Microstructural heterogeneities such as dislocations, grain boundaries, inclusions, voids, interfaces, impurity atom clusters

dislocations





Grain boundaries



inclusions

θ_T = trap occcupancy
α = number of sites per trap.
N_T = number of traps/m^3.

- **Hydrogen populations in NILS and trapping sites are assumed to be in equilibrium according to Oriani's theory**

$$\frac{\theta_T}{1-\theta_T} = \frac{\theta_L}{1-\theta_L}\exp\left(\frac{W_B}{RT}\right)$$

W_B = Trap binding energy
T=Temperature
R=gas constant

  - Trap density may evolve dynamically with plastic straining

- **Hydrogen Transport Equation**

$$\frac{D}{D_{eff}}\frac{dC_L}{dt} = DC_{L,ii} - \left(\frac{DV_H}{3RT}C_L\sigma_{kk,i}\right)_{,i} - \alpha\theta_T\frac{\partial N_T}{\partial\varepsilon^p}\frac{d\varepsilon^p}{dt}$$

  - Note the effect of stress and plastic strain

d/dt = time differentiation
C = Hydrogen concentration
D = diffusion coefficient
D_{eff} = Effective diffusion
$= D/(1+\partial C_T/\partial C_L)$ accounting for trapping
σ_{kk} = hydrostatic stress
ε^p = plastic strain
V_H = partial molar volume of H
N_T = trap density
$(\ )_{,i} = \partial(\ )/\partial x_i$

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Material: X70/80 acicular ferrite microstructure

$$C = K\sqrt{f} \qquad f = P\exp\left(\frac{Pd}{RT}\right) \qquad d = 15.84\ \mathrm{cm^3/mol}$$

$$K = 6.54696\times10^{18}\ \frac{\mathrm{H\ atoms}}{\mathrm{m^3}\sqrt{\mathrm{Pa}}}$$

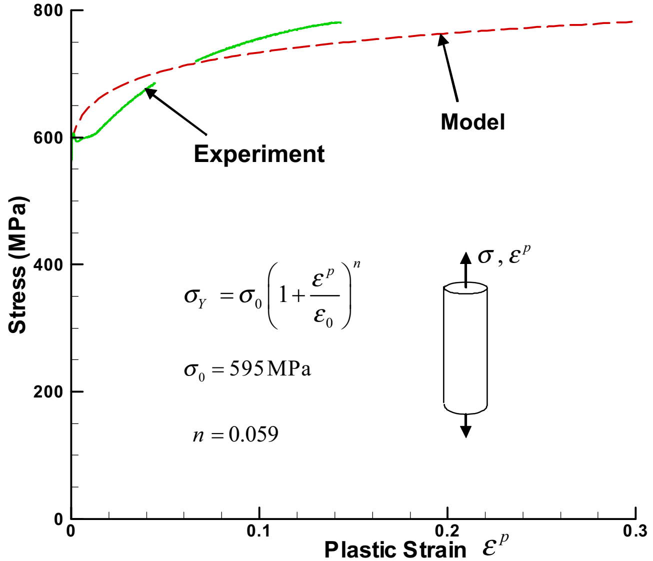
$$C_0 = 2.084\times10^{21}\ \mathrm{H\,atom/m^3} \qquad P = 1\ \mathrm{atm}$$

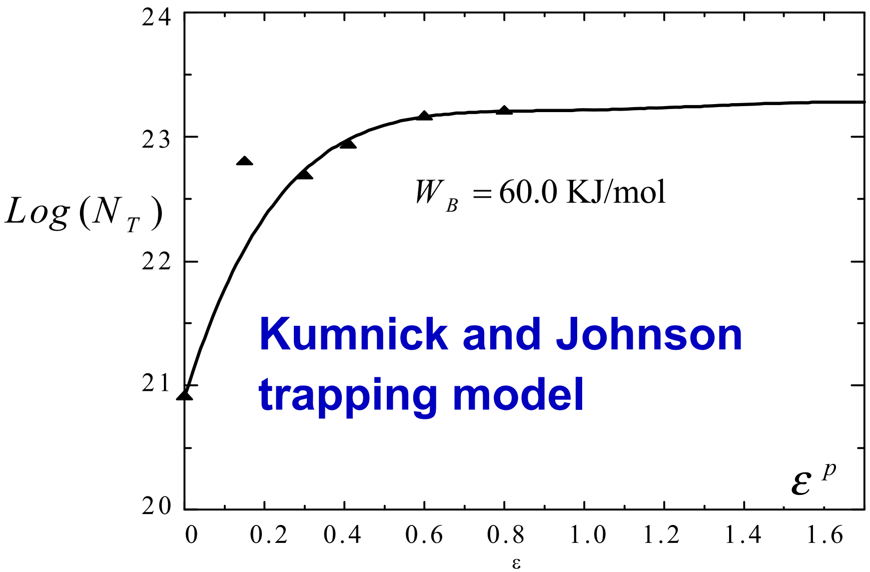
$$C_0 = 2.65932\times10^{22}\ \mathrm{H\,atom/m^3} \qquad P = 15\ \mathrm{MPa}$$

Lattice diffusion coefficient

$$D = 1.271\times10^{-8}\ \mathrm{m^2/s}$$

Stress-strain





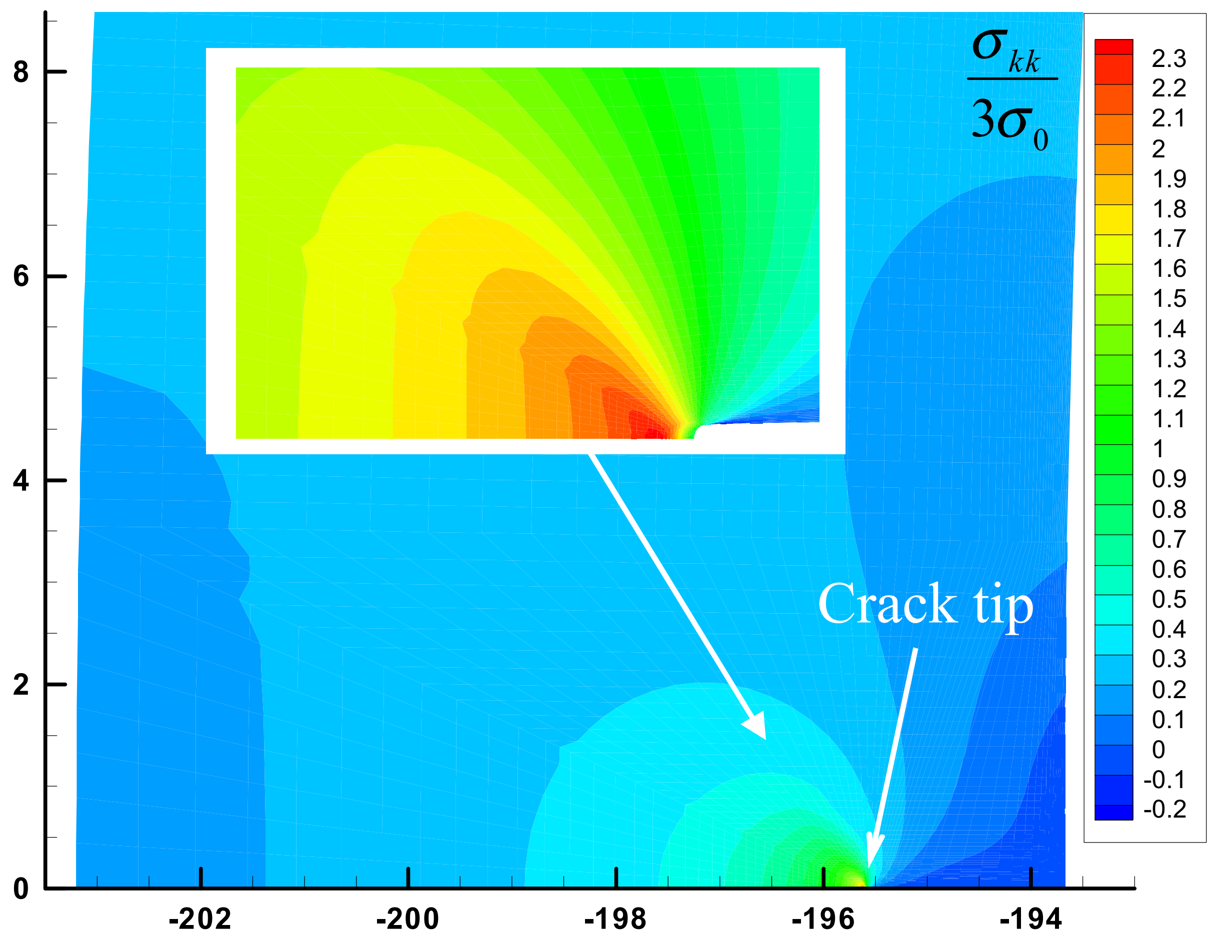
Dislocation trapping modeling

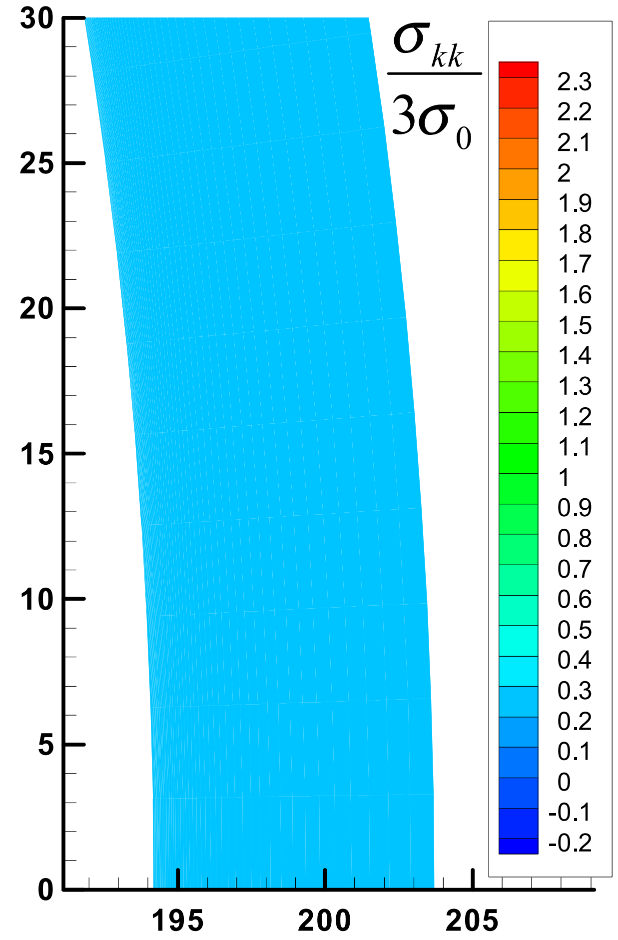
$$N_T = \frac{\sqrt{2}\rho}{a} \qquad W_B = 20.2\ \mathrm{KJ/mol}$$

$$\rho = \begin{cases} \rho_0 + \dfrac{\gamma}{0.15}\varepsilon^p & \varepsilon^p \le 0.15 \\ \text{const.} & \varepsilon^p > 0.15 \end{cases}$$

$$\rho_0 = 10^{10}\,m^{-2},\ \gamma = 10^{16}\,m^{-2}$$

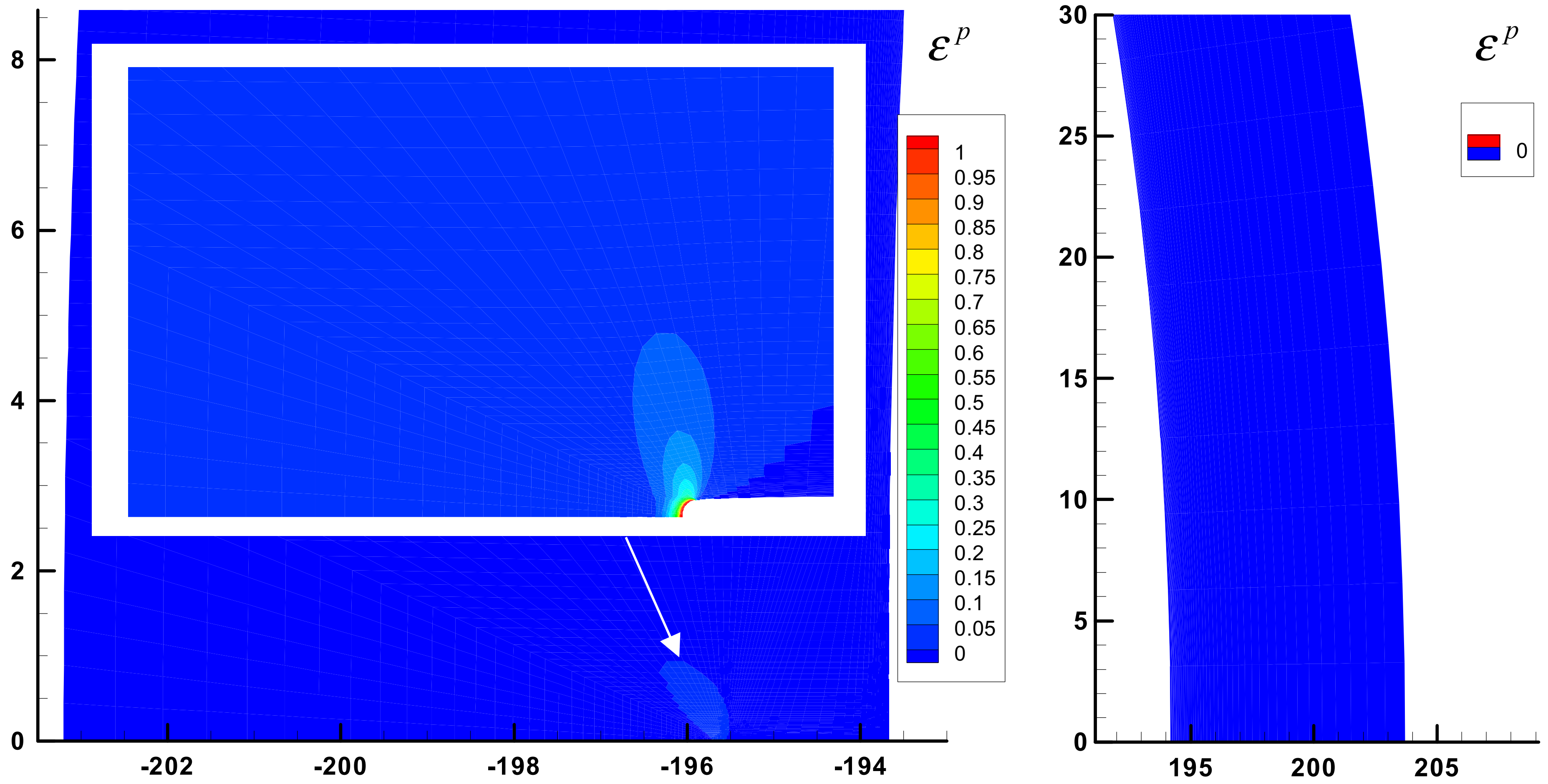
Hydrostatic Stress at Pressure 15 MPa





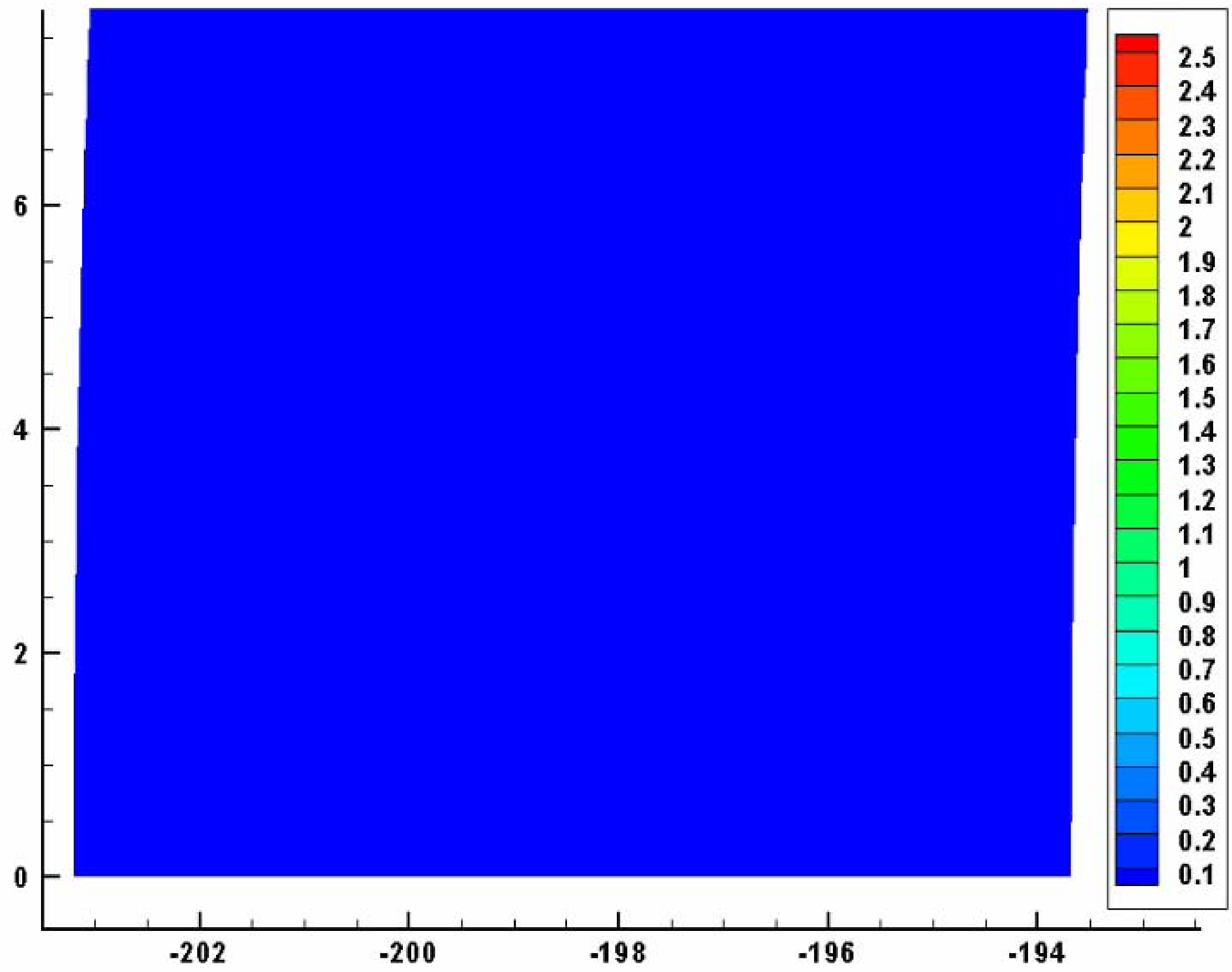
Geometric dimensions are in mm

Plastic Strain at Pressure 15 MPa



Geometric dimensions are in mm

Lattice Concentration Toward Steady State



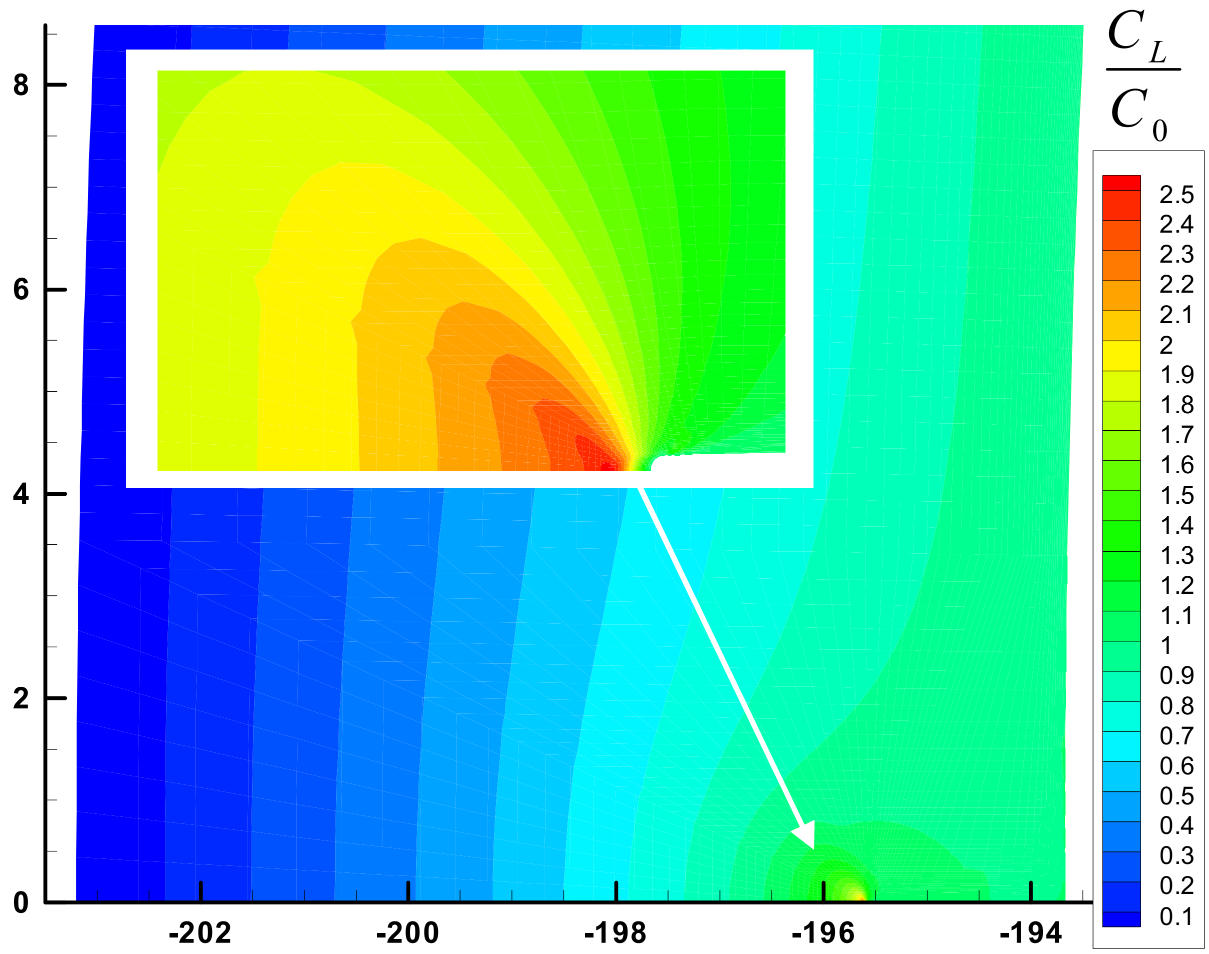
C_L / C_0

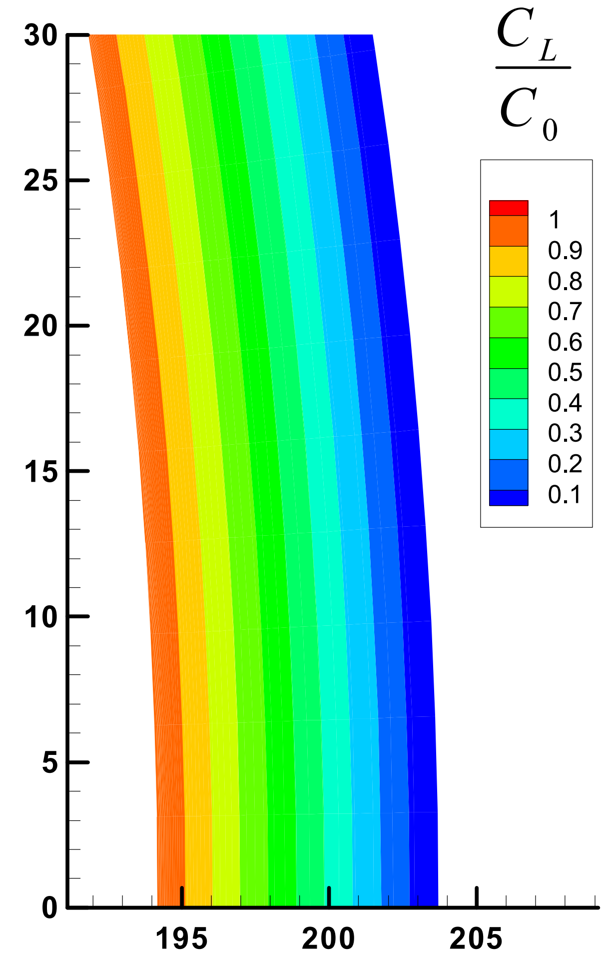
Lattice Hydrogen Concentration at Steady State

Kumnick and Johnson trapping model

Time to steady-state: 2.0 hrs

$$t_{ss} = 8 \ \text{min} \ 40\,\text{sec}$$





$C_0 = 2.65932 \times 10^{22}\ \text{H atom}/\text{m}^3$ $\qquad P = 15\ \text{MPa}$

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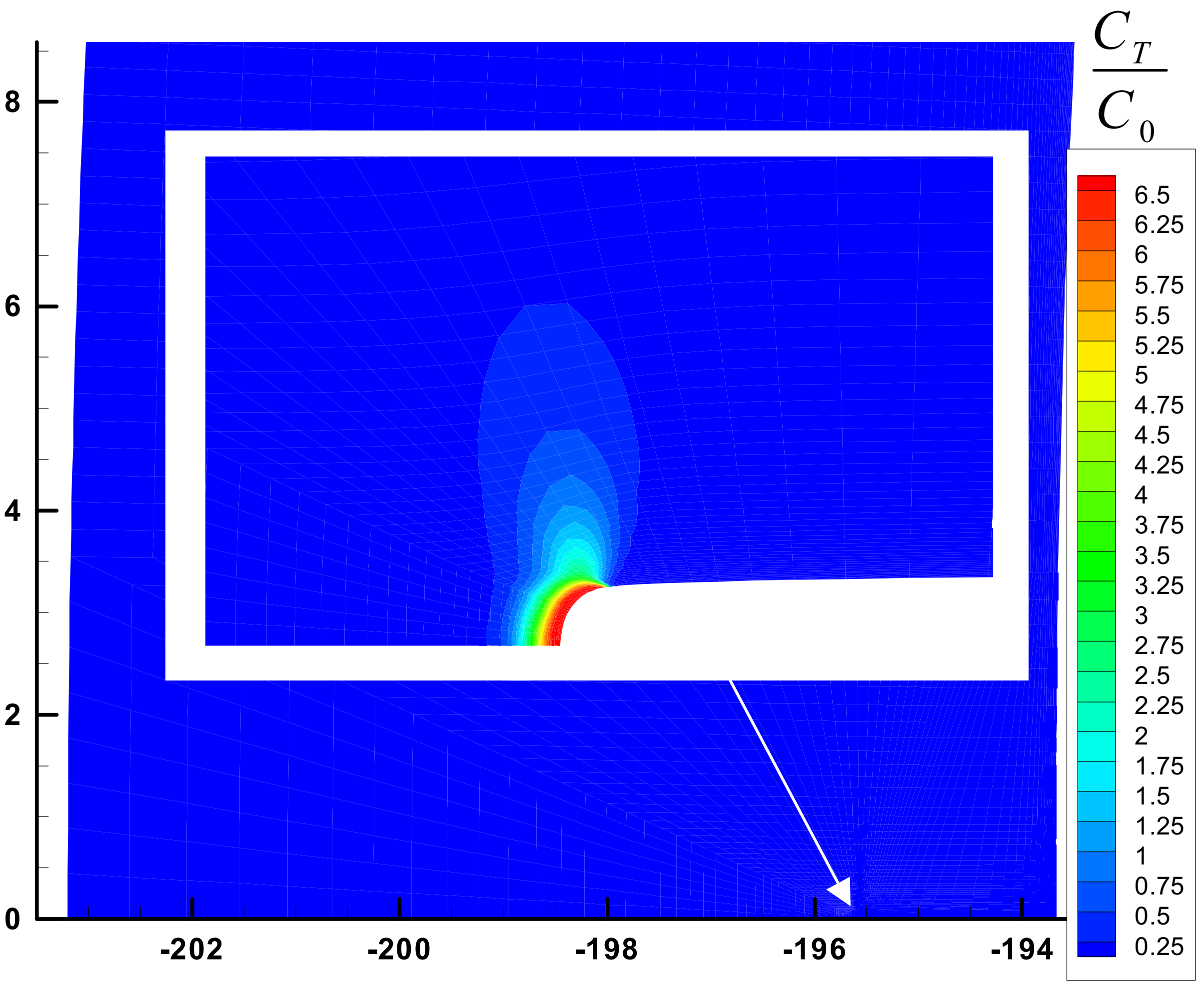
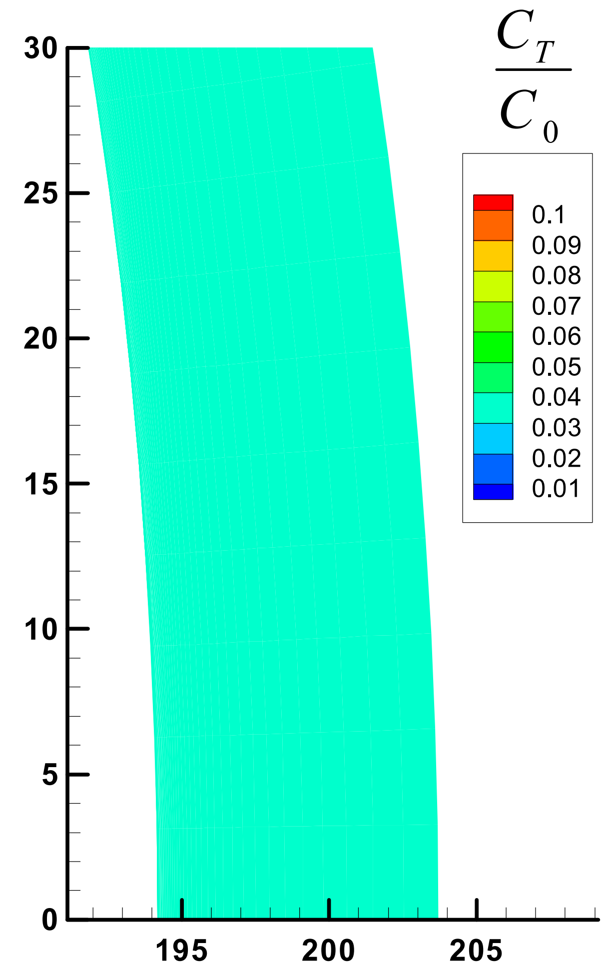
Trapped Hydrogen Concentration at Steady State

Kumnick and Johnson trapping model





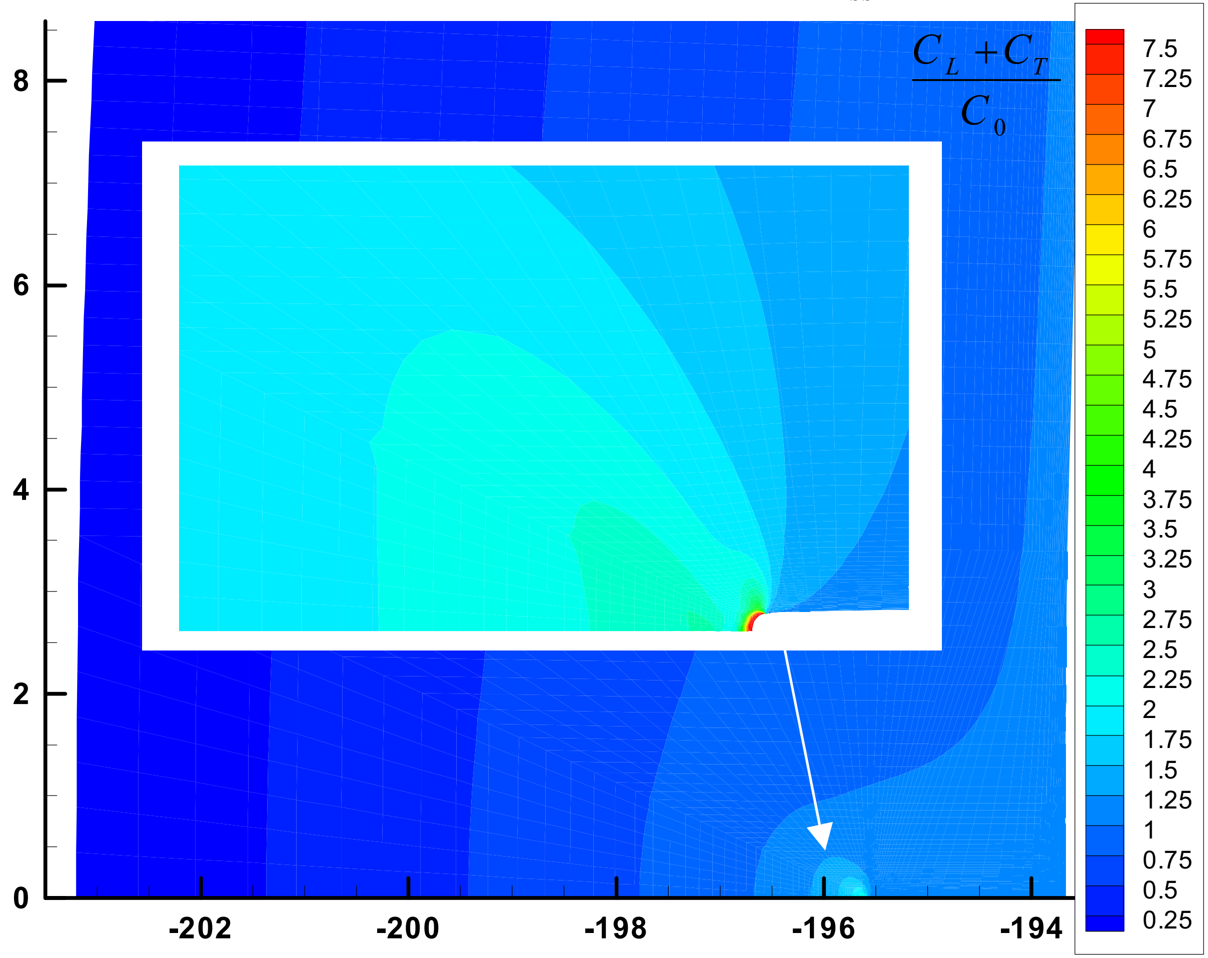
$C_0 = 2.65932 \times 10^{22}\ \text{H atom/m}^3 \qquad P = 15\ \text{MPa}$

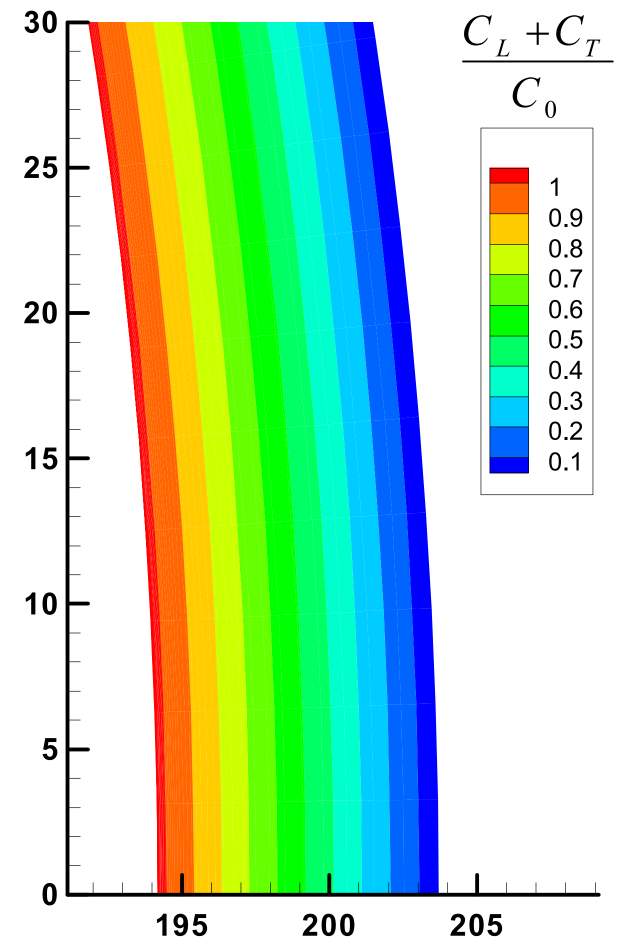
Total Hydrogen Concentration at Steady State

Kumnick and Johnson trapping model

Time to steady-state is 2.0 hrs

$$t_{ss} = 8 \ \min 40 \sec$$





$$C_0 = 2.65932 \times 10^{22} \ \text{H atom} / \text{m}^3 \qquad P = 15 \ \text{MPa}$$

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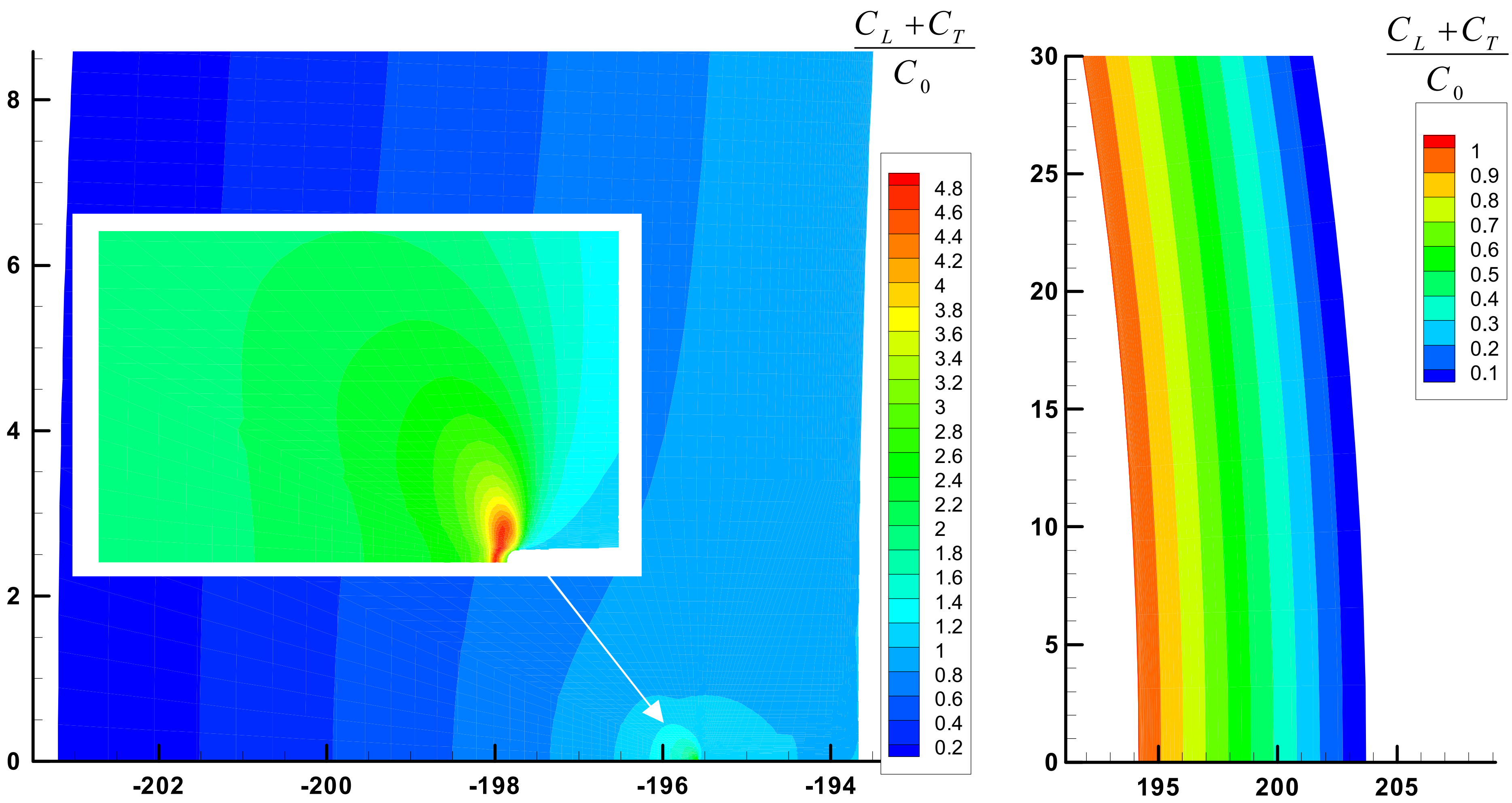
Total Hydrogen Concentration at Steady State

Dislocation trapping model



$C_0 = 2.65932 \times 10^{22}$ Hatom / m^3 $\quad P = 15$ MPa

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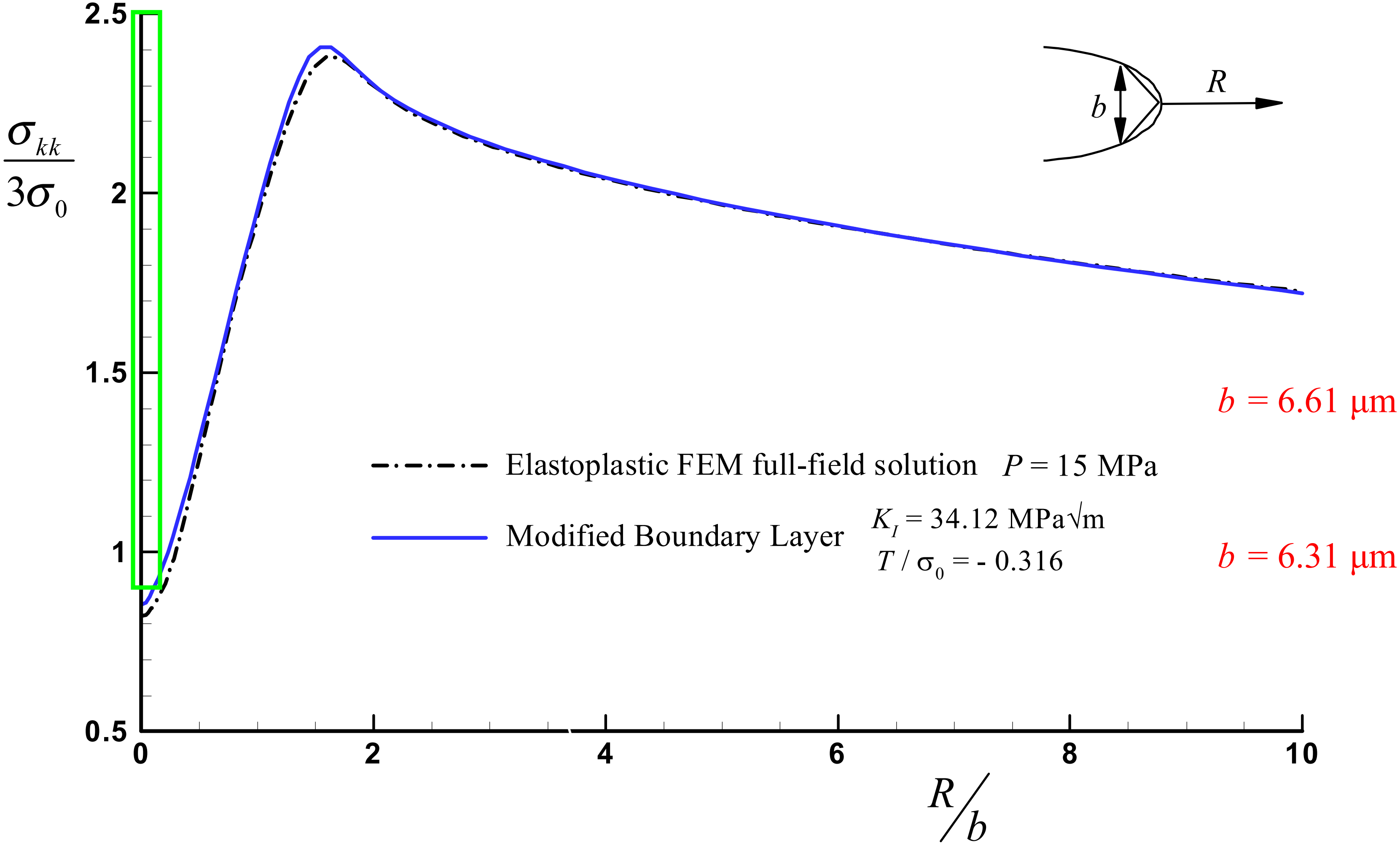
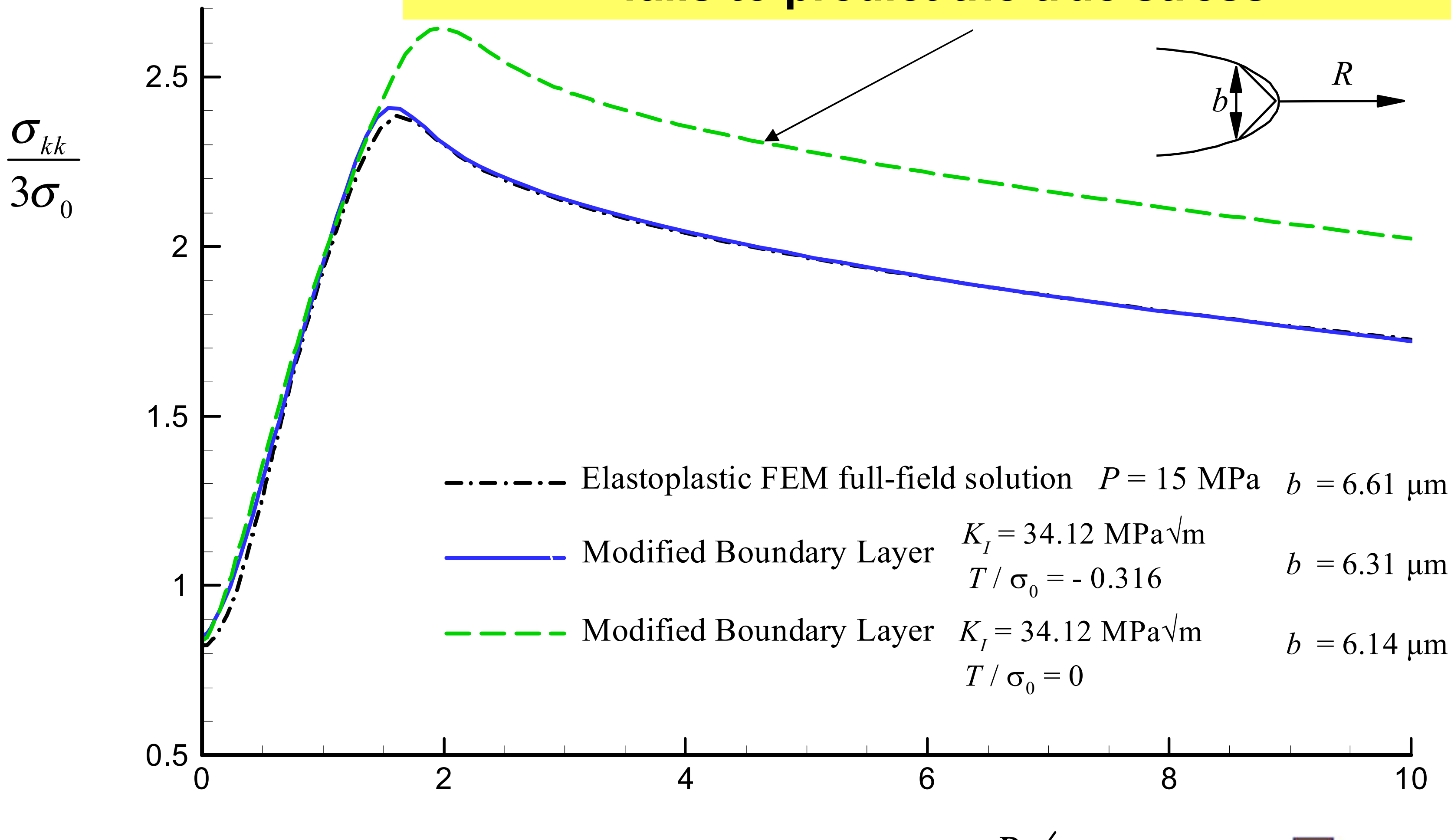
Full Field (pipeline) vs Boundary Layer Solution (laboratory specimen)



$a/h = 0.2$

Full Field (pipeline) vs Boundary Layer Solution (laboratory specimen)

Neglecting the *T*-stress in the MBL formulation fails to predict the true stress



$a/h = 0.2$

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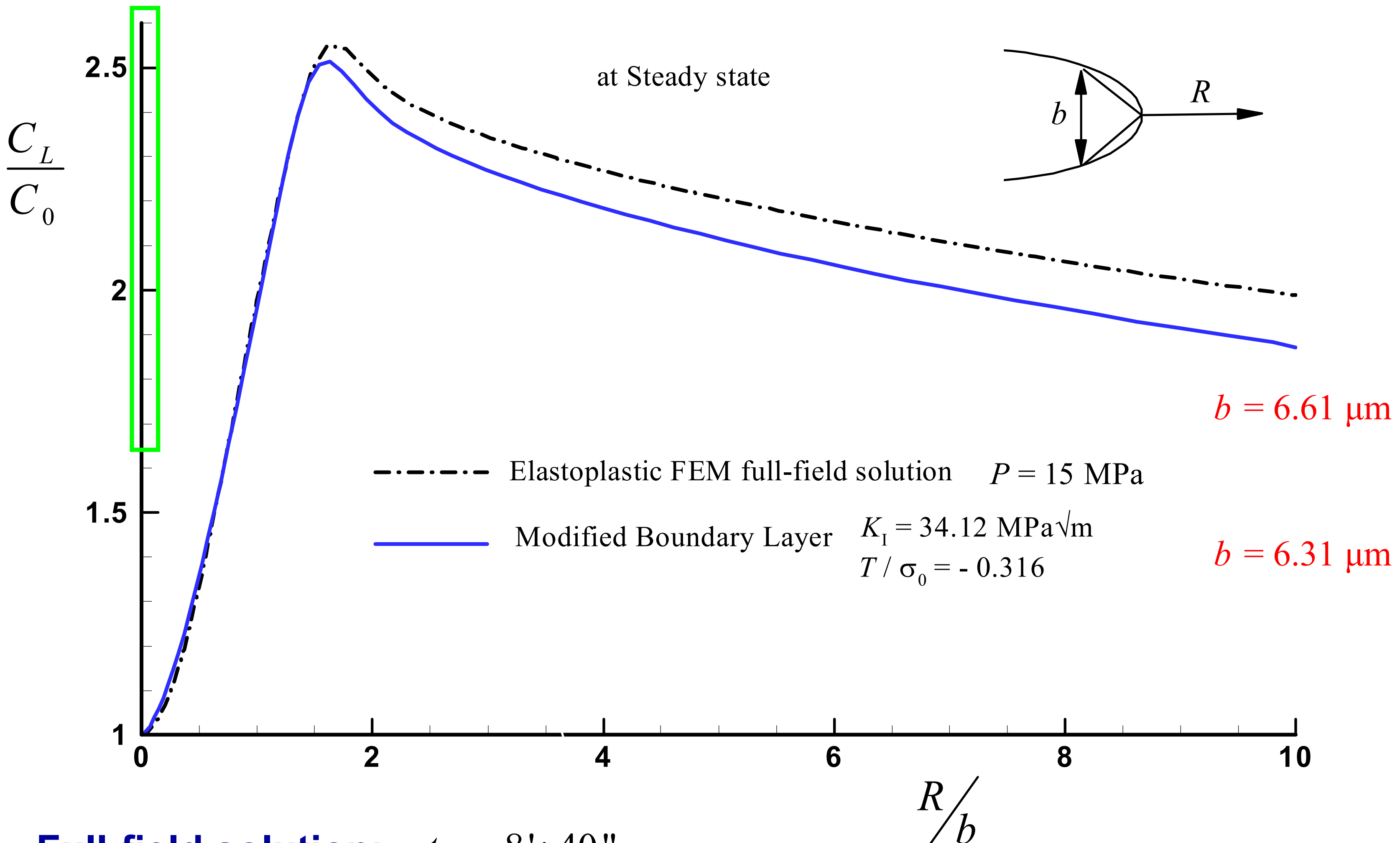
Full Field (pipeline) vs Boundary Layer Solution (laboratory specimen)



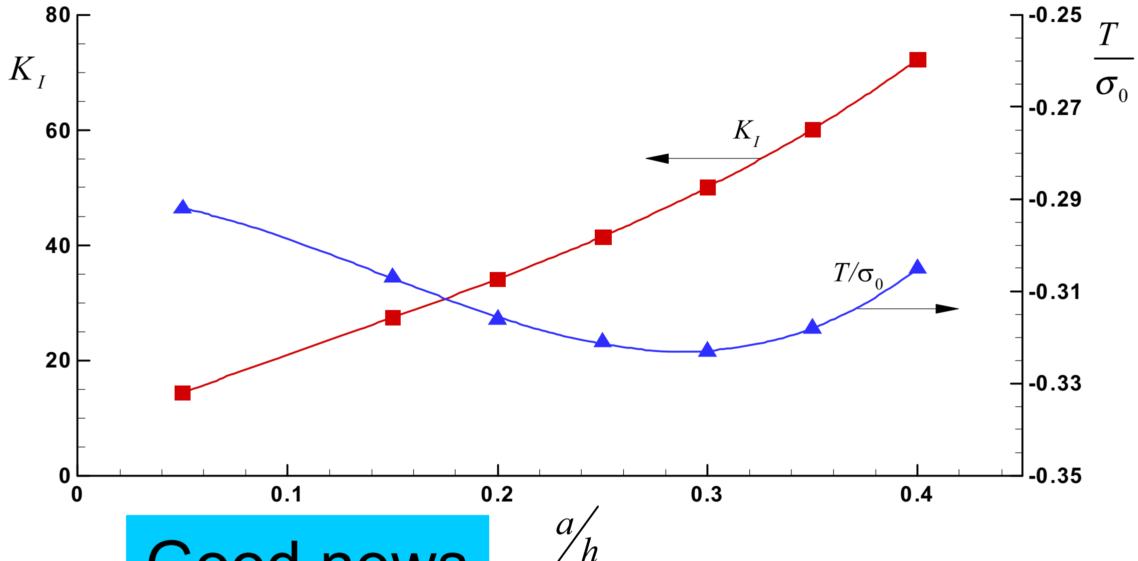
Full-field solution: $t_{ss} = 8':40''$

MBL approach: $t_{ss} = 6':40''$

$a/h = 0.2$

Fracture Mechanics Assessment

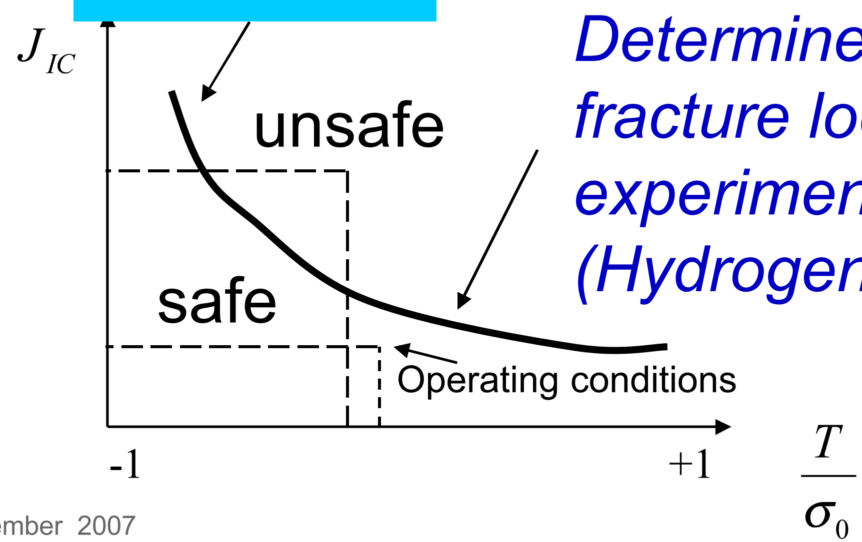
Constraint based fracture mechanics: J-T controlled fracture



Laboratory Specimens

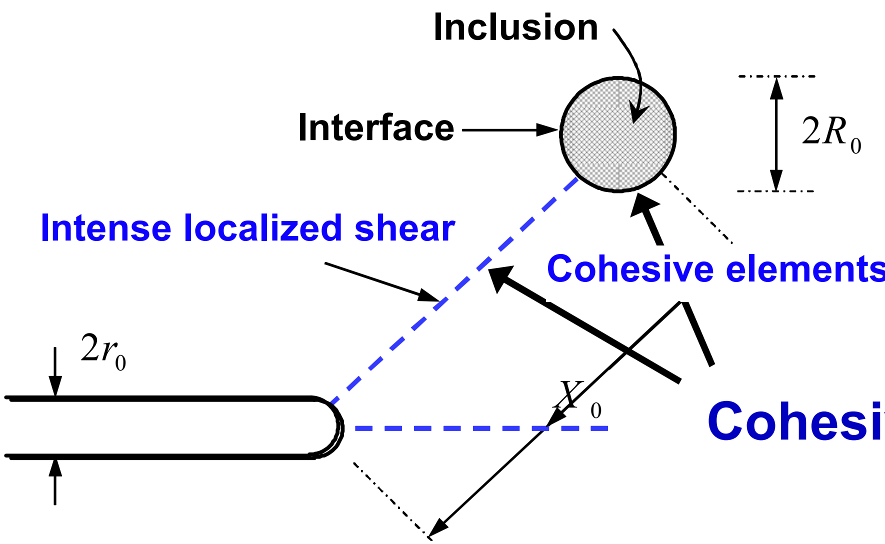
- **The deep-notch toughness data in the presence of hydrogen need not necessarily lead to a conservative fracture toughness assessment for shallow cracked geometries as is commonly assumed in the absence of hydrogen**
- **Shallow crack are attracting hydrogen by plasticity so they , too, are degraded**
- **Deep-notch cracks are attracting hydrogen by the hydrostatic constraint constraint**

Good news



Determine this fracture locus experimentally (Hydrogen effect?)

Modeling the Fracture Process



Cohesive elements

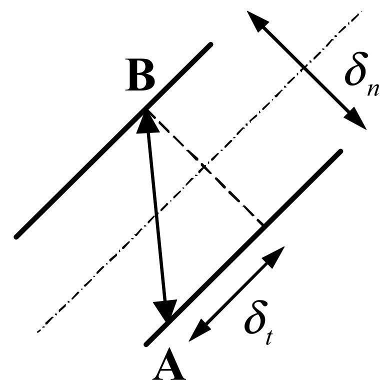
$$T_n = \frac{\sigma(c,q)}{q}\frac{u_n}{\delta_n}$$

$$T_t = \frac{\delta_n}{\delta_t}\frac{\sigma(c,q)}{q}\frac{u_n}{\delta_t}$$

$$q = \sqrt{\left(\frac{u_n}{\delta_n}\right)^2 + \left(\frac{u_t}{\delta_t}\right)^2}$$

Transient separation

[Mishin *et al*., 2002]



$$\sigma(c,q) = \frac{27}{4}\sigma_{\max}\left[1+(\kappa-1)c\right]q(1-q)^2$$

$\sigma_{\max}$ **: Maximum cohesive stress**

$$\kappa = \frac{\text{cohesive energy with } c=1}{\text{cohesive energy with } c=0}$$

First Principles Calculations

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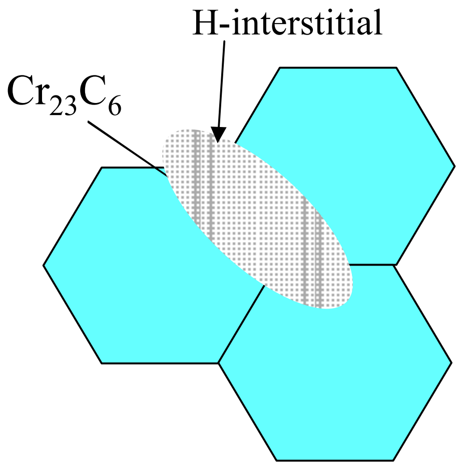
First Principles Calculations

- **Assessment of interfacial strength of second-phase particles in pipeline steels in hydrogen**
  - Ferrite-based alloys have $Cr_{23}C_6$ and MnS precipitates at grain boudnary interfaces. Substitutional solutes (e.g. Cr, Mn, Si) or interstitials (e.g. H, N, C) modify structure and stability
    - H (N of C) interstitials alter bonding and cohesion
    - Cr is depleted near $Cr_{23}C_6$ interface while Fe preferentially occupies Cr sites not bonded to C
  - Obtain cohesive energies via first-principles, Density Functional Theory (DFT) calculations with distribution of atoms near interfaces based on periodic cell approximations

- **Calibration of phenomenological parameters in the thermodynamic theory of decohesion of Mishin et al. (200)**

- **Validation of ab-initio calculations for decohesion energy calculations**
  - Unrelaxed binding energies (eV) and their differences for H in Fe grain boundary (GB) and free surface (FS) calculated by VASP PAW-GGA and FLAPW (Zhong *et al*., 2000).



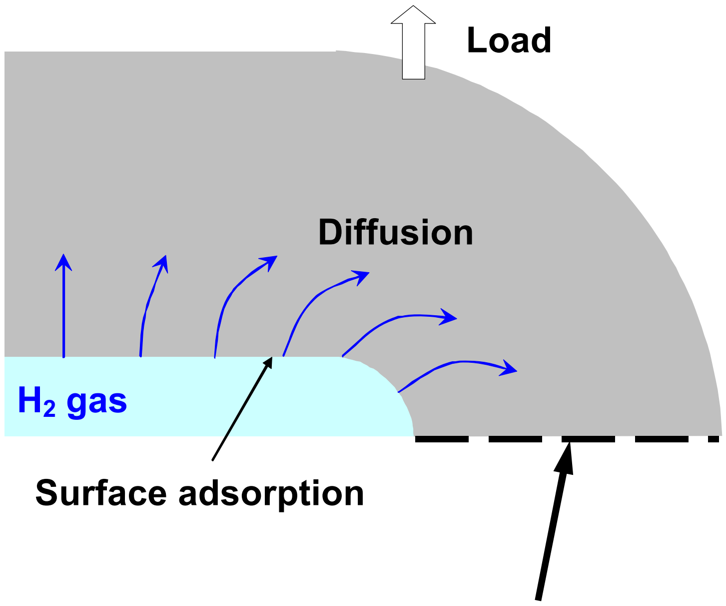
		GB	FS	GB-FS
Unrelaxed binding energies	VASP PAW-GGA	-3.23	-3.57	+0.34
	FLAPW GGA (Zhong *et al*., 2000)	-3.09	-3.42	+0.33

Time Scales

t_a : **characteristic time of adsorption**

t_L : **loading rate**

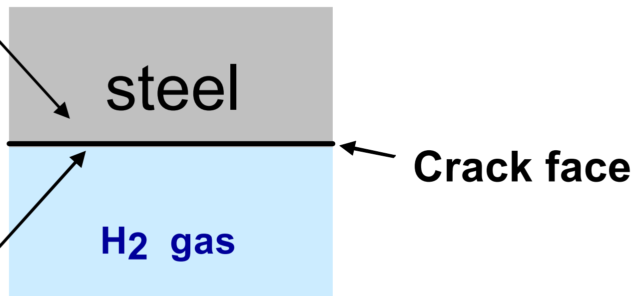
t_D : **characteristic diffusion time** $\propto \dfrac{1}{D_{eff}}$



Effect of time scales on mechanics of crack initiation and growth

Hydrogen Adsorption

$$\mu = \mu_0(\Theta) + R\,\Theta \ln(c_L) - \sigma_{kk} V_H / 3$$



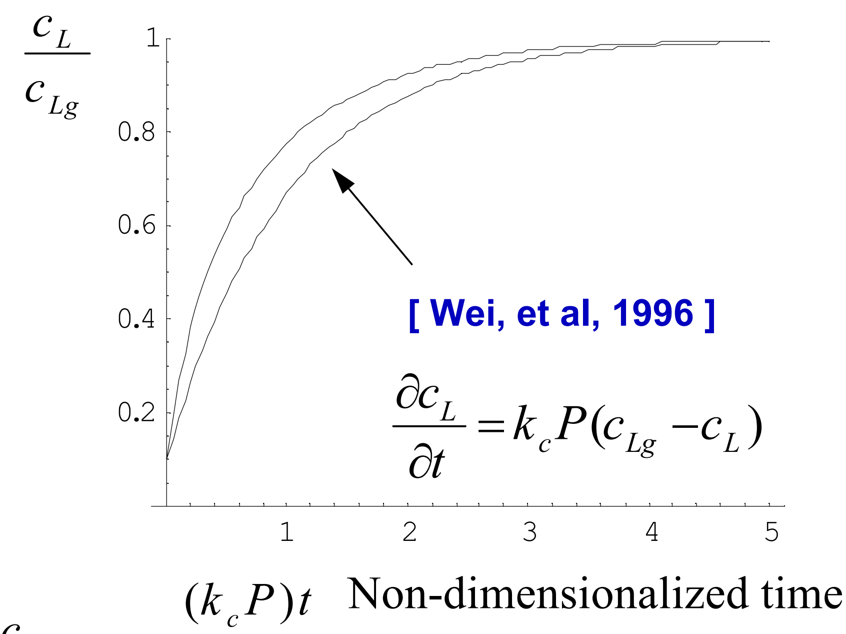
$$\mu_g = \mu_0(\Theta) + R\,\Theta \ln(c_{Lg})$$

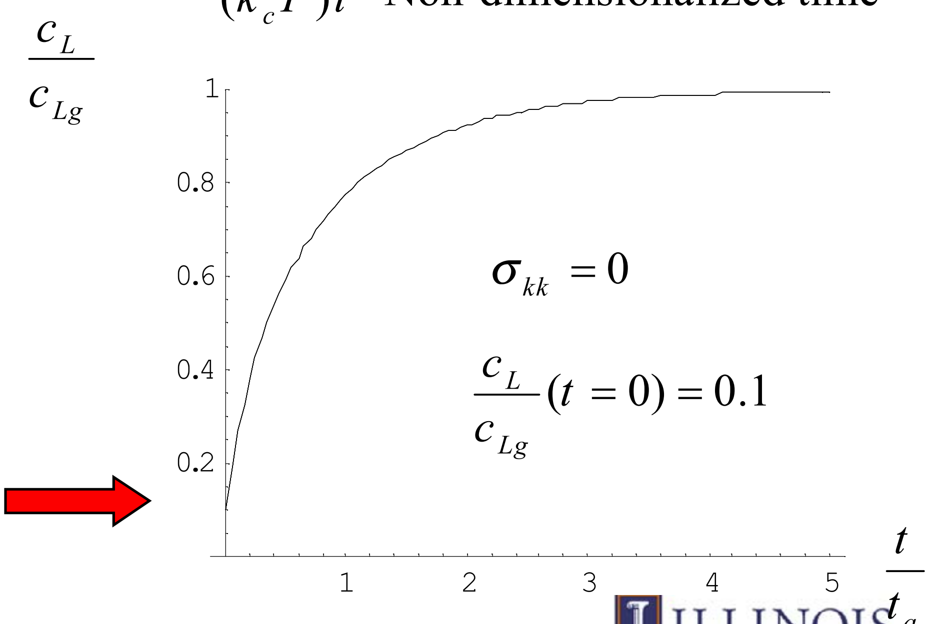
$$c_{Lg} \propto \sqrt{f}$$

$$\frac{\partial c_L}{\partial t} = \frac{1}{t_a R\,\Theta}(\mu_g - \mu)$$

t_a **: characteristic adsorption time**

$$\frac{\partial c_L}{\partial t} = \frac{1}{t_a}\left[\ln(c_{Lg}/c_L) + \sigma_{kk} V_H / 3R\,\Theta\right]$$

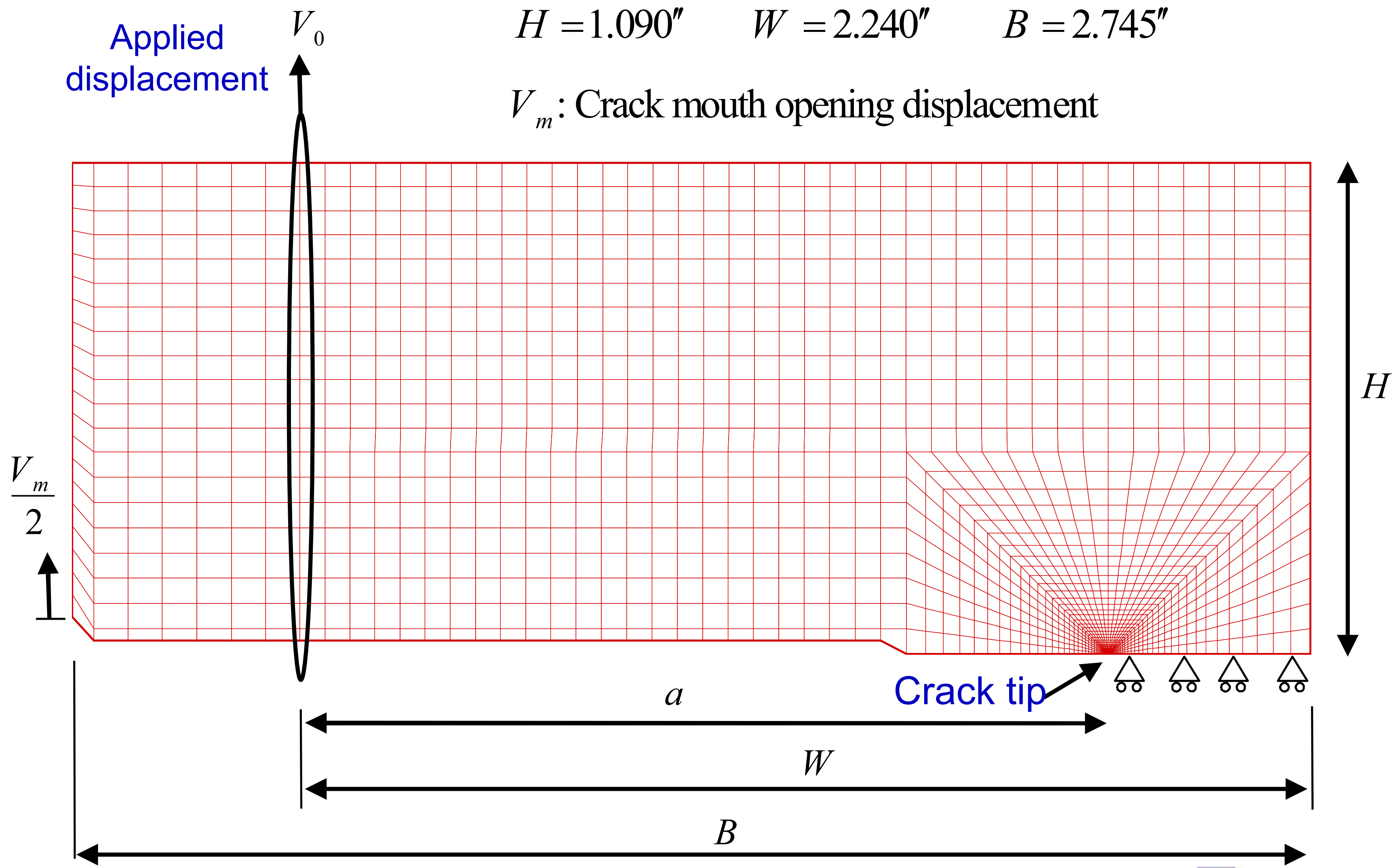




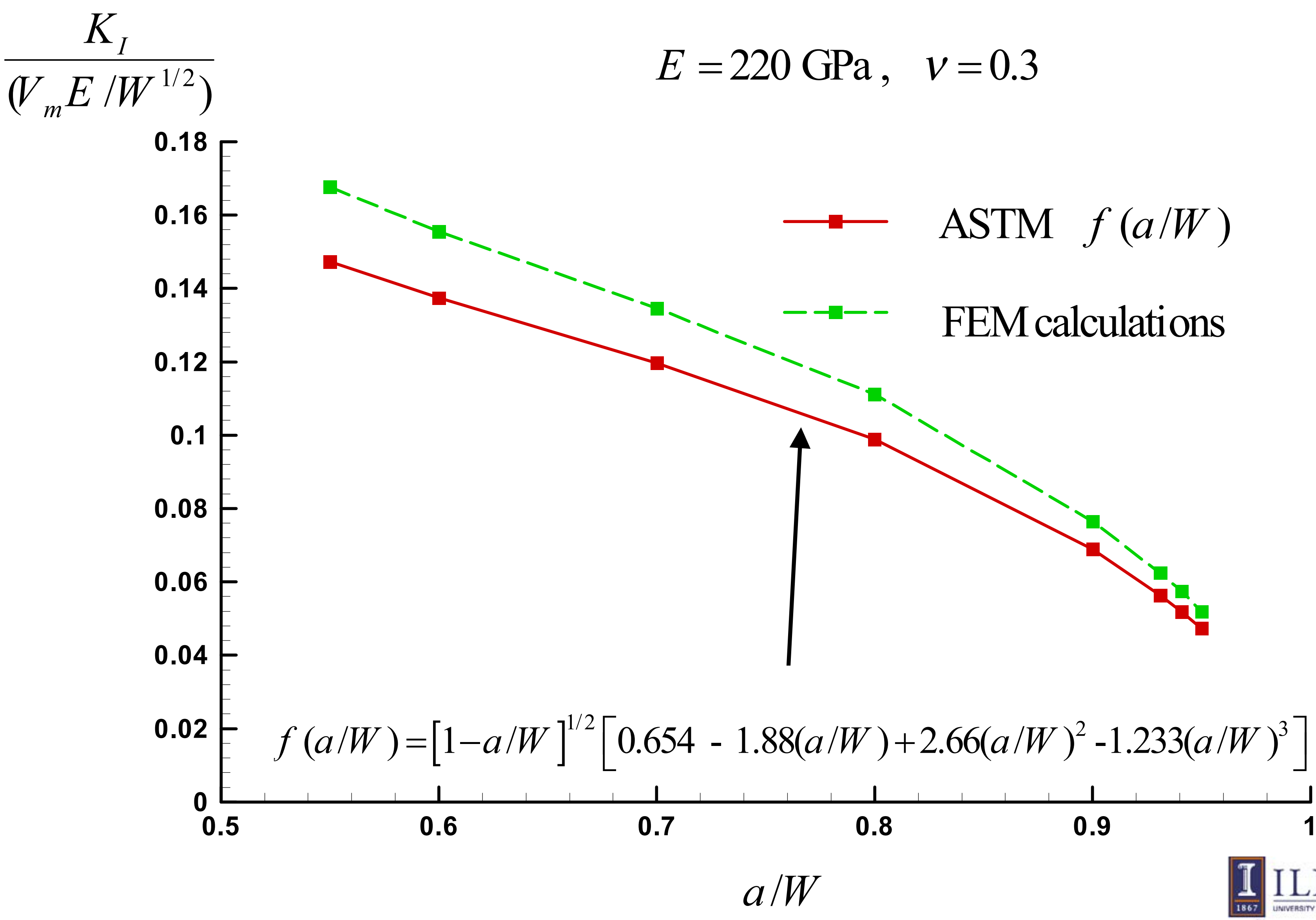
WOL Specimen for Subcritical Crack Growth Finite Element Mesh

$H = 1.090''$ $W = 2.240''$ $B = 2.745''$

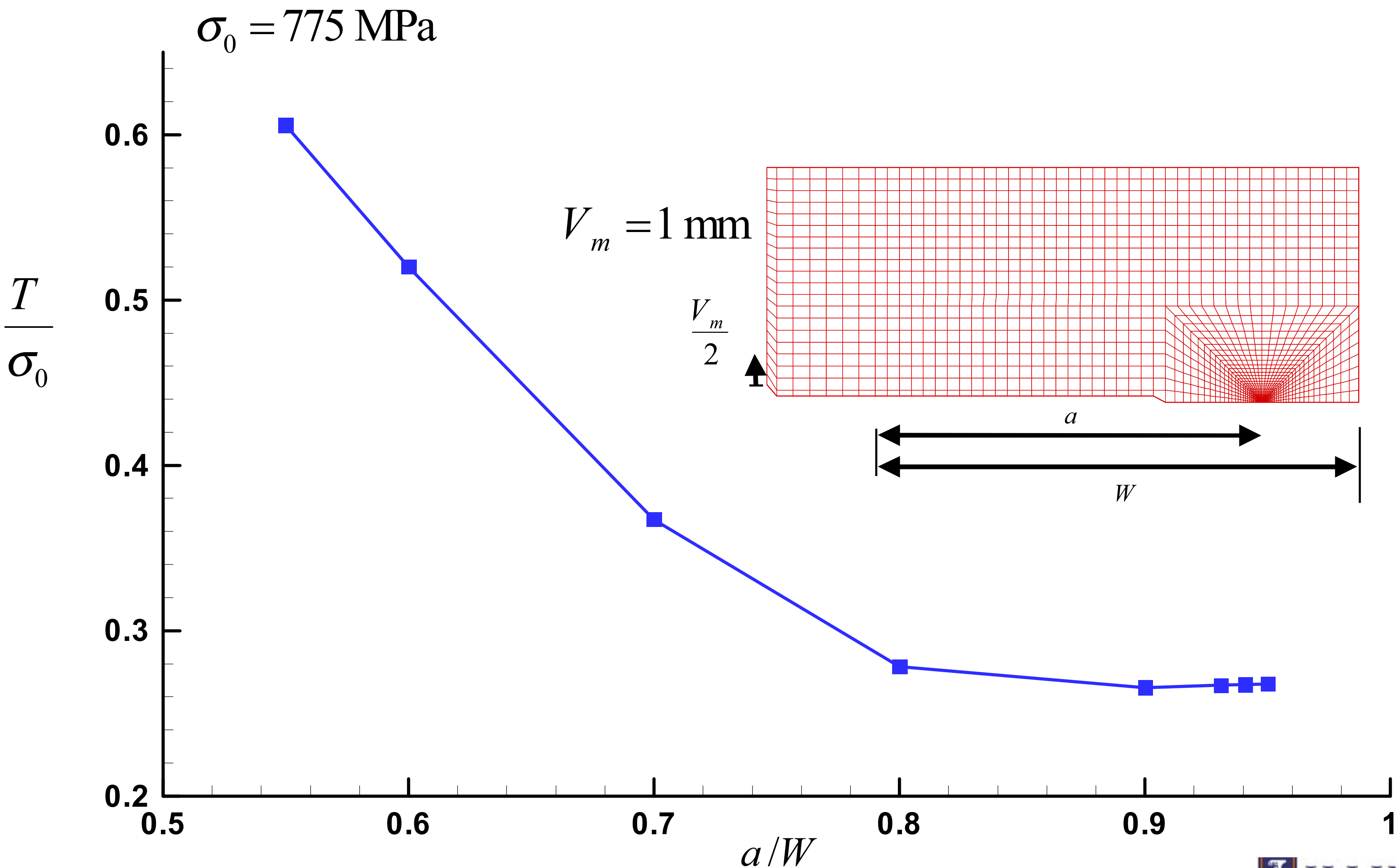
V_m: Crack mouth opening displacement



Comparing FEM Result with ASTM Equation



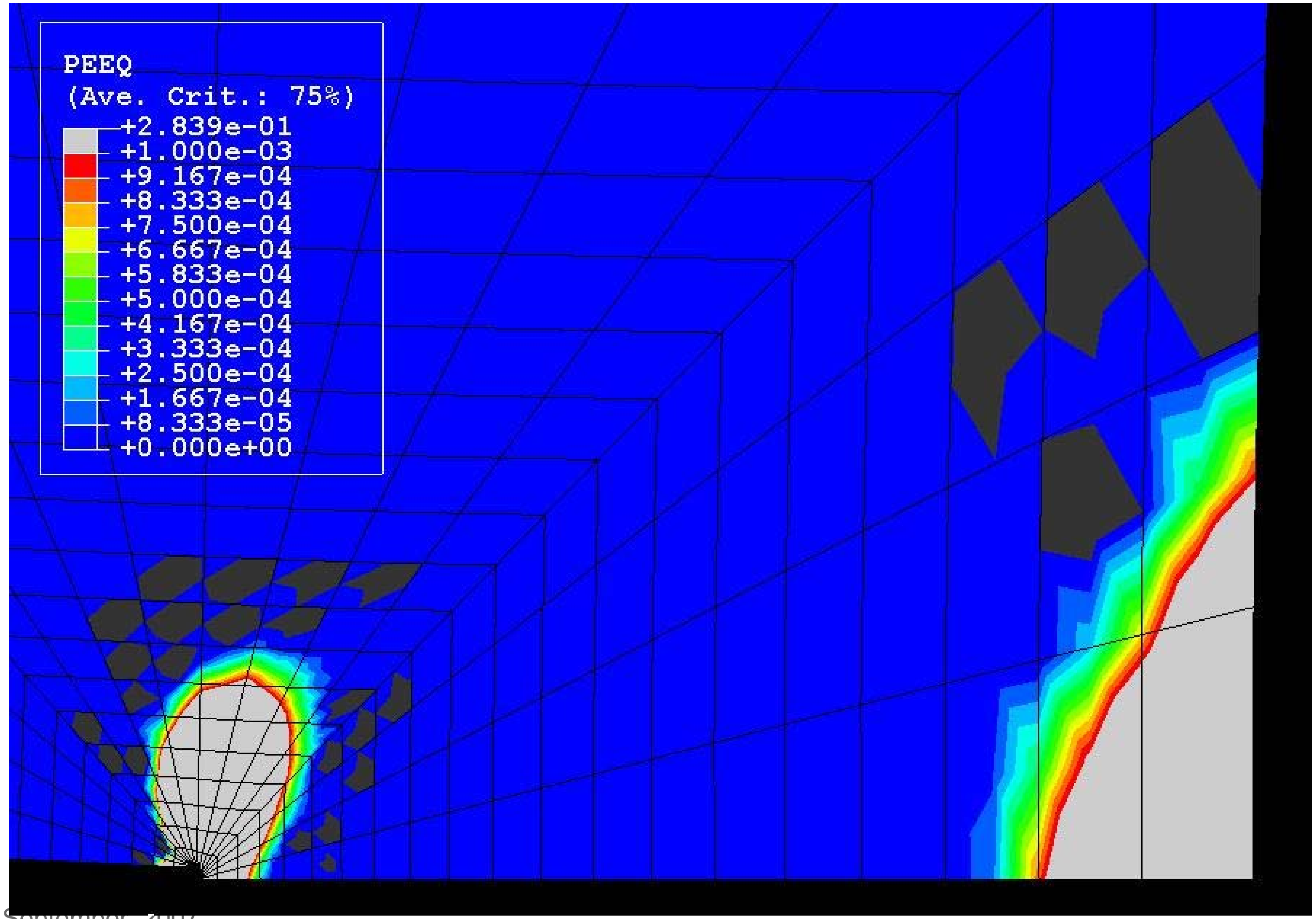
Normalized T-stress for specific V_m – FEM Calculations



Plasticity in WOL: Issue of *K*-dominance

$V_m = 1.204\text{mm}$ $\quad a/W = 0.9408$ $\xrightarrow{\text{ASTM}}$ $K_I = 57.5 \text{ MPa}\sqrt{\text{m}}$

$\xrightarrow{\text{FEM}}$ $K_I = 63.8 \text{ MPa}\sqrt{\text{m}}$



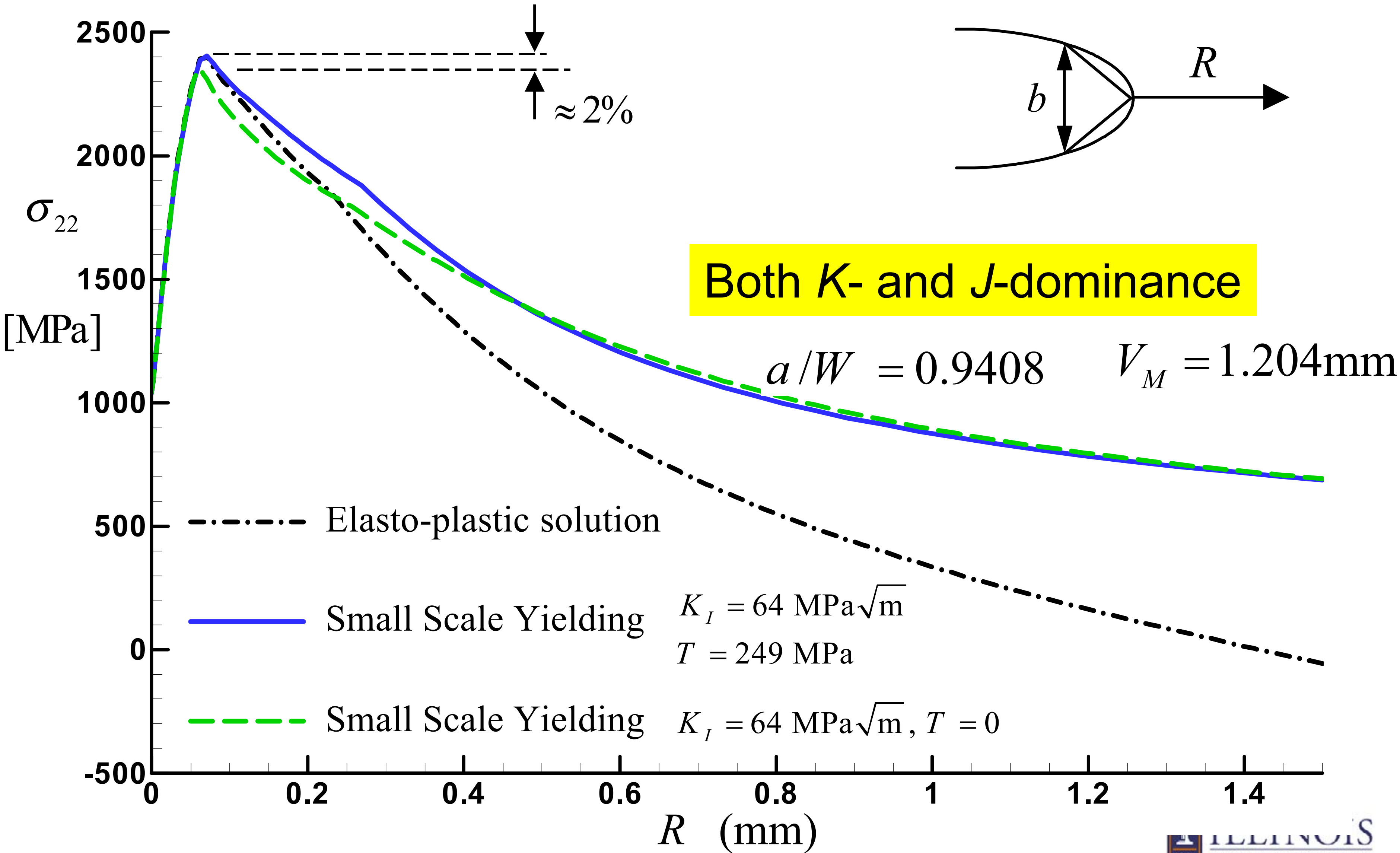
$\xrightarrow{\text{FEM (Plastic)}}$

$$J = 16008 \text{ N/m}$$

$$K_I = \sqrt{\frac{JE}{1-\nu^2}}$$

$$K_I = 62.2 \text{ MPa}\sqrt{\text{m}}$$

Stresses in WOL: Issue of *K*-dominance



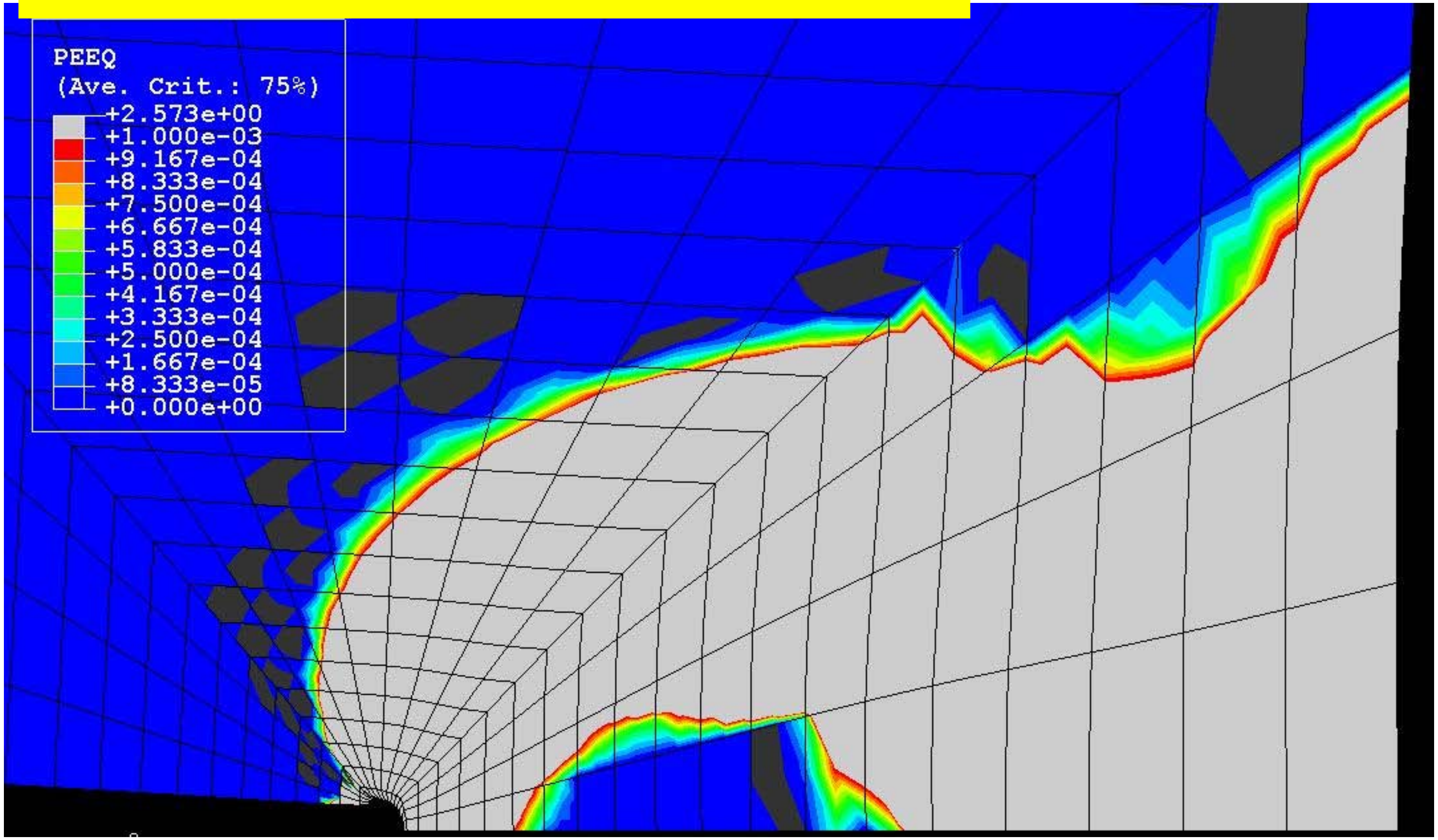
FEM Results for increased load of SNL Exp-2

$V_m = 4.9582\text{mm}$ $\quad a/W = 0.9408$

$\xrightarrow{\text{ASTM}}$ $K_I = 236.9 \text{ MPa}\sqrt{\text{m}}$

$\xrightarrow{\text{FEM}}$ $K_I = 261.8 \text{ MPa}\sqrt{\text{m}}$

Loss of both *K*- and *J*-dominance



$\xrightarrow{\text{FEM (Plastic)}}$

$$J = 124000 \text{ N/m}$$

$$K_I = \sqrt{\frac{JE}{1-\nu^2}}$$

$$K_I = 170 \text{ MPa}\sqrt{\text{m}}$$

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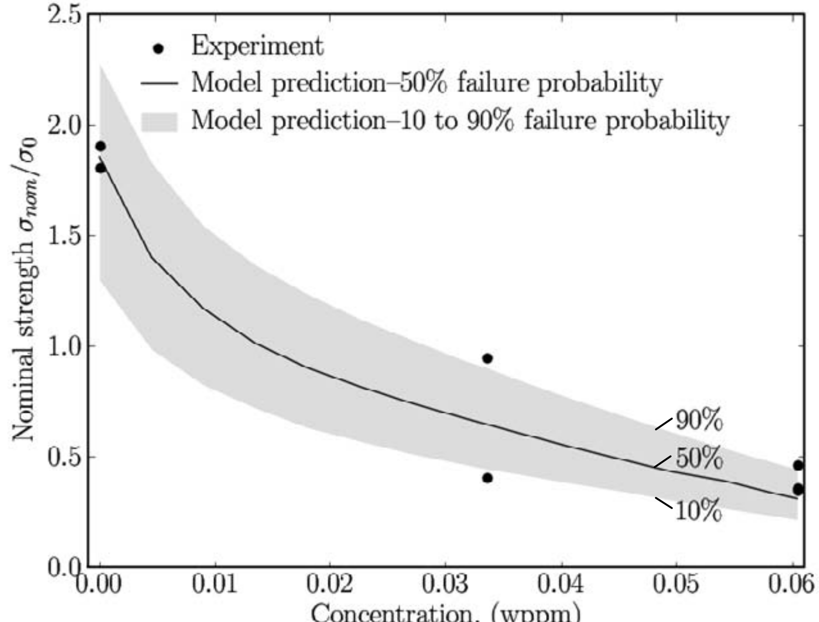
Conclusions and Future Work

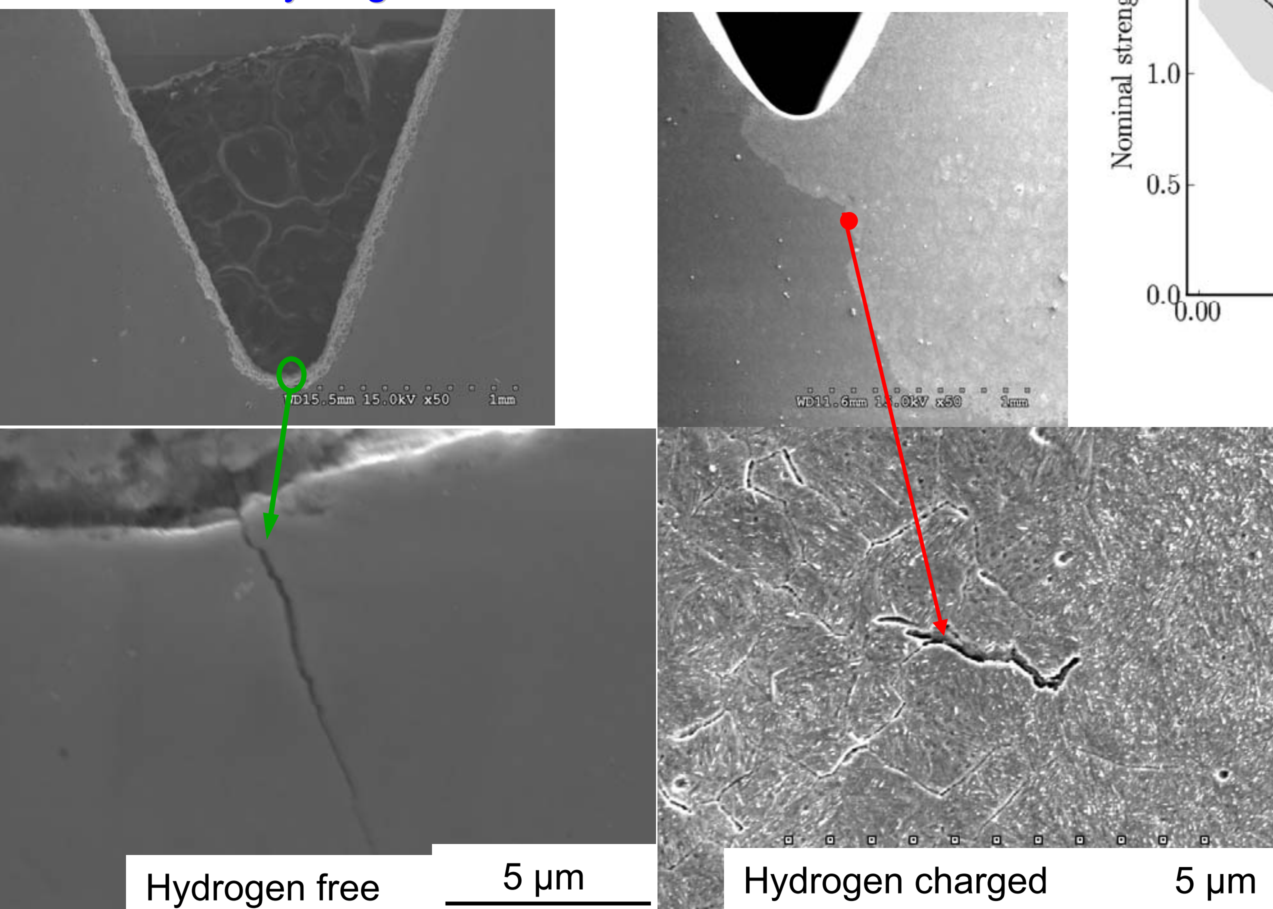
- **Hydrogen adsorption and transport methodology**
  - Interaction of time scales
  - Possible effects on remediation
- **Mechanisms of fracture (microstructural characterization)**
  - Material system dependence
    - Steel microstructure
    - Weldment
  - Load mode dependence (static vs fatigue)
  - Mode of hydrogen uptake (subcritical crack growth)
- **Coupling mechanisms with transport to understand**
  - Crack initiation
  - Crack propagation
  - Devise fracture criteria with predicting capabilities
    - Possibly a J_{IC}-T locus
- **Fracture mechanics/mechanism-based approach to design**
  - As opposed to the SMYS approach

Hydrogen-Induced Degardation in 4340 Steel

- Studies on the mechanical properties of high-strength steel (AISI 4340) characterize the marked deterioration in fracture strength with increase in hydrogen concentration.
- Mechanical properties are used in the statistical model of hydrogen-assisted fracture

Results for 4-point Bend Single Notched Specimens: Experiment vs Modeling





Mechanistic Aspects

- double-notch bend testing shows that without H, fracture is *strain*-controlled, *i.e.*, initiation occurs at the notch (left)
- with H, fracture is inter-granular and *stress*-controlled; initiation occurs ahead of the notch (right)

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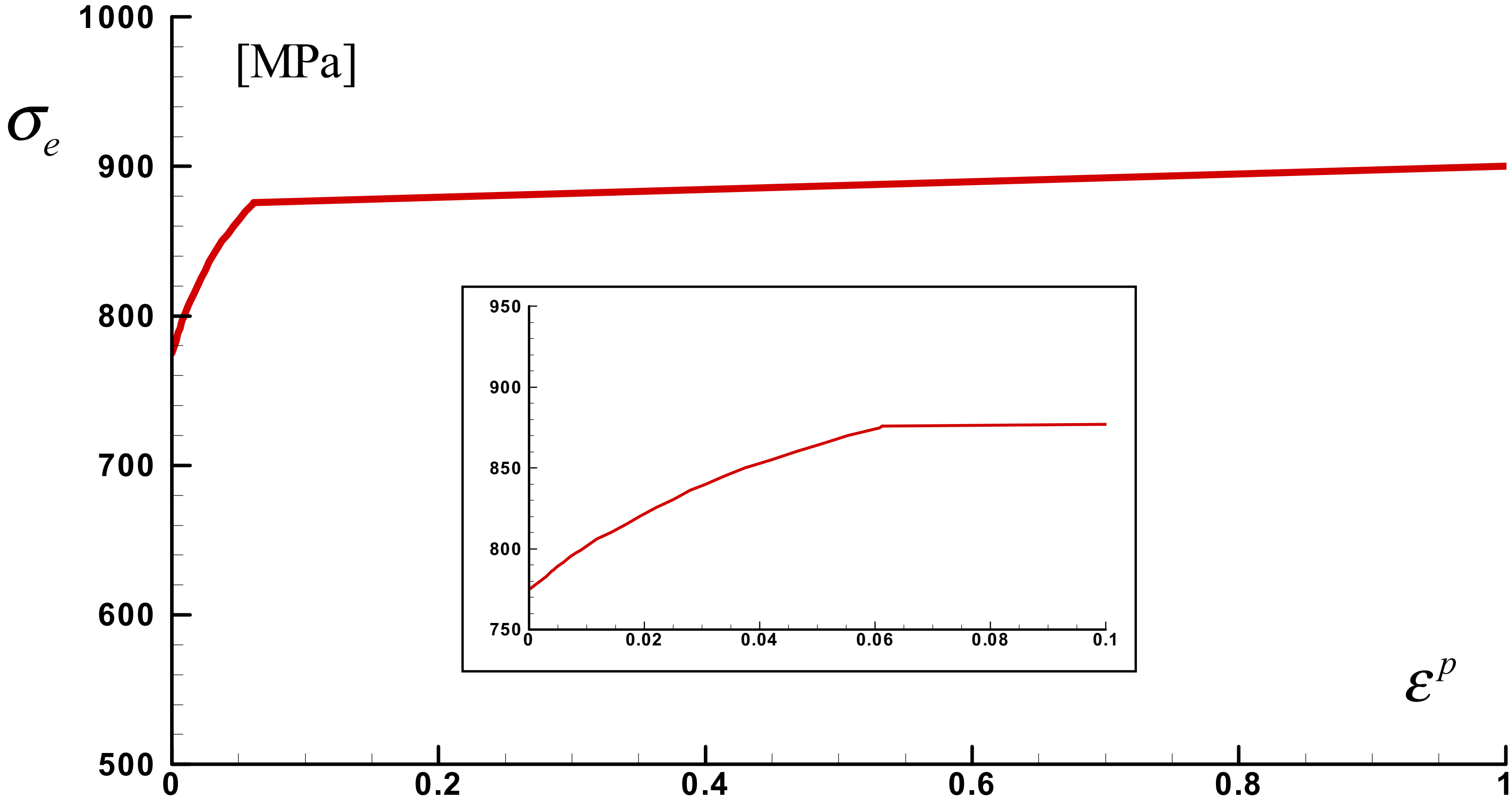
Additional slides

Conclusions on WOL

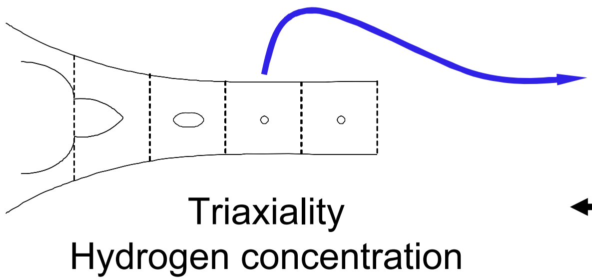
- Abaqus result on K seems to be correct
  - See comparison with the compact tension specimen which we “assume” has a more accurate calibration function
- We do have K dominance even for a crack of a/w=0.94
  - This is not the case for X-52 at such large a/w
- An important outcome is that we have both K and T. In combination with the experiment we can explore criticality conditions based on two parameter characterization
  - Study the hydrogen effect on this two-parameter characterization

Stress – plastic strain curve

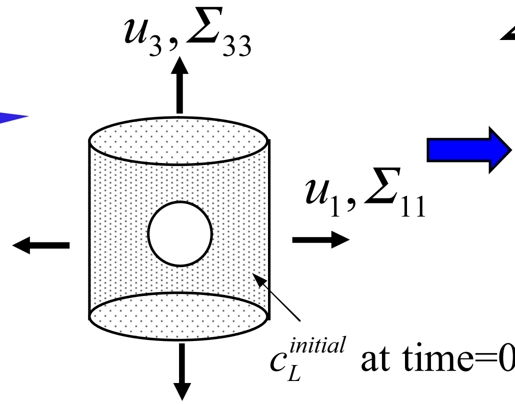


Long Term Objective: Multiscale Fracture Approach

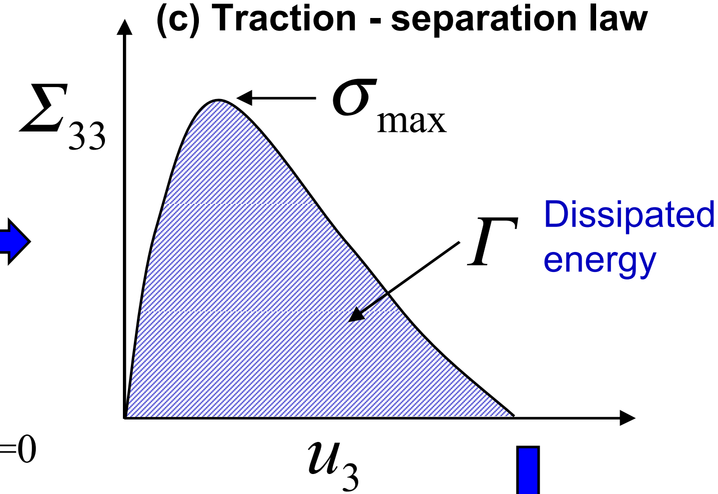
(a) Crack tip fracture process zone

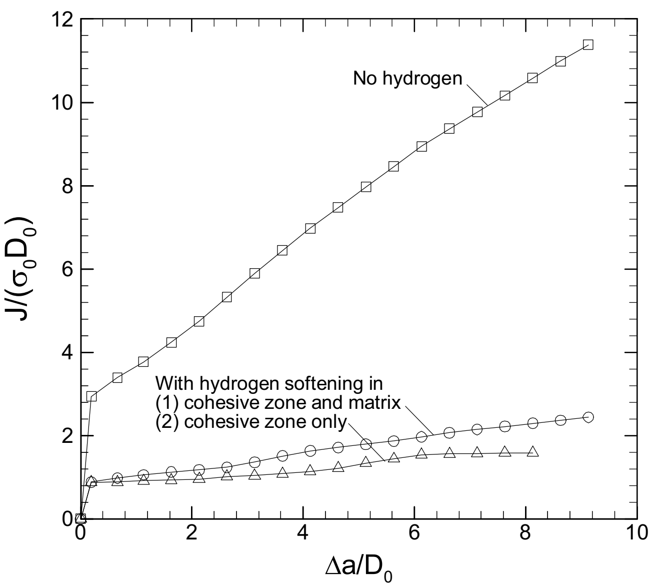


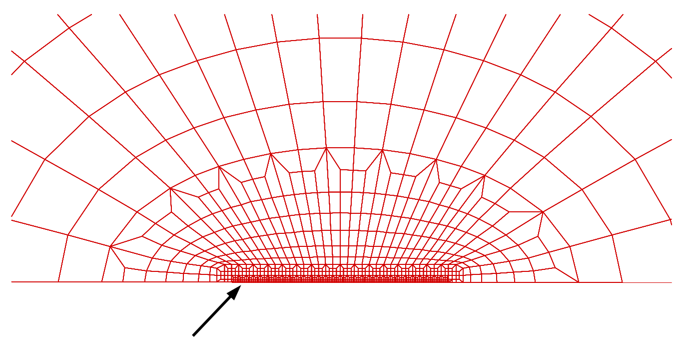
(b) Axisymmetric unit cell model



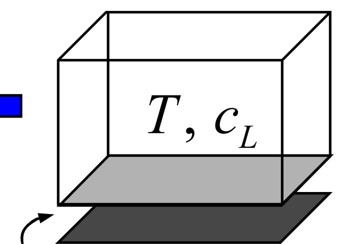
(c) Traction - separation law







Adjacent finite element

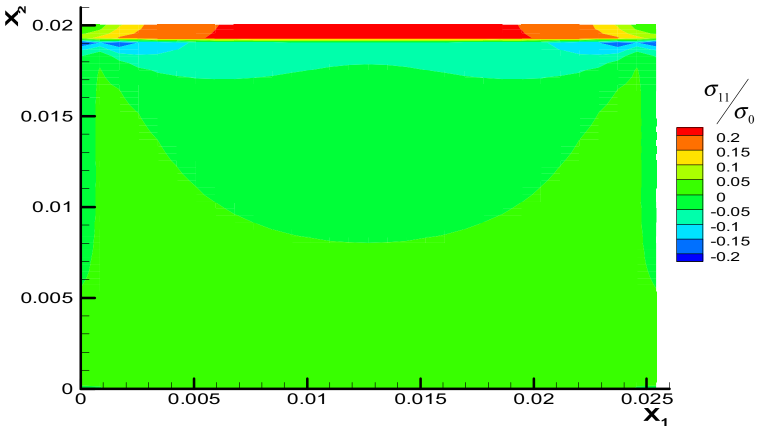


(d) Cohesive element

(e) Cohesive elements characterized by a traction-separation law based on the unit cell model

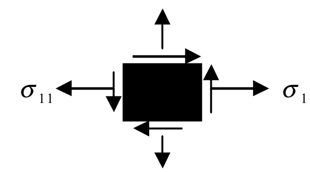
Future Work

- **Other Activities**
  - **Finite element analysis of residual stresses of a Schott Coating sitting on the substrate**



Average tensile stress σ_{11} in the coating is 125 MPa

Note that substrate is under large compression (-100Mpa) at the edges (possible delamination cause)

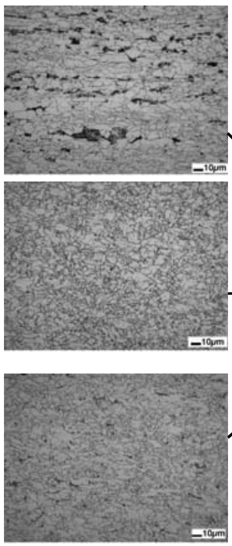


  - **Continue collaboration with ASME on establishing guidelines for codes and standards**
- **Continue our ongoing collaboration with the Japan program for materials solutions for the Hydrogen Economy**
  - **Hydrogen National Institute for Use and Storage (Hydrogenius)**
    - **Kyushu University (Prof. Y. Murakami)**
- **Continue our ongoing collaboration with the NATURALHY Project sponsored by the European Union**
  - **Interaction of hydrogen in a pipeline with a corrosion induced-crack on the external wall**

Future Work

Experiment

- **Establish the diffusion characteristics of existing and new pipeline steel microstructures**
  - Existing pipeline steel samples provided by Air Liquide and Air Products. Specimens are in our laboratory
  - New micro-alloyed steels (new microstructures) provided by Oregon Steel Mills through DGS Metallurgical Solutions, Inc.



	API/ Grade	C	Mn	Si	Cu	Ni	V	Nb	Cr	Ti	
A	X70	0.08	1.53	0.28	0.01	0.00	0.050	0.061	0.01	0.014	Typical natural gas pipeline steel
B	X70/80	0.05	1.52	0.12	0.23	0.14	0.001	0.092	0.25	0.012	Ferrite/acicular ferrite
C	X70/80	0.04	1.61	0.14	0.22	0.12	0.000	0.096	0.42	0.015	Ferrite/acicular ferrite
D	X52/60	0.03	1.14	0.18	0.24	0.14	0.001	0.084	0.16	0.014	Ferrite/low level of pearlite

  - **Collaboration with ORNL and Schott North America for coating of our samples**

- **Determine uniaxial tension macroscopic flow characteristics in the presence of hydrogen**

- **Carry out fracture testing: Collaboration with Sandia, Livermore**

- **SEM and TEM studies on existing and new pipeline material microstructures**
  - Fracture surfaces, particle, dislocation, and grain boundary characterization

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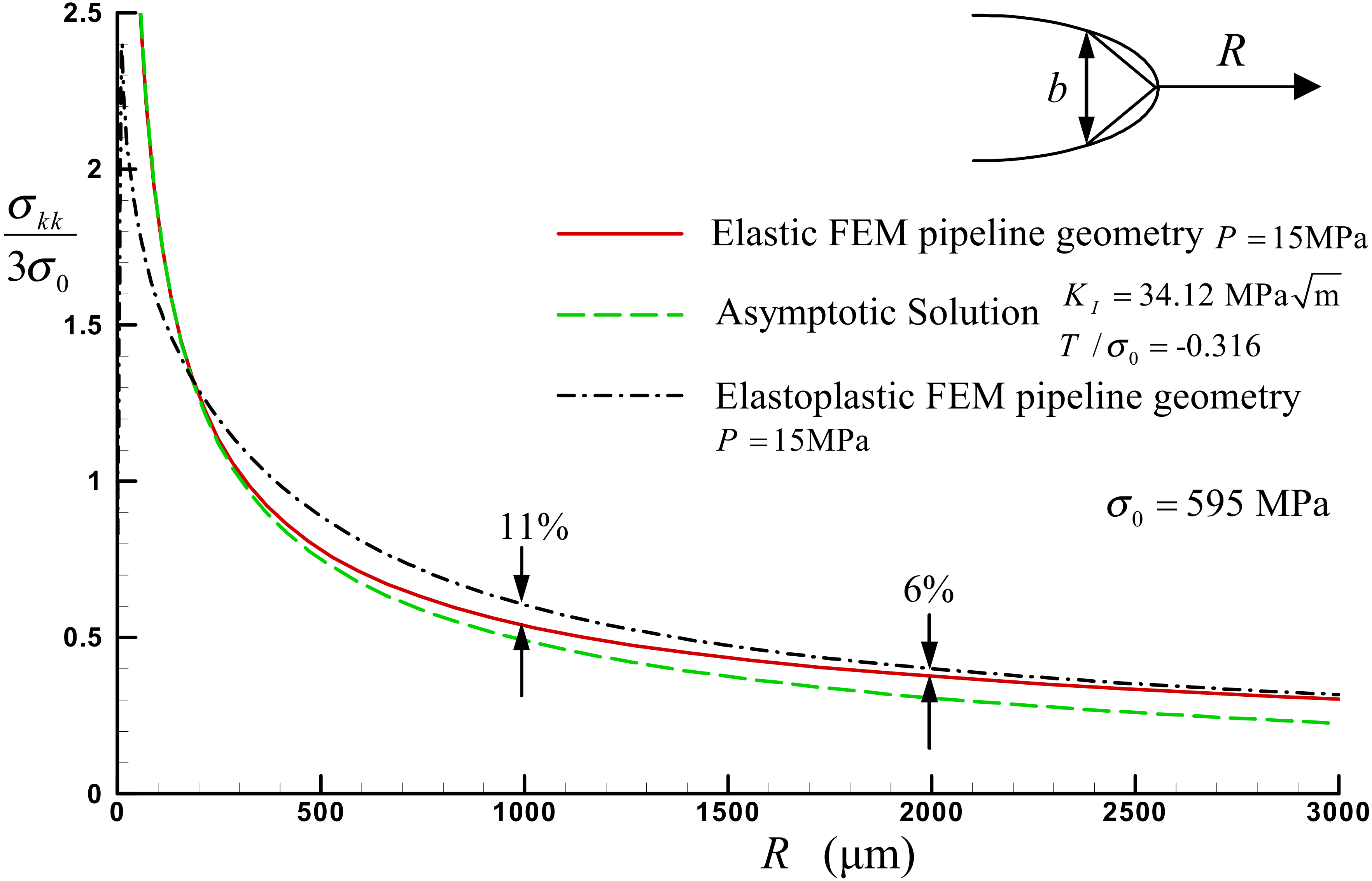
Additional slides

Critical Assumptions and Issues

- **Hydrogen-induced cracking in existing pipeline steels initiates at second phase particles by hydrogen-induced decohesion followed by shear localization of ligaments**
  - **Fracture toughness testing and SEM/TEM studies will verify this assumption**
- **Embrittlement of acicular ferrite initiates at the needle-pearlite/ferrite interface**
  - **Fracture toughness testing and SEM/TEM studies will verify this assumption**
- **Hydrogen dramatically degrades the resistance of steel to fatigue crack growth. Possible remediation by water vapor and oxidation**
  - **Experiments to study the oxidation effects**
- **Lack of funding does not allow**
  - **Hire personnel**
  - **Construct experimental devices**
  - **Carry out testing**

Ahead of the crack tip



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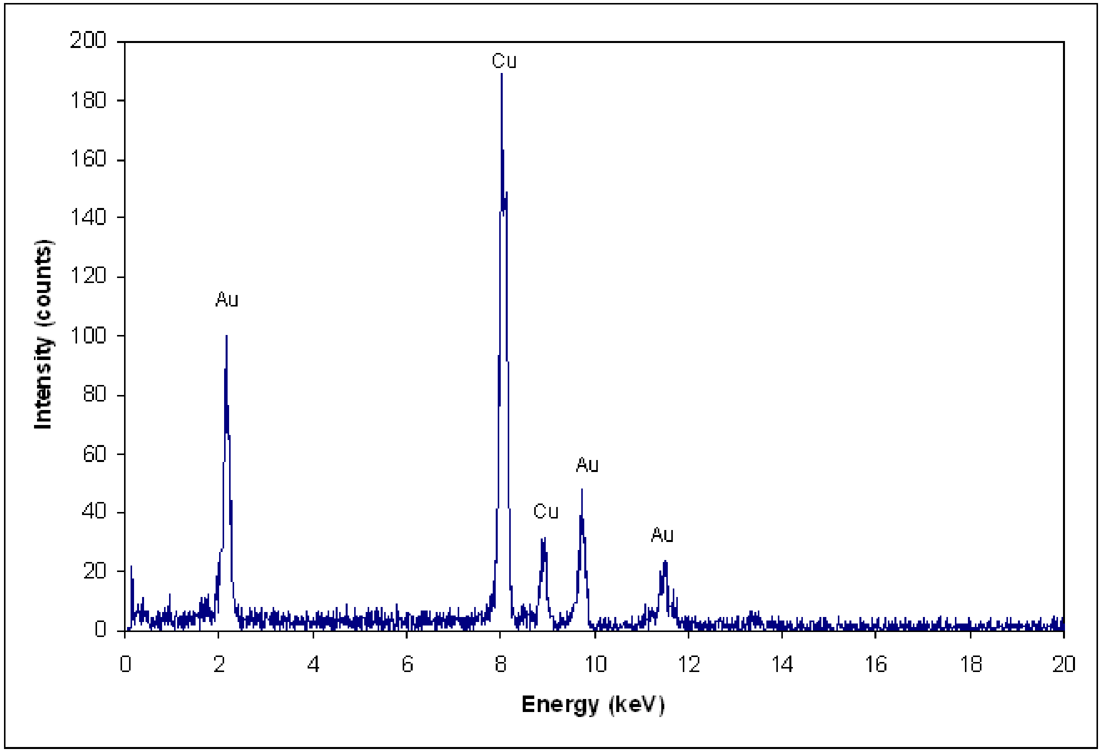
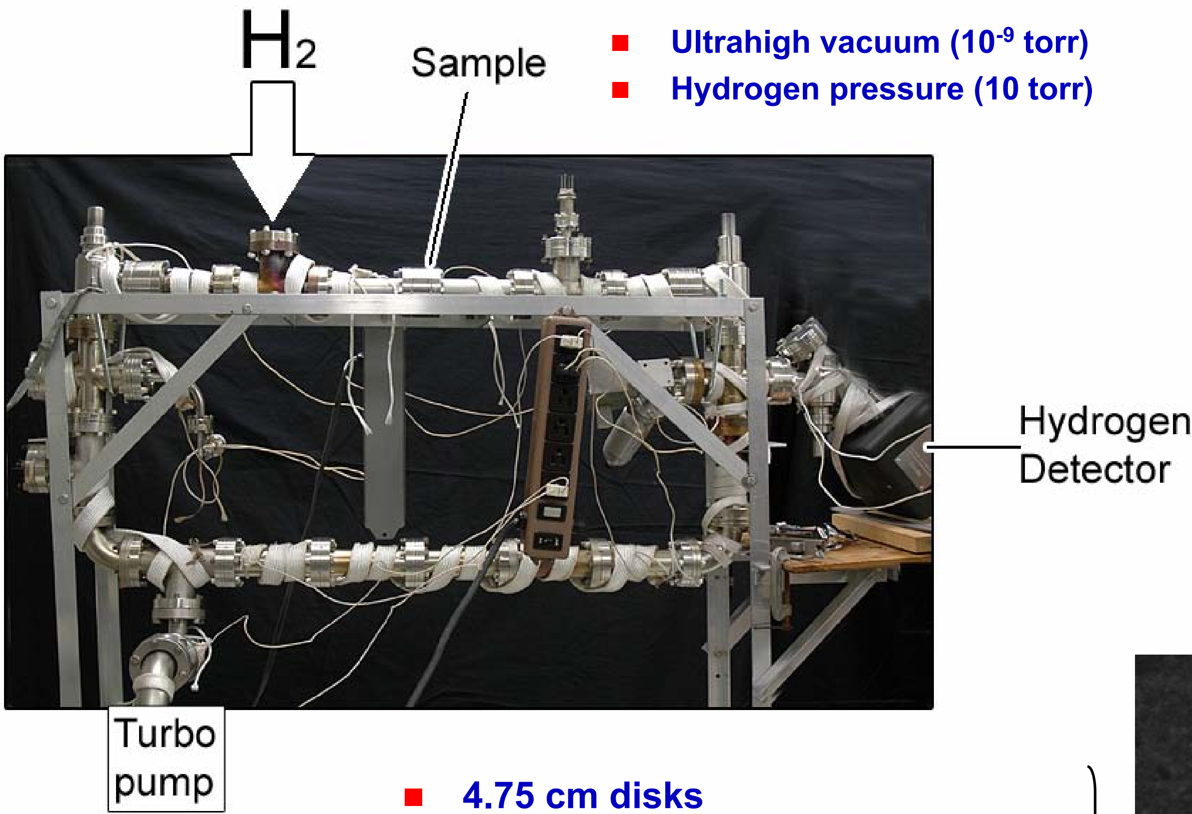
EDS reference



EDS of gold sample showing copper peaks from sample holder

Permeation

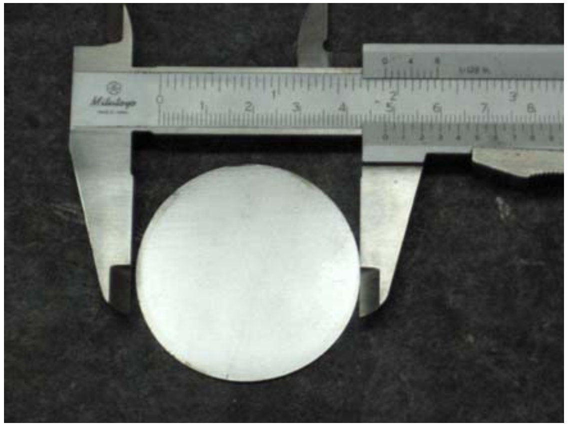


- Ultrahigh vacuum (10^{-9} torr)
- Hydrogen pressure (10 torr)

- **Hydrogen is introduced on one side of the sample**
- **Permeates through sample**
- **Detected by ion pump**

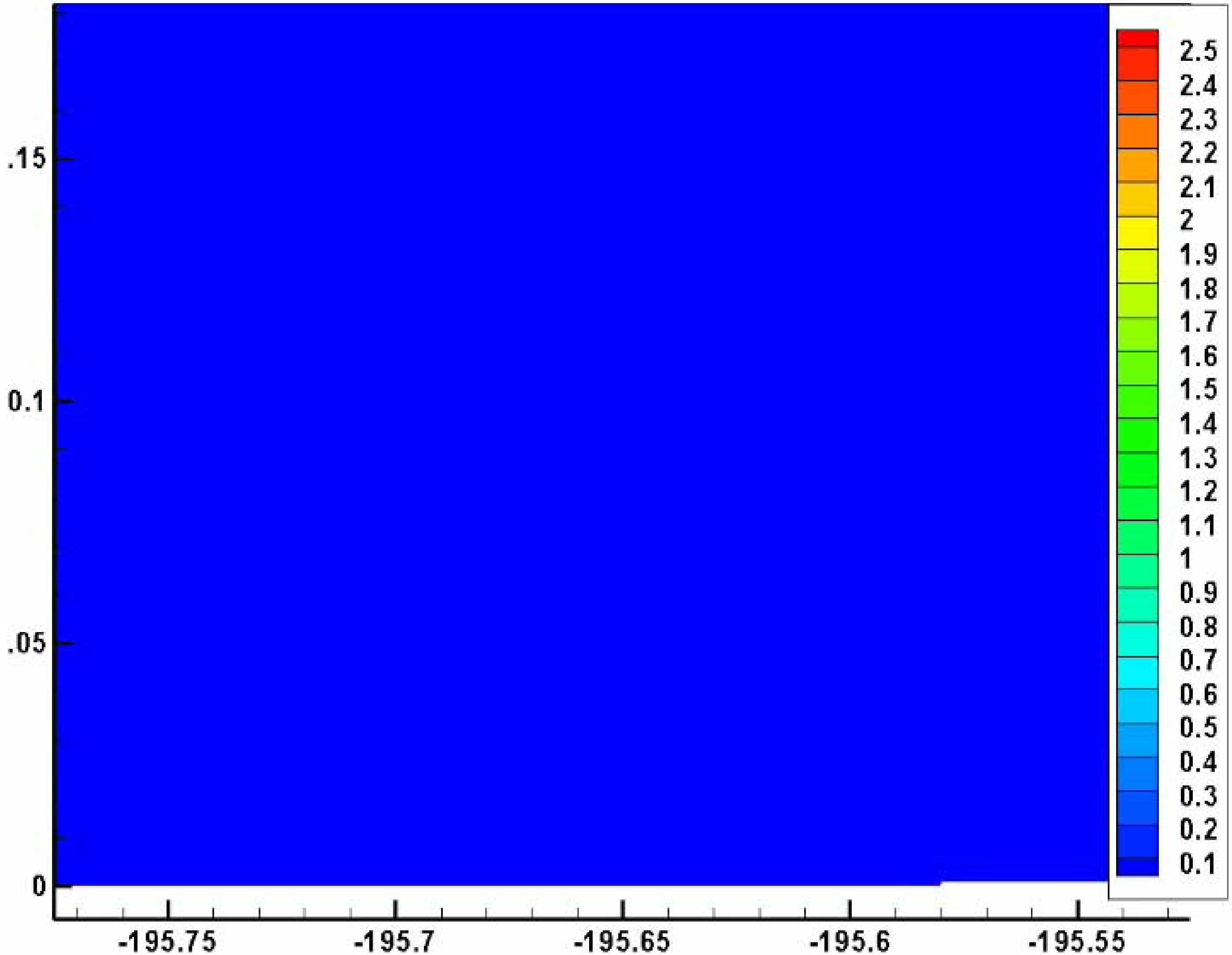
- **4.75 cm disks**
- **100 micron thickness**

- **Palladium coating on exit side**
- **Testing coatings on hydrogen side**



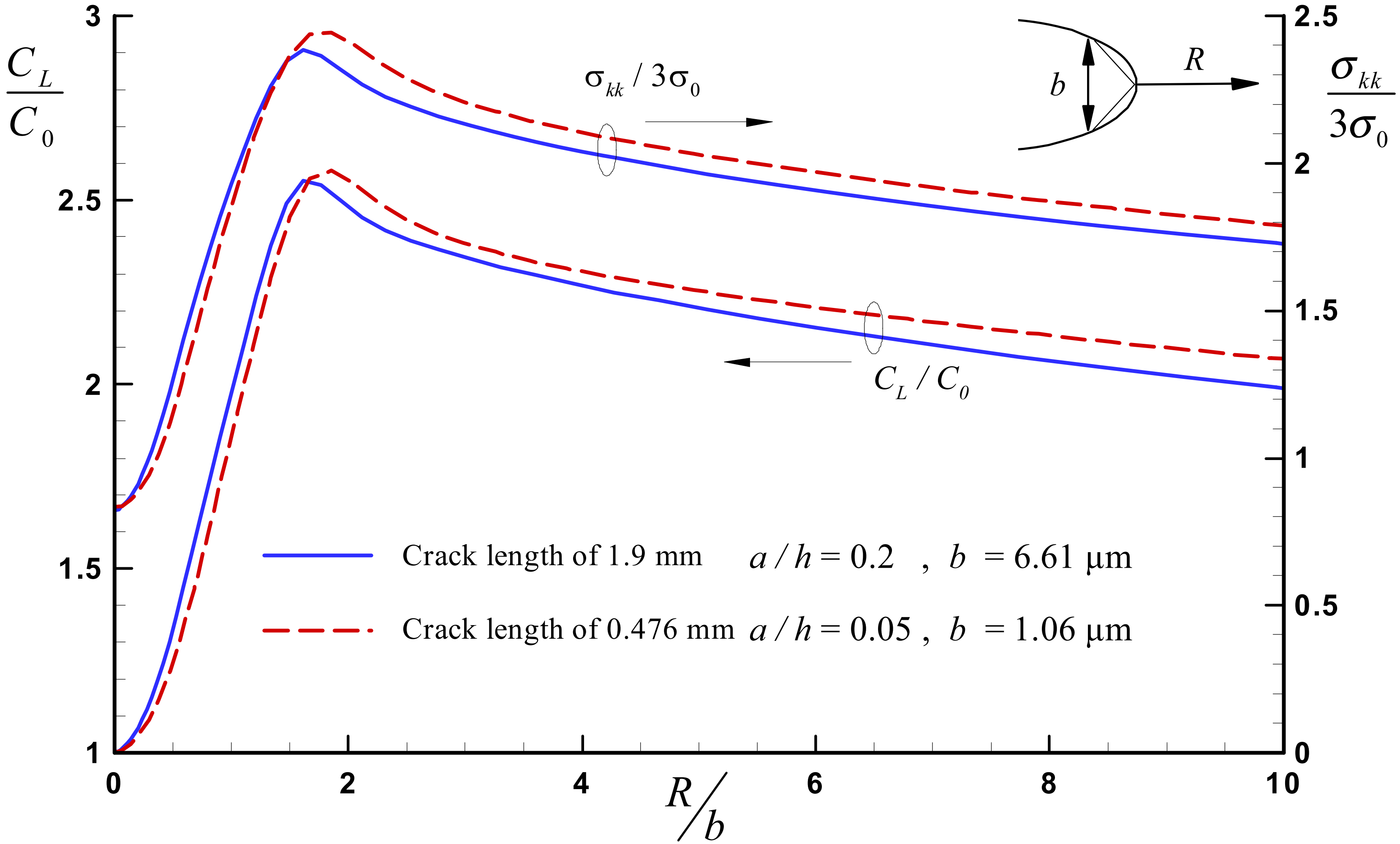
Real-world pipeline specimens are in our possession for testing
Air Liquide and Air Products provided the coupons

Transient to Steady State - Lattice Concentration



C_L / C_0

Full Field (pipeline) vs Boundary Layer Solution (laboratory specimen)



$a/h = 0.2$

$K_I = 34.12 \text{ MPa}\sqrt{\text{m}}$

$T/\sigma_0 = -0.316$

$a/h = 0.05$

$K_I = 14.38 \text{MPa}\sqrt{\text{m}}$

$T/\sigma_0 = -0.292$

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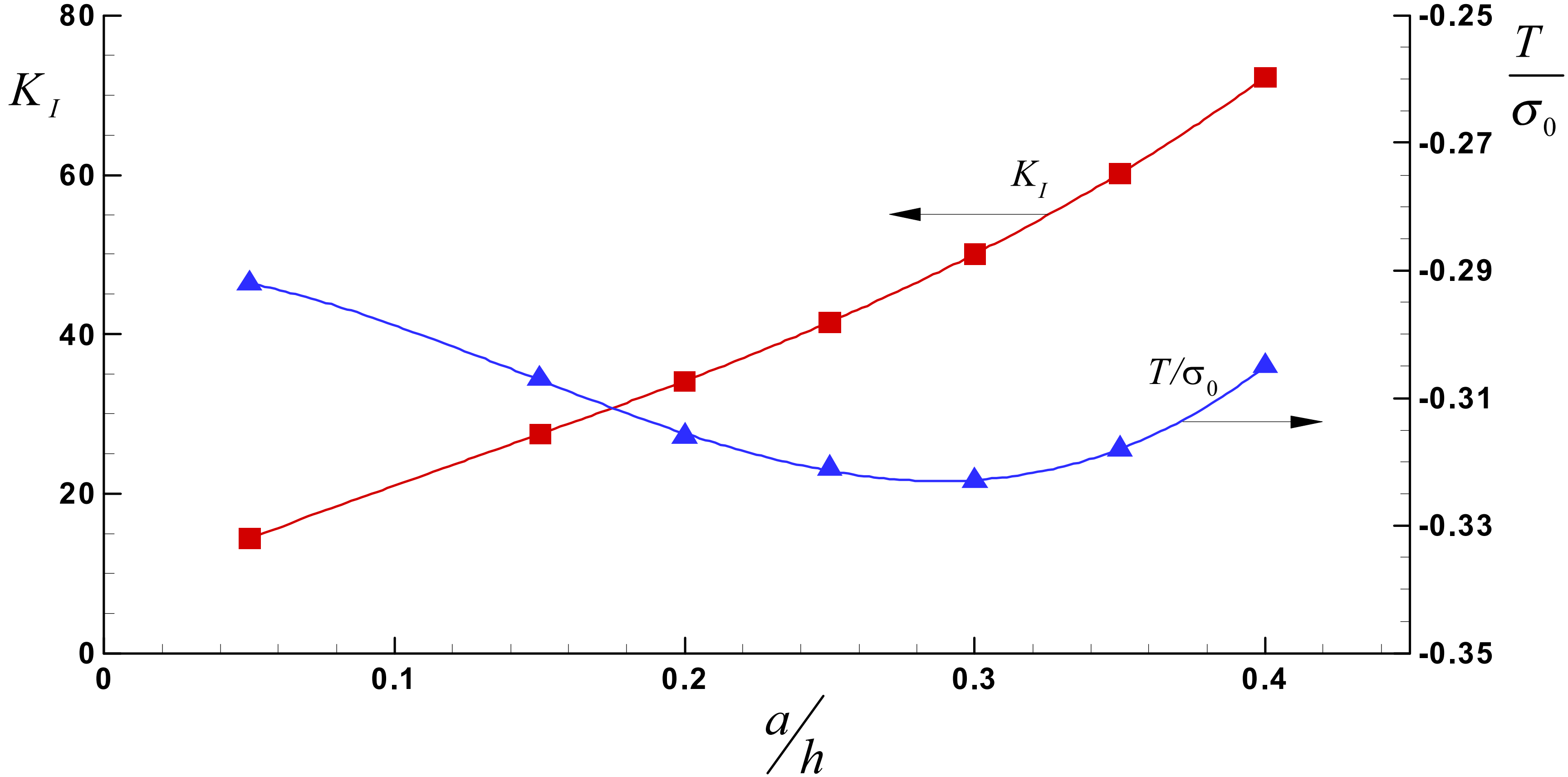
Fracture Assessment

From the full pipeline to laboratory specimens

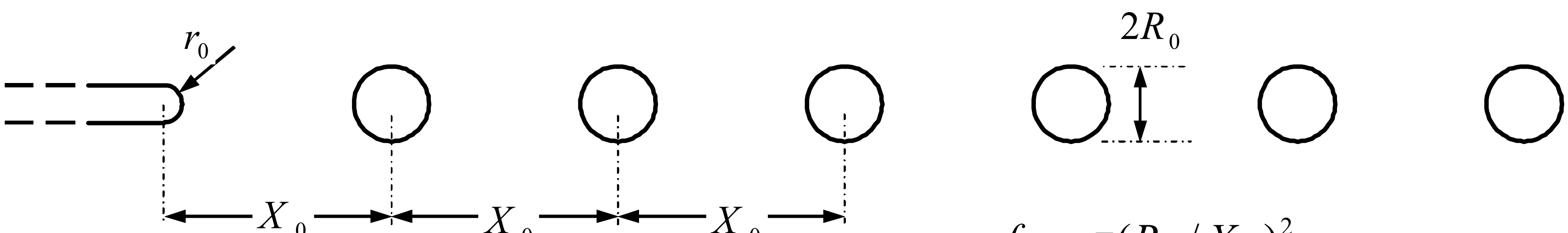


Crack depth/pipeline thickness

Hydrogen effect on ductile crack growth

- crack growth mechanisms
  - Void by void growth
  - Multiple void growth

void population



$$f_0 = \pi (R_0 / X_0)^2$$

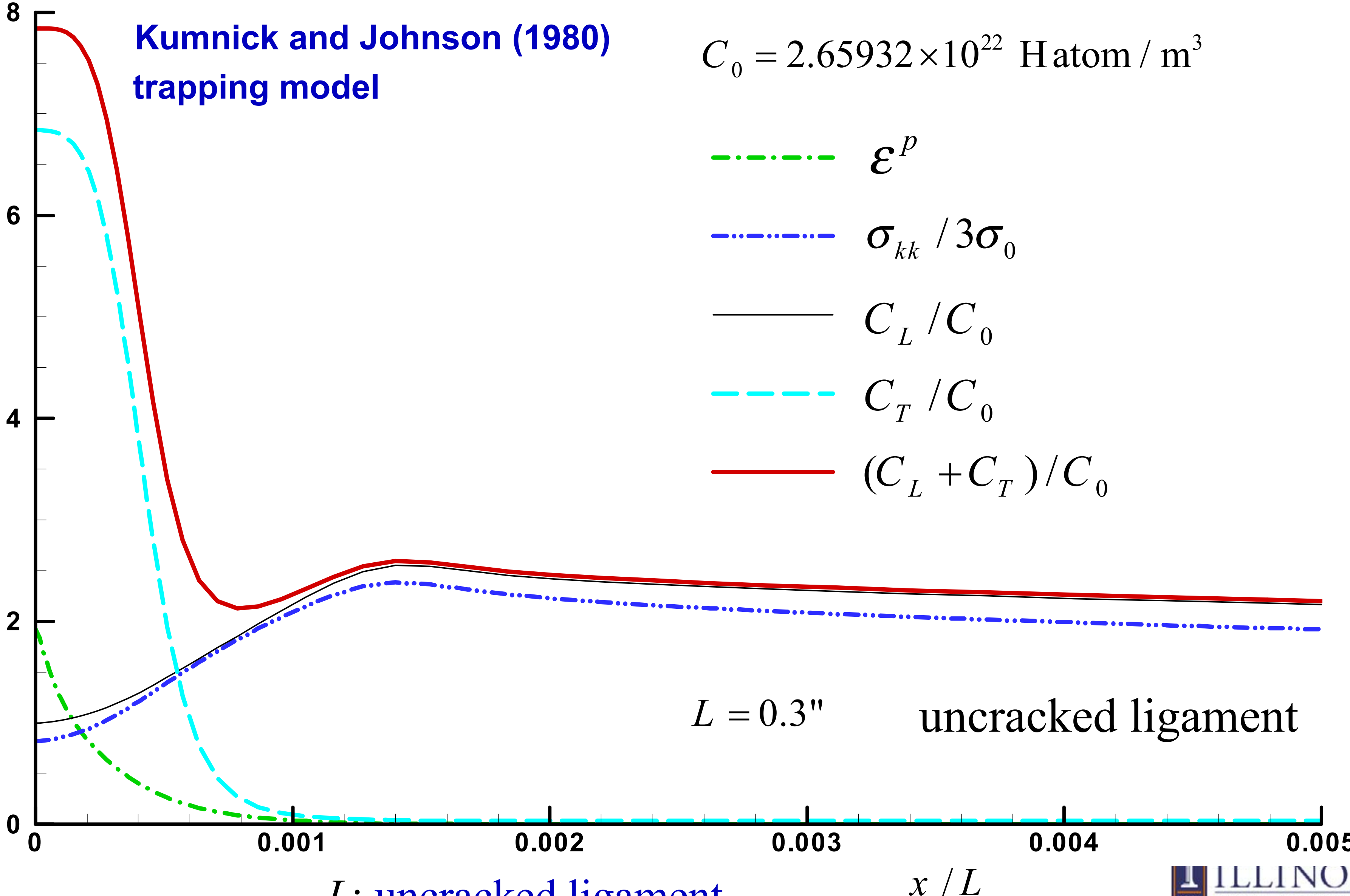
**[Tvergaard and Hutchinson, 2002
Petti and Dodds, 2005]**

- **Effect of hydrogen softening and dilatation**
- **Identifying the range of f_0 that each mechanisms is operative**

Ab-initio

- We have completed several necessary validation “computer experiments” on the binding energies for H in Fe grain boundary and free surface using a pseudopotential based plane-wave method via projected-augmented wave basis functions, as implemented in the Vienna *ab initio* Simulation Package. A subset of our validation results provides unrelaxed binding energies for H in Fe for GB/FS equal to -3.23/-3.57 eV, and the binding energies difference of the GB and FS equal to +0.34 eV, in good agreement with values in literature [4].

Ahead of the crack tip at steady state



L: uncracked ligament

Compact Tension Specimen: FEM Result vs Handbook

$$f\left(\frac{a}{W}\right) = \frac{2+\frac{a}{W}}{\left(1-\frac{a}{W}\right)^{3/2}}\left[0.886 + 4.64\left(\frac{a}{W}\right) - 13.32\left(\frac{a}{W}\right)^2 + 14.72\left(\frac{a}{W}\right)^3 - 5.6\left(\frac{a}{W}\right)^4\right]$$