Modelling of Iodine induced Stress Corrosion Cracking (I-SCC) of zirconium alloys with MFRONT

11th MFront User Meeting – 2025-11-20

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Outline

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   Iodine induced Stress Corrosion Cracking (I-SCC)
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3. **Implentation in MFRONT**
   One element in tension
   Cyclic behavior
4. **Applications**
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   Polycristalline simulations
5. **Conclusions and Perspectives**

1. Context

Pellet Cladding Interaction (PCI)

Iodine Induced Stress Corrosion Cracking (I-SCC)

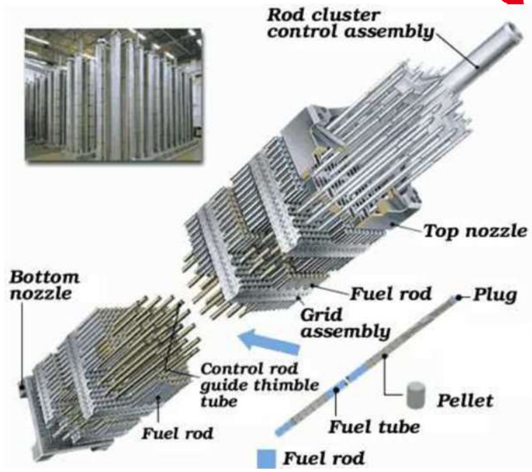
Context

Fuel cladding and Pellet-Cladding Interaction (PCI)

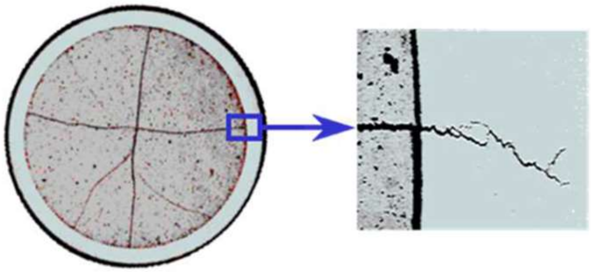
- **Zirconium alloys** are widely used in the nuclear industry as **fuel cladding material** due to their good properties. They are the primary containment barrier for fuel pellets and fission products in pressurised water reactors (PWR).
- During incidental power transients in the reactor, the fuel pellets increase in temperature and expand. Each pellet exerts a high stress on the fuel cladding, and this phenomenon is known as **Pellet-Cladding Interaction (PCI).**

Iodine-Induced Stress Corrosion Cracking (ISCC)

- During large power variations or incidental situations, the combination of **the mechanical load imposed** on the cladding and **the corrosive environment** could lead to a risk of **Iodine-Induced Stress Corrosion Cracking (ISCC)**



Scheme of Pressurized Water Reactor fuel assembly

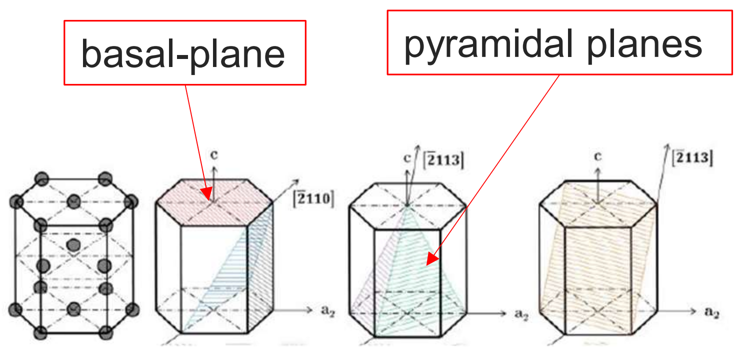


Fuel partitioning in in the fuel pellet (radial cracks) and ISCC crack [Davies, 1977].

Context

Iodine-Induced Stress Corrosion Cracking (ISCC)

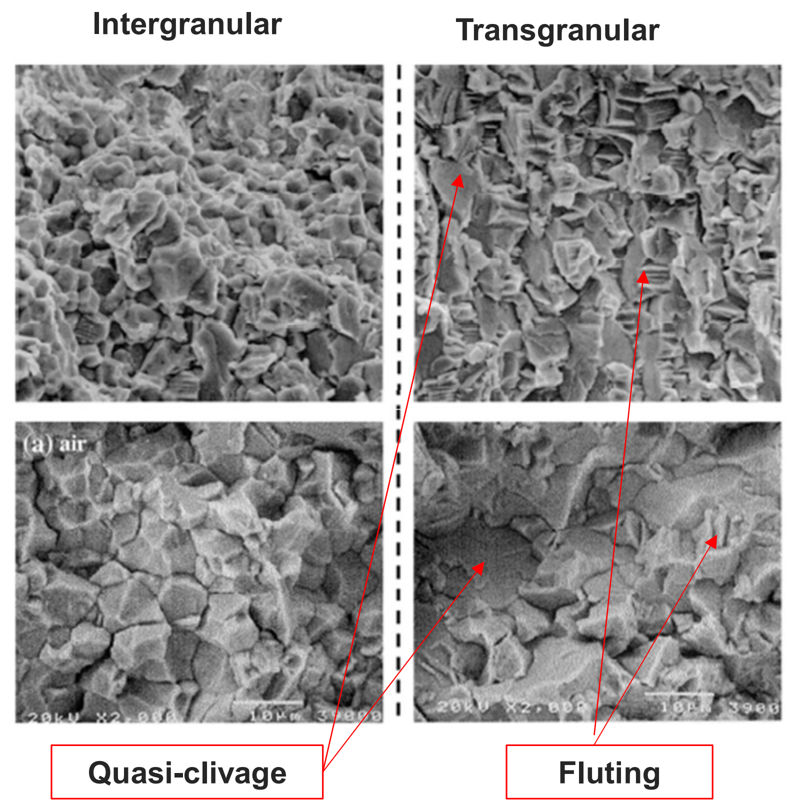
- The initiation of an ISCC crack is mainly intergranular
- The propagation is mainly transgranular
  - Quasi-clivage on basal-planes
  - Fluting on pyramidal planes



Tenckhoff 2005; Linga Murty et Charit 2006

Essai en rampe au GETR d'une gaine de Zircaloy-2 (Davies 1977)

Essai de laboratoire sur Zy-4 RX (Frégonèse 1999)



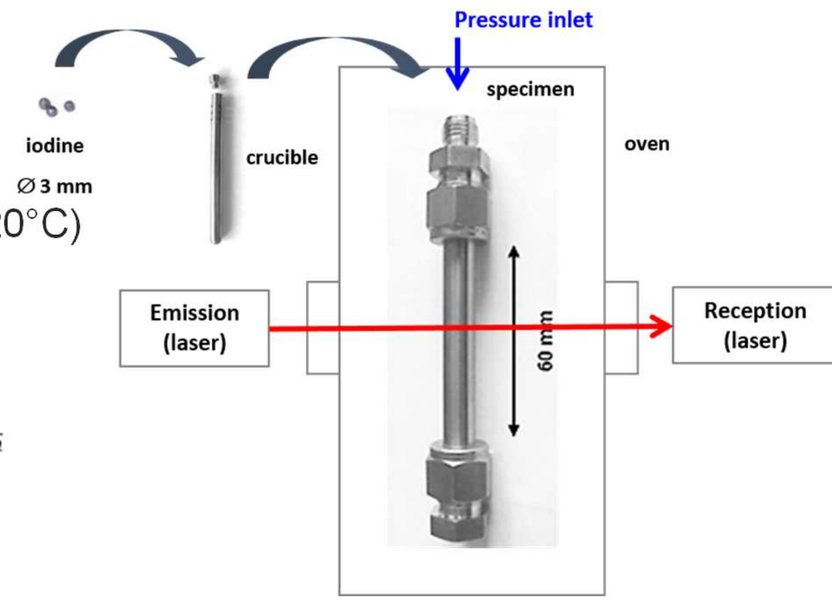
2. Laboratory tests

Inner Pressure tests in iodine vapor

Laboratory tests (example)

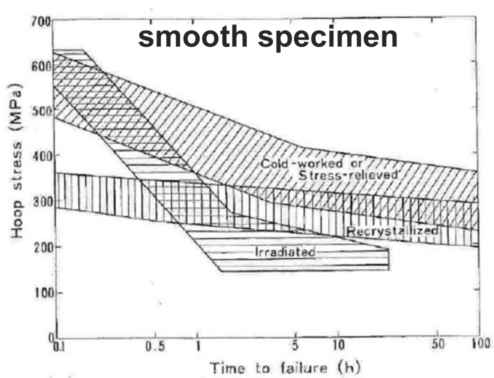
Inner Pressure tests with iodine vapor

- Inner Pressure P experimentally controlled
- At PWR's temperature of the inner wall of the cladding (320°C-420°C)
- On smooth specimen ➔ initiation of I-SCC cracks
- On pre-cracked specimen ➔ Propagation of I-SCC cracks



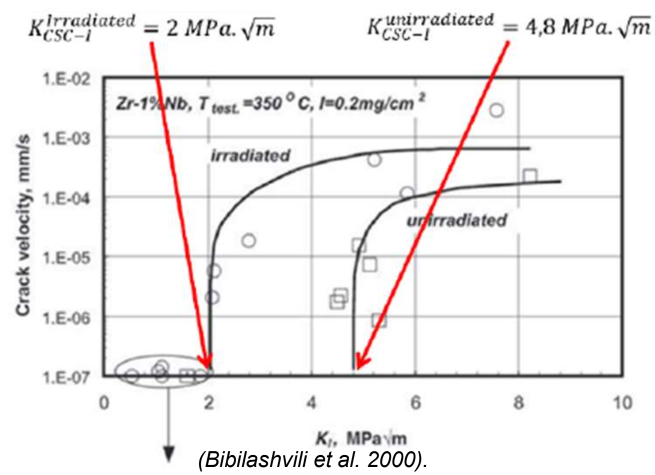
$$\sigma_{\theta\theta} = P.\frac{(R_{out} + R_{in})}{2.e}$$

$$pI_2 \approx 300\ 000\ Pa$$



Influence de la contrainte tangentielle sur le temps de rupture pour différentes nuance de Zr (Une 1983)

pre-cracked specimen



(Bibilashvili et al. 2000).

3. I-SCC modelling

Kachanov’s damage law

KACHANOV's damage law (1/2)

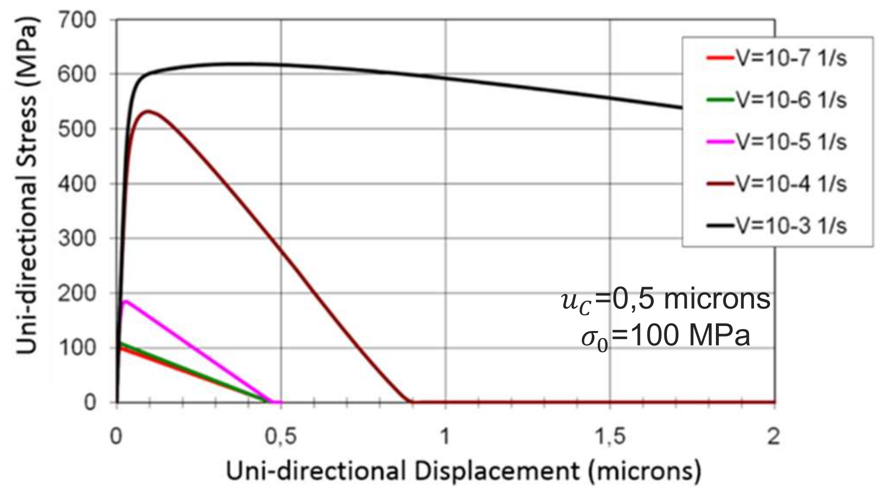
- Coupled to viscoplastic models presented after
- KACHANOV's law suits well for brittle time-dependent failure modes.
  - The parameters depend on the local Iodine quantity.
  - It defines a local isotropic damage variable D to simulate the initiation and the propagation of an I-SCC crack

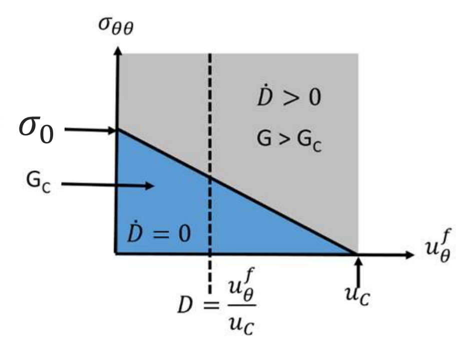
$$\dot{D} = A(I).e^{-\frac{Q}{T}}.\left\langle \frac{\sigma_D}{1-D} - \sigma_0(I) \right\rangle^B$$

$$\sigma_D = \sqrt{< \sigma_{\theta\theta} >^2 + \beta\left(\sigma_{R\theta}^2 + \sigma_{Z\theta}^2\right)}$$

- A cracking strain is added ε_f to apply a cracking energy $G_C(I)$ in the calculations
  - The cracking strain is added to the other strains of the material (viscoplasticity, thermal dilatancy, …).
  - Is defined with the opening u of the crack and a parameter with is the local size of the element of the mesh $L0$
  - It allows to define a critical opening $u_C(I)$ of the I-SCC crack

$$\varepsilon_f = \frac{u}{L0} ; \mathrm{D} = \frac{u}{u_C(I)} \qquad G_C(I) = \frac{1}{2}.\sigma_0(I).u_C(I)$$



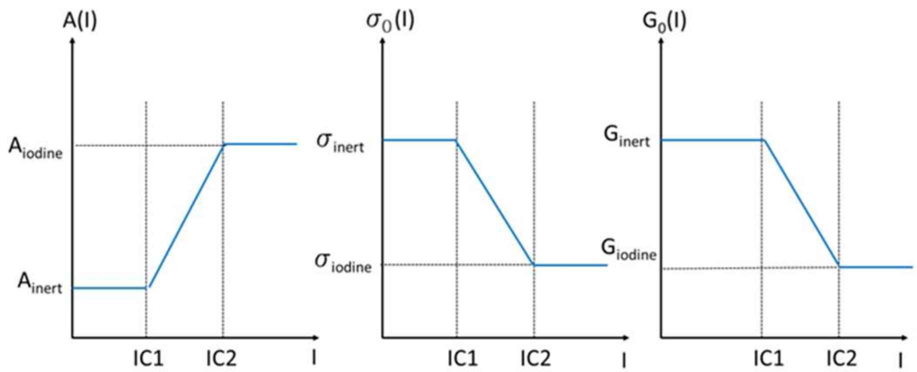


KACHANOV's damage law (2/3)

- Kachanov's model with embrittlement functions according to the iodine content
- Embrittlement functions according iodine content "I":
  - When "I" is lower than a threshold of iodine content "IC1", there is no embrittlement of the material. The Kachanov's model is supposed to model the damage of the material under an inert environment.
  - When "I" is higher than a saturation iodine content "IC2", the I-SCC susceptibility of the material does not change.
  - The local iodine content "I" and the parameters IC1 and IC2 can be physical quantities or dimensionless quantities.

$$\dot{D} = A(I).e^{-\frac{Q}{T}}.\left\langle \frac{\sigma_\theta}{1-D} - \sigma_0(I) \right\rangle^B$$

$$G_0(I) = \frac{1}{2}.\sigma_0(I).u_C(I)$$

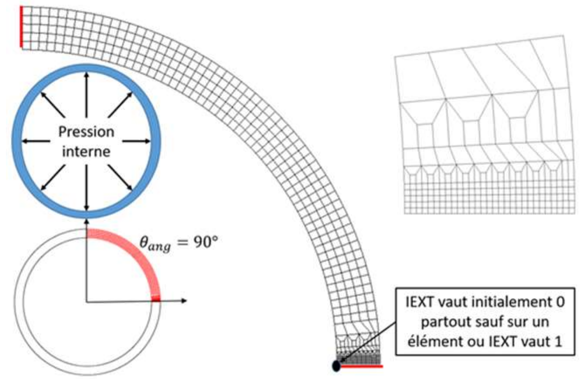


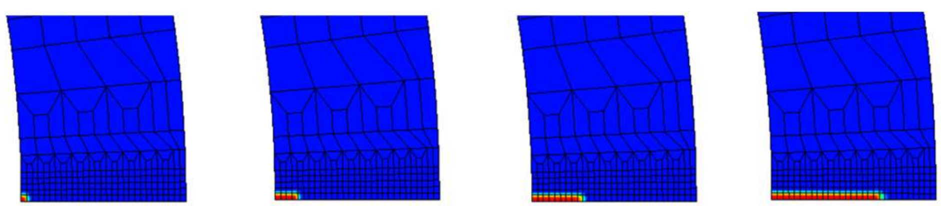
KACHANOV's damage law (3/3)

- The local iodine content "I" is assumed to follow I-SCC Miller's model
  - Based on Fick's law (diffusion)
  - Assuming that iodine does not diffuse in the zirconium, except in the I-SCC crack or at the tip of a crack, the Fick's law can be written, in 2D-Rθ, as:

$$\frac{dI}{dt} = \frac{1}{\tau}(I_{EXT} - I)$$

- τ is a period of time characteristic of the diffusion of iodine in the crack and the tip of a crack, in the zirconium.
- External iodine load "I_{EXT}" and the local iodine content "I" are fields of values defined on all the elements of the mesh in the FE simulations.
  - I_{EXT} is 0 everywhere, except in the crack or at the tip of the crack.
  - I_{EXT} is updated after each step of calculation in CAST3M according to the updated position of the I-SCC crack.





Viscoplastic behavior’s law (1/3)

- Cladding’s viscoplastic model for PCI conditions
  - Implemented in MFRONT
  - Zy-4 (Annie SONIAK, 1996) and M5 (Annie SONIAK, 2001)
  - Primary and secondary orthotropic viscoplastic creep strain combined
  - $\dot{\varepsilon}_{eq}^{vp} = V_s + (V_p - V_s).exp\left(-\frac{\varepsilon_{eq}^{vp}}{\epsilon_0}\right)$
  - $V_p = V_{p0}(\sigma_{Hill}, T).V_{pf}(\emptyset_t)$

$$V_{p0}(\sigma_{Hill}, T) = VP00.exp\left(-\frac{Q_{p0}}{T}\right).sinh\left(\frac{\sigma_{Hill}}{\sigma_{p0}}\right)$$

$$V_{pf}(\emptyset_t) = VPF1.exp\left(-\frac{\emptyset_t}{PHI1}\right) + (1 - VPF1).exp\left(-\frac{\emptyset_t}{PHI2}\right)$$

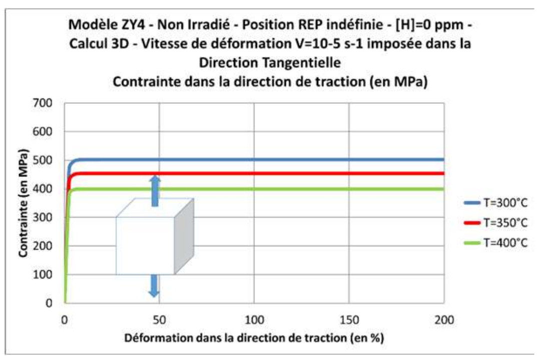
  - $V_s = V_{s0}(\sigma_{Hill}, T).V_{sf}(\emptyset_t)$

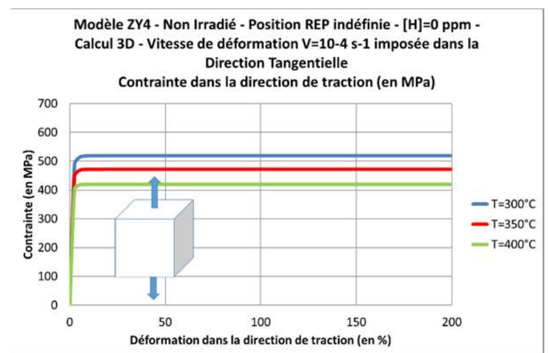
$$V_{s0}(\sigma_{Hill}, T) = VS00.exp\left(-\frac{Q_{s0}}{T}\right).sinh\left(\frac{\sigma_{Hill}}{\sigma_{s0}}\right)$$

$$V_{sf}(\emptyset_t) = VSF1 + (1 - VSF1).exp\left(-\frac{\emptyset_t}{PHI1}\right)$$

Viscoplastic behavior’s law (2/3)

- Claddings’ viscoplastic models for Reactivity Injection Accident (RIA)
  - Implemented in MFRONT
  - ZY4 (Matthieu LE SAUX, CEA, 2008) and CROCORIA (Elodie BOSSO, EDF, 2015)
    - Orthotropic Lemaître’s law
    - $\dot{\varepsilon}_{eq}^{vp} = \left(\frac{\sigma_{Hill}}{K.L\left(\varepsilon_{eq}^{vp}\right)}\right)^{1/m}$





Viscoplastic behavior's law (3/3)

- Effective stress
  - $\sigma_{Hill}^{eff} = \frac{\sigma_{Hill}}{1-D}$
- Viscoplastic models coupled to Kachanov's law
  - The effective stress acts on the material
    - $\dot{\varepsilon}_{eq}^{vp} = (1 - D)\left(\frac{\sigma_{Hill}^{eff}}{K.L\left(\varepsilon_{eq}^{vp}\right)}\right)^{1/m}$
  - Assuming $\sigma_{Hill}^{eff}.\, \dot{\varepsilon}_{eq}^{eff} = \sigma_{Hill}.\, \dot{\varepsilon}_{eq}^{vp}$ it allows to define an effective equivalent strain $\dot{\varepsilon}_{eq}^{eff}=(1-D).\dot{\varepsilon}_{eq}^{vp}$
    - $\dot{\varepsilon}_{eq}^{eff} = (1 - D)\left(\frac{\sigma_{Hill}^{eff}}{K.L\left(\varepsilon_{eq}^{eff}\right)}\right)^{1/m}$

3. Implementation in MFRONT

Strain rate and cyclic behavior

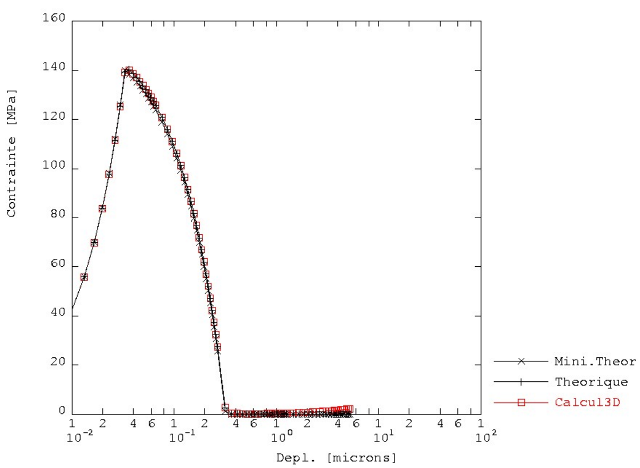
Implementation

- Damage allowed in the Radial-Axial plane of the cladding only
  - To avoid rotations of the principal stress coordinate system that are un-usefull for our needs
- Solved by Newton-Raphson in MFRONT
  - θ-method with θ=0,5.
  - Jacobian calculated
  - Jacobian validated with the CompareToNumericalJacobian compilation option of MFRONT

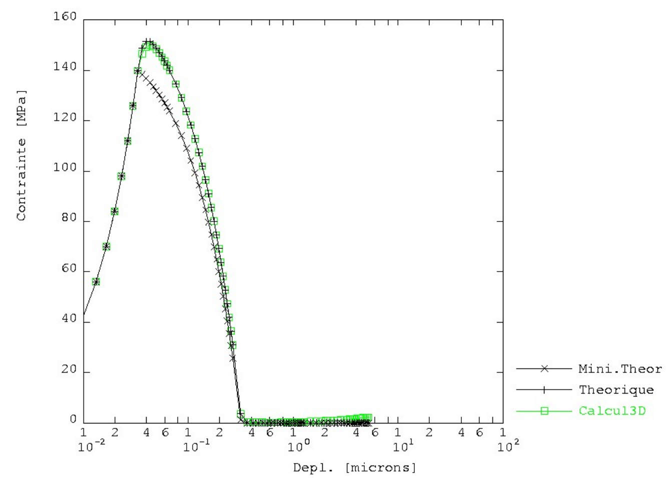
$$[\underline{J}] = \begin{bmatrix} \frac{\partial f\underline{eel}}{\partial \Delta \underline{eel}} & \frac{\partial f\underline{eel}}{\partial \Delta p} & \frac{\partial f\underline{eel}}{\partial \Delta D} & \frac{\partial f\underline{eel}}{\partial \Delta I} \\ \frac{\partial fvp}{\partial \Delta \underline{eel}} & \frac{\partial fvp}{\partial \Delta p} & \frac{\partial fvp}{\partial \Delta D} & \frac{\partial fvp}{\partial \Delta I} \\ \frac{\partial fD}{\partial \Delta \underline{eel}} & \frac{\partial fD}{\partial \Delta p} & \frac{\partial fD}{\partial \Delta D} & \frac{\partial fD}{\partial \Delta I} \\ \frac{\partial fI}{\partial \Delta \underline{eel}} & \frac{\partial fI}{\partial \Delta p} & \frac{\partial fI}{\partial \Delta D} & \frac{\partial fI}{\partial \Delta I} \end{bmatrix}$$

Example on 1-element (1/3)

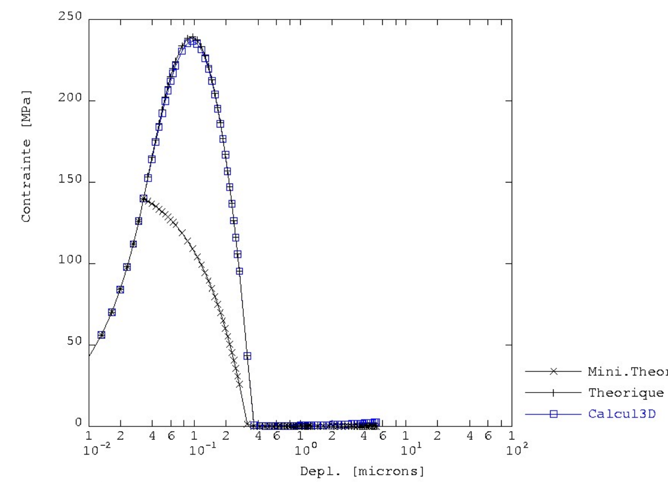
- Viscoplastic model + KACHANOV
- Comparison of the solution calculated with MFRONT compared to an analytical solution
  - One element loaded in constant strain rate in 3D (tested in pure shear too).
- The « Mini.Theor » solution is the theoretical solution obtained with the KACHANOV's law for an infinitelly slow applied strain rate.
  - This solution defines an minimal mechanical energy required to lead the material to failure.
  - This solution is recalled on all the figures.



T=320 Celcius, F=100E24 n/m2, V= 1.E-8 1/s



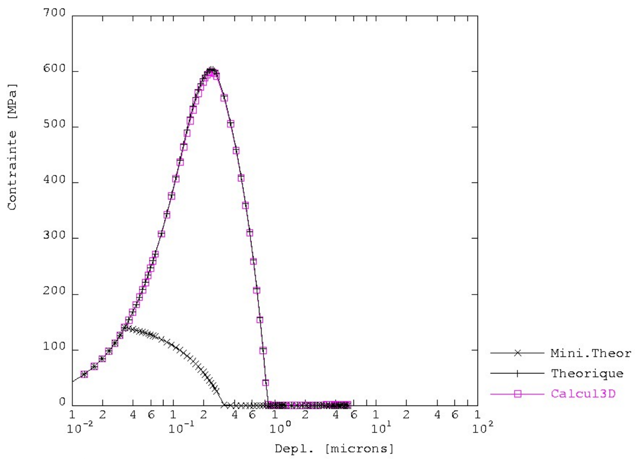
T=320 Celcius, F=100E24 n/m2, V= 1.E-7 1/s



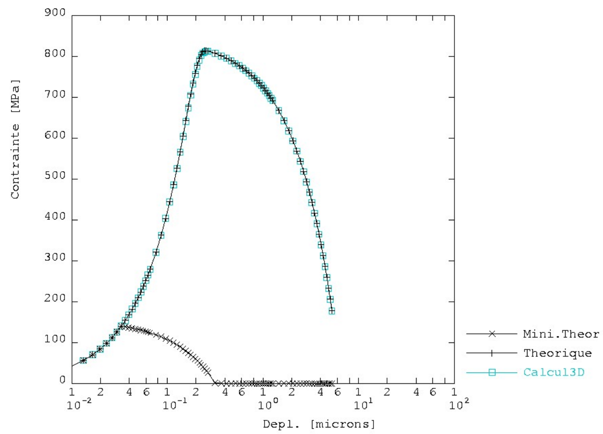
T=320 Celcius, F=100E24 n/m2, V= 1.E-6 1/s

Validation de KACHANOV sur un élément (2/3)

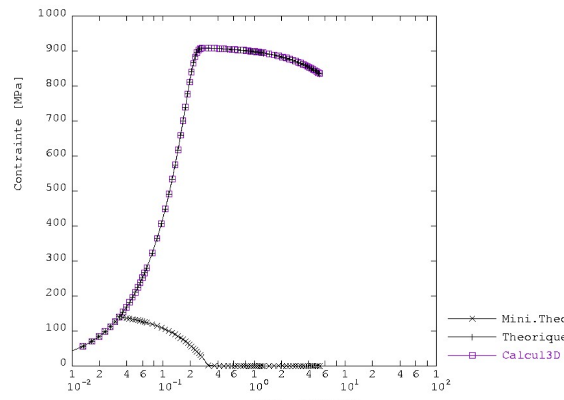
- Viscoplastic model + KACHANOV
- Comparison of the solution calculated with MFRONT compared to an analytical solution
  - One element loaded in constant strain rate in 3D (tested in pure shear too).
- The « Mini.Theor » solution is the theoretical solution obtained with the KACHANOV's law for an infinitelly slow applied strain rate.
  - This solution defines an minimal mechanical energy required to lead the material to failure.
  - This solution is recalled on all the figures.



T=320 Celcius, F=100E24 n/m2, V= 1.E-5 1/s



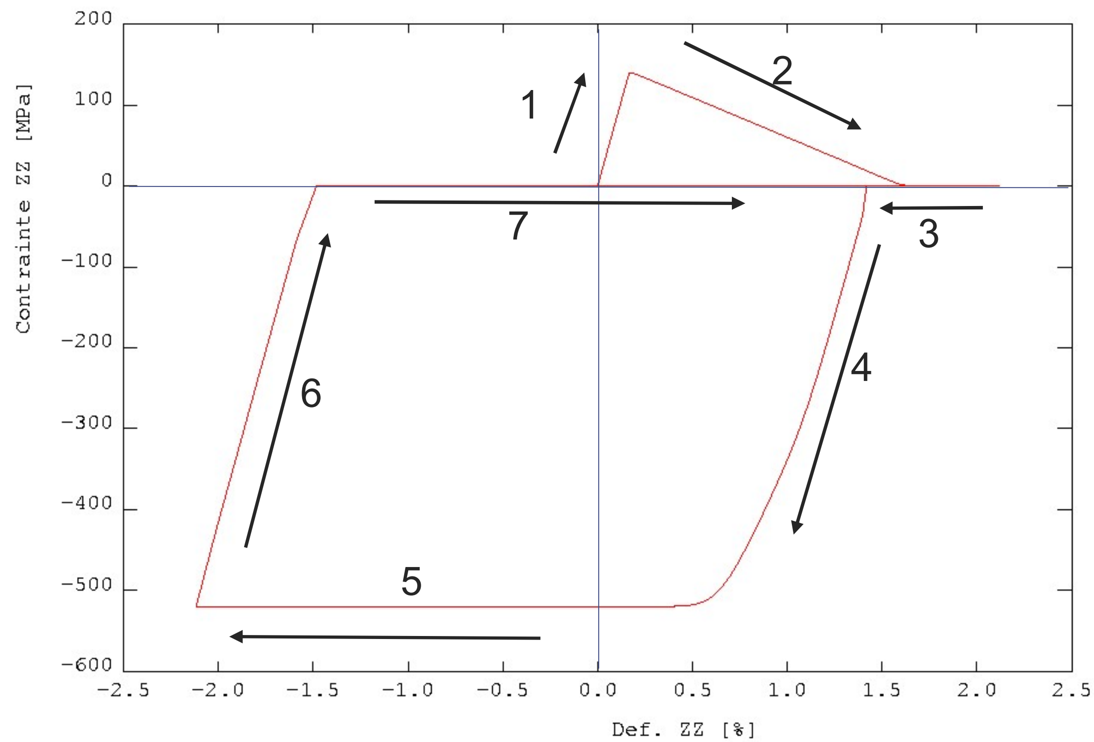
T=320 Celcius, F=100E24 n/m2, V= 1.E-4 1/s



T=320 Celcius, F=100E24 n/m2, V= 1.E-3 1/s

Cyclic behavior(3/3)

- Example of cyclic behavior
  1. Elasto-viscoplastic load in traction
  2. Progressive dammage to final failure
  3. Un-load of the failed element
  4. Eleastic re-load in compression
     1. From the cracking-deformation-to-failure and the viscoplastic déformation (neglectible in this example)
  5. Viscoplastic déformation in compression
  6. Compressive elastic un-load
  7. Elastic load of the failed element in tension

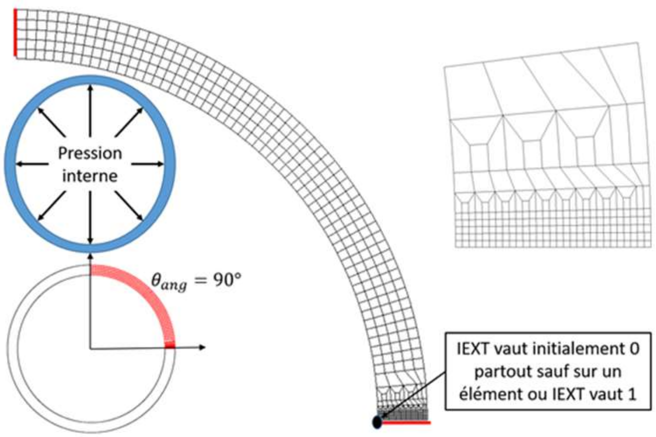


Contrainte - Deformation Totale, T=320 C, F=100E24 n/m2

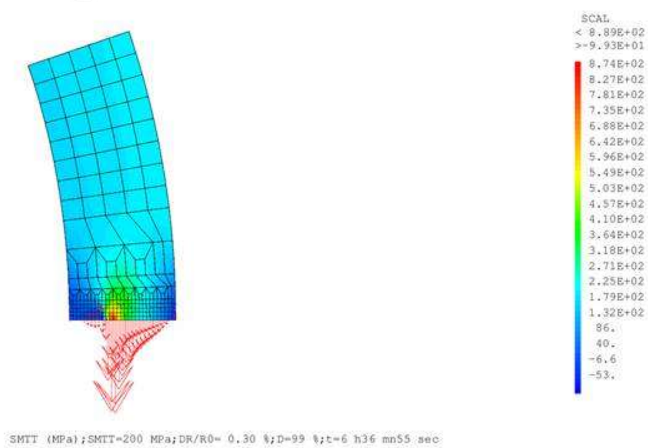
4. Examples of application

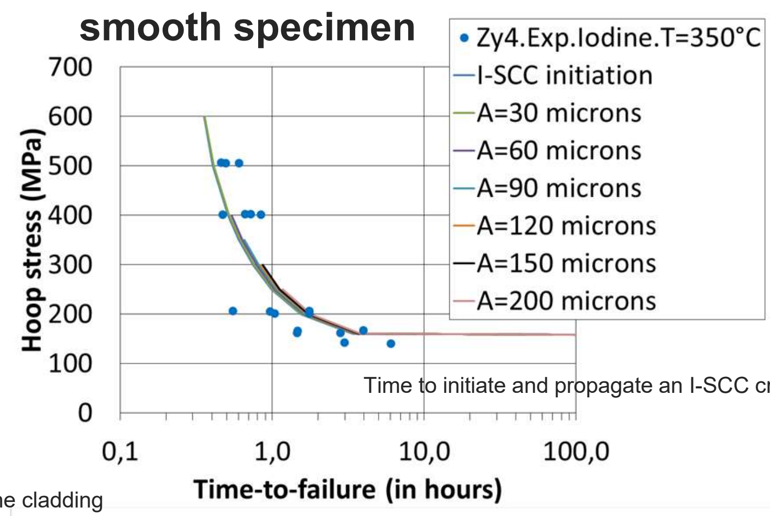
Inner Pressure tests, polycristalline simulations

Inner Pressure Tests

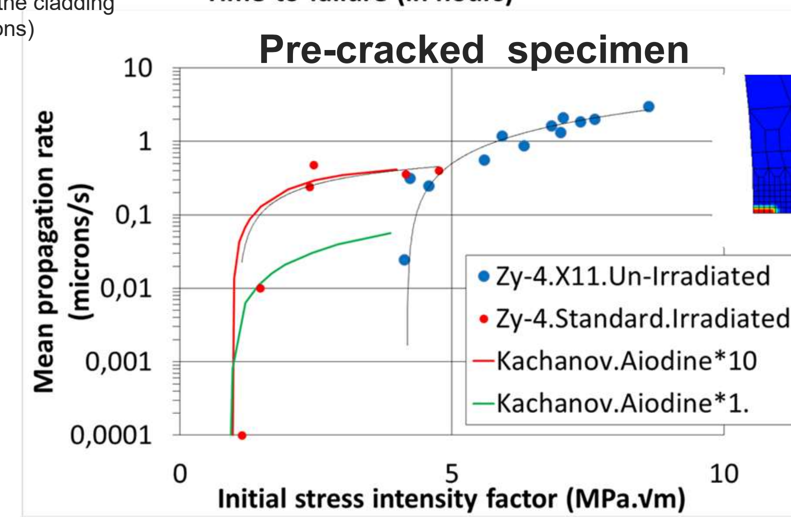


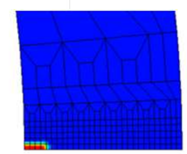
Constant pressure applied inside the cladding
(experiment and simulations)





Time to initiate and propagate an I-SCC crack of depth A

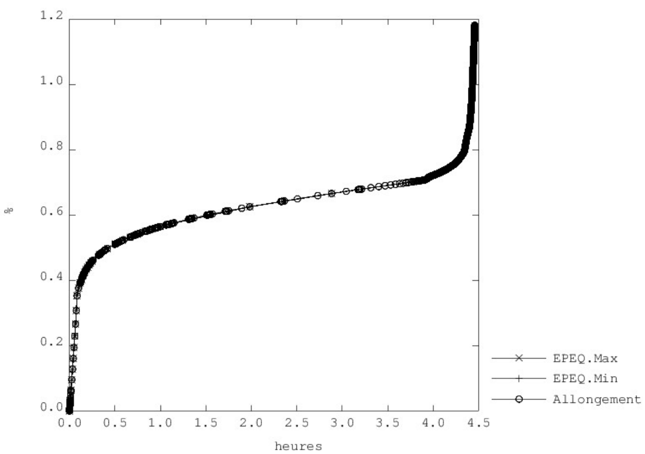




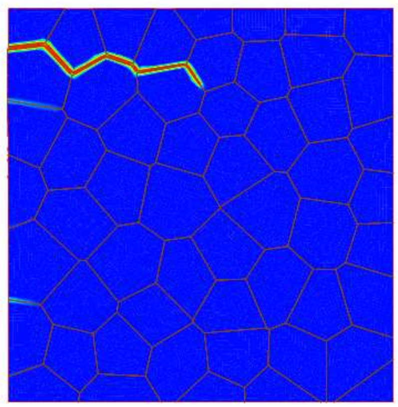
Results presented at OECD-NEA - PCI WORKSHOP – 22-24 june 2016 – Lucca,

Polycristalline simulations

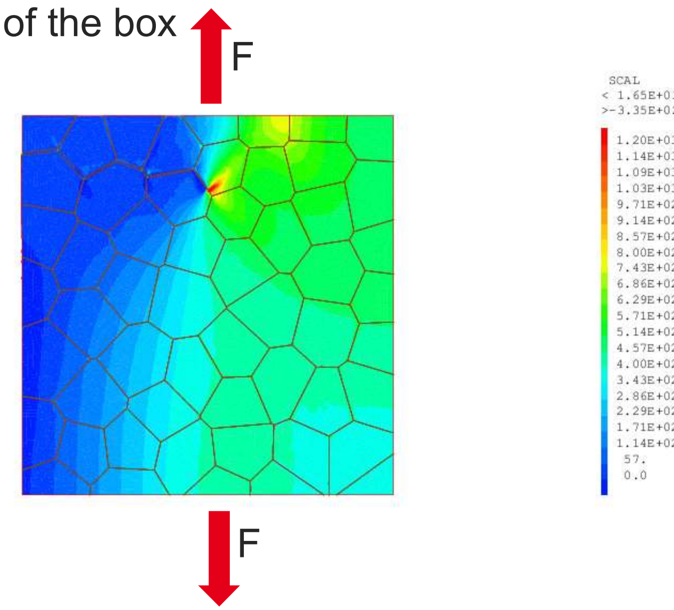
- To simulate the intergranular initiation of an I-SCC crack.
  - The KACHANOV-MILLER model has been implemented in the Grain-Boundaries of a polycristalline mesh
  - Orthotropic viscoplastic models in the grains.
  - Constant resulting force F applied at the upper and lower boundaries of the box



Vertical elongation of the box as a function of the time



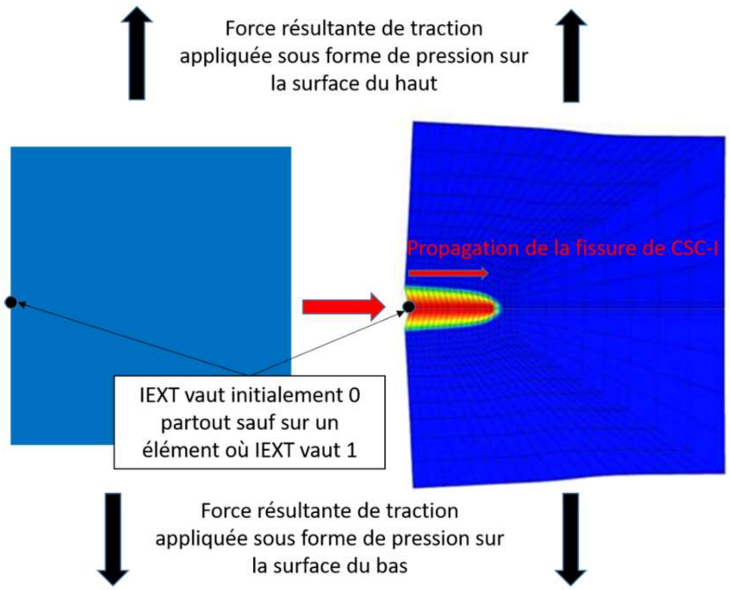
I-SCC intergranular crack at 4h27mn



Local vertical stress at 4h27mn

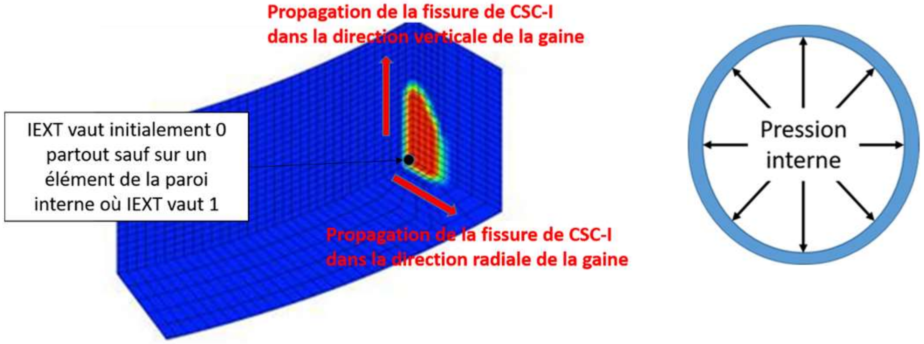
Example on a plate and a tube

- Plate in tension a 2D



- Portion of cladding in inner pressure in 3D
  - Miller's diffusion law generalised to 3D

$$\dot{I} = \left(\frac{n_R}{\tau_R} + \frac{n_Z}{\tau_Z}\right)(I_{\mathrm{EXT}} - I)$$



4. Conclusions

Perspectives

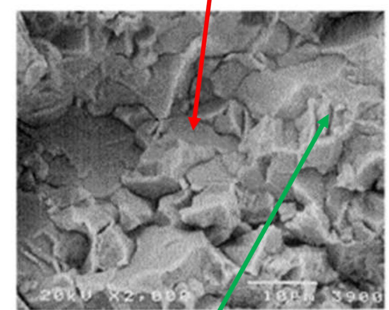
Conclusions and perspectives

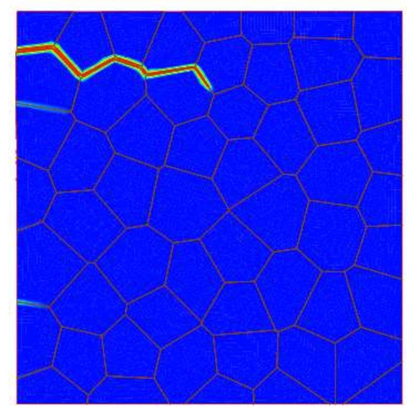
- KACHANOV implemented in MFRONT
  - KACHANOV was implementd in MISTRAL before
    - MISTRAL is a catalogue of behavior’s law. It pre-allocates 99 parameters and 99 inner variables in the computer’s memory whatever the behavior’s law of the catalogue
  - KACHANOV works faster with MFRONT
- Coupled to a simplified diffusion of iodine to simulate the initiation and the propagation of an I-SCC crack
  - At a macroscopic scale (in the frame of homogeneous and continuous media)
  - At a polycristalline scale (to simulate the intergranular initiation)
- Perpectives
  - Replacing the MILLER’s simplified diffusion model by a physical diffusion model.

$$\frac{\partial \mathrm{I}}{\partial \mathrm{t}} = -\mathrm{D}_{\mathrm{Zr}}.\left(\nabla \mathrm{I} + \frac{\mathrm{I}Q^{*}}{\mathrm{RT}^{2}}\nabla \mathrm{T} - \frac{\mathrm{I}\overline{\mathrm{V}}}{\mathrm{RT}}\nabla \mathrm{P}\right)$$

  - The implementation in MFRONT makes it possible to simulate the transgranular propagation at the polycristalline scale
    - Using the model, coupled with an orthotropic model, in each grains

$$\sigma_D = \sqrt{\underbrace{< \sigma_{\theta\theta} >^{2}}_{\text{Quasi-clivage}} + \underbrace{\beta\left(\sigma_{R\theta}^{2} + \sigma_{Z\theta}^{2}\right)}_{\text{Fluting}}}$$





Thank you

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Laboratory tests (example)

Inner Pressure tests with iodine vapor

- Inner Pressure P experimentally controlled
- At PWR's temperature of the inner wall of the cladding (320°C-420°C)

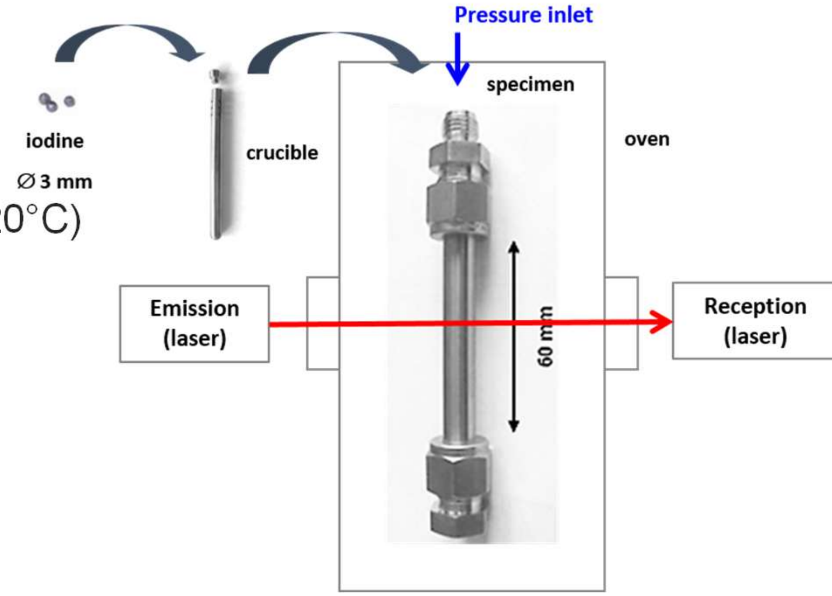
- pI2 is very big in these tests and pO2 is not controlled !!!
  - Difficult to go lower in iodine content

$$pI_2 \approx 3\ bars = 3.10^5\ Pa$$

$$\frac{nI_2}{n_{Argon}} \approx 1\ \%$$

$$pO_2\ evaluated\ to\ 3000\ Pa\ (Jezequel, 2017)$$

$$\frac{nO_2}{n_{Argon}} \approx 0{,}01\ \%$$



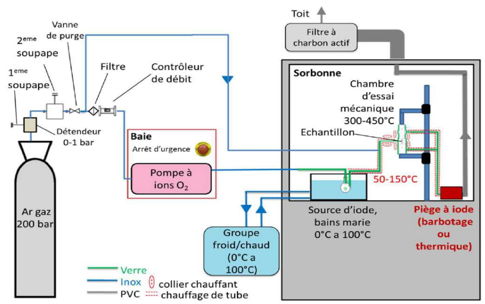
$$\sigma_{\theta\theta} = P.\frac{(R_{out} + R_{in})}{2.e}$$

$$P \approx 300\ bars$$

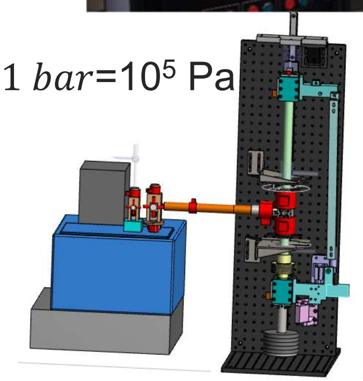
$$\sigma_{\theta\theta} \sim 300\ MPa$$

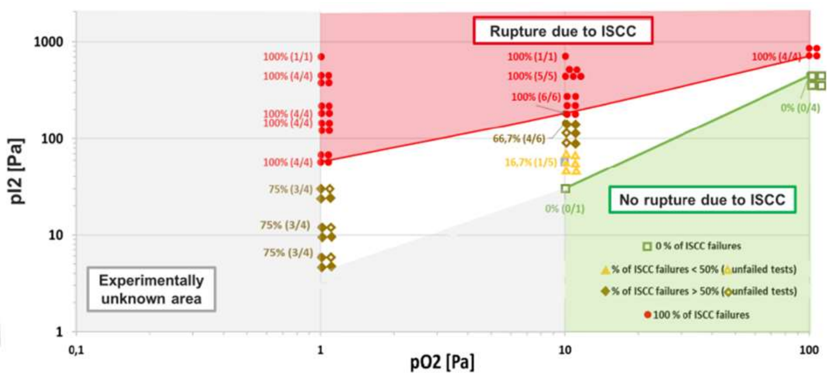
New laboratory tests

- To better simulate the PWR physico-chemical environment in laboratory



$P \approx 1\ bar$=10^5 Pa





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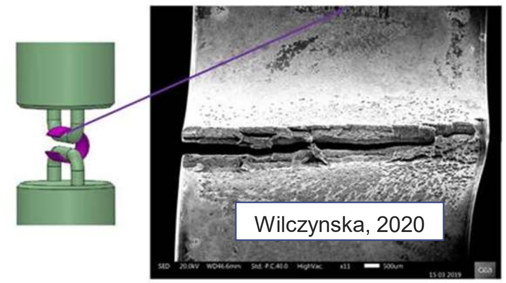

- Device in quartz to avoid chemical interactions with iodine
- Low pO_2 controlled (above 1-10 Pa)
  - Possibility to go lower under study
- Low pI_2 controlled (above 1-10 Pa)
  - Possible to go lower
- Temperature controlled

$$pI_2 \approx 10\ Pa \qquad pO_2 \approx 10\ Pa$$

$$\frac{nI_2}{n_{Argon}} \approx 0{,}01\ \% \qquad \frac{nO_2}{n_{Argon}} \approx 0{,}01\ \%$$

PWR simulations (ALCYONE)

- The polycristalline scale is better to study PCI/I-SCC failures in PWR ?
  - No experimental device to study that scale, under vapor iodine, today➔ Simulations instead ?