FRACTURE MODELS FOR RPV AND FOR THE IASCC OF INTERNALS MULTISCALE MODELLING

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(with extensive contributions from SOTERIA WP5.3)

This project received funding under the Euratom research and training programme 2014-2018 under grant agreement N° 661913

Overview

- This presentation provides an overview of the ongoing activities within the SOTERIA Project related to fracture predictions.

- The aim is to provide an overview of Local Approach (LA) process and the various fracture models being considered.

- The aspects being examined and extended are then introduced.

Models considered

- These fracture aspects are focused on the estimates of fracture in both ferritic steels and Irradiation Assisted Stress Corrosion Cracking (IASCC) in austenitic stainless steels, under irradiated conditions.

- Cleavage fracture is being considered by a range of modelling estimates including:
  - the Beremin Model [1],
  - the Bordet Model [2],
  - the JFJ Model [3],
  - the Micro-structurally Informed Brittle Fracture (MIBF) Model [4, 5].

- IASCC is being modelled through the INITEAC code.

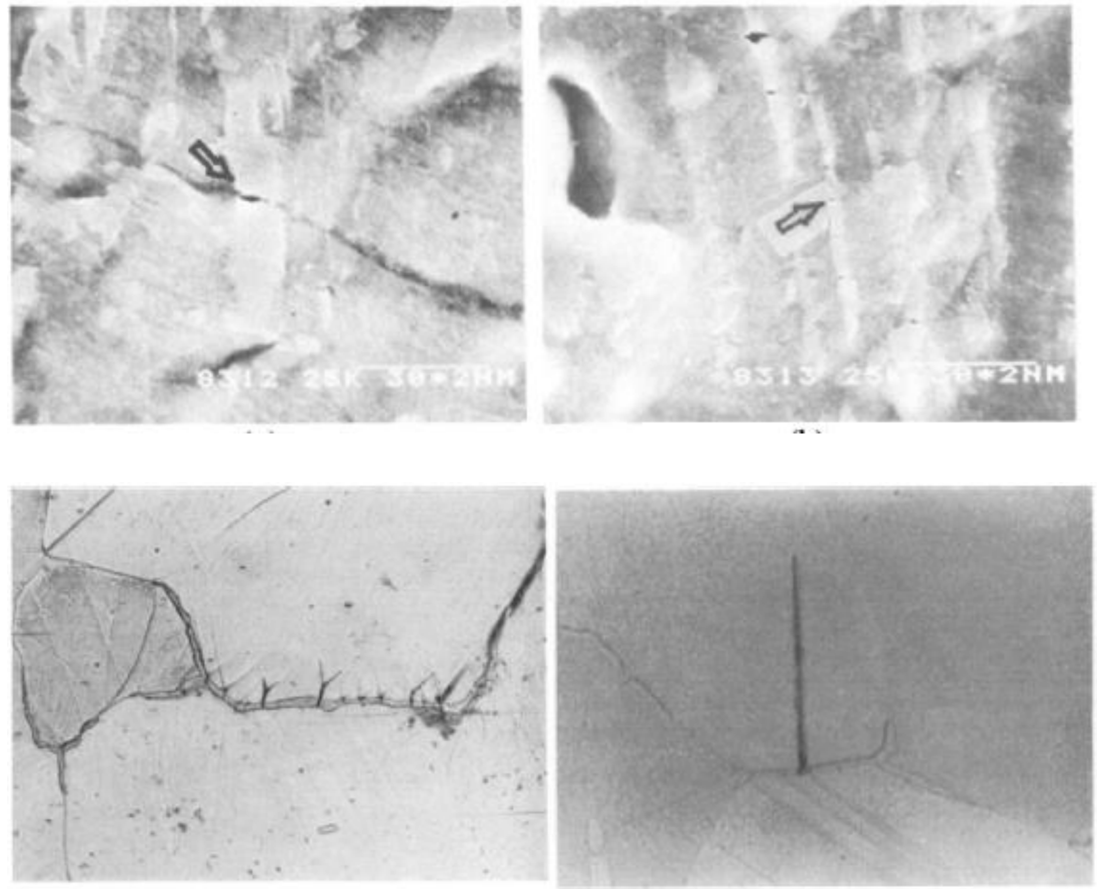
- Background to these (cleavage) models is included here before an overview of the ongoing activities in SOTERIA is provided.

Background…

1) Local Approach (LA) Theory

2) Cleavage Fracture LA Models in SOTERIA:
   1) Beremin Model
   2) Bordet Model
   3) JFJ Model
   4) MIBF Model

3) INITEAC Model for IASCC

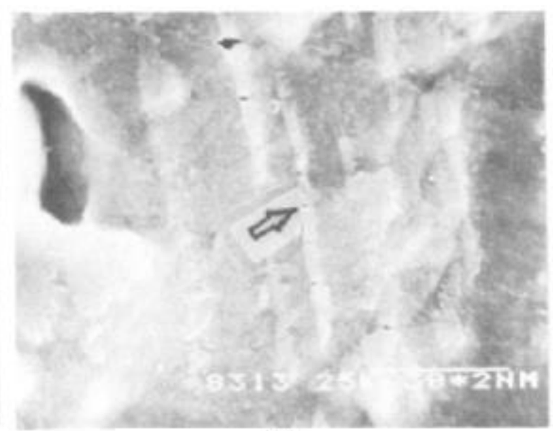


Cleavage fracture process (1)

- Cleavage fracture is normally considered to include a number of stages to the fracture event. These include:

  1) Yielding of the matrix surrounding initiating particles (normally assumed to be carbides, but can be any elastic-brittle particle in the matrix).
  2) Brittle particle failure, leading to a micro-crack being formed.
  3) Propagation of the micro-crack through the ferritic matrix.

Micro-crack from plastic slip [6]



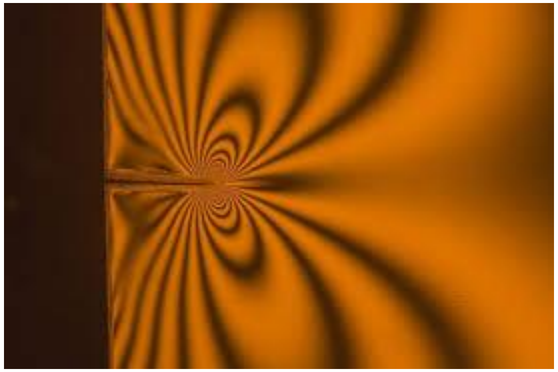
Micro-crack from shear stress [6]

Local approach models (1)

- The use of LA methods to predict fracture are generally recognised from the 1980's (Beremin model).

- LA models have two main assumptions:
  1) Global failure is a weakest link event,
  2) The probability of failure is a governed by the local mechanical (stress and strain) fields and the local microstructure.

     Shifts in fracture toughness, T_0 etc, are therefore considered an effect of the change of tensile properties.



Local approach models (2)

- There is a general formulation that most LA models share to describe the local probability of failure (for a point, *i*):

$$p_{f,i} = \int_{r_{c,i}}^{\infty} p_{c,i} f(r) dr$$

  - *r* is the particle radius, $r_{c,i}$ is the critical micro-crack for propagation, $p_{c,i}$ is the probability of micro-crack nucleation and *f(r)* is the probability density of the initiators size.

- Assuming all events for *i* are independent, using the weakest link argument, the global probability of failure is:

$$P_f(V) = 1 - \prod_{i=1}^{N} (1 - p_{f,i})$$

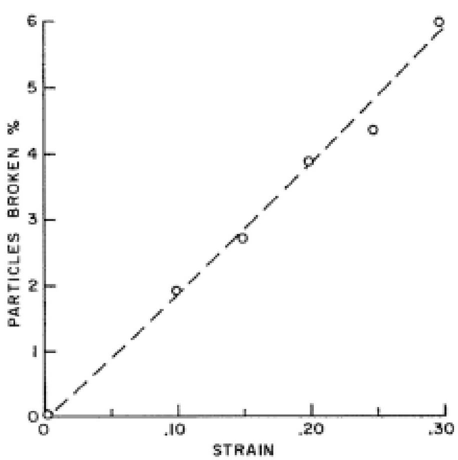
- *N* is the number of possible links in the volume *V* (generally used in finite element analyses with *i* taken from each integration point).

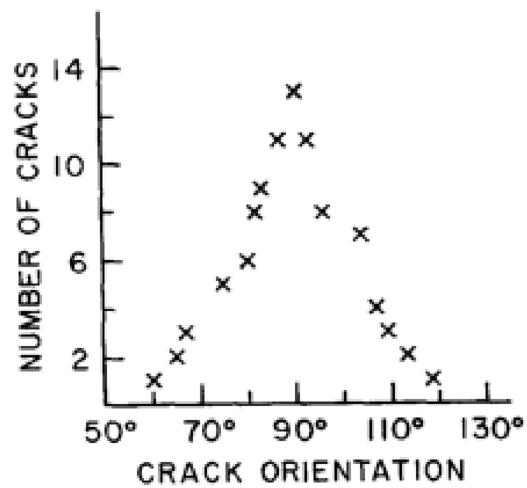
Physical basis of LA models (1)

- $p_{C,i}$, the term that describes the probability of micro-crack nucleation event captures both:
  - the loading applied to the initiating particles and
  - the subsequent formation of a micro-crack (i.e. stages 1 and 2 previously).

- Generally observed to follow:
  - The number of failed particles follows the plastic strain (with cracks forming normal to the loading direction).
  - Larger particles are seen to fail before smaller particles.

Relationship between plastic strain and % particles broken [7]





Frequency of micro-cracks relative to loading orientation [7]

Physical basis of LA models (1)

- r_c is the critical micro-crack for propagation through the matrix (stage 3 of the cracking process).

- Generally assumed that the cracks behave as Griffith cracks – follows that a crack extends when the elastic strain energy is greater than a critical value (normally assumed to be the surface energy (density) of the matrix, γ_s). Critical stress / critical radius can then be provided as:

$$\sigma_f = \sqrt{\frac{\pi E \gamma_s}{2(1-\nu^2)r}} \qquad\qquad r_c = \frac{\pi E \gamma_s}{2(1-\nu^2)\sigma_1^2}$$

where σ_f is the critical stress, E is the materials elastic modulus, ν is Poisson's ratio and σ_l is the opening/applied stress.

Beremin model (1)

- The Bermin model assumes the initiating particles follow:
  - $f(r) = \alpha / r^{\beta}$ (where α and β are scaling parameters)
  - There needs to be plasticity to form a micro-crack ($p_{c,i}$ = 1 or 0).
  - Cracks will extend via the Griffiths criteria.

- This can be used to show:

$$p_{f,i} = \int_{r_{c,i}}^{\infty} p_{c,i} f(r) dr = \left[\frac{\alpha}{(1-\beta) r^{\beta-1}} \right]_{r_c}^{\infty} = \frac{\alpha}{\beta - 1} \left(\frac{E\gamma_s}{2\pi(1-\nu^2)} \right)^{1-\beta} \sigma_1^{2\beta-2}$$

- If $m = 2\beta - 2$ and $\sigma_u = \left(\frac{1-\beta}{\alpha \rho_0 V_0} \right)^{\frac{1}{2\beta-2}} \sqrt{\frac{E\gamma_s}{2\pi(1-\nu^2)}}$

$$\boxed{P_f(V_p) = 1 - \exp\left[-\left(\frac{\sigma_w}{\sigma_u} \right)^m \right] \qquad \sigma_w = \sqrt[m]{\int_{V_p} \sigma_1^m \frac{V_i}{V_0}}}$$

Beremin model (2)

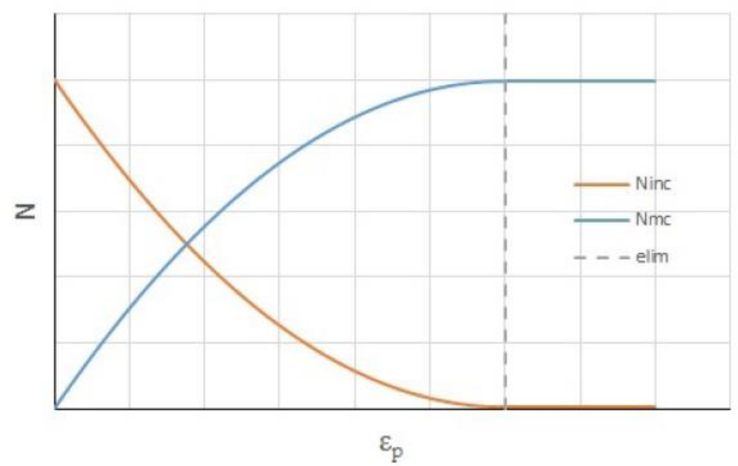
- Generally implemented using maximum principal stress for that volume to the current time.
- There are therefore two parameters to calibrate: *m* and $\sigma_u V_0^{\frac{1}{m}}$
- A slight alteration was also included to the model, called the Modified Beremin Model [1], to include plastic strain (constraint effects) to the calculation by changing the σ_w term:

$$\sigma_w = \sqrt[m]{\int_{V_p} \sigma_1^m \exp\left(-\frac{m\varepsilon_p}{k}\right) \frac{V_i}{V_0}}$$

Bordet model

- The Bordet model is a variation of the Beremin model such that:
  - The nucleation process is a continual process (not 1 or 0) with plastic strain.
  - Micro-cracks that do not initially propagate blunt (controlled by a threshold stress for propagation).

Relative number of intact particles / microcracks with plastic strain



$$\sigma_w^* = \sqrt[m]{\int_{V_p} \left[\int_0^{\varepsilon_{peq,i}} \frac{\sigma_Y(T,\dot{\varepsilon})}{\sigma_{y0}} \max\left(\sigma_1^m - \sigma_{th}; 0\right) \exp\left(\frac{\sigma_Y(T,\dot{\varepsilon})}{\sigma_{y0}} \frac{\varepsilon_p}{\varepsilon_{p,0}} \right) d\varepsilon_p \right] \frac{V_i}{V_0}}$$

JFJ model

- The JFJ model looks to improve on the Beremin approach by:
  - Allowing for a measured distribution of initiating particles (current work uses the Ortner distribution for Euro Material A but this can be modified).
  - A micro-crack nucleation term based on strain energy.

$$p_{c,i} = 1 - \exp\left[-\left(\frac{r}{r_0}\right)^3 \frac{\psi_1}{\psi_0}\right]$$

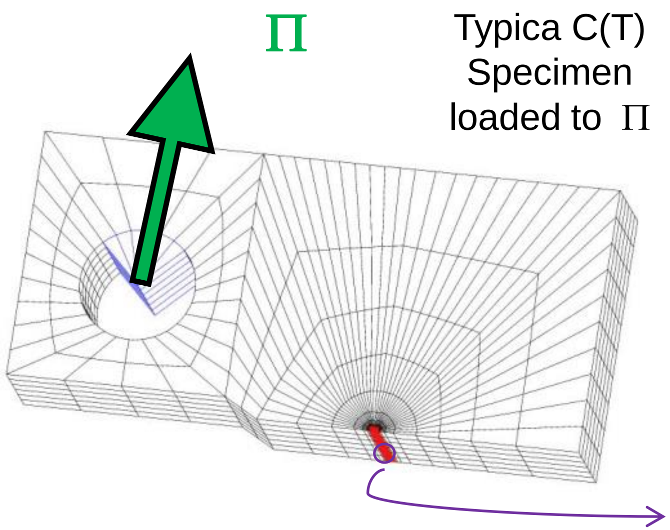
    - where the r_o is the normalising carbide size in the size distribution, ψ_1 is the strain energy normal to the principal stress and ψ_0 is a scaling term.

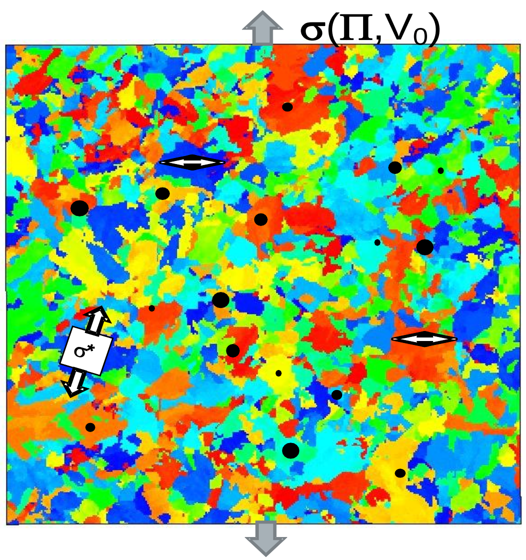
  - A modification to the Griffiths term to account for micro-crack blunting, depending on the level of plastic strain.

$$r_c^* = \frac{\pi E \gamma_s}{2(1-\nu^2)\sigma_1^2} \sqrt{1 + \left[\frac{\pi E \varepsilon_1^p}{2(1-\nu^2)\sigma_1}\right]^2}$$

MIBF model (1)

- The MIBF model looks to include the effect of a variable stress field resulting from the bainitic microstructure of the RPV steel ahead of the crack (other models assume a homogeneous material).





- Here variations in the stress field, in the volume V_0, from the microstructure are captured from crystal plasticity modelling.

MIBF model (2)

- A distribution of principal stresses are then used as an input to the LA modelling.
- The basic approach in the MIBF model is then similar to the Bermin model (nucleation based on plasticity and propagation based on the Griffiths term).
- The implementation allows a range of *f(r)* laws to be used.

Summary of LA models considered

- The LA method is well established and many models follow the same underlying assumptions.

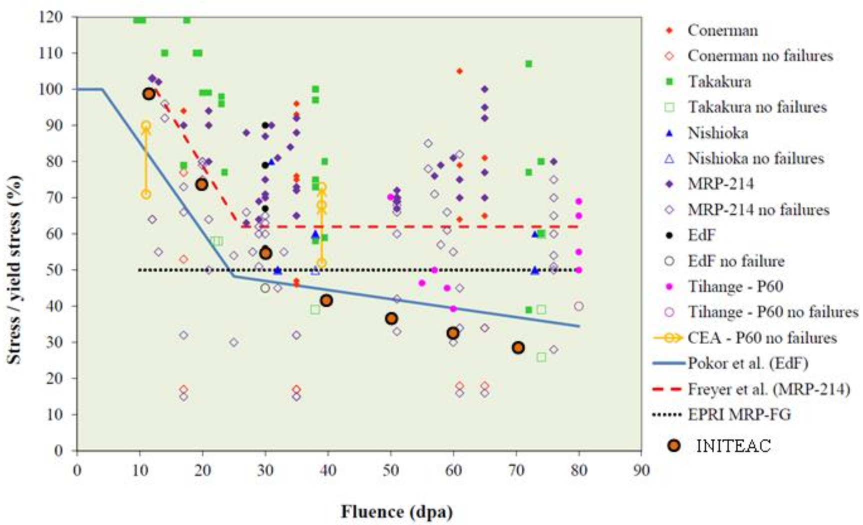
- The Beremin model was initially developed and is still used.

- Further models have looked to improve different aspects of this:
  - How to include plasticity in the nucleation process.
  - How to best include plasticity / blunting in the micro-crack propagation.
  - Ability to include a measured particle distribution.
  - How to better account for stress variability.

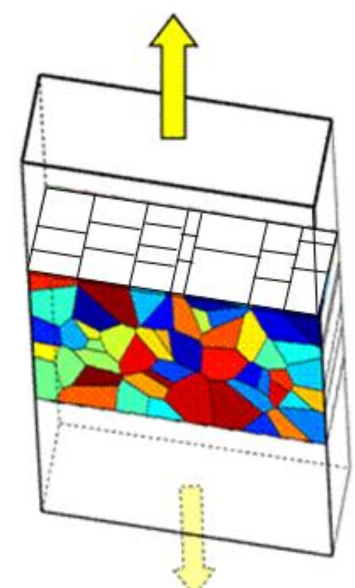
- *Worth noting that further models (WST, Bernaeur etc) are also available (with slightly different assumptions).*

INITEAC code for IASCC

- Also covered in the fracture codes is the INITEAC code for IASCC.
  - This has been covered extensively yesterday (*so only briefly noted here*).



Example results of INITEAC model



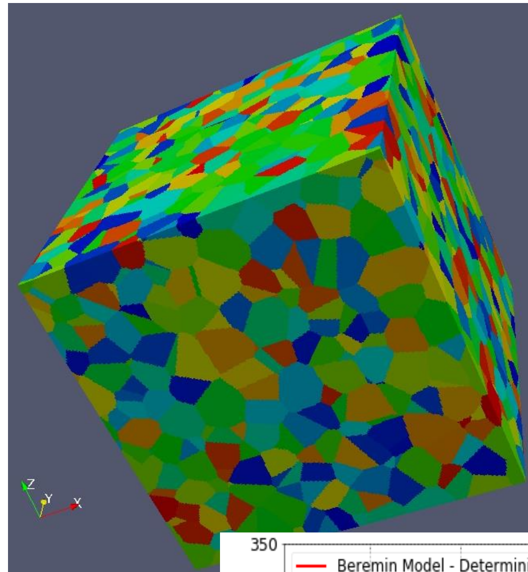
2.5 D schematic of INITEAC model

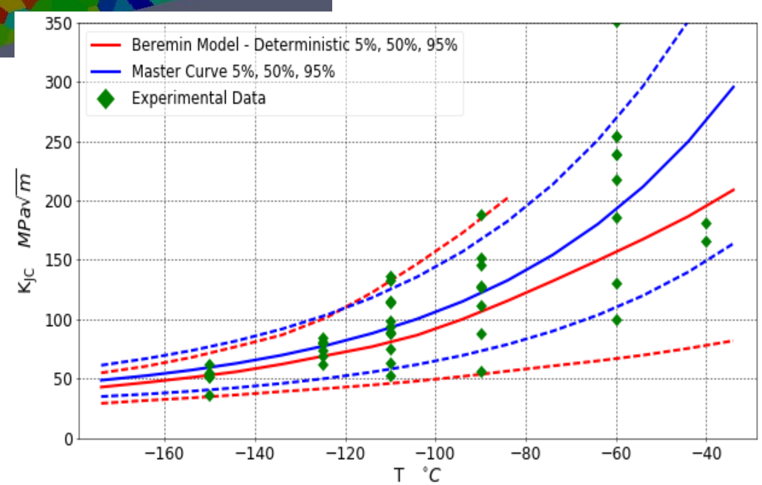
Activities in SOTERIA

1) LA Fracture Models:
   1) Plasticity in cleavage fracture,
   2) Outlying results,
   3) Experimental validation / comparison of models.

2) INITEAC Model for IASCC

3) Summary





Activities in SOTERIA – Fracture

Main objective is to develop micro-structurally informed models for the final stage of the multi-scale simulation process.

This means there is a need to use, better understand and develop the process to model fracture. As noted this relates to:

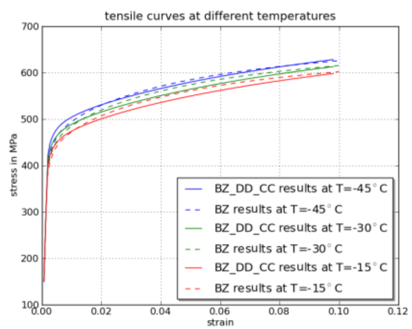
- Fracture Models for RPV – This typically uses a range of Local Approach models to predict the cleavage fracture toughness.

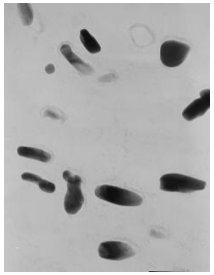
- Fracture Models for Internals – In SOTERIA this is linked to the INITEAC code for Irradiation Assisted Stress Corrosion Cracking (IASCC).

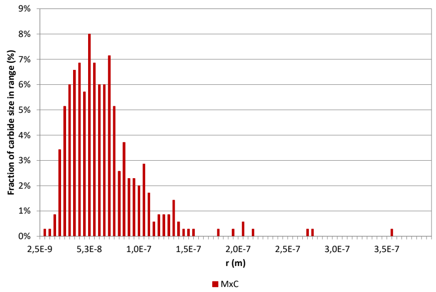
Cleavage fracture models

- To consider final stage of multi-scale modelling – fracture;
  - Review effect of plasticity on cleavage fracture models,
  - Improve understanding of variation / outlying results,
  - Further experimental validation / comparison of models.

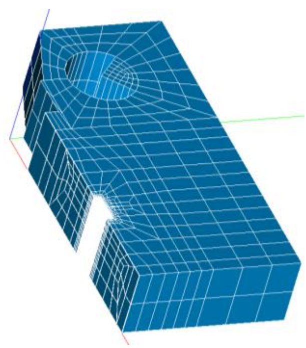
Tensile Curves

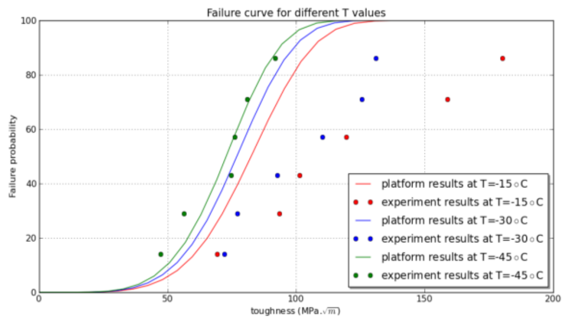






Carbide Distributions





EFFECT OF PLASTICITY

Review effect of plasticity on cleavage fracture models

Plasticity in LA models (1) (CEA)

- **Review of the treatment of plasticity in existing fracture models**

- This deliverable conducted a review of different brittle fracture models while focussing on different items:
  - How do they model the nucleation of the micro-defects that will lead to cleavage?
  - How do they model the propagation of these micro-defects towards a macroscopic crack?
  - How are the initiation sites for these micro-defects modelled?
  - What role does plastic strain play in the various assumptions of the model?

Plasticity in LA models (2) (CEA)

Carbide size distribution	
Non explicit power law β/r^{α}	Beremin Mod Beremin Bernauer CN Bernauer DBT Bordet
Explicit asymptotic power law	MIBF
Lee	MIBF
Jayatilaka	WST MIBF
Ortner	JFJ MIBF (Mathieu)
Normalized power law	MIBF
Explicit carbide population	Mathieu

Nucleation	
Plasticity induced	All
Carbide strength distribution	Promethey
Continuous nucleation	Bordet
Continuous nucleation	Bernauer CN
Energy density	WST
Energy density	JFJ
Debonding of carbides	Bernauer DBT

Propagation	
Griffith	All except Promethey
Deterministic propagation	Promethey
Truncating	Bordet
Blunting	JFJ

Ductile propagation	
GTN	Bernauer DBT

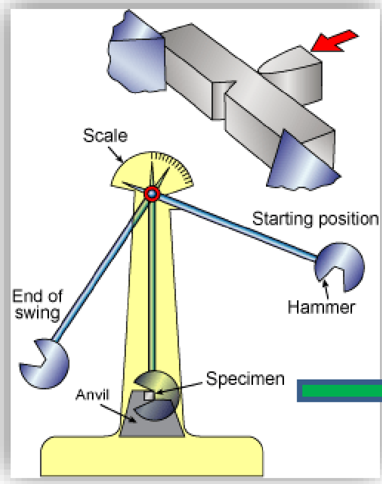
Crystal plasticity	
Bainitic microstructure	MIBF
Explicit bainitic microstructure	Mathieu

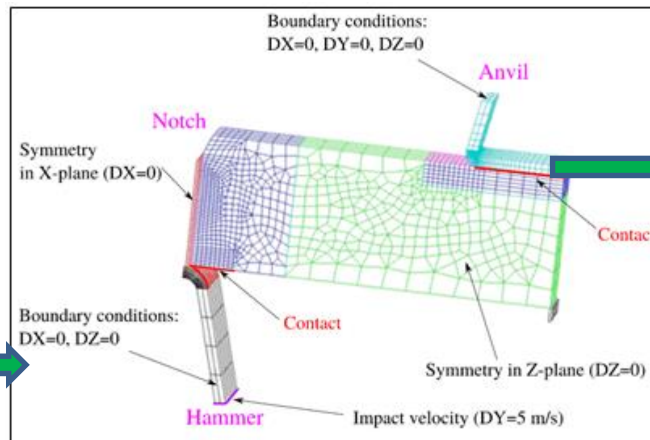
Reported comparison table for different LA models

It has been shown than all models are compatible with the MIBF model (which also allows crystal plasticity to be considered).

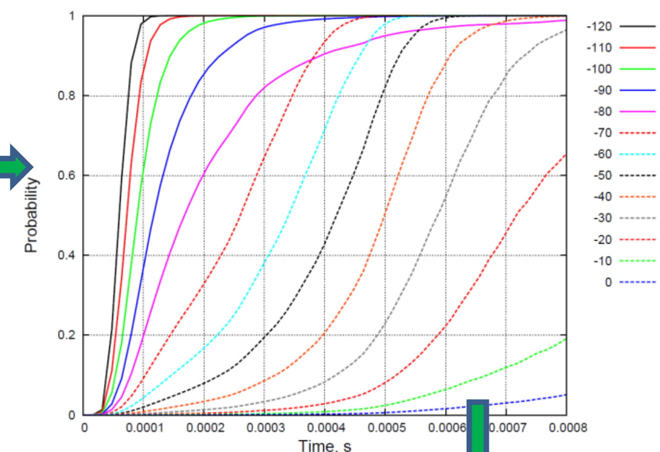
Including ductile damage in prediction (EDF)

- Modelled Charpy test with elastic-viscoplastic behaviour for brittle fracture and post-processing for cleavage with Beremin model
- Similar to exercise considered.



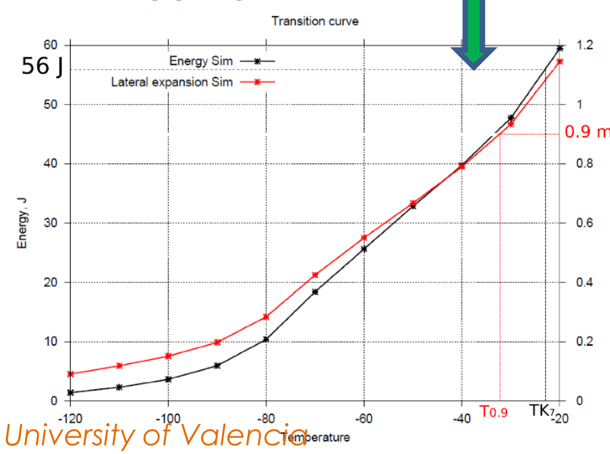


Probability of failure P_f vs. t for different T



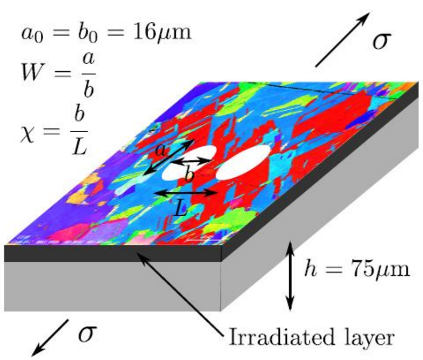
- Range of assumptions for material properties
- Promising results, and good prediction of ΔT
- Looking to introduce the model of the ductile tearing with the use of Gurson model to be able to construct the full DBTT curve (in process)

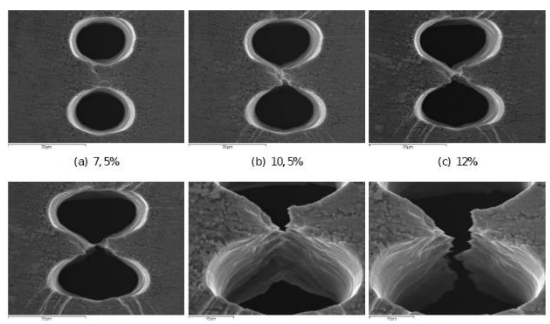
DBTT curve

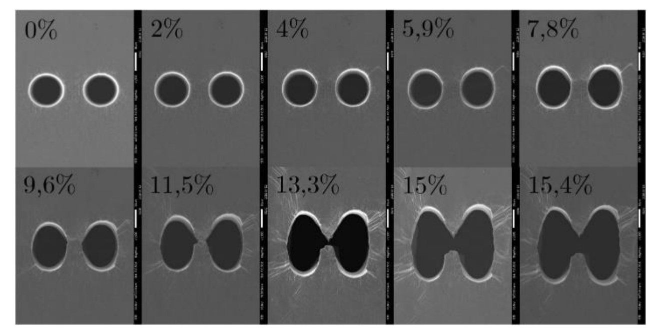


Void growth and coalescence (CEA)

- To provide experimental data on void growth and coalescence in irradiated materials. These data would also be useful to calibrate constitutive equations for irradiated austenitic stainless steels.
- Ion-irradiated thin tensile samples - Focused Ion Beam (FIB) drilling of cylindrical holes. SEM observations of the evolution of void dimensions under tensile loading.







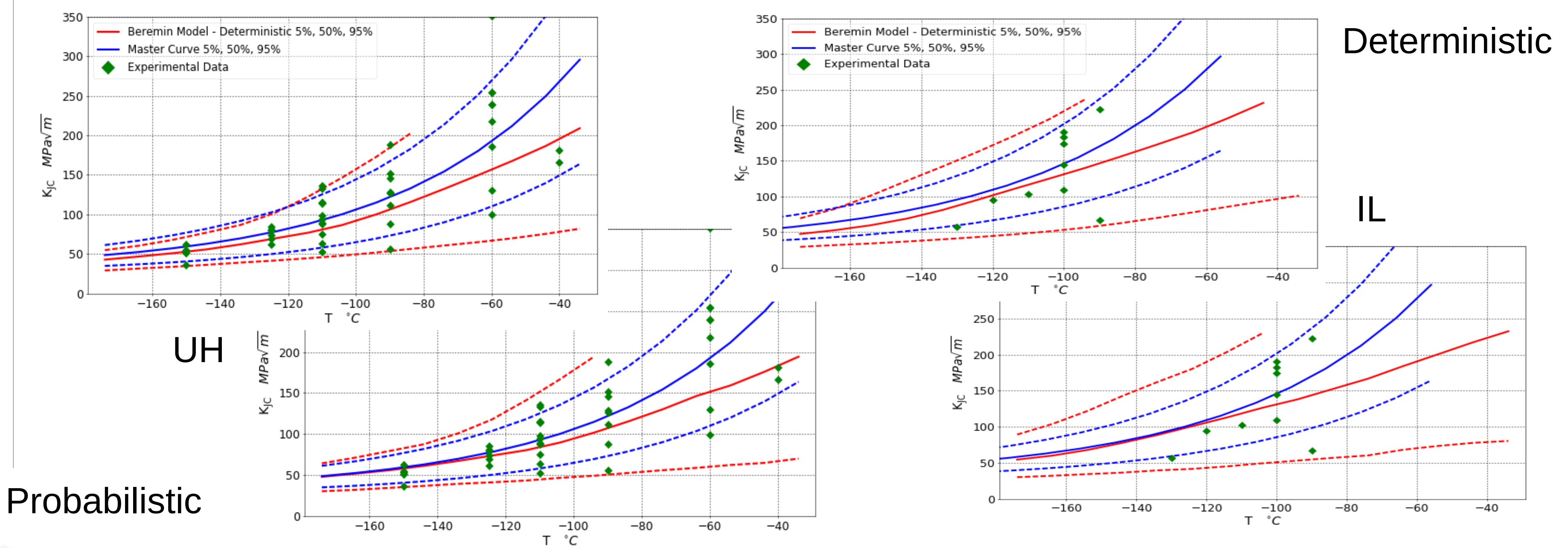
- Strong dependence of void deformation to crystallographic orientations.
- Strong influence of activated slip systems on void coalescence.
- Now in position to progress to stainless steel experiments.

OUTLYING RESULTS

Improve understanding of variation / outlying results

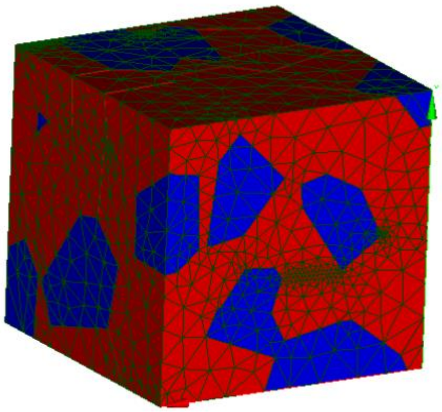
Monte Carlo implementation of LA models (Wood)

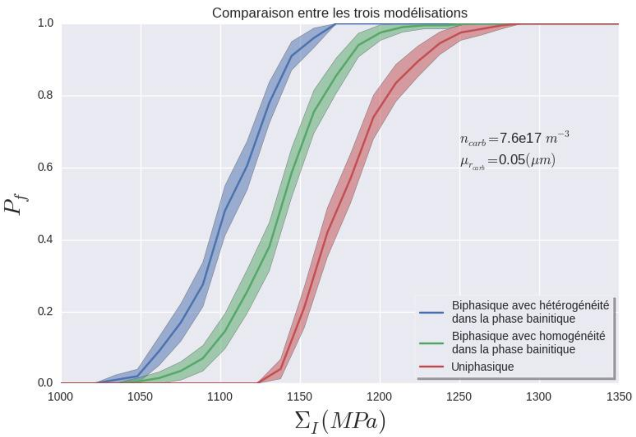
- To consider variation in the material initiating particles and their impact on fracture toughness. Probabilistic assessments considering localised variation in the calibration parameters of the brittle fracture model(s).
- Successful use of Beremin and JFJ LA models in a deterministic and probabilistic methods.
- For reference case materials selected within the programme (parent and weld materials).



Location of carbides (EDF)

- Determine the influence of the spatial distribution of carbides in a RPV steel in a LA to fracture model, and to assess for the influence of stress heterogeneities at grain boundaries to the onset of brittle fracture.
- The aggregate has 98 grains with a non-regular mesh. Two versions of this aggregate are available:
  - A monophasic one (with only bainite);
  - A biphasic one (with bainite and ferrite):
    - Carbides homogenously in bainite phase.
    - Carbides sample in the bainite phase only and preferentially near the interface.





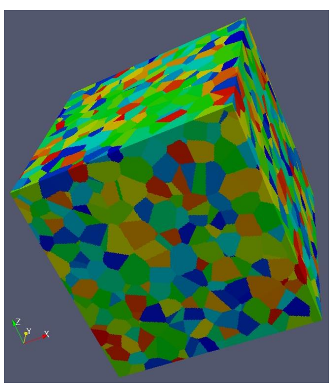
- Indicates that the spatial location of the carbide may need to be considered (need to consider further)

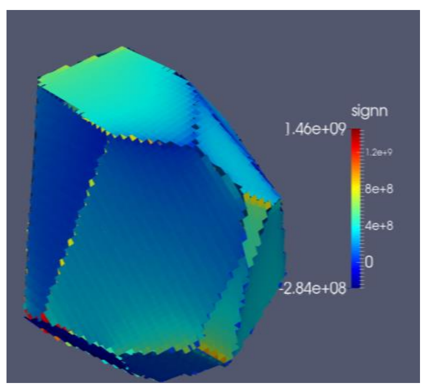
Influence of inter-granular fracture (CEA)

- A version of the MIBF model (IG-MIBF) has been developed to specifically consider the effect of grain boundary fracture.
- This may help explain extreme lower bound fracture data.
- There is a need to consider:
  - The grain-boundary stress / strain field
  - Estimate of the distribution of initiating particles on the GB
  - An estimate of the critical stress to cause a failure event.

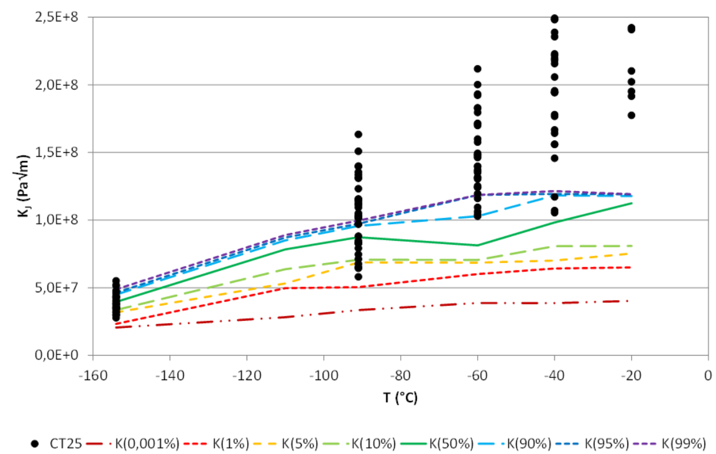
$$P_i(V_p, \Pi) = 1 - \exp \int_{V_p} n_p S_v \cdot \ln\left(1 - P_\gamma\left(\sigma_n^* > \sigma_i\right)\right) dV$$

Characteristic failure size parameter	Grain boundary area per volume unit	Grain boundary stress distribution	Intergranular critical stress





Ductile to brittle transition curve for Euro Material A, for (cleavage) MIBF model combined to (inter-granular) IG-MIBF model with critical stress = 2500 MPa



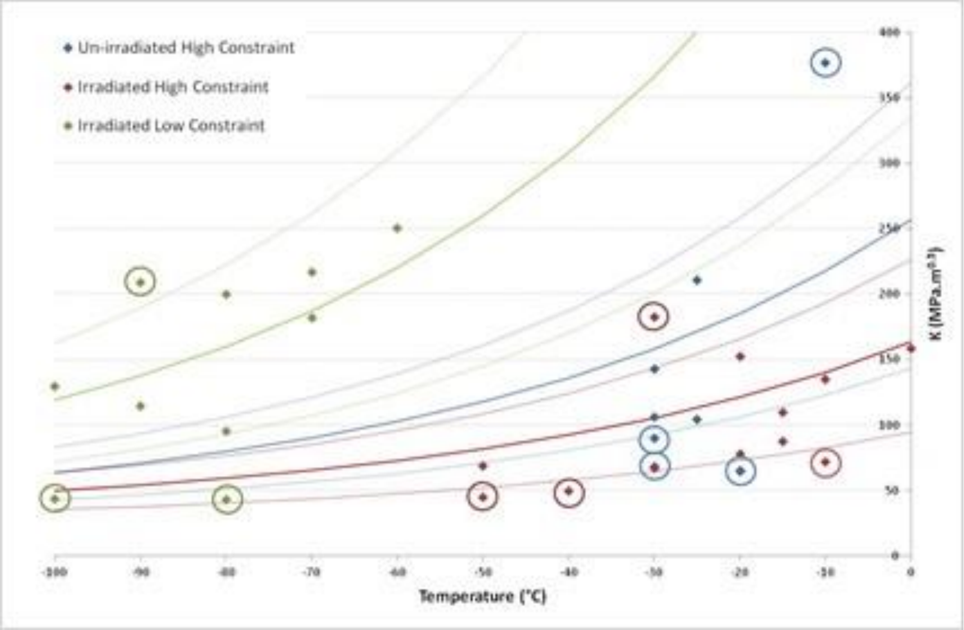
VALIDATION

Further experimental validation / comparison of models

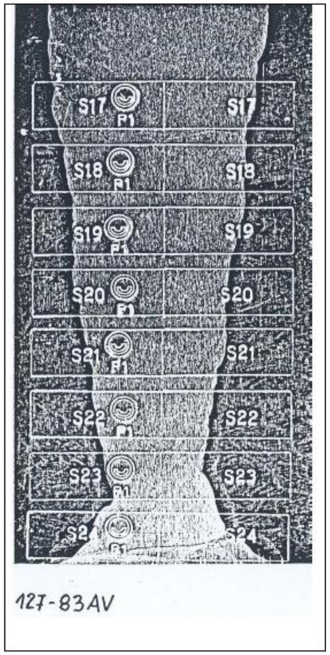
Reference materials for comparison (Framatome)

- Two materials have been considered for validation purposes (parent and weld – referenced as ANP1 [*20MnMoNi5-5*] and ANP2 [*S3NiMo1/OP41 TT*]).
- Chosen as parent conforms to Master Curve, Weld less so. Data readily available from Framatome.
- Comparisons ongoing (with different LA models identified above)

Weld Material Comparison to MC



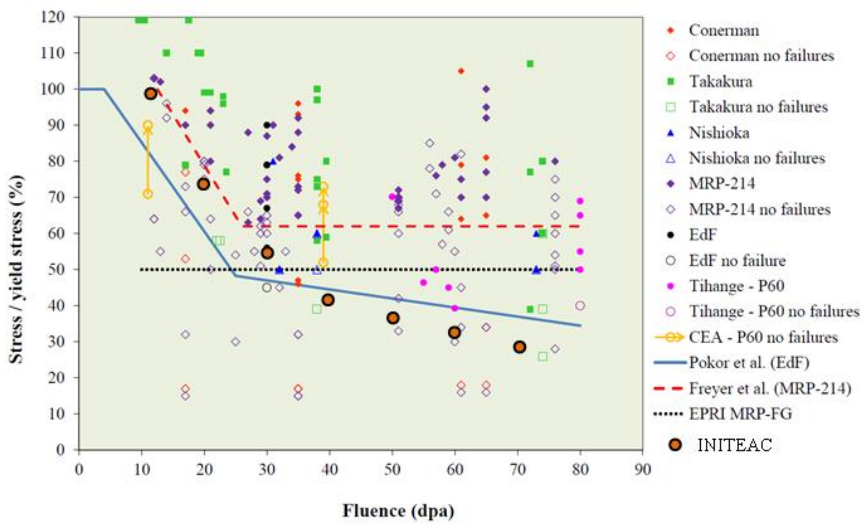
Extracted locations of weld data

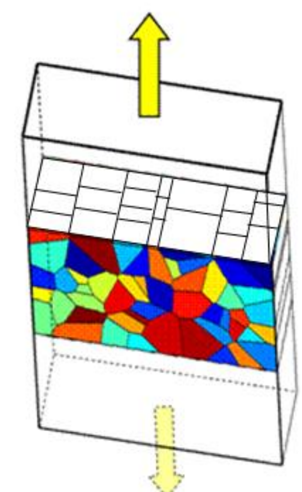


INITEAC

IASCC modelling

- To further develop physically based models to encapsulate physical understanding of current IASCC processes;
  - Update models (e.g. INITEAC) to include understanding from elsewhere within SOTERIA,
  - Further develop local/grain sized modelling approaches to allow improved modelling of IASCC processes.
  - *Work to consider this is dependent on understanding from elsewhere and is only starting to be considered (not reported here).*





Summary

- This presentation provides an overview of the final stage of the multi-scale process, i.e. available fracture models.
- The presentation also provides an overview of the ongoing activities within the SOTERIA Project related to fracture predictions.
- The Cleavage Fracture LA models have considered:
  - Review effect of plasticity on cleavage fracture models,
  - Improve understanding of variation / outlying results,
  - Further experimental validation / comparison of models.
- The development for IASCC (INITEAC) is to focus on:
  - Update INITEAC to include understanding from elsewhere within SOTERIA,
  - Further develop local/grain sized modelling approaches to allow improved modelling of IASCC processes.

References

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