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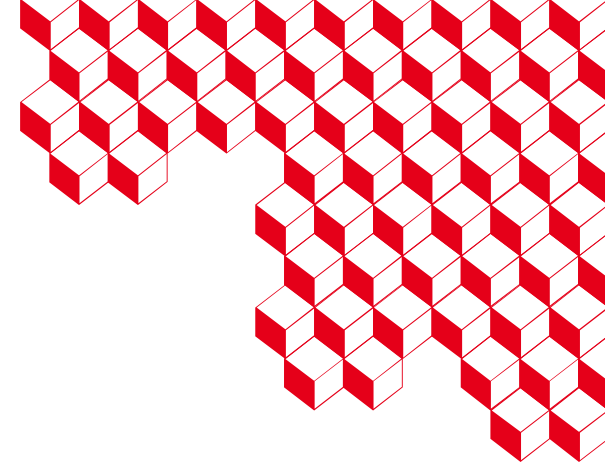
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A probabilistic modeling of the brittle fracture of low alloy steels constituting the heavy components of nuclear reactors

Ludovic VINCENT, Bernard MARINI, Pierre FORGET

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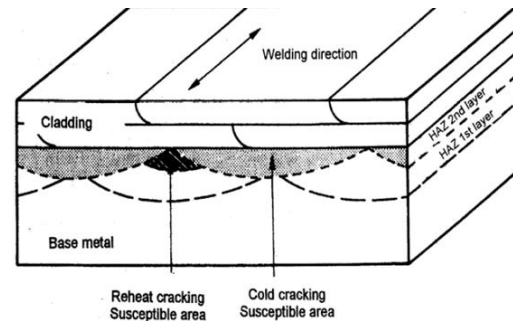
ludovic.vincent@cea.fr

Industrial context: Reactor Pressure Vessel

- Total : 58 Reactor Pressure Vessels (RPVs)
- Manufacturer: Framatome (Areva), Westinghouse license except N4 and EPR
- 1 PWR unit (300 MWe) stopped in 1991 : Chooz A
- 1 PWR unit under construction : EPR , Flamanville 3
- Typical operating conditions for the vessel: 290°C - 150 bars – $6 \cdot 10^{19}$ n/cm² endlife
- Vessel material :
 - Forged low alloyed steel : 16MND5 (yield stress, fracture properties, weldability, cost)

C _{max}	Mn	P _{max}	S _{max}	Si	Ni	Cr _{max}	Mo	Va _{max}	Cu _{max}	Al _{max}	Co _{max}
0.22	1.15-1.60	0.008	0.005	0.10-0.30	0.50-0.80	0.25	0.43-0.57	0.01	0.08	0.04	0.03

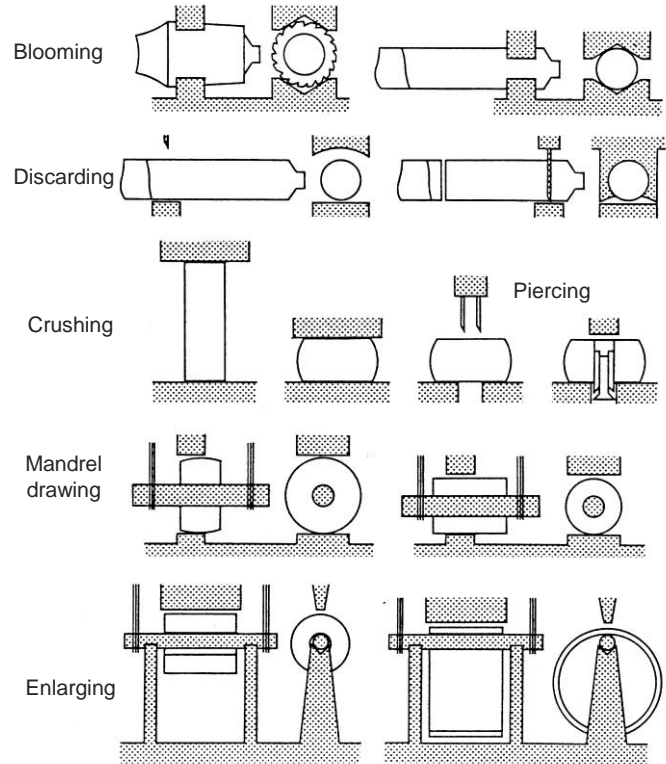
- Inner cladding in austenitic steel



Industrial context: Forging and Heat treatments

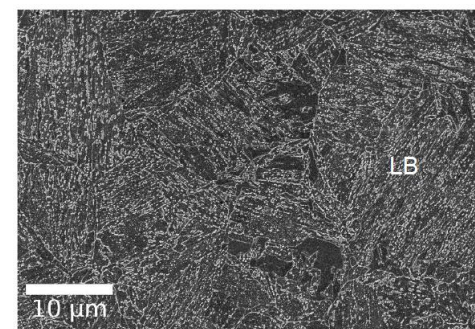
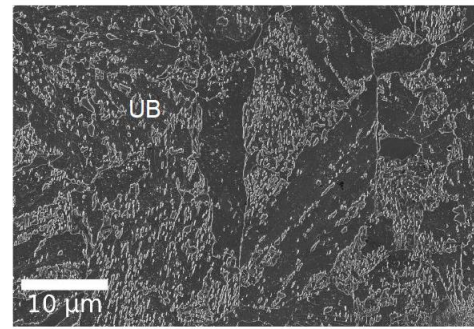
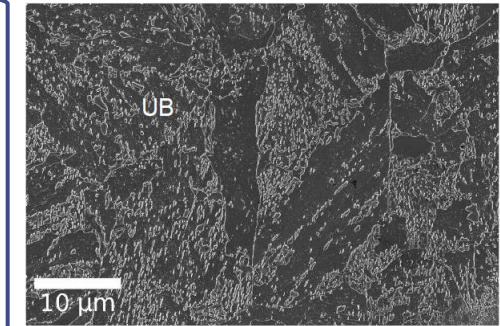
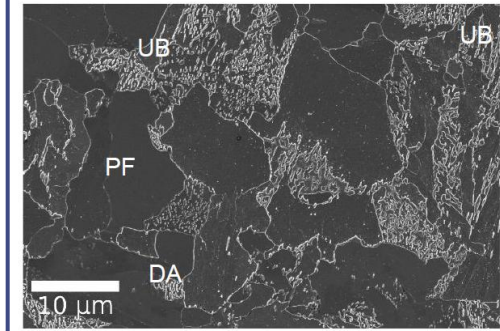
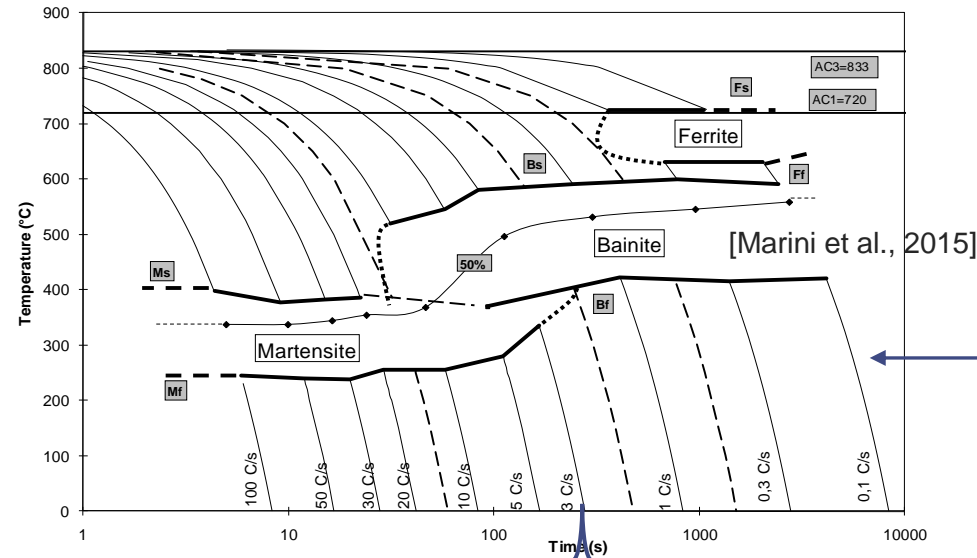


A) Hot Forging



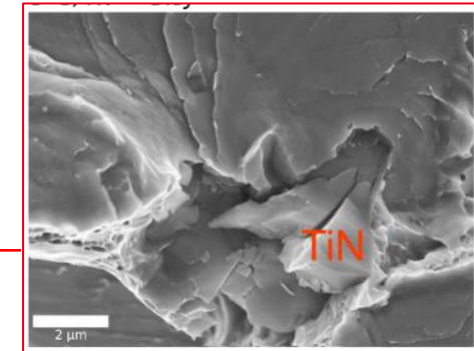
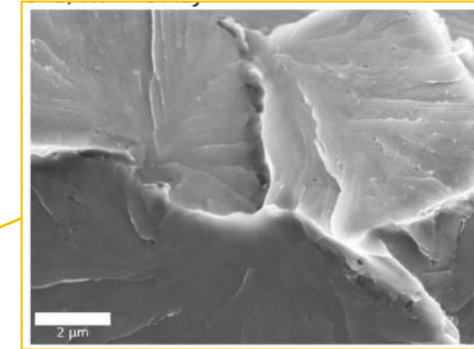
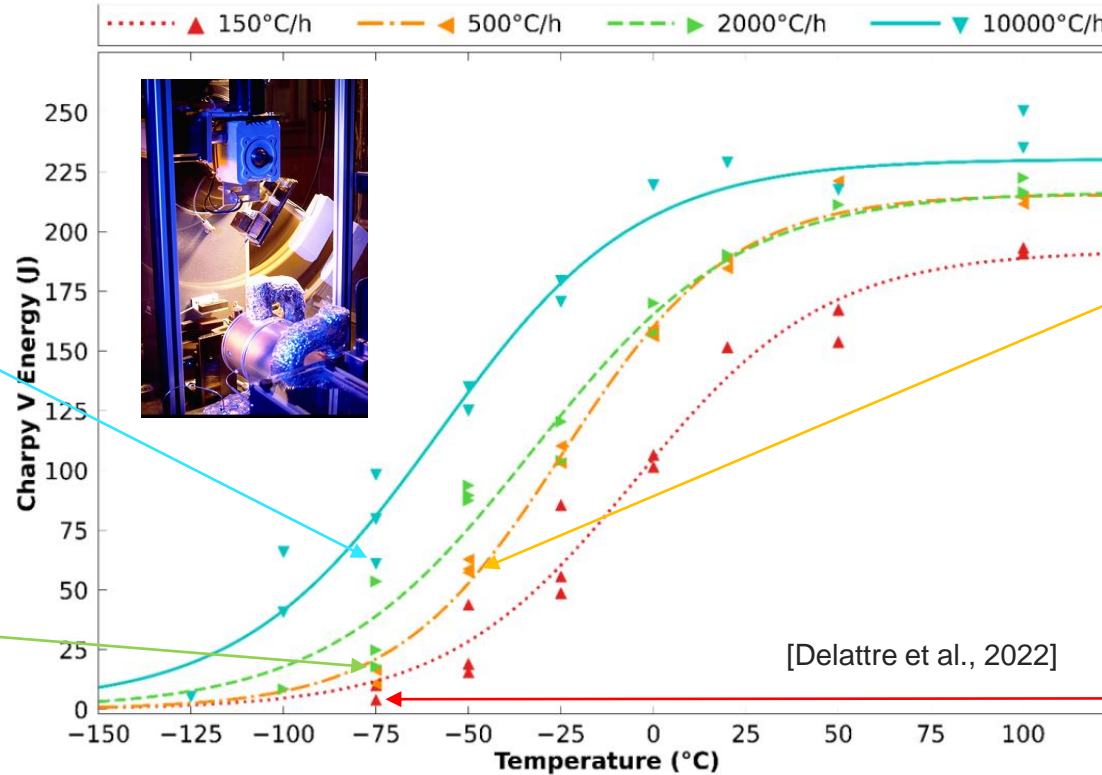
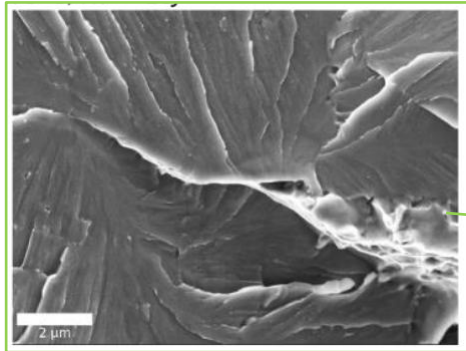
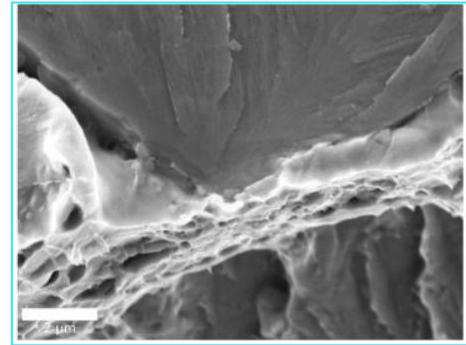
B) Heat Treatments :

- 1) First austenization at high temperature to dissolve carbides precipitated during the relatively slow cooling rate after forging
- 2) Second austenization at lower temperature followed by water quenching to obtain the desired microstructure and grain size
- 3) Stress relieving heat treatment at lower temperature to obtain good ductility and toughness properties



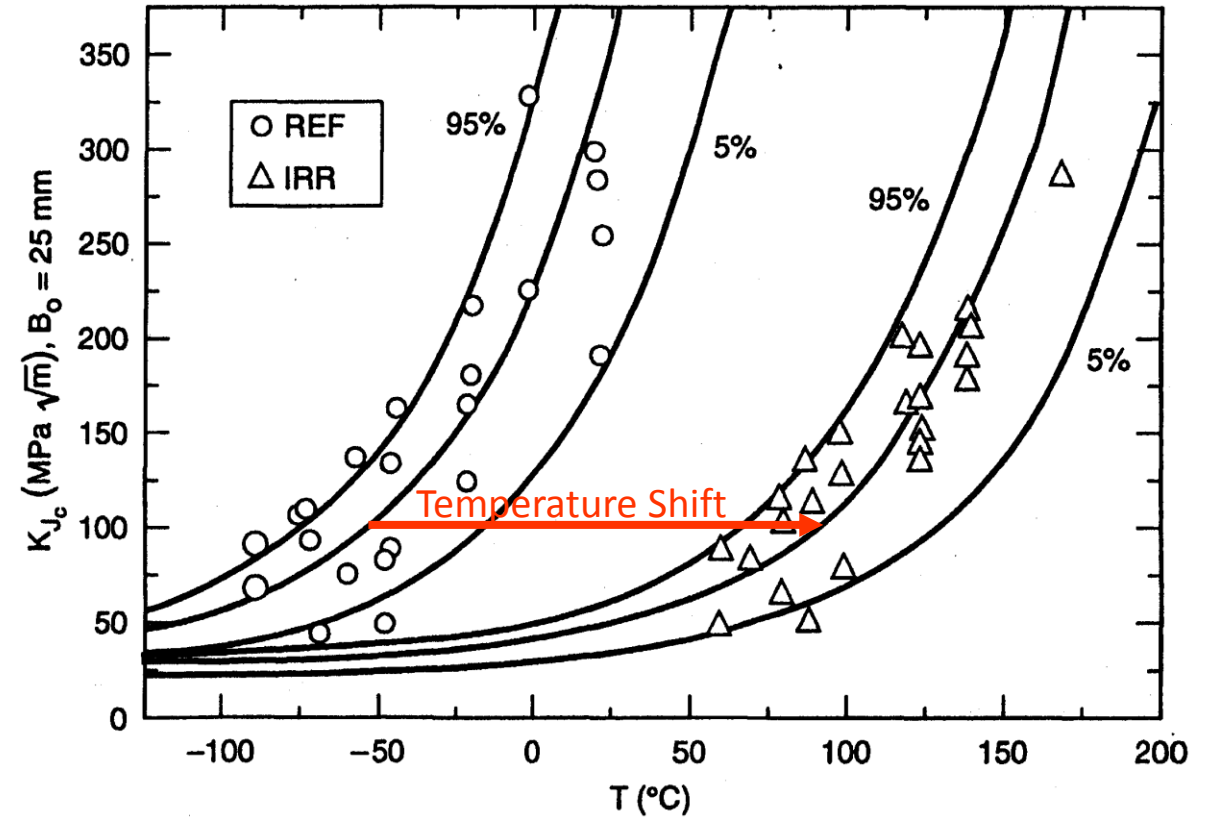
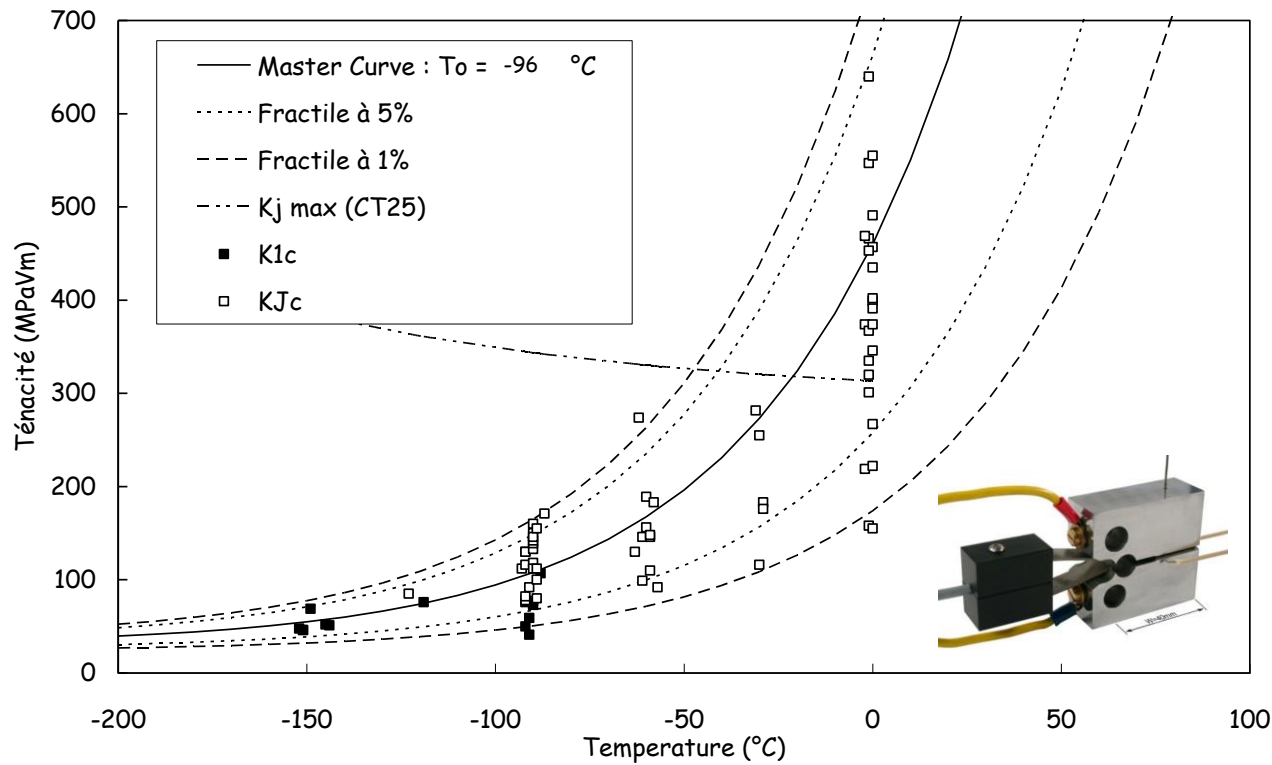
[Delattre et al., 2022]

Industrial context: Effect of quenching rate on Impact properties



- Lower Tempered Bainite: good compromise between strength and ductility
- Cleavage fracture at the onset Ductile to Brittle Fracture transition
- Generally initiates close to Grain Boundaries, usually from carbides or precipitates

Industrial context: Material toughness properties



- **Large variations of fracture toughness values in the Ductile-Brittle transition**
- **Irradiation embrittlement -> similar to a temperature shift**

Industrial context: accidental scenario

Thermal shock on low alloy RPV steel 16MND5

Reference flaw

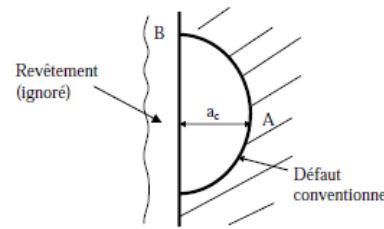
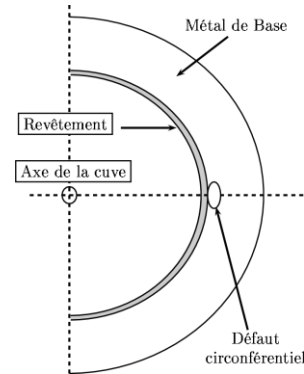
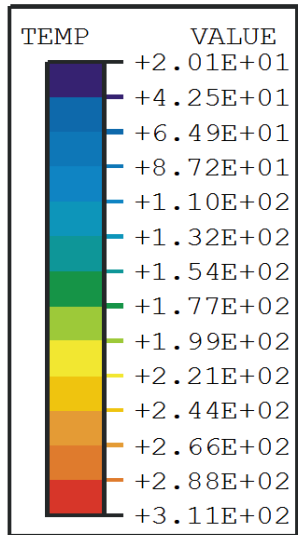


FIGURE Z G 3210. DÉFAUT CONVENTIONNEL

For French RPV :

➤ Subclad flaws :

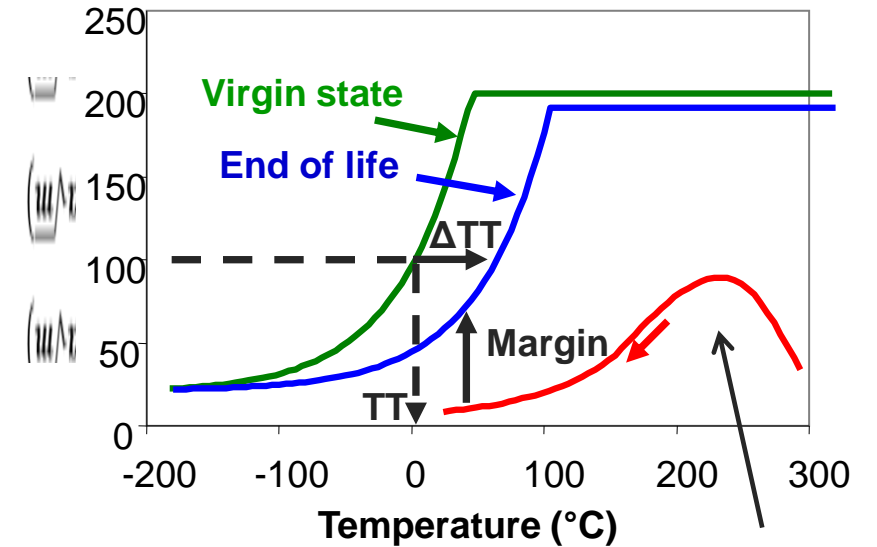
✓ 900 MWe

6 mm * 60 mm (for subclad flaws)

✓ 1300 MWe

6 mm * 30 mm (for subclad flaws)

➤ Flaws located in 1st layer of cladding 4 mm depth



K_I variation due to emergency cooling

End of life of nuclear reactors based on DBTT shift predictions of RPV steels

Outline

- 1) Industrial Context
- 2) Microstructure Informed Brittle Fracture modelling
- 3) “Recent” developments
- 4) Conclusions / Prospects

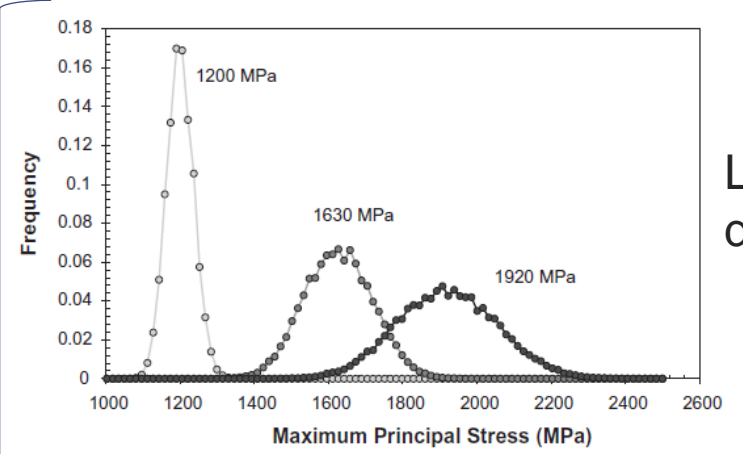
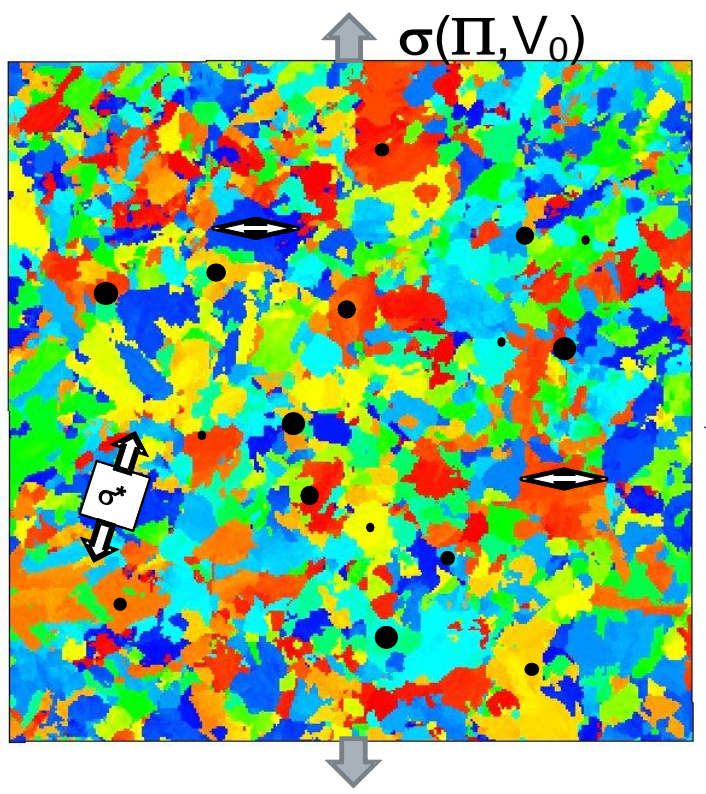
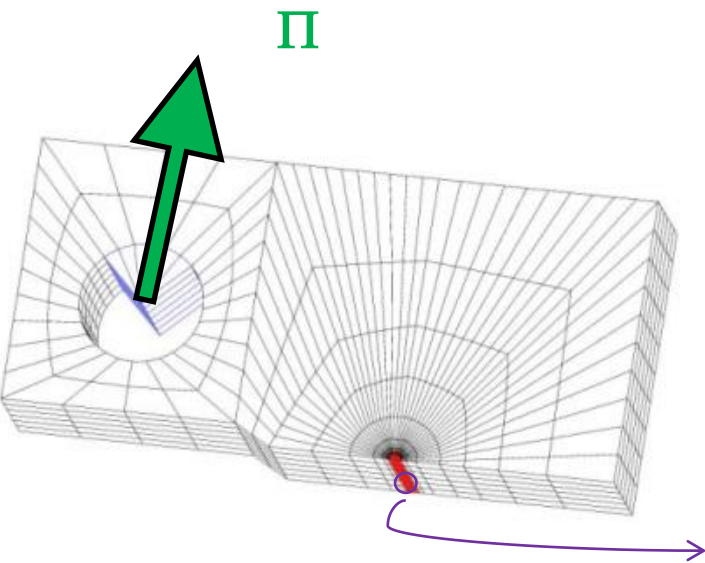




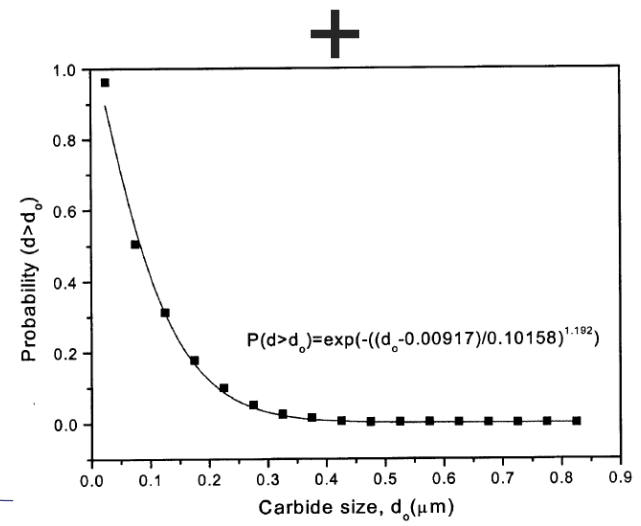
2 **M**icrostructure **I**nformed **B**rittle **F**racture model (MIBF)

2.1 **G**eneral principles and initial formulation

2.2 **F**irst results



Local stress distribution



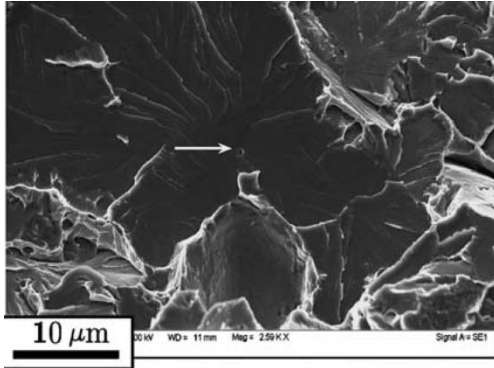
Defect size distribution

2.1 General principles and initial formulation

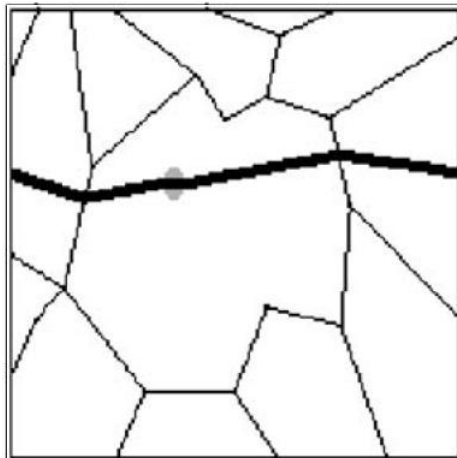


Probabilistic model of brittle fracture

Rupture : initiation + propagation



[Tanguy et al., 2005]



[Pineau, 2006]

Initiation hypothesis: initiation on carbides, when plastic strain starts.

➔ ε_{min}^p

Propagation hypothesis:

- No crack arrests on grain boundaries.
- Propagation following Griffith criterion at the grain scale:

Let be a semi-elliptical crack of size r , submitted to a local maximum principal stress σ_I (averaged on the grain)

➔ Propagation if : $\sigma_I = \sigma_c(r) = \sqrt{\frac{\pi E \gamma_s}{2(1-\nu^2)r}}$

γ_s : Surface creation energy
 E : Young modulus
 ν : Poisson coefficient

Probabilistic model of brittle fracture

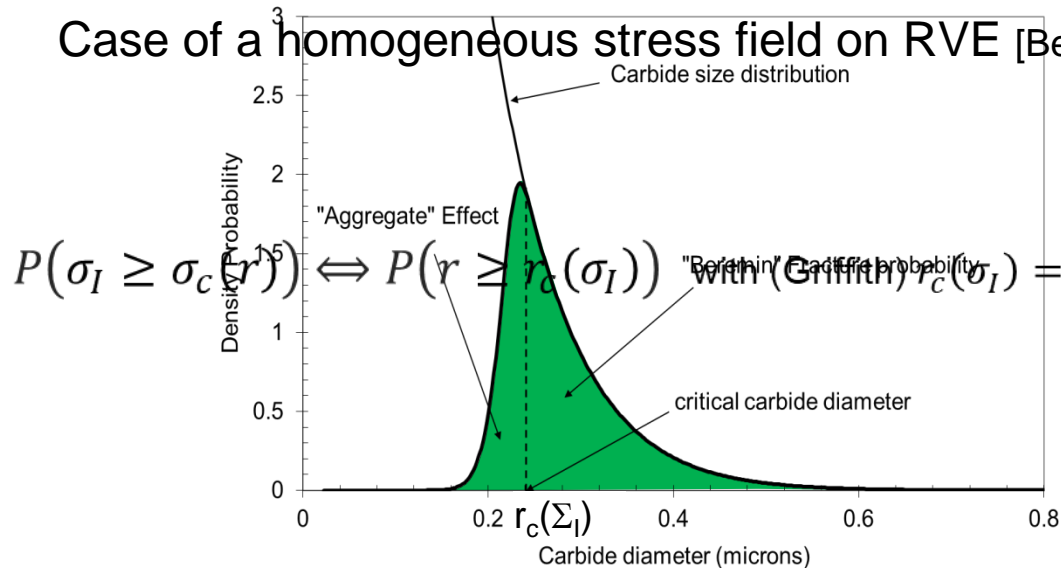
Crack initiation hypothesis : initiation on carbides, when plastic strain starts.

Size distribution of carbides inside RPV steel : $f(r)$

➔ Fracture probability of one carbide:

$$p_f(carb, \sigma_1) = \int_0^{+\infty} f(r) P(\sigma_I \geq \sigma_c(r)) dr \quad \text{with} \quad \sigma_c(r) = \sqrt{\frac{\pi E \gamma_s}{2(1-\nu^2)r}}$$

Case of a homogeneous stress field on RVE [Beremin, 1983]



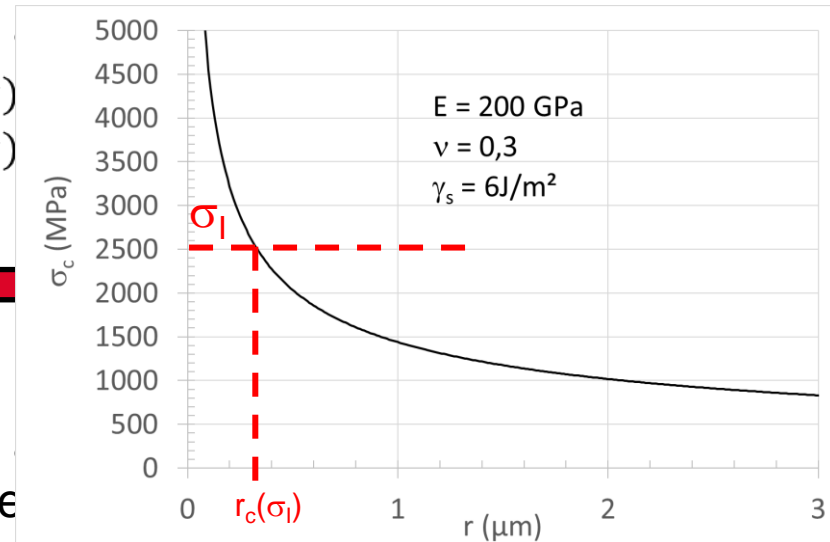
Case of

$$P(\sigma_I \geq \sigma_c(r))$$

$$P(\sigma_I \geq \sigma_c(r))$$

$$P(\sigma_I \geq \sigma_c(r)) = \frac{\pi E \gamma_s}{2(1-\nu^2)\sigma_I^2}$$

Case of an aggregate



[Beremin, 1983]

$$r_c(\sigma_I) = \frac{\pi E \gamma_s}{2(1-\nu^2)\sigma_I^2}$$

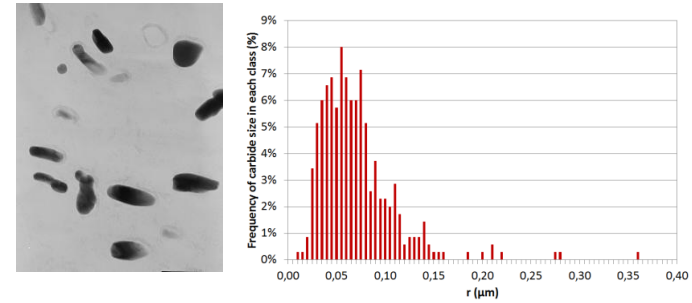
Weakest link hypothesis



From the Fracture probability of one carbide to the Fracture probability of a grain loaded under local stress $\underline{\sigma}$

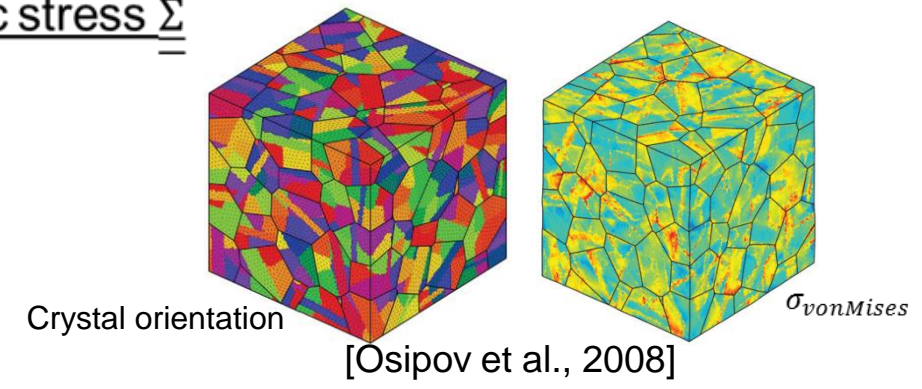
$$1 - p_f(g, \sigma_1) = \prod_{N_c V_g} \left(1 - p_f(carb, \sigma_1) \right)^{N_c V_g}$$

N_c : number density (mm⁻³)
 V_g : Grain volume



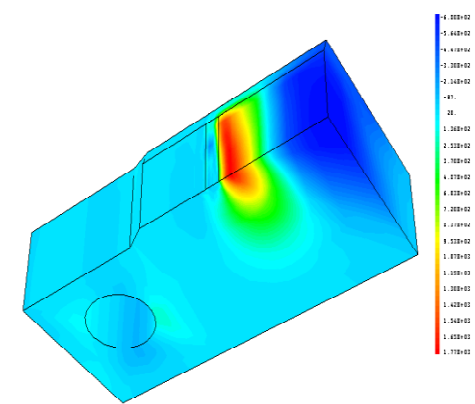
Fracture probability of an aggregate of volume V_0 loaded at a macroscopic stress $\underline{\Sigma}$

$$1 - P_f(V_0, \Sigma_1) = \prod_{g \in V_0} \left(1 - p_f(g, \sigma_1) \right)$$



Fracture probability of a structure loaded at a force F :

$$1 - P_f(V, F) = \prod_{V_0 \in V_p} \left(1 - P_f(V_0, \Sigma_1) \right)$$



Probabilistic model of brittle fracture

$$P_g(V_p, \Pi) = 1 - \exp \int_{V_p} n_c \ln \left(1 - \int_{r=0}^{+\infty} P_\chi(\sigma^* > \sigma_c(r)) \frac{dF}{dr} dr \right) dV$$

Densité volumique de carbures

Distribution de contraintes dans les grains

Critère de Griffith

Distribution de taille de carbures

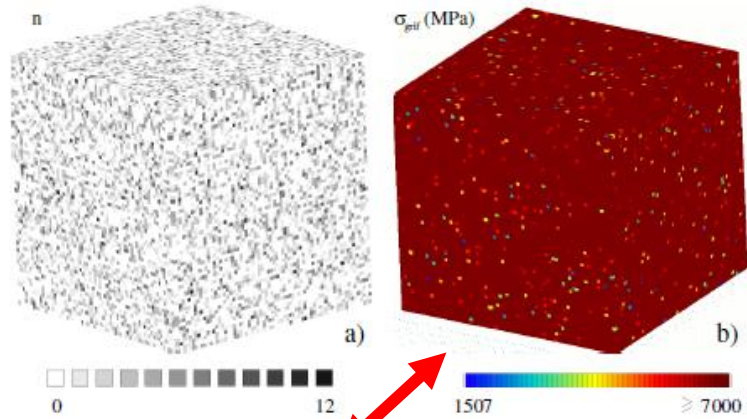
MIBF : Versatile probabilistic model

Stochastic model of brittle fracture [Mathieu, 2006]

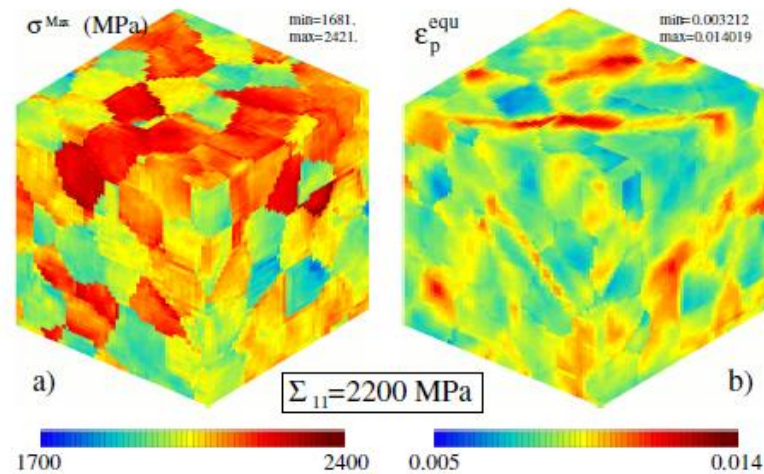
Alternative, yet similar approach: submodelling



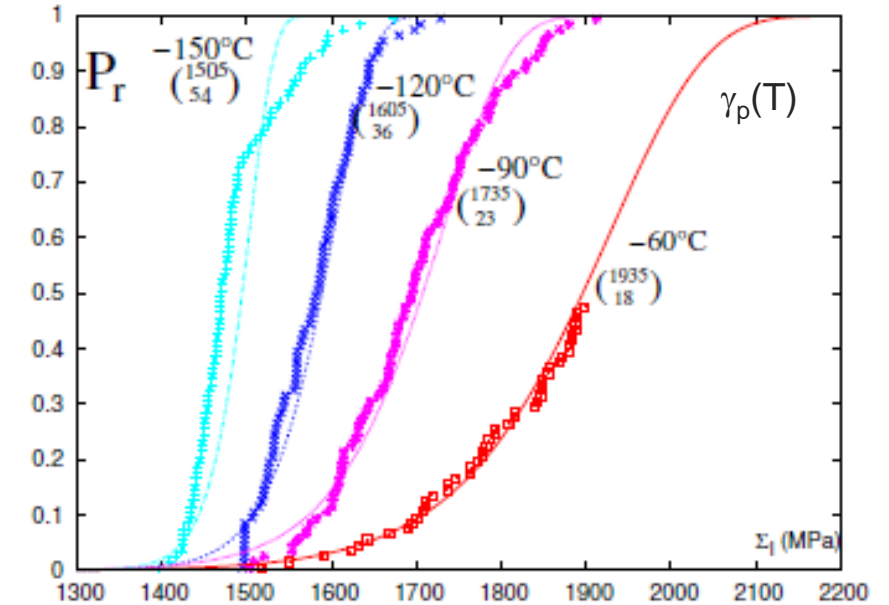
Random drawing of the number and size of carbides



Corresponding Griffith critical stress field



Material behavior of Bainite : composite (ferrite + carbides)



Plastic strain field (initiation criterion)





2.2 First results

Crystal plasticity modeling [Sekfali, 2004, Libert 2007]

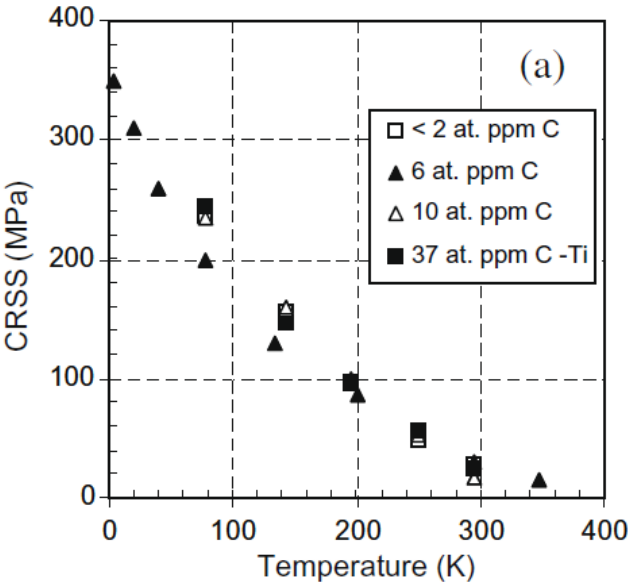


Thermally activated behavior

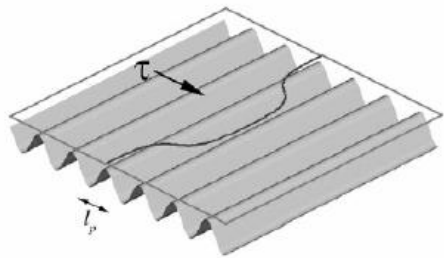
Effective stress $\tau_{eff}^s = |\tau^s| - \tau_c^s$ $\tau_c^s = \tau_F + \frac{(\mu b)^2 \sum_u a^{su} \rho^u}{\tau^s - \tau_0}$ [Rauch, 1993]

Flow rule $\dot{\gamma}_{nuc}^s = \dot{\gamma}_0 \exp\left(-\frac{\Delta G_0}{kT} \left(1 - \left(\frac{\tau_{eff}^s}{\tau_0}\right)^p\right)^q\right) \text{sign}(\tau^s)$ [Kocks et al., 1975]

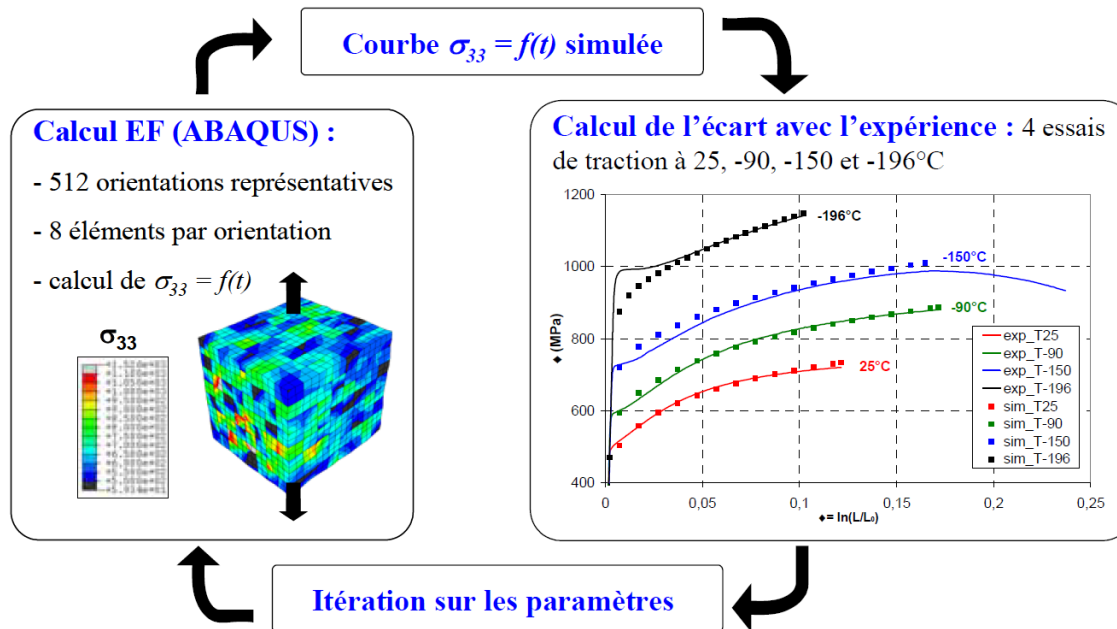
Dislocation density evolution $\dot{\rho}^s = \frac{|\dot{\gamma}^s|}{b} \left(\frac{1}{\Lambda^s(T)} - \gamma^s(T) \rho^s\right)$ avec $\frac{1}{\Lambda^s(T)} = \frac{1}{D_{lath}} + \frac{\sqrt{\sum_{u \neq s} \rho^u}}{K(T)}$ [Tabourot, 1992]



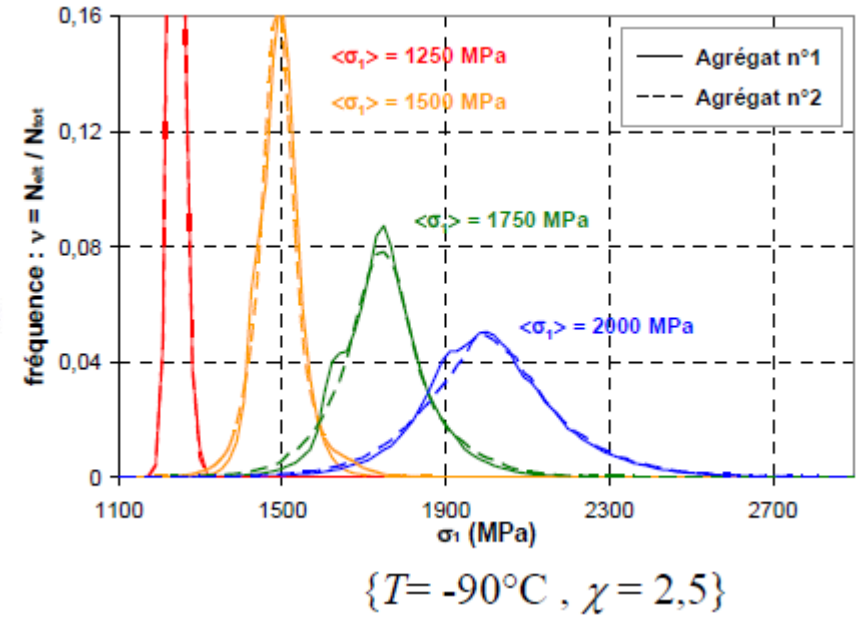
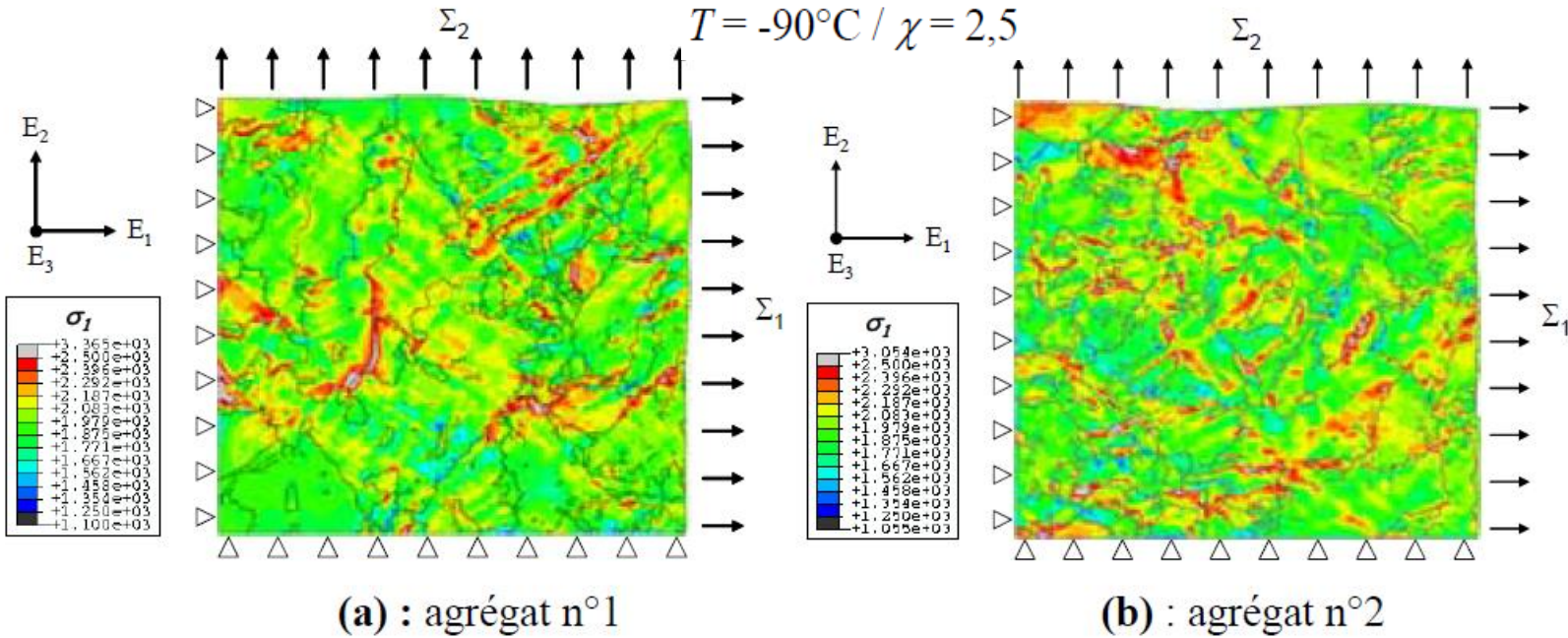
[Quesnel et al., 1975, Spitzig, 1973, Kuramoto et al., 1979, Spitzig et Keh, 1970] dans [Naamane et al. 2010]



[Stainier et al., 2002]

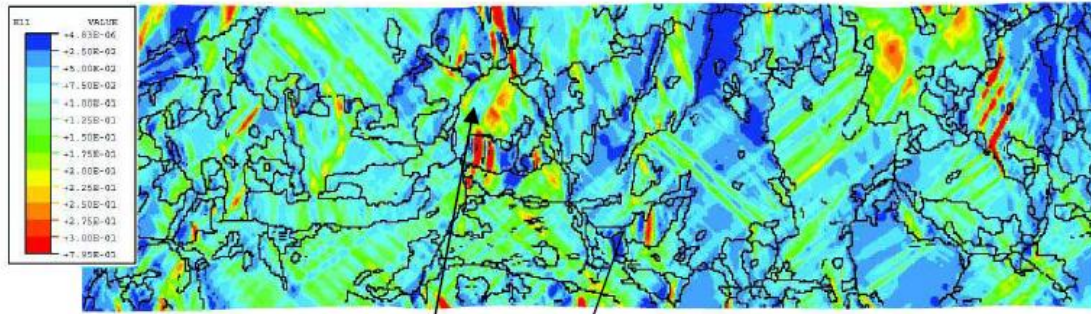


Mesososcopic stress fields [Libert 2007]

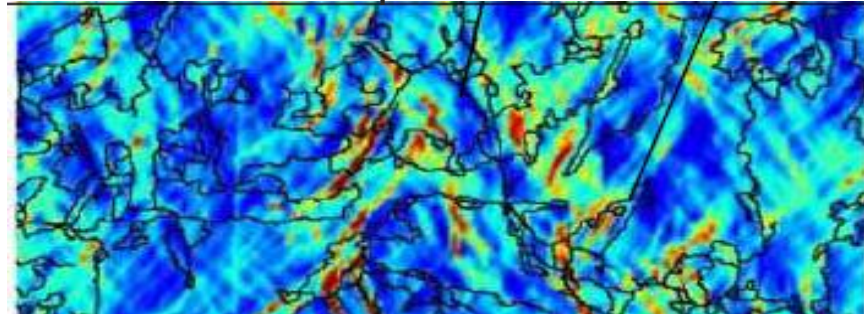


Simulated strain fields can be compared to experimental ones observed at the surface of in-situ tensile tests [Sekfali, 2004] (poor predictions due to lack of knowledge of the underlying microstructure ☹)

Simulation

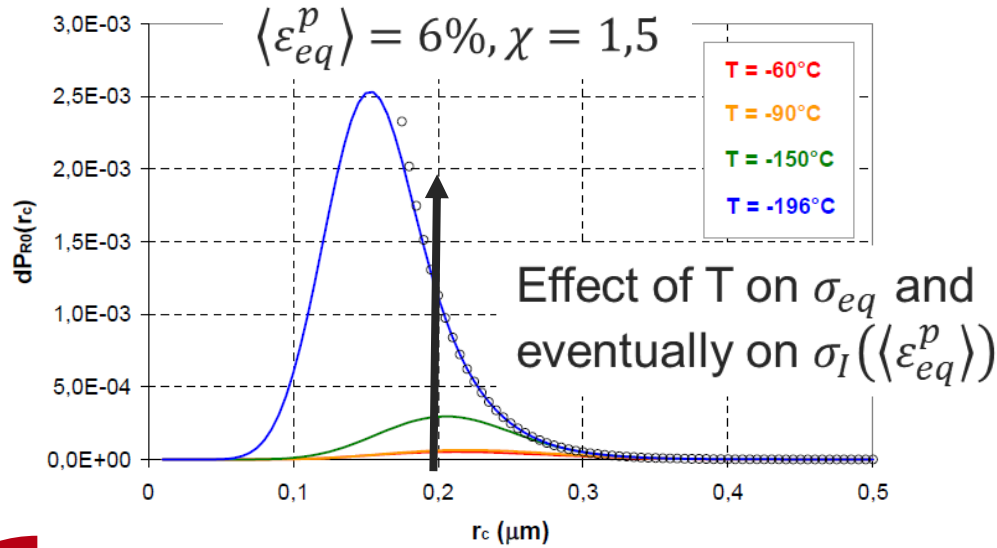


Experimental

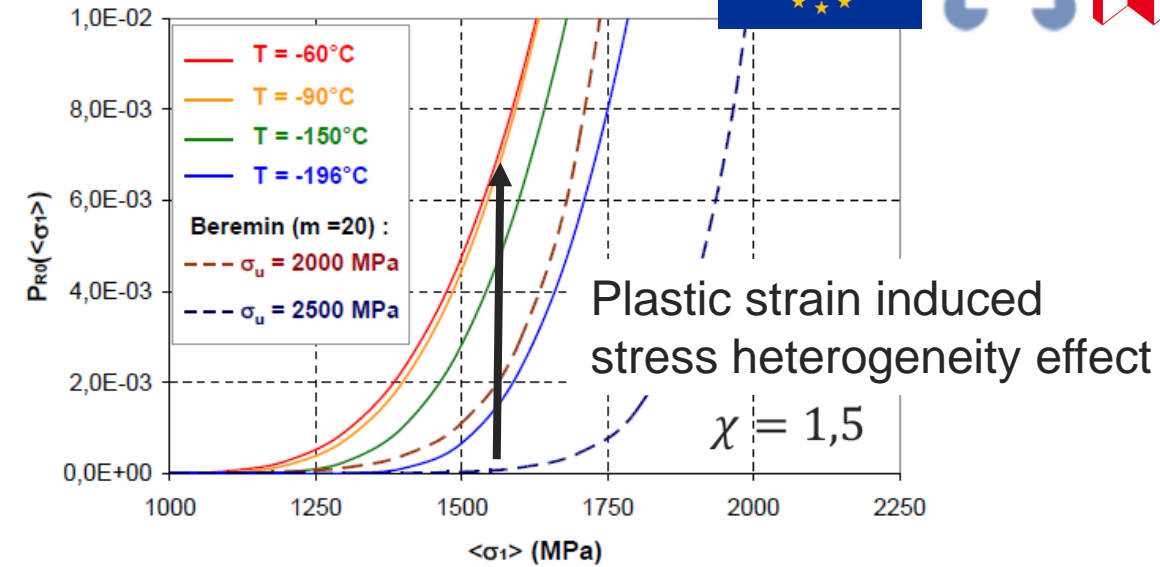


Fracture probability of RVE

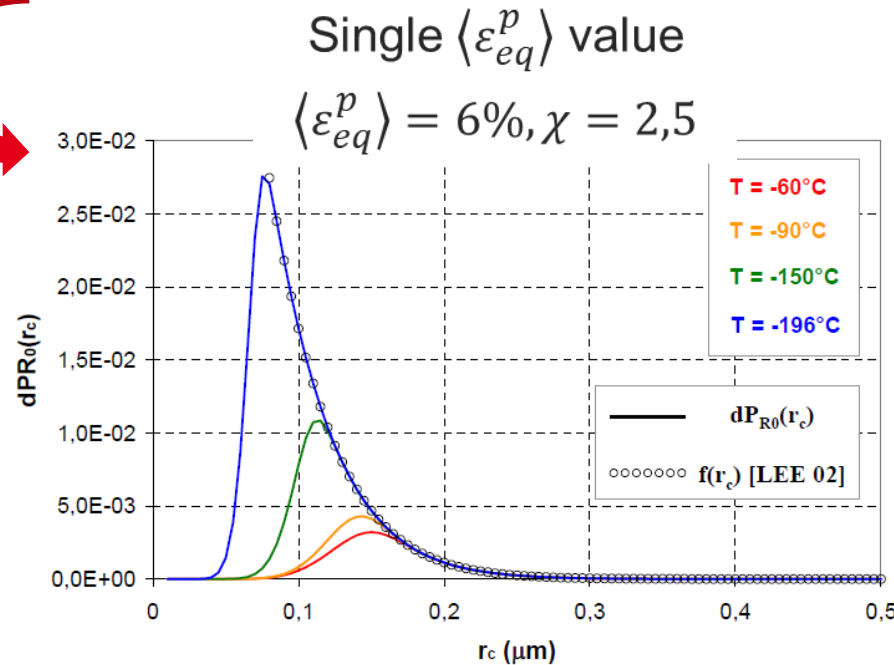
$$\chi = \frac{\sigma_{kk}}{3\sigma_{eq}}$$



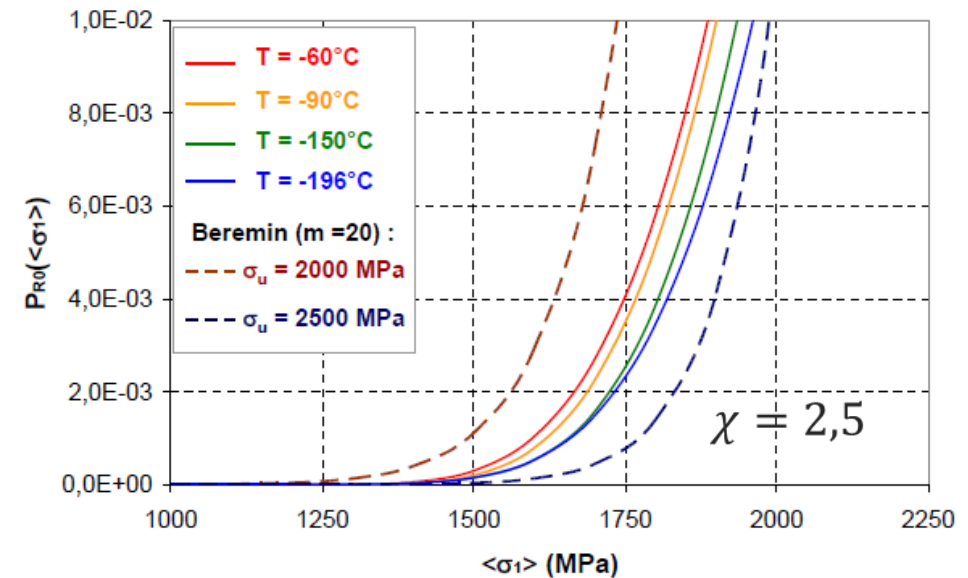
[Libert 2007]



Effect of χ on $\sigma_I(\langle \epsilon_{eq}^p \rangle)$



Increasing σ_1



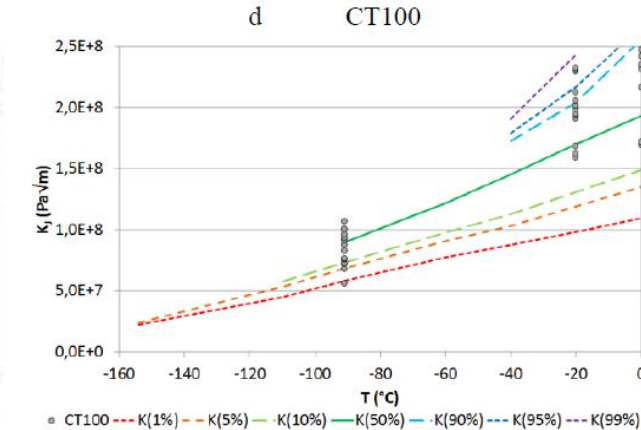
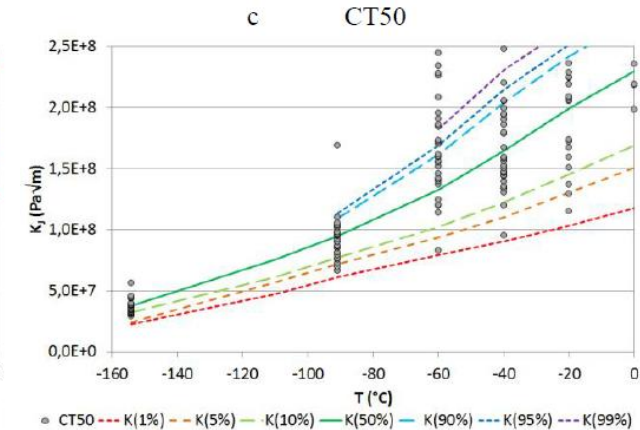
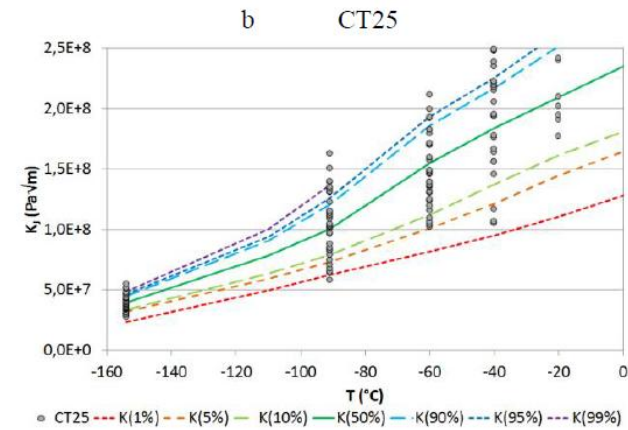
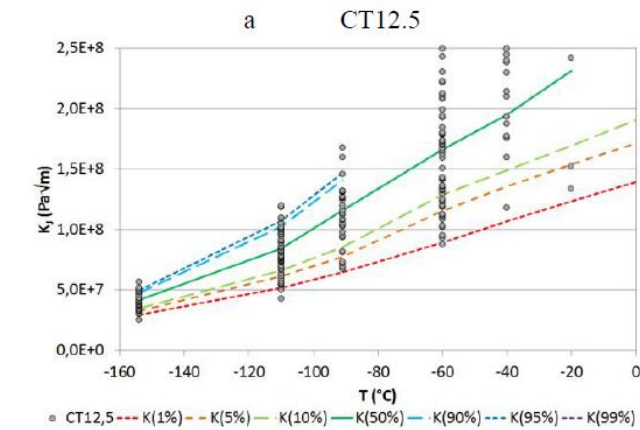
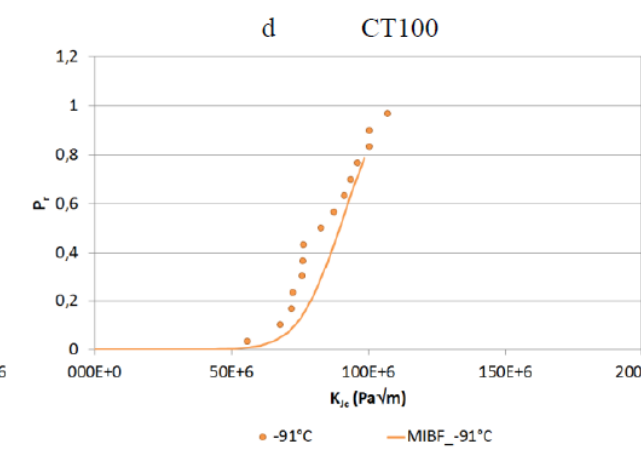
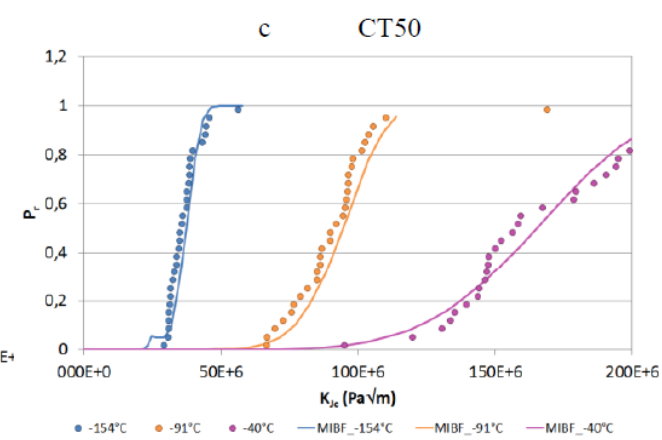
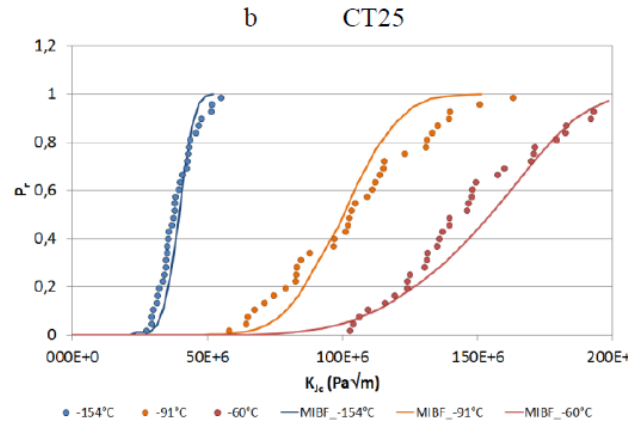
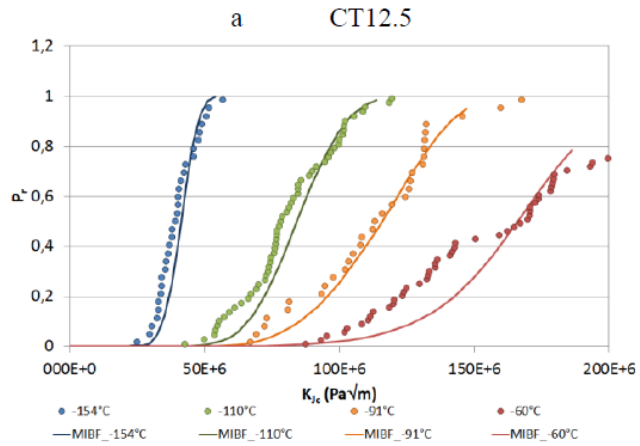
Size and temperature effects on fracture toughness



[Forget et al., 2016]



MIBF Application on CT specimens



Outline

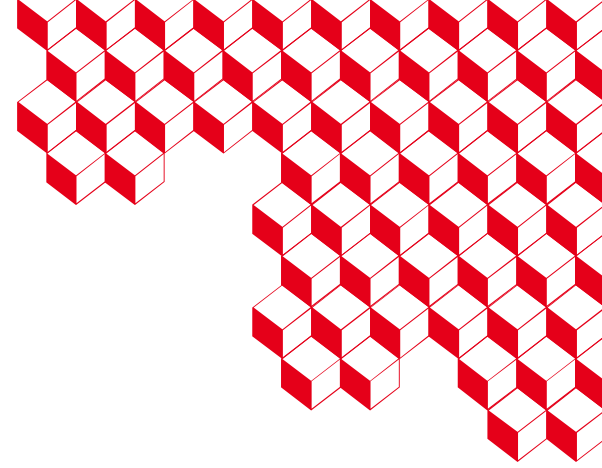
1) Industrial Context

2) Microstructure Informed Brittle Fracture modelling

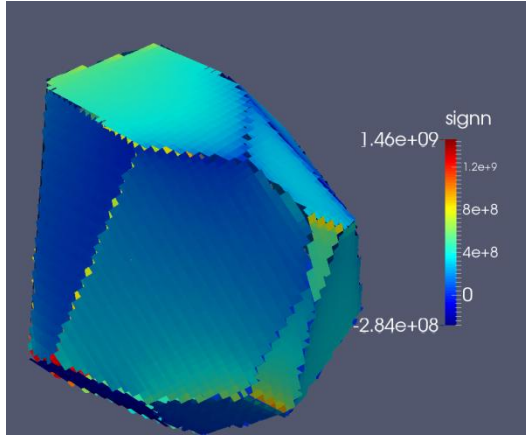
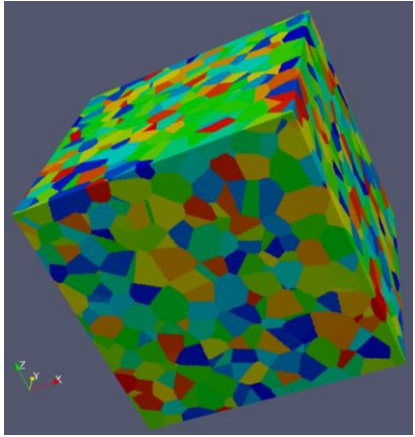
3) “Recent” developments

4) Conclusions / Prospects





Intergranular fracture [Forget et al., 2018]

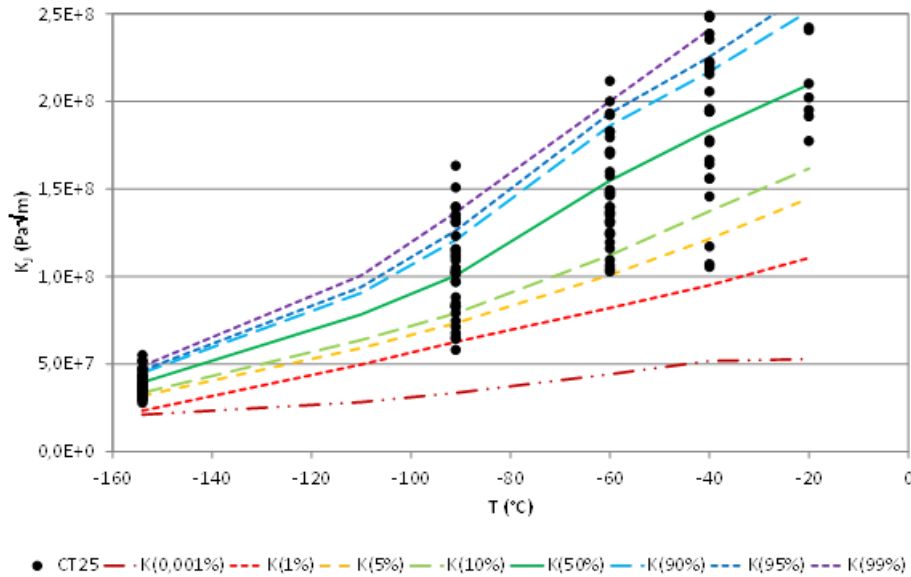


$$P_i(V_p, \Pi) = 1 - \exp \int_{V_p} n_p \cdot S_v \cdot \ln(1 - P_\gamma(\sigma^* > \sigma_i)) dV$$

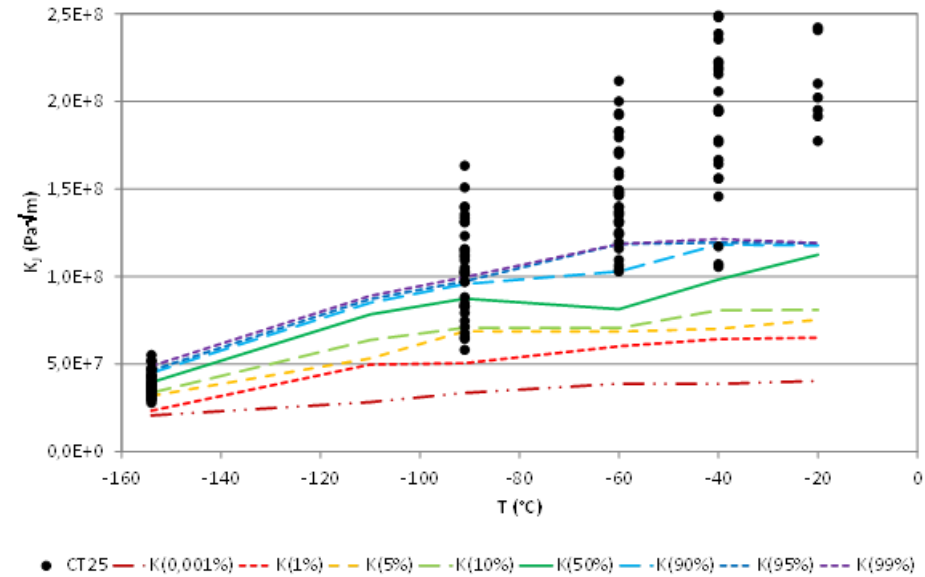


AMITEX

No intergranular brittleness: cleavage only



Intergranular brittleness: reduction of K_Ic



Macrosegregation

[Ren et al., 2022]



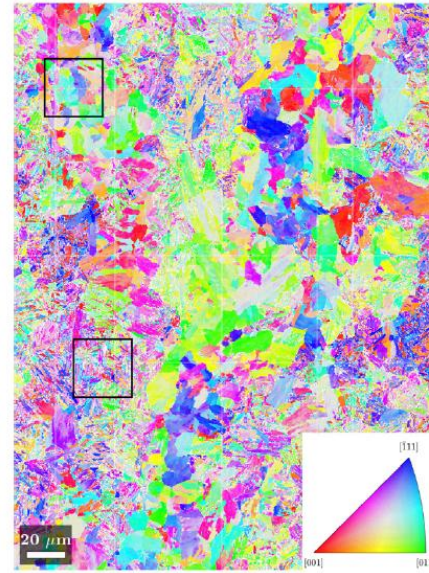
framatome



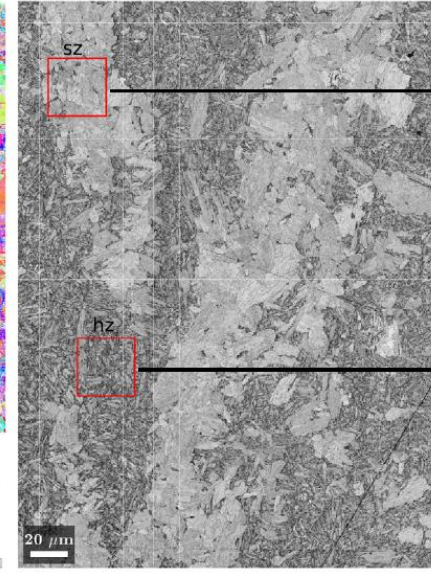
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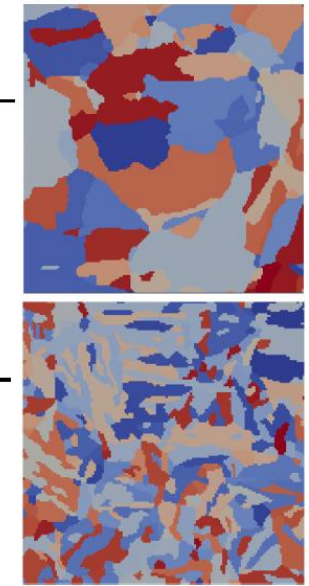
0.29%C



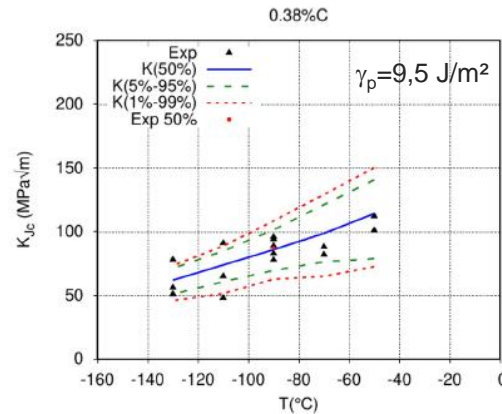
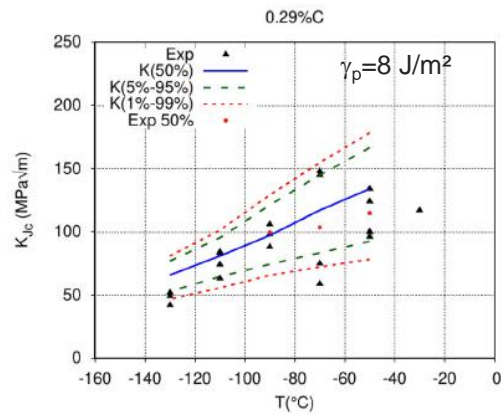
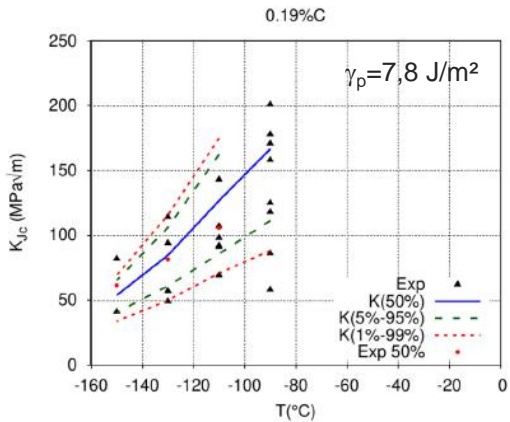
0.38%C



unit cells used in FFT simulations



30 x 30 μm
150 voxels
in y z
1 voxel in x





4 **Conclusions Prospects**

Conclusions

- A Microstructure Informed Brittle Fracture model is proposed: \approx Beremin model with the effective carbide size distribution + intragranular stress distribution
- One « tuning » parameter: the surface energy γ_s
- The predictions of the model rely on the correct description of initiators (carbides?) and of mechanical behavior at the grain scale (efficient cristal plasticity law at the slip plane level ?)

Limitations / Prospects



RPV steels : not an ideal Fe-C model alloy

- Carbides not uniformly distributed inside the microstructure and not always at the origin of brittle fracture
- Cleavage fracture generally initiates close to grain boundaries
- Real microstructure very complex to model: local texture, grain shapes, minor and major segregations, ...

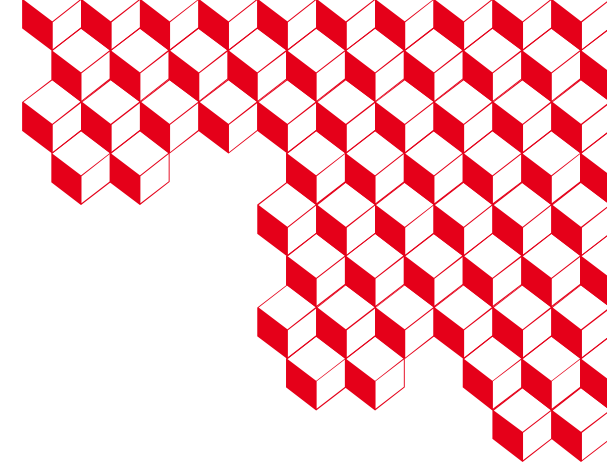
Improvements of current mechanical modeling:

- To better identify irradiation microstructures and their effective strength in RPV steels by multiscale approaches.
- To improve current polycrystal plasticity modelling to better describe strain localizations, size effects and stress fields close to grain boundaries (with precipitates, carbide clusters) where cleavage generally initiates
- To introduce in MIBF model size effects of the microstructure (on stress fields and critical stress), segregation effects, ductile tearing,...



isqs

Thank you



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