MODELLING OF CRACKING IN UO_2 AND ITS APPLICATIONS IN FUEL PERFORMANCE CODES

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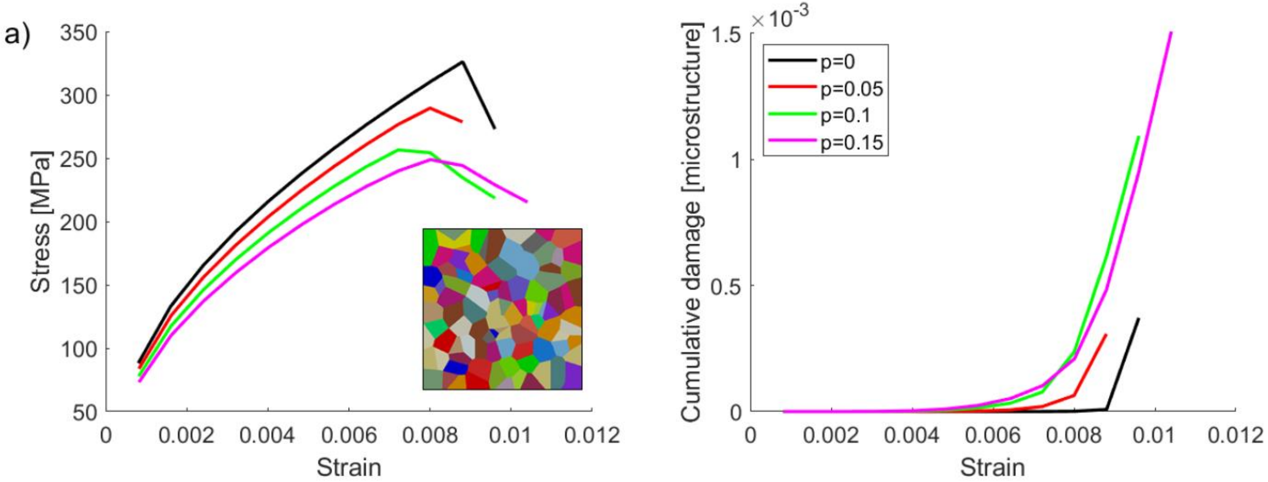
Outline

- Common goals in crystal plasticity modelling of UO_2 under NKS-POMMI project
- Plasticity model parametrization
- Development of a fracture model
- Reactivity-initiated accident (RIA) modelling with the BISON code
- Current status of mechanical modelling in BISON
- Conclusions

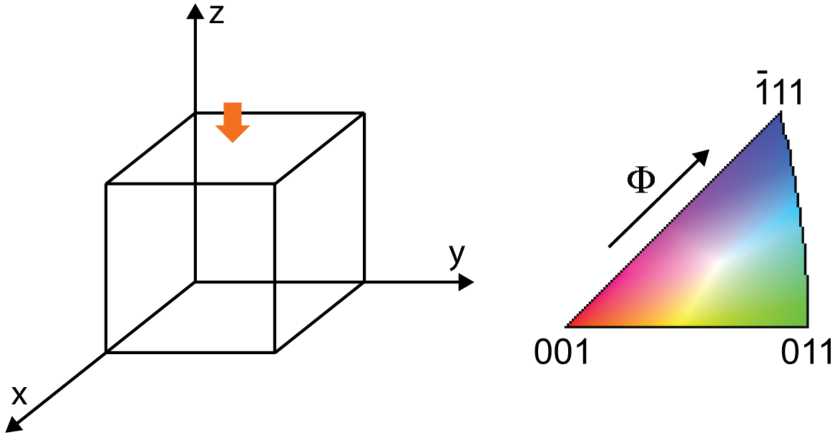
NKS-POMMI goal: A crystal plasticity framework for UO_2 fracture modelling

- Plastic deformation mechanisms
  - Dislocation density-based formulation was used to describe plasticity due to dislocation slip systems
  - Develop a model for brittle failure related to cleavage type fracture in the material
- Microstructure and porosity based on SEM-EBSD data
- The strength of the material as a function of increasing porosity in a tensile test

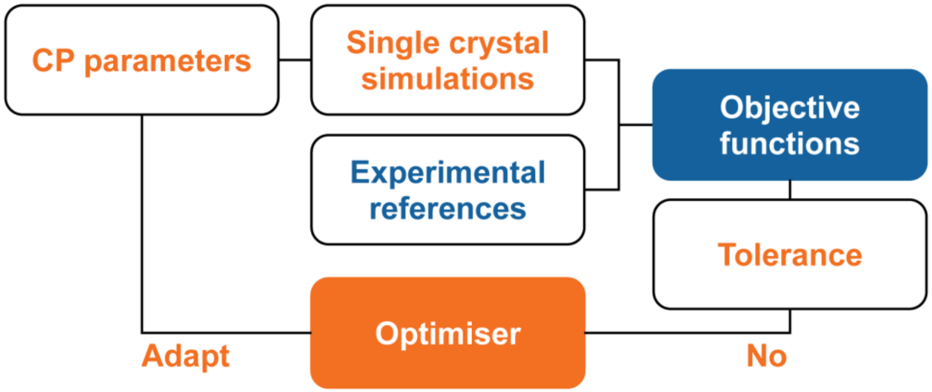


Stress-strain response with damage, p is the volume fraction of pores in the mesh

Parameterisation of the CP model

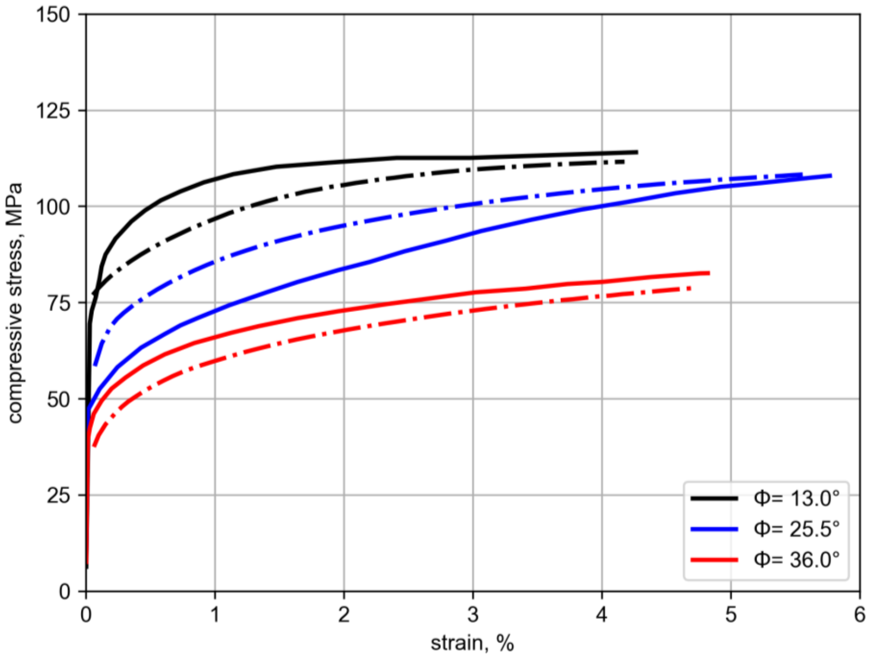


Compression simulations of single crystals

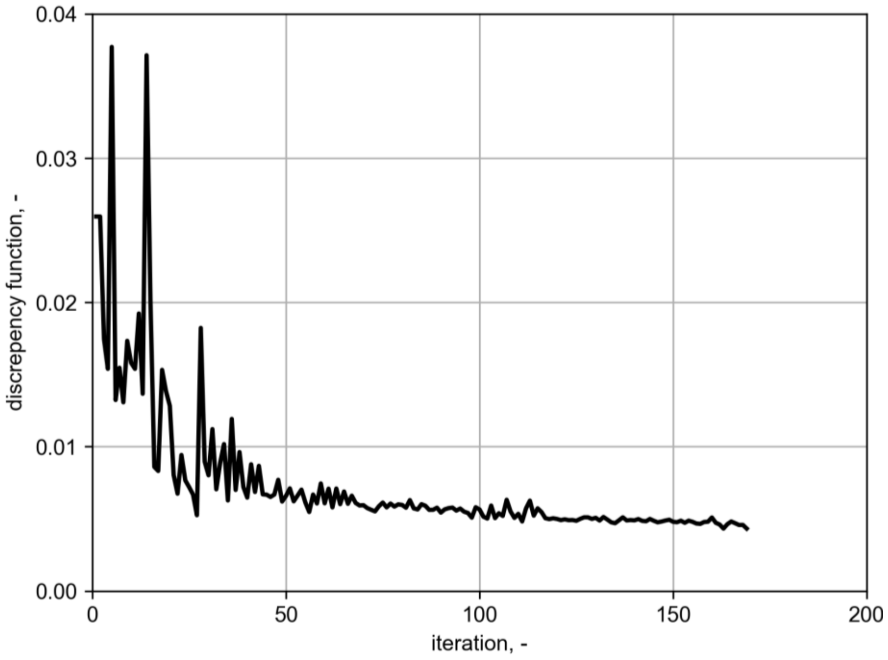


CP parameterisation workflow

Parameterisation of the CP model



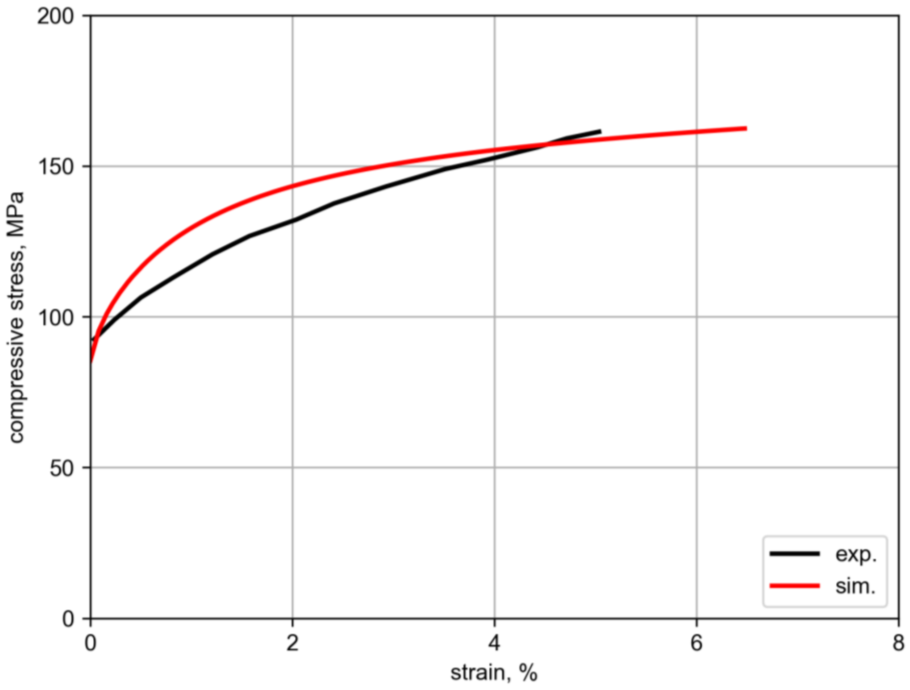
Flow curve comparison



Evolution of objective function

Validation with polycrystal simulation

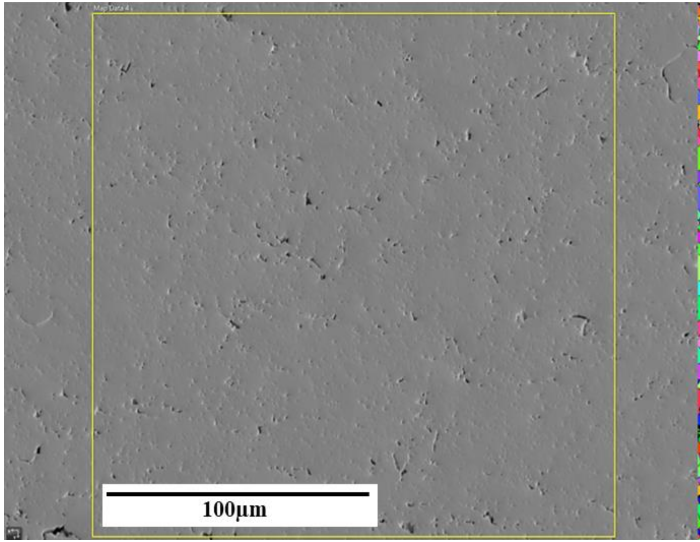
- Uniaxial compression simulation of polycrystal with ~250 grains
- Using optimised parameters
- Changing grain size to match characterisation data
- Further studies have been conducted to account the temperature and strain rate effects



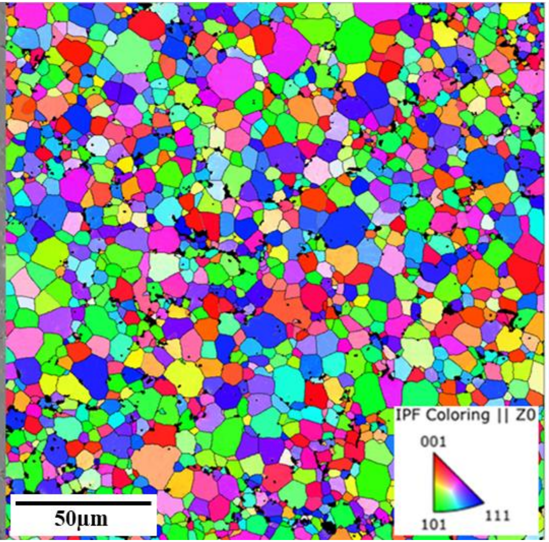
Electron backscatter diffraction (EBSD) analyses of a standard uranium dioxide pellet, done at KTH

- SEM-EBSD examinations at 1000X of magnification of a standard UO_2 fuel

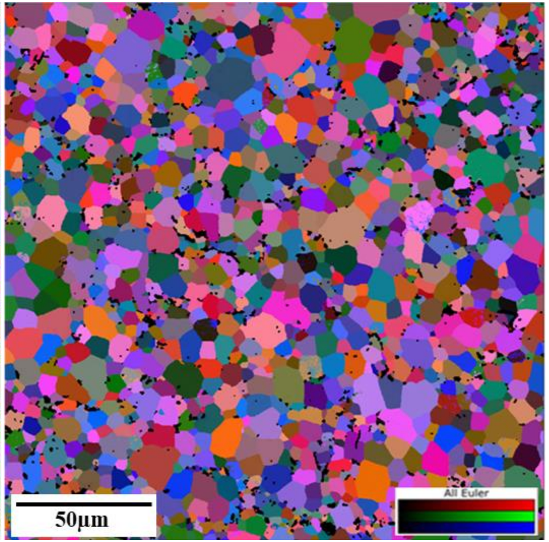
microstructure morphology (SEM-SE image)



inverse pole figure (IPF) map in the direction Z0

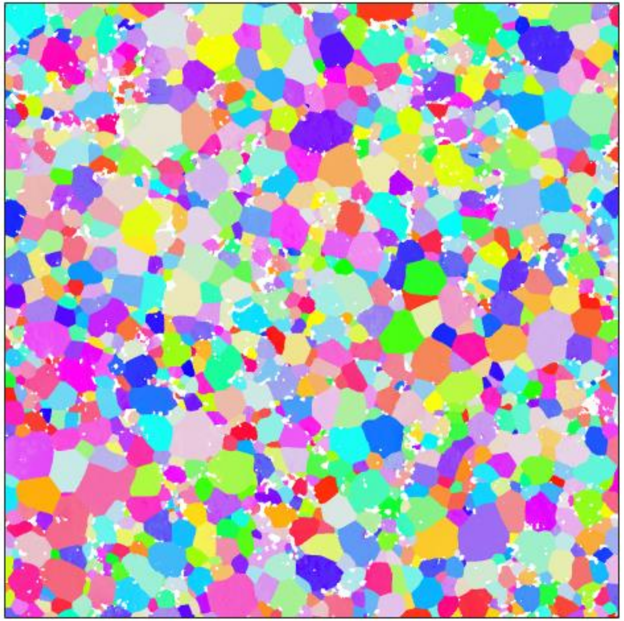


Euler angle (EA) map

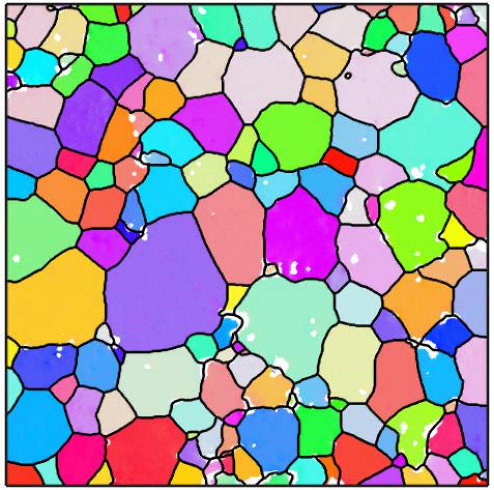


Identifying grains

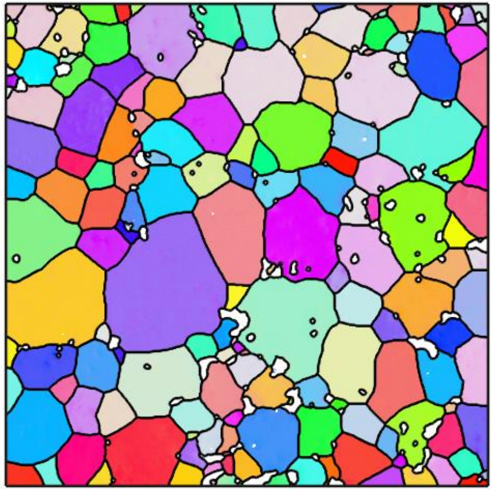
- Sample2: 200umx200um



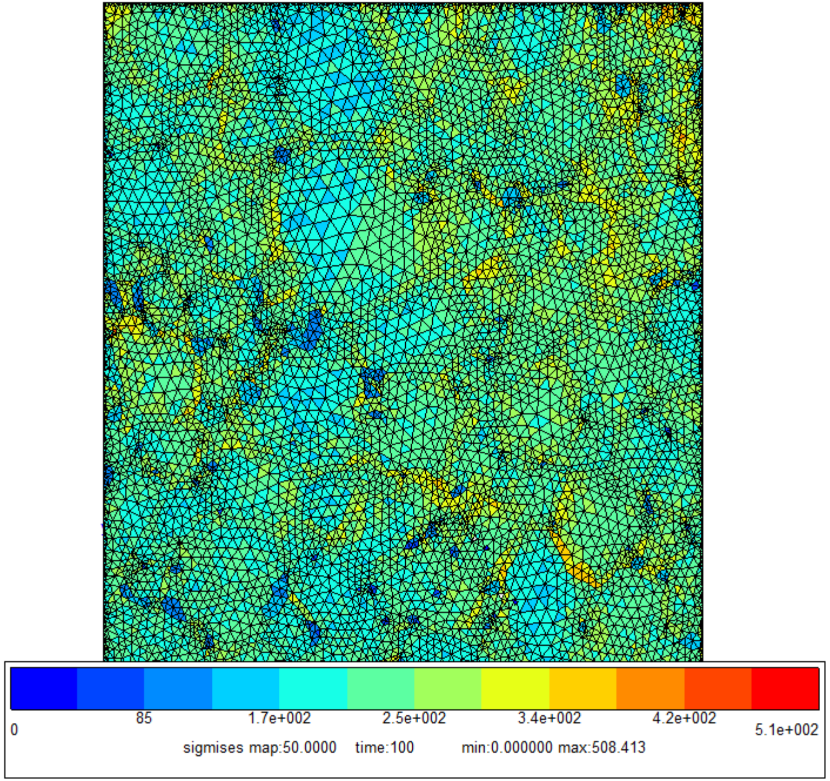
- Reconstructing grain boundaries
- Threshold angle: 5 degrees
- Allow grains to grow to non-indexed regions

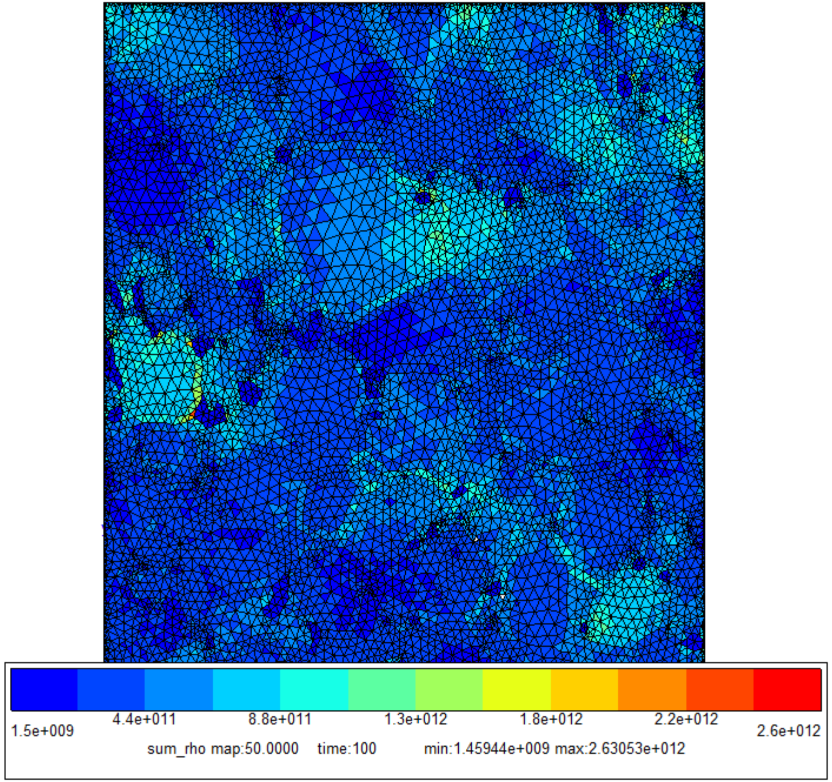


- Threshold angle: 5 degrees
- Non-indexed regions are grained
- Filtering of small grains

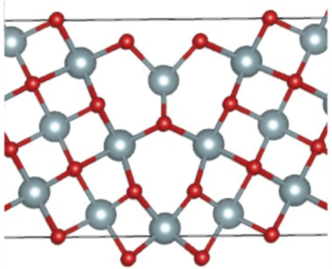


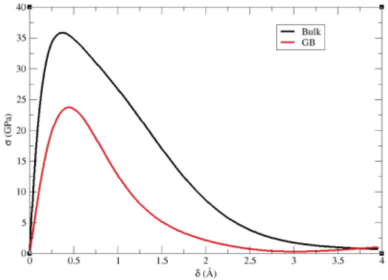
Stress and plastic deformation





From atomic scale to continuum damage model





DFT

Cleavage resistance:

$$Y_C^{d1/d2} = Y_0 \exp\left(-\beta \sum_{S=1}^{N^S} \nu^S\right) + Hd$$

Damage evolution:

$$\dot{\delta}_C^{d1/d2} = \left\langle \frac{|\sigma_{dc}| - Y_C^{d1/d2}}{K_d} \right\rangle^{n_d} \text{sign}(\tau_{dc}) \quad \text{with} \quad \sigma_{dc} = \underline{n}_d^{d1/d2} \cdot \underline{M} \cdot \underline{n}_d^{d1/d2}$$

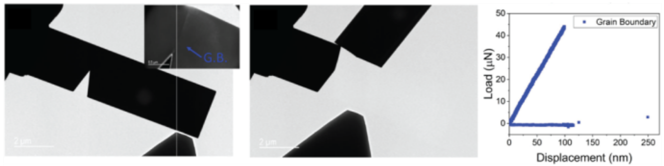
Rate of damage accumulation:

$$\dot{d} = \sum_{d1=1}^{N_{100}} \left|\dot{\delta}_C^{d1}\right| + \sum_{d2=1}^{N_{111}} \left|\dot{\delta}_C^{d2}\right|$$

Softening due to damage:

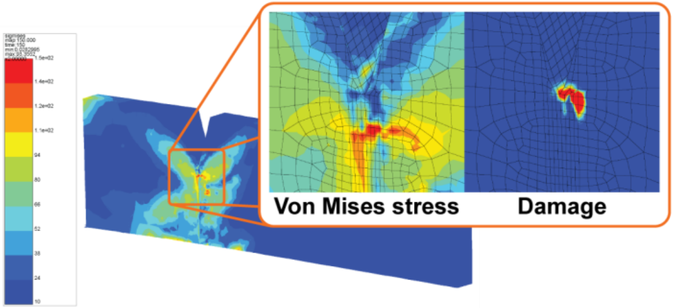
$$\tau_c^s = \tau_0^s + \mu b^s \sqrt{\sum_{s=1}^{6} a_{100}^{sj}\rho^j + \sum_{s=7}^{12} a_{110}^{sj}\rho^j + \sum_{s=13}^{24} a_{111}^{sj}\rho^j} - Y_0 \beta d \exp(-\beta \nu^S)$$

Microscopic damage model



Source: Feng et al. JOM 2020

Bending of microcantiliver beam of UO_2



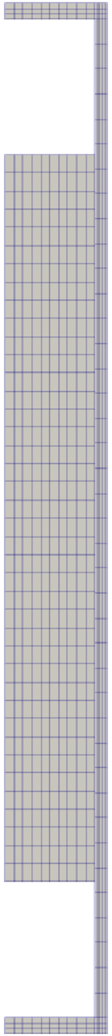
Microcantiliver beam simulation

Validation with experimental references

Scale-bridging law

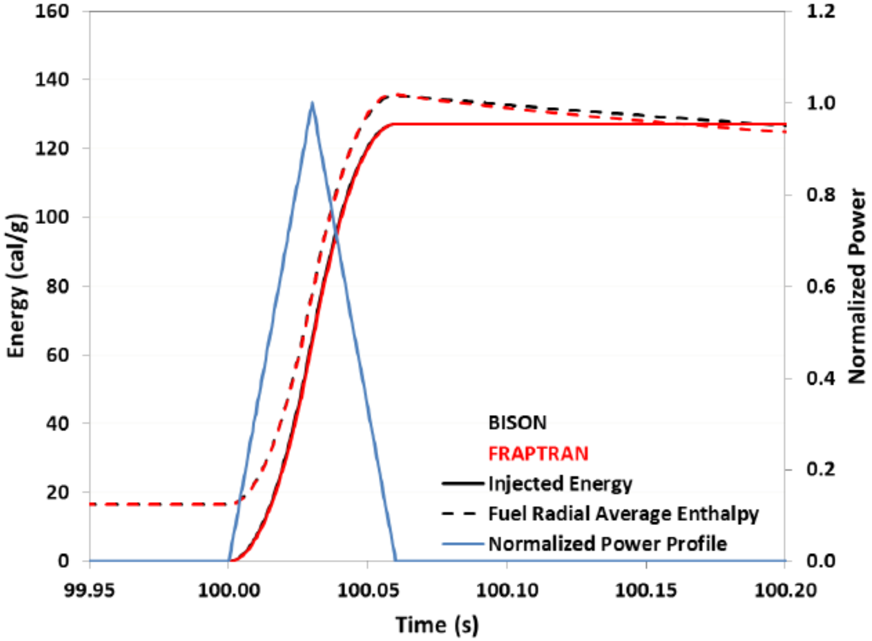
Loading conditions during Reactivity-Initiated Accident (RIA)

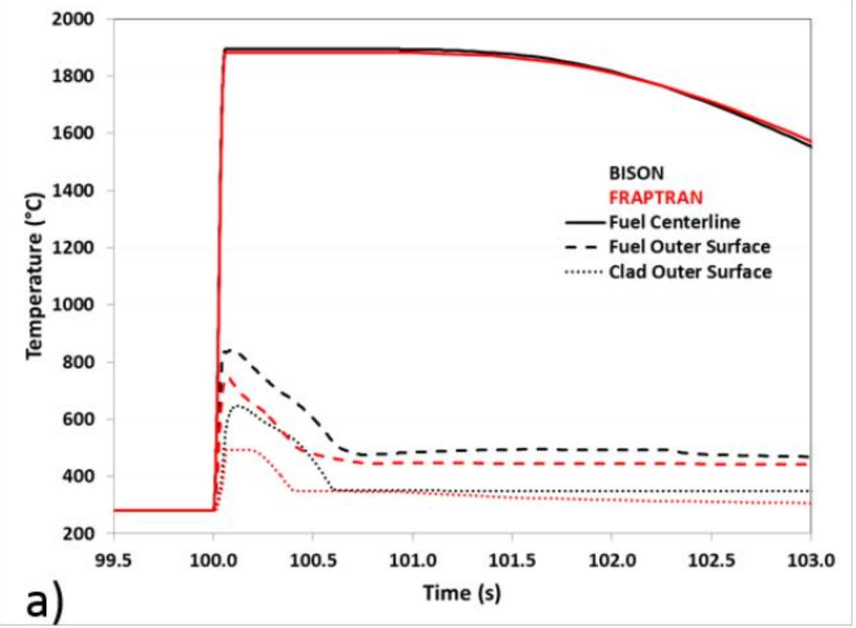
- OECD/NEA/WGFS RIA Fuel Codes Benchmark Case 5
  - A fresh fuel case without experiments
  - Pellet-cladding gap closed
  - Porosity 4%
  - The fuel is modeled using an Elastic model with a Modulus of Elasticity of 200 GPa,
  - a Poisson ratio of 0.345 and thermal expansion coefficient as defined in MATPRO



Boundary conditions for fuel performance modelling

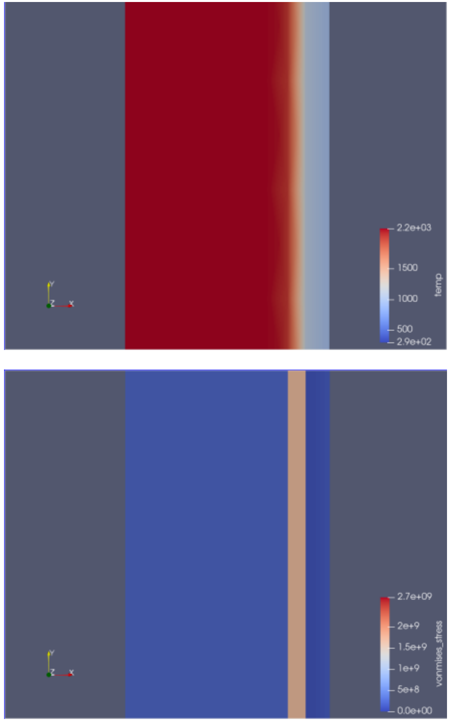
- The power pulse starts from zero power at t=100 s and is approximated with a triangular shape. The pulse width is 30 ms full width at half max (FWHM)
- The maximum power was defined as 1.0 MW, aimed at initiating departure from nucleate boiling (DNB)
- The power pulse will result in 531.6 J/g (127.06 cal/g) of energy injected into the fuel.


160
140
120
100
80
60
40
20
0
Energy (cal/g)
1.2
1.0
0.8
0.6
0.4
0.2
0.0
Normalized Power
99.95
100.00
100.05
100.10
100.15
100.20
Time (s)
BISON
FRAPTRAN
Injected Energy
Fuel Radial Average Enthalpy
Normalized Power Profile

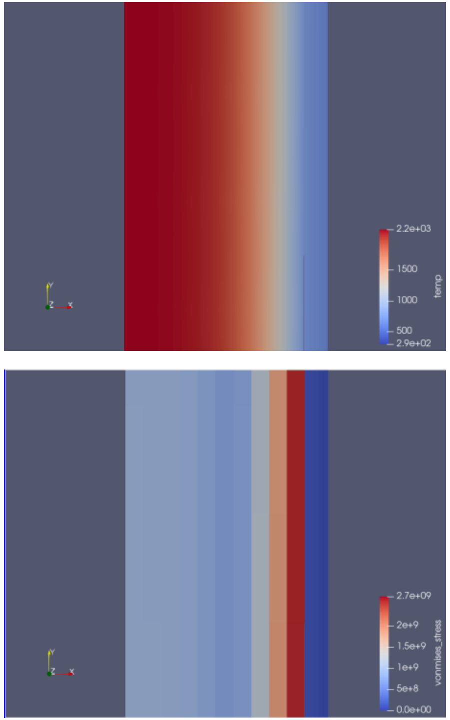

2000
1800
1600
1400
1200
1000
800
600
400
200
Temperature (°C)
99.5
100.0
100.5
101.0
101.5
102.0
102.5
103.0
Time (s)
BISON
FRAPTRAN
Fuel Centerline
Fuel Outer Surface
Clad Outer Surface
a)

Temperature and von Mises stress during the transient

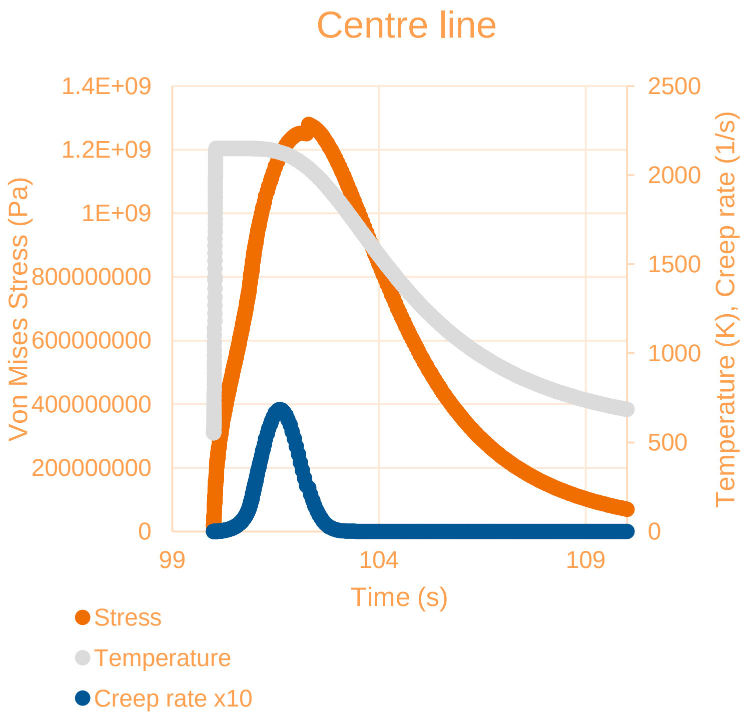
t = 100.079 s

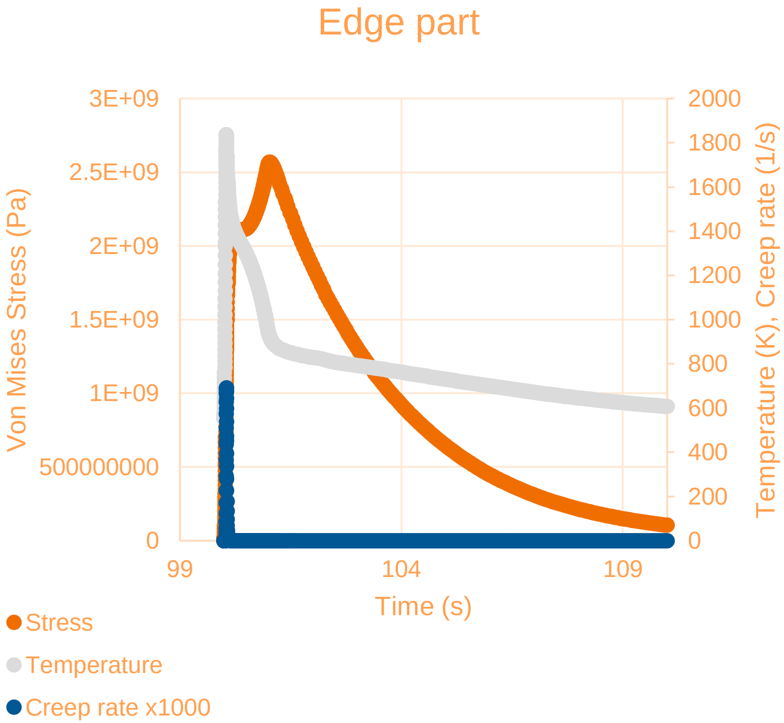


t = 101.38 s



Current status of mechanical modelling of pellets in the BISON fuel performance code





Conclusions

- Impactful results of the NKS-POMMI project
  - Plastic behaviour of polycrystalline UO_2 can be understood better -> tools for modelling of future fuels too
  - Traction-separation modelling of UO_2 bulk and grain boundaries with atomistic simulations
  - Future work: fracture model development and scaling of results from atomistic calculations
- BISON models provide currently high stresses in the fuel pellet -> improvement of the plasticity and damage models required
- What next?
  - Research work continues especially with the European partners