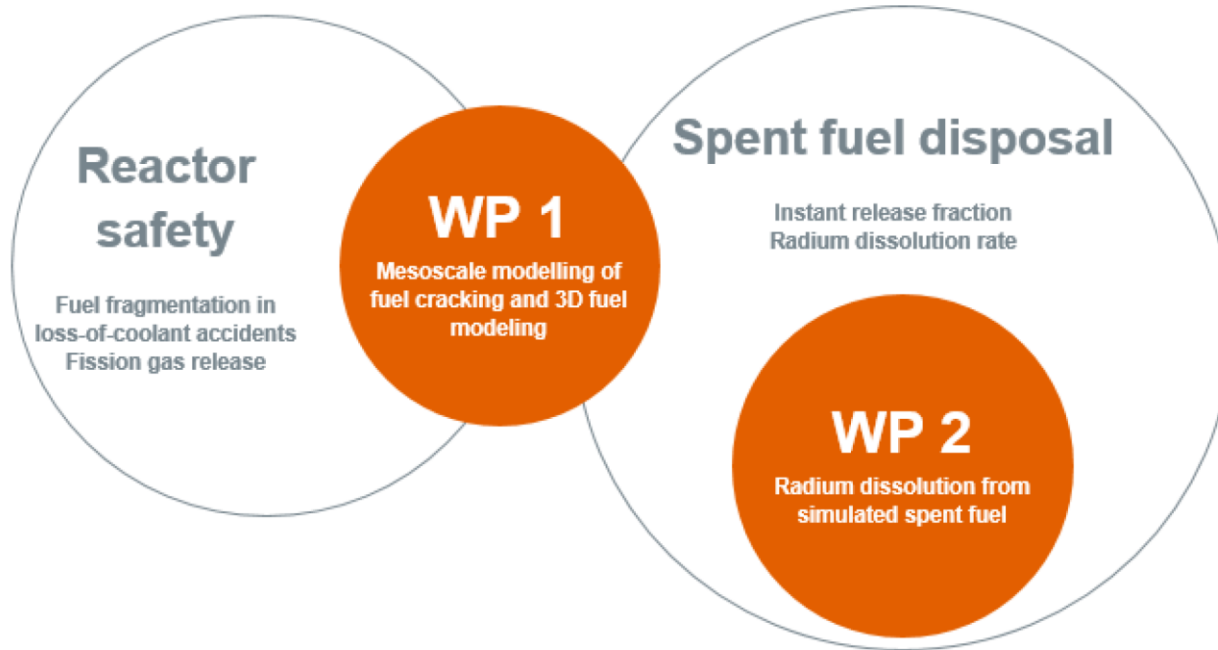


**KYT2022-SAFIR2022  
PORA  
Interim webinar**

**Janne Heikinheimo**

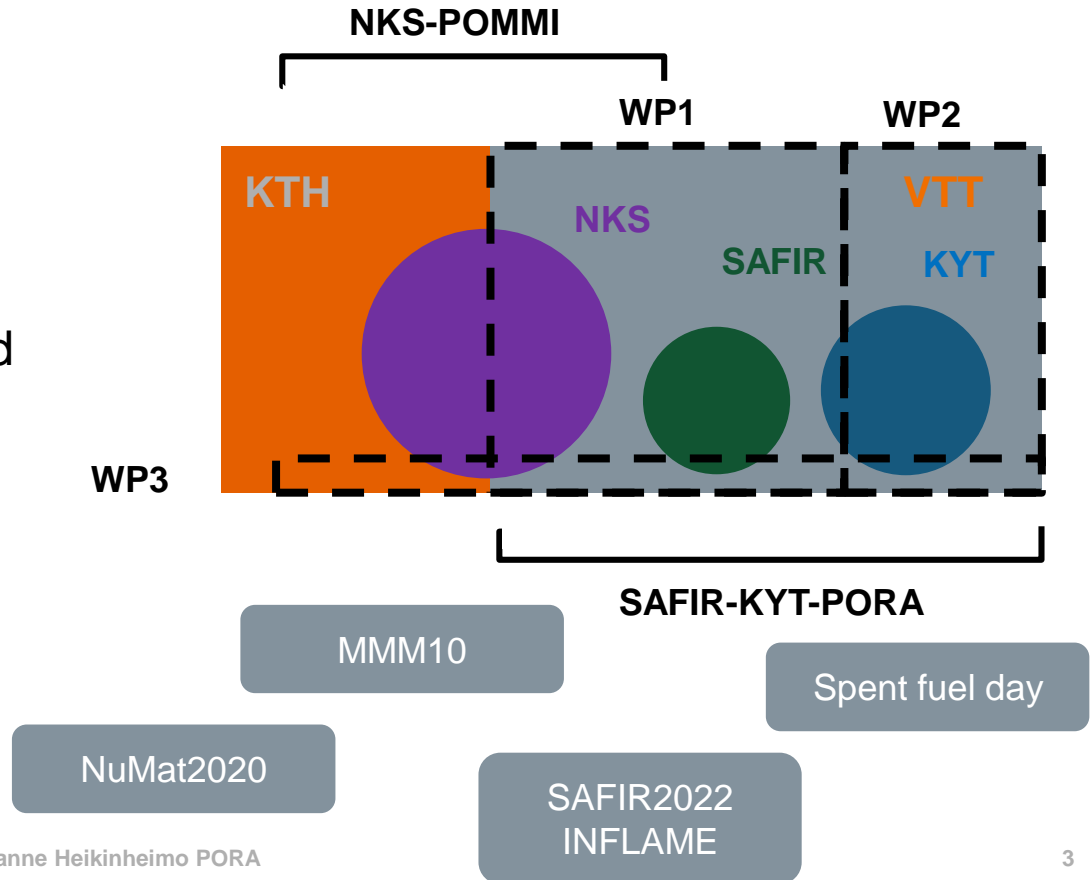
18/3/2021

# PORA – Fuel microstructure and radium solubility (Polttoaineen mikrorakenne ja radiumin liukoisuus)



# Work packages, connections and funding

- WP1 Modelling of fuel microstructural cracking behaviour
  - Mesoscale modelling
  - Macroscopic modelling
- WP2 Radium dissolution and interaction with bentonite or bentonite/zeolite mixture
  - Radium experiments
  - Molecular dynamics calculations
- WP3 Project management

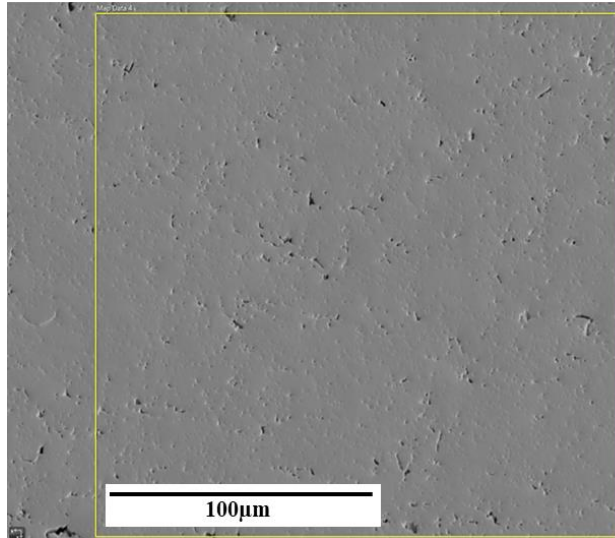


# WP1 Modelling of fuel microstructural cracking behaviour

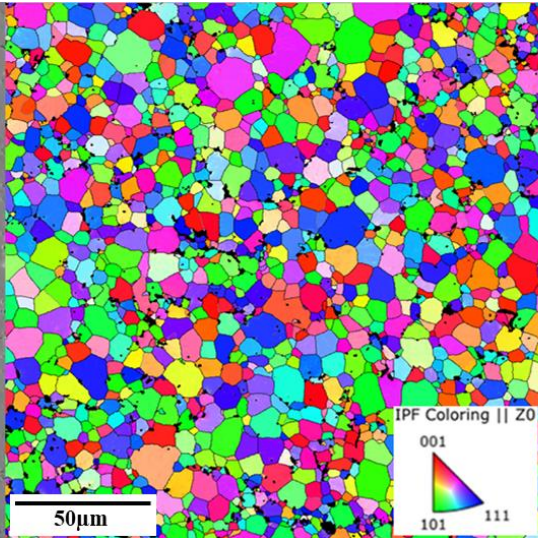
# Electron backscatter diffraction (EBSD) analyses of a standard uranium dioxide pellet, done at KTH

- SEM-EBSD examinations at 1000X of magnification of a standard  $\text{UO}_2$  fuel

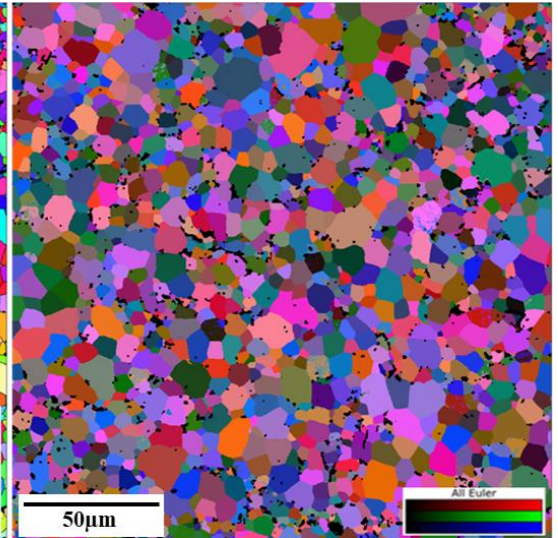
microstructure  
morphology (SEM-SE image)



inverse pole figure (IPF)  
map in the direction Z0

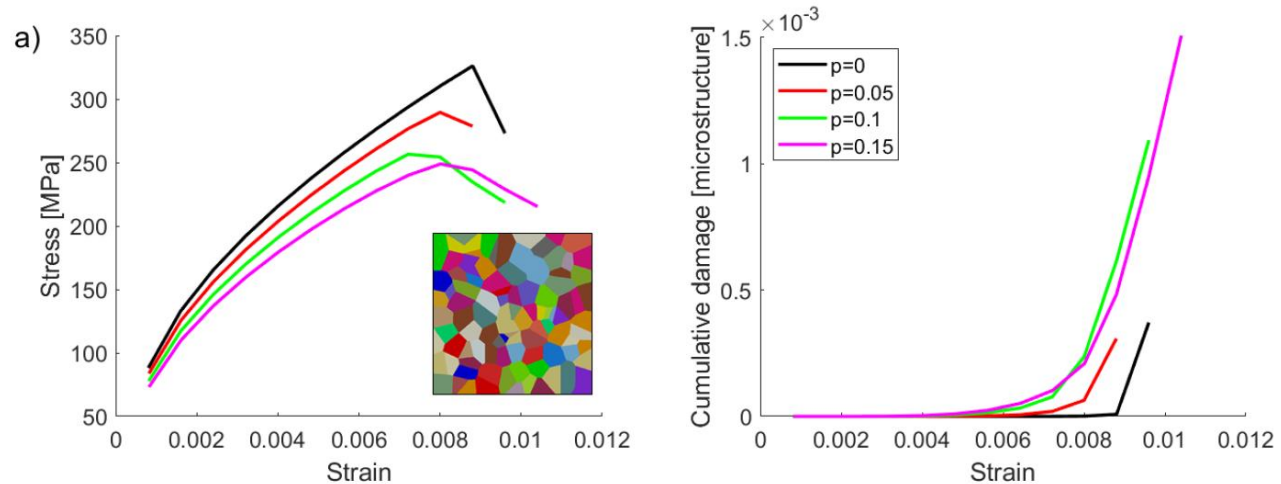


Euler angle (EA) map



# A crystal plasticity framework for $\text{UO}_2$ fracture modelling

- Plastic deformation mechanisms
  - Dislocation density based formulation was used to describe dislocation slip deviated plasticity
  - 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

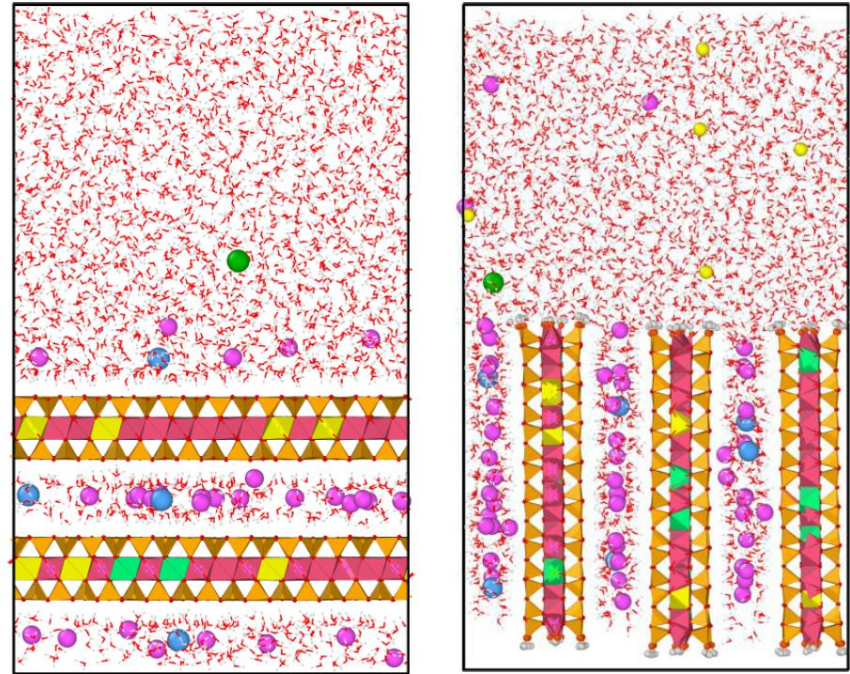


Stress-strain response with damage,  $p$  is the volume fraction of pores in the mesh

# WP2 Radium dissolution and interaction with bentonite or bentonite/zeolite mixture

# Approach to radium dissolution and interaction with bentonite or bentonite/zeolite mixture

- Leaching experiments for SIMFUEL pellets in disposal conditions
  - Ra/Ba released
- Interaction experiments of Ra and bentonite or bentonite/zeolite mixture
- Molecular dynamics modelling and calculations of equilibrium constant  $K_D$  for  $\text{Ra}^{2+}$  in the surfaces of MX-80 type montmorillonite and zeolite A minerals



Adsorption process onto the interlayers/terminal surface of MX-80 type montmorillonite (MD modelling)



# bey<sup>0</sup>nd

## the obvious

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