Multiscale modelling of cracking in CeO_2 and UO_2 pellets

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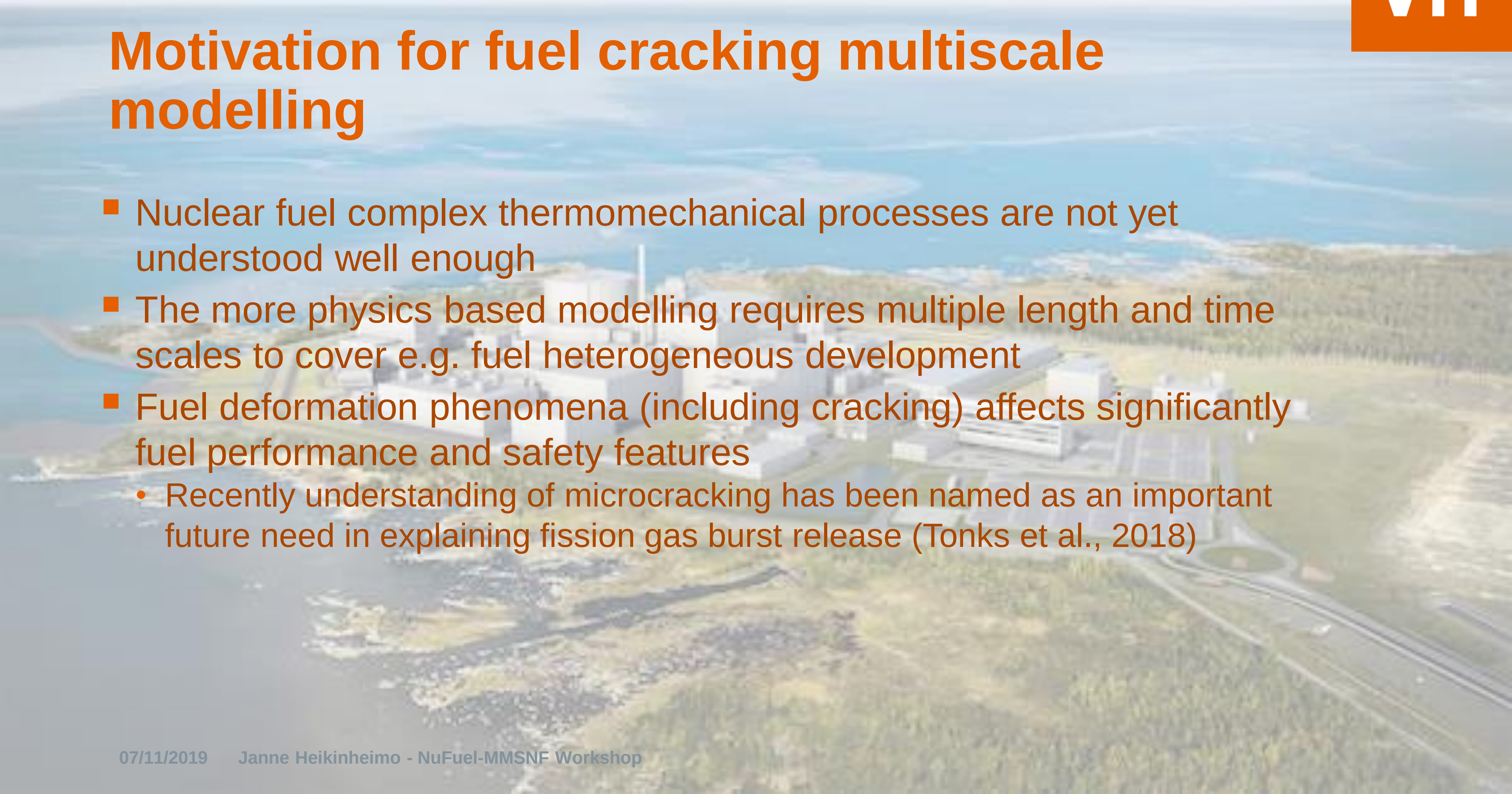
Outline

- Motivation for fuel cracking multiscale modelling
- What is properTune?
- Crystal plasticity modelling
- Case example with modelling: Martensite steel cracking
- Model development for UO_2 and CeO_2 cracking
- Experimental comparison
- Future plans

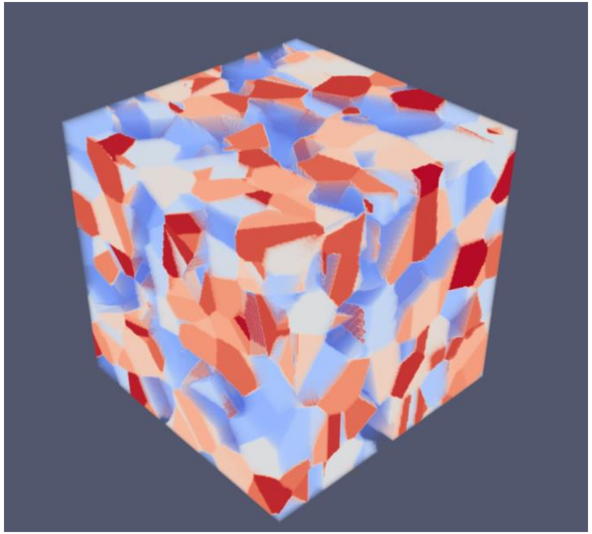
Motivation for fuel cracking multiscale modelling



- Nuclear fuel complex thermomechanical processes are not yet understood well enough
- The more physics based modelling requires multiple length and time scales to cover e.g. fuel heterogeneous development
- Fuel deformation phenomena (including cracking) affects significantly fuel performance and safety features
  - Recently understanding of microcracking has been named as an important future need in explaining fission gas burst release (Tonks et al., 2018)

What is properTune?

- Collection of tools used in solving thermomechanical properties of different materials
- Applies the MOOSE framework
- Covers length and time scales from MD to component scale
- Applied so far successfully in steel cracking modelling under stress: ductile to brittle transition (DBT)
- Development for ceramic cracking modelling ongoing

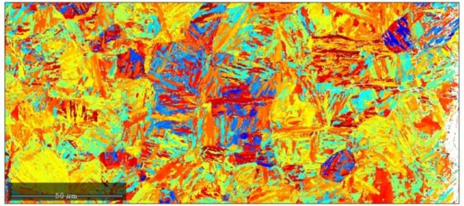


Lindroos, M., et al. Comput. Mater. Sci. 170, 109185, 2019

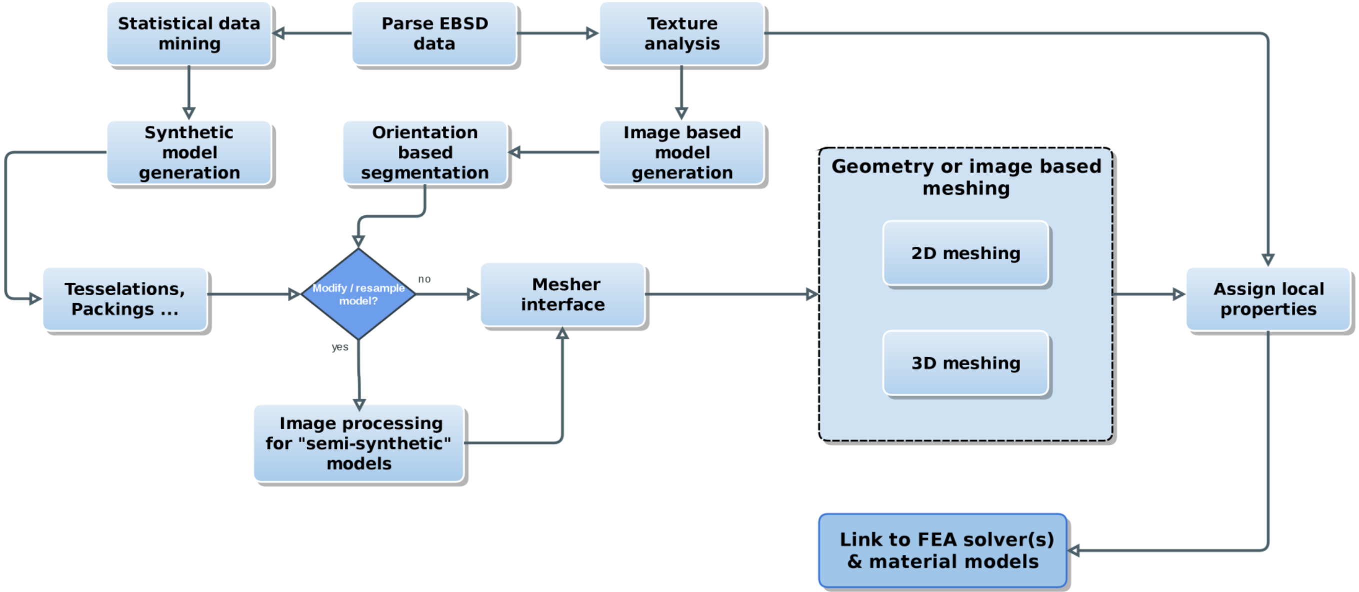
Crystal plasticity modelling

1) Preferably SEM EBSD characterization as input. Information about the grain morphology and possible texture is needed

2) 3D microstructural model geometry from a stack of 2D EBSD images as input (utilizing FIB for serial sectioning) if available.



- Finite element type approach
- Thermomechanical properties depend on the crystal orientation



Statistical data mining

Parse EBSD data

Texture analysis

Synthetic model generation

Orientation based segmentation

Image based model generation

Tesselations, Packings ...

Modify / resample model?

no

yes

Mesher interface

Image processing for "semi-synthetic" models

Geometry or image based meshing

2D meshing

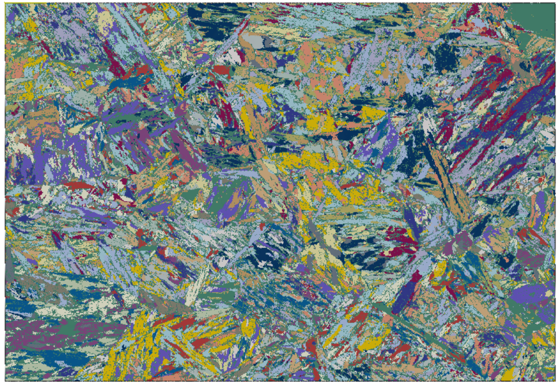
3D meshing

Assign local properties

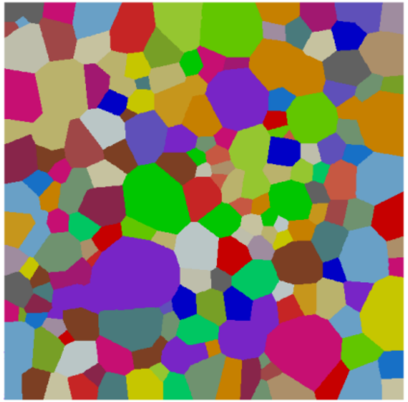
Link to FEA solver(s) & material models

Electron backscatter diffraction (EBSD) based mesh model

- EBSD inverse pole figure (IPF) map
- Realistic microstructure



- Synthetic models



Crystal plasticity model with ”cleavage damage”

$$\dot{\gamma}^s = \dot{\nu}\, sign(\tau^s) = \left\langle \frac{|\tau^s - x^s| - r^s - \tau_0}{K} \right\rangle^n sign(\tau^s - x^s)$$

Phenomenological slip rate formulation

$$x^s = c\alpha_s \;;\; \dot{\alpha}_s = (sign(\tau^s - x^s) - d\alpha^s)\dot{\nu}^s$$

Kinematic hardening parameter

H is softening modulus

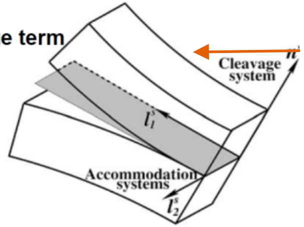
$$r^s = Q\sum_r H_{rs}\{1 - exp(-bv^r)\} + H\beta^2\nu + H\beta d$$

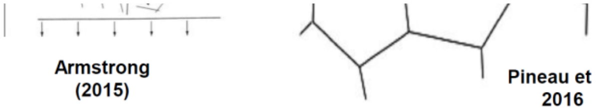
Damage term

Plasticity term

Beta is coupling factor

Isotropic hardening and softening arising from the contribution of damage





Armstrong (2015)

Pineau et al. 2016

$$\underline{\dot{\epsilon}}^{in} = \underline{\dot{\epsilon}}^p + \underline{\dot{\epsilon}}^d$$

$$\underline{\dot{\epsilon}}^d = \sum_{s=1}^{N_{damage}} \underbrace{\dot{\delta}_c^s \underline{n}_d^s \otimes \underline{n}_d^s}_{\text{Opening}} + \underbrace{\dot{\delta}_1^s \underline{n}_d^s \otimes \underline{l}_{d1}^s}_{\text{Shear M II}} + \underbrace{\dot{\delta}_2^s \underline{n}_d^s \otimes \underline{l}_{d2}^s}_{\text{Shear M III}}$$

Crack growth

where $\dot{\delta}_c^s$, $\dot{\delta}_1^s$, $\dot{\delta}_2^s$ are the strain rates for mode I, mode II, and mode III crack growth, respectively.

$$\tau_{dc} = \underline{n}_d^s \cdot \underline{M} \cdot \underline{n}_d^s$$

$$\dot{\delta}_c^s = \left\langle \frac{\tau_{dc} - Y_c^s}{K_d} \right\rangle^{n_d} sign(\tau_{dc})$$

Background in Aslan(2011) and Sabnis(2016) for FCC and soft BCC materials

while the mode II and mode III shearing is computed similarly.

$$\tau_{di} = \underline{n}_d^s \cdot \underline{M} \cdot \underline{l}_{di}^s$$

$$\dot{\delta}_i^s = \left\langle \frac{\tau_{di} - Y_i^s}{K_d} \right\rangle^{n_d} sign(\tau_{di}), \;\; with \;\; (i = 1, 2)$$

Cleavage systems in BCC operate on [100] planes

$$Y := Y_0 + Hd + H\beta\gamma$$

Initial cleavage threshold

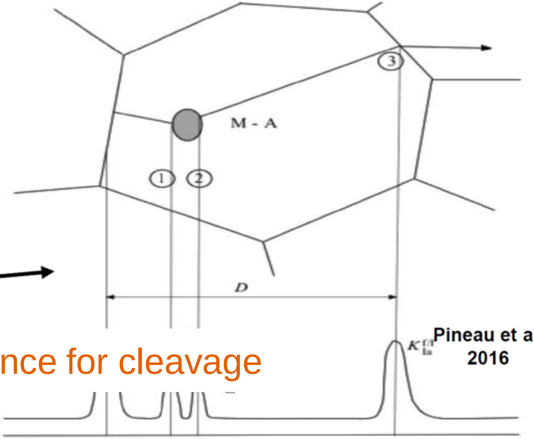
Softening by damage itself

Softening by plasticity

Damage variable (d) is strain based instead of scalar [0,1]

Therefore, crack opening strain is tracked and it can go back to zero (crack is closed)

Local cleavage resistance is dependent on microstructure and local defects



Pineau et al. 2016

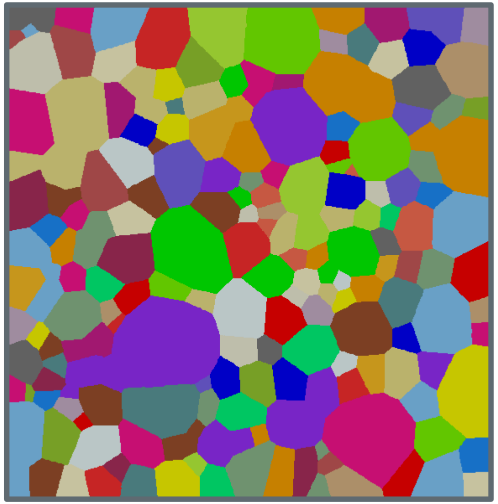
Resistance for cleavage

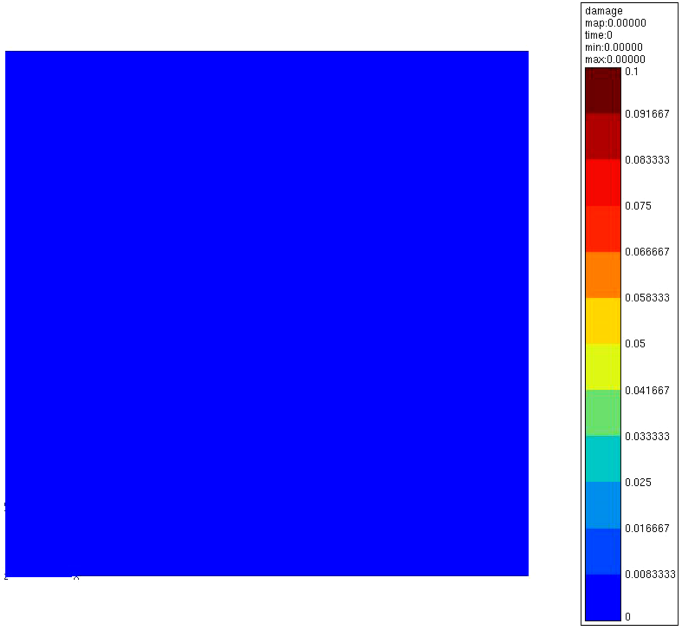
Damage model parameters

- Plasticity
  - Initial critical resolved shear stress, τ_0 (slip families 110, 112)
  - Hardening coefficient, Q
  - Interaction matrix (slip-slip), H_1-H_8
  - Strain rate parameters, K, n
  - Kinematic hardening parameters, C, D
- Damage
  - Softening parameters, H_i (for each damage mode)
  - Plasticity-damage coupling parameter, β
  - Cleavage opening threshold, τ_{cl}
  - Cleavage shear mode II threshold, τ_{sl}
  - Cleavage shear mode III threshold, τ_{sh}
  - Viscous parameters (growth rate)
  - Limiting compression strength, α
  - Hardening limit (damaged zones)

Case example with modelling: Martensite steel cracking

- Tensile test
- Damage evolution



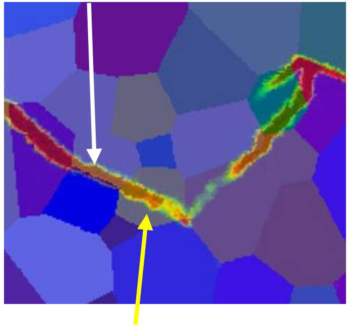


Case example with modelling: Martensite steel cracking

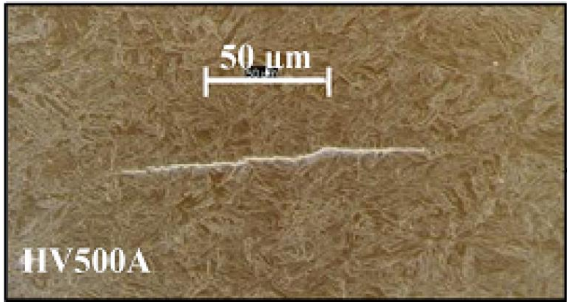
- Damage initiates near grain boundaries, usually at triple points
- Damage propagates intra grain and inter grain, e.g., at grain boundaries and within grains
- Shear localization affects damage path

Triple point GB

Grain boundary propagation

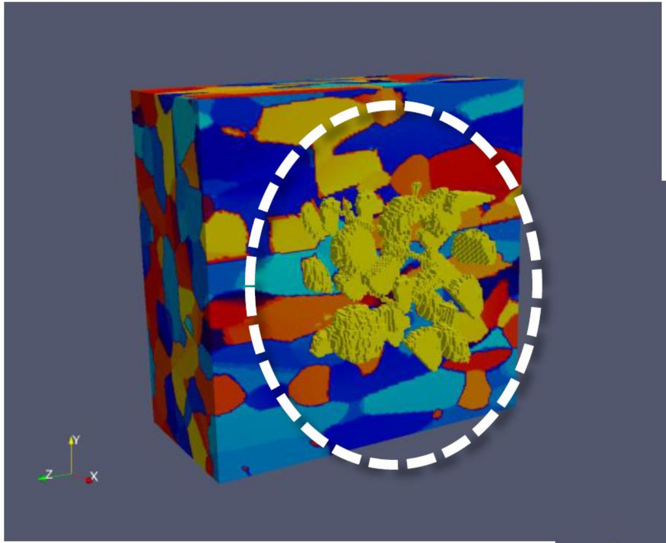


Intra-grain propagation

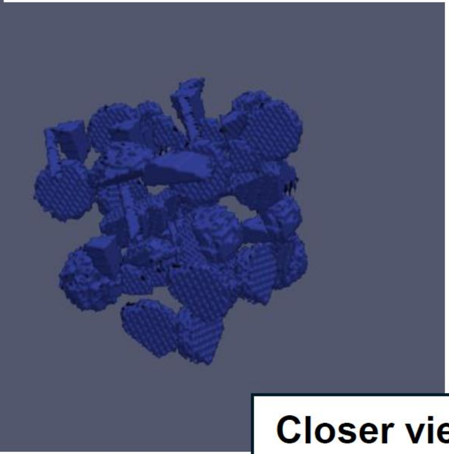


Model development for UO_2 and CeO_2 cracking

- Inclusions: gas bubbles at grain boundaries, porous phases
- Crystal plasticity: Discontinuities can be taken into account as geometrical objects with different or absent material properties or as field variable in FE analysis.
- Coupled phase field modelling: size evolution of porous phases



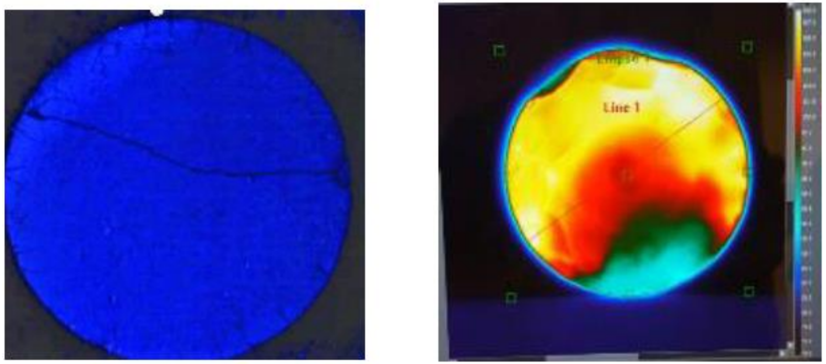
Inclusion cluster in an anisotropic oriented microstructure



Closer view of cluster inclusion phase

Experimental comparison

- Induction heating applying Ar as cooling gas
- Simultaneous optical and infrared imaging
- Different temperatures and temperature gradients



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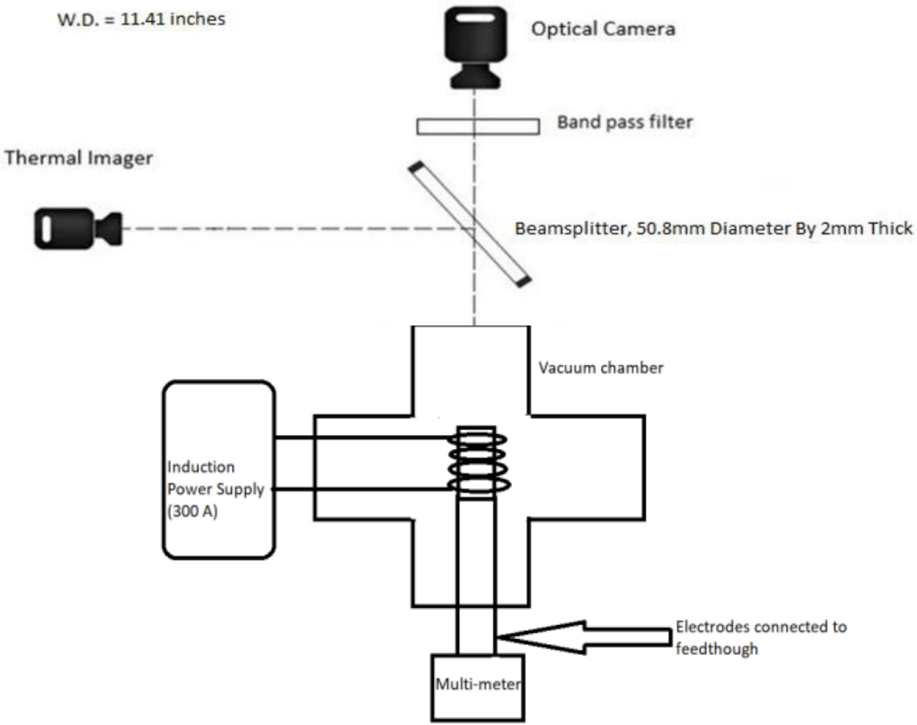

Future plans

- CeO_2 and UO_2 EBSD imaging and crystal model construction
- Test crystal plasticity modelling to reference fuel materials
- Add porosity and/or fission gas bubbles to the grain boundaries and apply phase field modelling together with the crystal plasticity approach
- Comparison of the obtained results to similar modelling at INL preferably with the MARMOT/BISON codes
- Comparison of the results with the upcoming experiments at INL

Thank you!

beyond
the obvious

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