Imperial College London

Centre for Nuclear Engineering

Peridynamic Modelling of Nuclear Materials

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Contents

- Introduction to peridynamics:
  - What is it?
  - What are the advantages over FE?
  - How do we do it?
- UO_2 fuel pellets.
- SiC/SiC accident-tolerant fuel.
- ZrO_2 cracking and Zr cladding oxidation.

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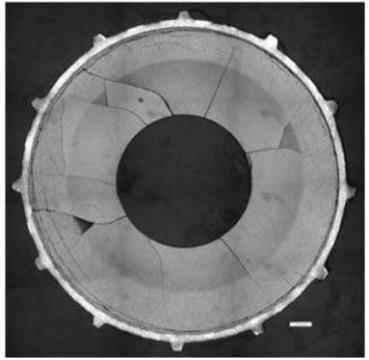
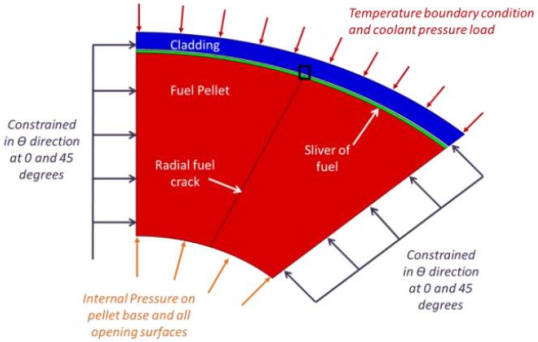
What are the Advantages of Peridynamics?

- Our previous work has used idealised assumed crack patterns.
- The real world isn't like this:
  - Branching cracks.
  - Separate regions.
  - Micro-cracks.
- XFEM only allows us to model crack opening, not the crack patterns.
- Peridynamics offers:
  - No discontinuities at crack tips.
  - Multiple cracks.
  - Growth, branching, retardation and coalesce.
  - Improved mesh-insensitivity.

Haynes TA, Ball JA, Shea JH, Wenman MR. Finite element modelling of pellet-clad interaction during operational transients. TopFuel 2015 Oral Transactions. 2015:62-71.

Kallstrom R, Karlsson JKH, Johansson J, Levy M, Minay J, Barker M, et al. Post-irradiation Examinations on AGR fuel pins in Studsvik. TopFuel Transactions, Manchester, UK, 2- 6 September. 2012:104-9.

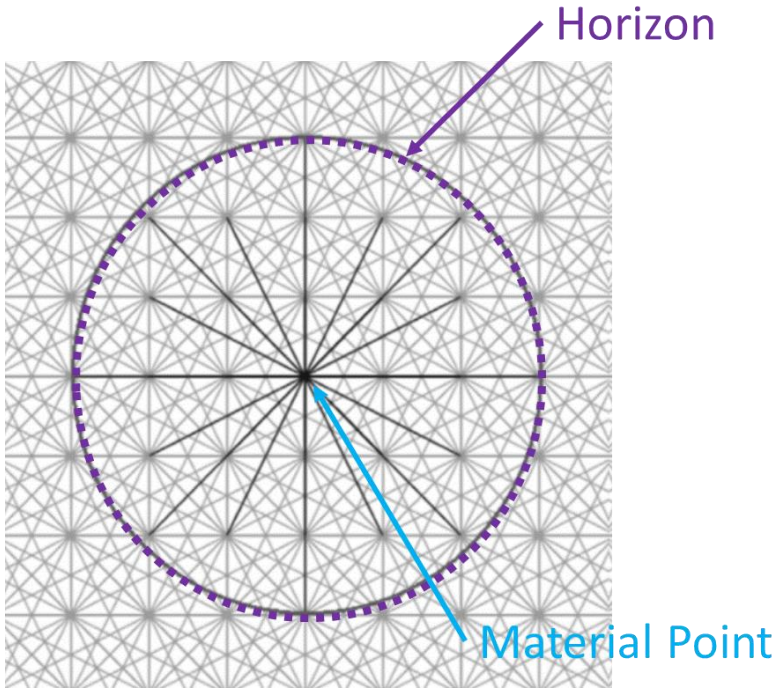




What is Peridynamics?

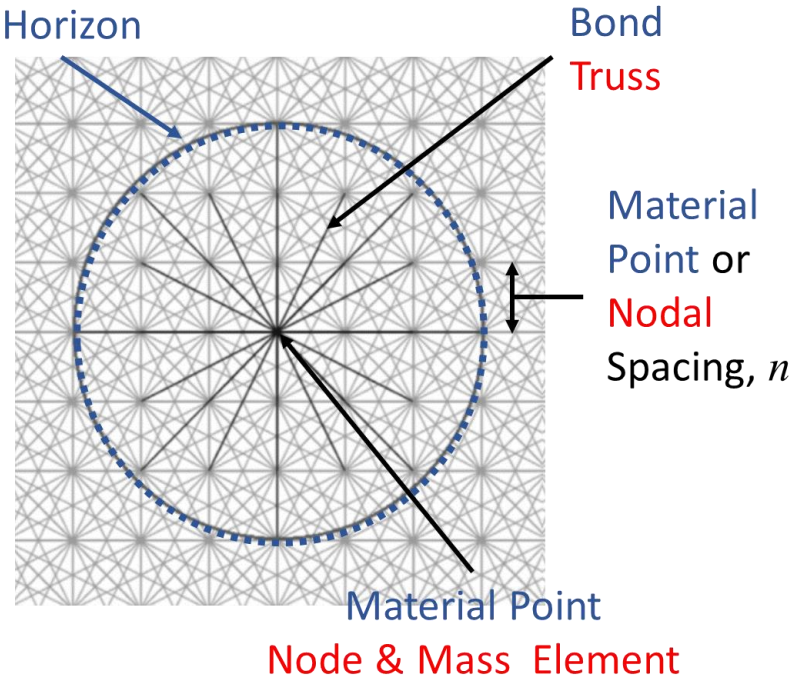
- A non-local modelling technique.
- ‘Force at a distance’.
- A horizon of material points.
- Reliance upon integrals rather than differentials.
- Can predict complex crack patterns.

Beckmann R, Mella R, Wenman MR. Mesh and timestep sensitivity of fracture from thermal strains using peridynamics implemented in Abaqus. Computer Methods in Applied Mechanics and Engineering. 2013;263:71-80.



Bond-Based Peridynamics in a Finite Element Code

- Key ideas:
  - Mass elements are placed upon nodes and represent material points.
  - Truss elements connect nodes and represent bonds.
  - Loads and boundary conditions are applied to nodes.
  - Trusses convey the internal forces.
  - Trusses can fail causing fracture.
- Separate pre-processing program.
- This allows a range of material properties to be easily applied.



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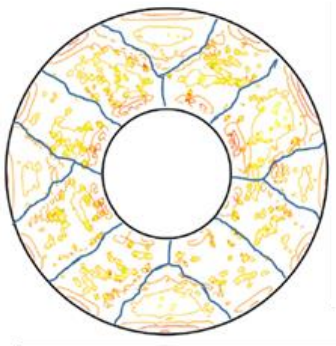
UO_2 Fuel Pellets – Initial Rise to Power

- Work carried out by Rizgar Mella whilst in our group.
- Peridynamics was carried out in LAMMPS.
- Cracking was predicted during initial rise to power.

Reproduced from Figure 4 in: Mella R, Wenman MR. Modelling fracture of nuclear fuel pellets during a power transient using peridynamics. J Nucl Mater. 2015;467:58–6



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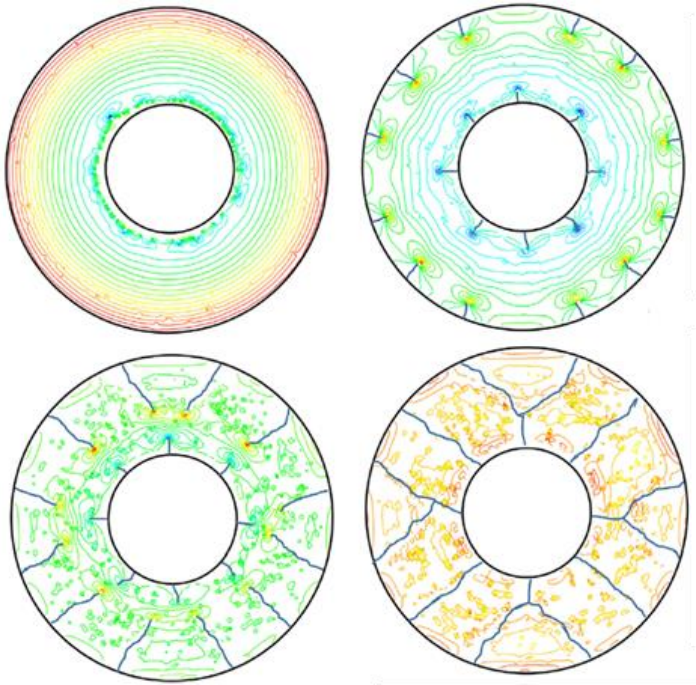
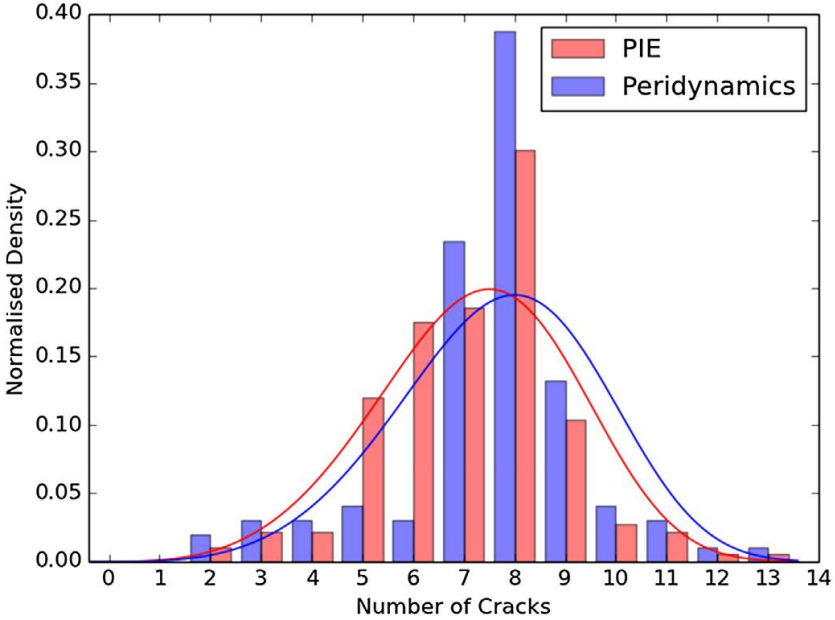


Reproduced from Figure 4 in: Mella R, Wenman MR. Modelling fracture of nuclear fuel pellets during a power transient using peridynamics. J Nucl Mater. 2015;467:58–6

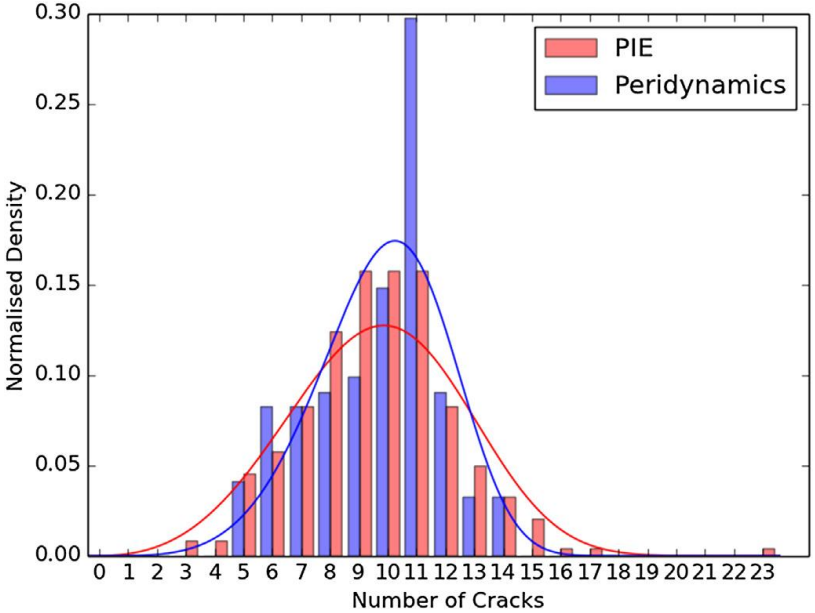
UO_2 Fuel Pellets – Validation

Reproduced from Figure 5 in:
Mella R, Wenman MR. Modelling fracture of nuclear fuel pellets during a power transient using peridynamics. J Nucl Mater. 2015;467:58–6

Inner Surface

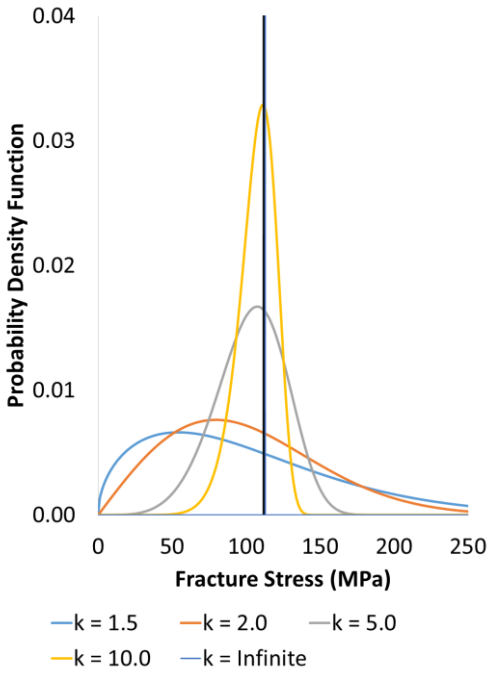


Outer Surface

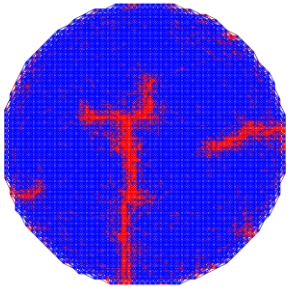
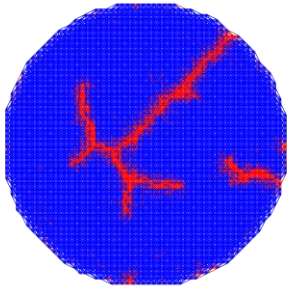
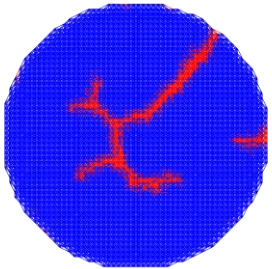
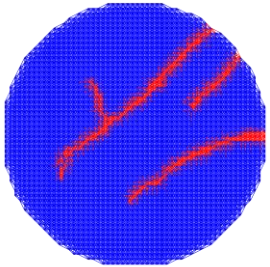


Current Work on Modelling LWR Fuel Pellets

- Lloyd Jones has focused upon the statistical treatment of failure.
- Ceramic samples typically fracture at a range of fracture stresses.
  - An Weibull distribution of fracture strains was applied to the bonds.
  - A characteristic strain, λ, was used, corresponding to fracture stress of 112.5 MPa.
  - A range of Weibull moduli, k were used.

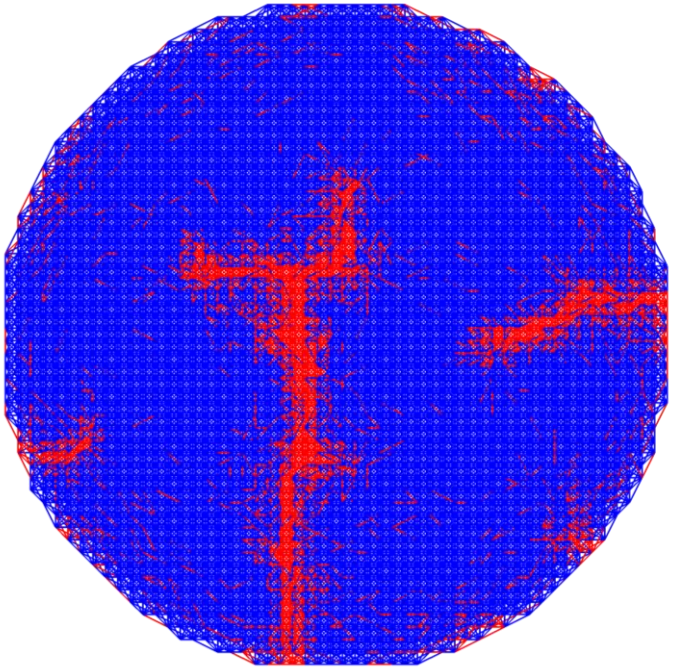


Varying the Weibull Modulus (Early Work)

 ***2.0***	 ***4.0***	***6.0***
 ***8.0***	 ***Infinite***	***Weibull Modulus***

Varying the Weibull Modulus

- Using a wider distribution of fracture stresses gives rise to more cracks on the pellet surface.
- It might be that greater cracking observed in doped fuels is due to a wider distribution of strengths.



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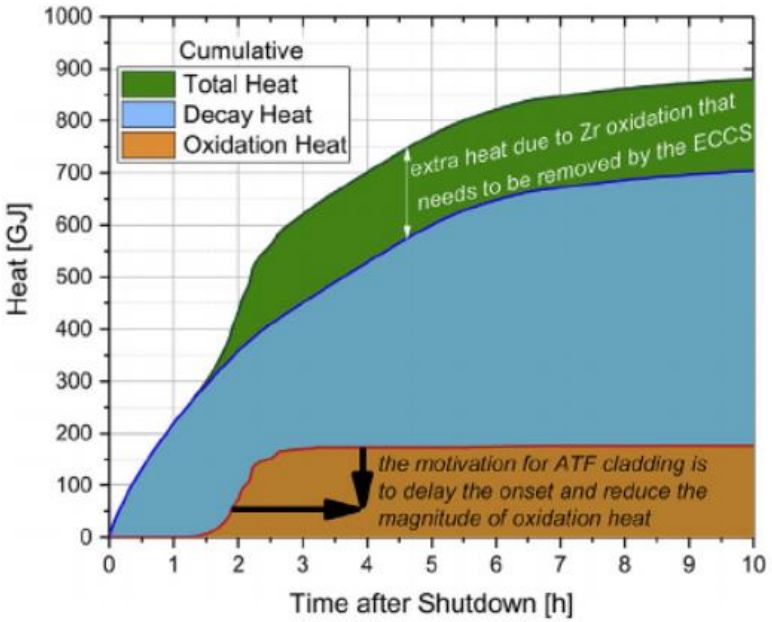
What are Accident Tolerant Fuels

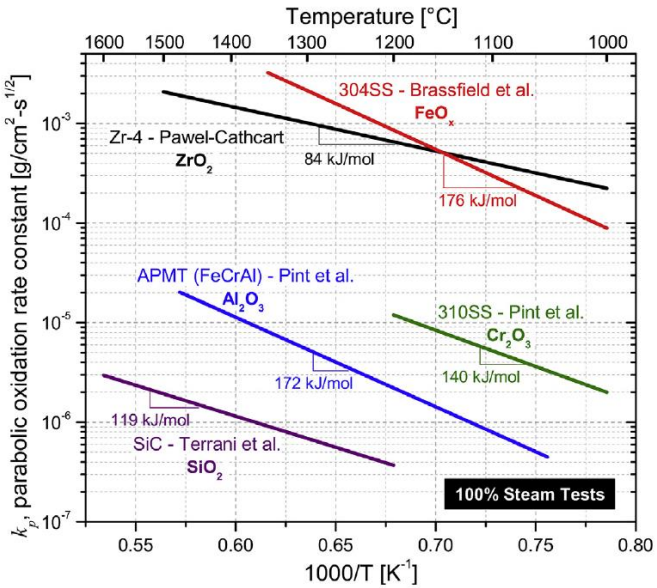
- Zirconium alloys offer excellent thermal, neutronic and corrosion performance during routine operation and DBAs.
- Their performance is less good during severe accidents:
  - Oxidization of the alloy is highly exothermic.
  - Hydrogen is produced.
  - The impact of the increased heat and hydrogen production were seen at Fukushima.



Reproduced from Figure 1 in:
Terrani KA. Accident tolerant fuel cladding development: Promise, status, and challenges. J Nucl Mater. 2018;501:13–30.

The Use SiC/SiC Cladding

- Why opt for Silicon Carbide Claddings?
  - SiC components are strong and are creep-resistant, reducing the ballooning seen in accidents.
  - SiC has been proposed for future reactor designs and is therefore comparatively well understood.
- Why not opt for Silicon Carbide Claddings?
  - SiC oxidises to for SiO_2.
  - SiO_2 is soluble in water.
  - Manufacturing and porosity challenges.
- Some of these challenges can be solved by controlled water chemistry.

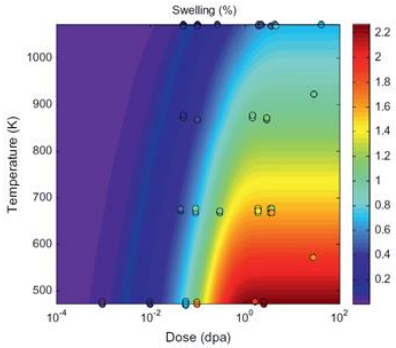


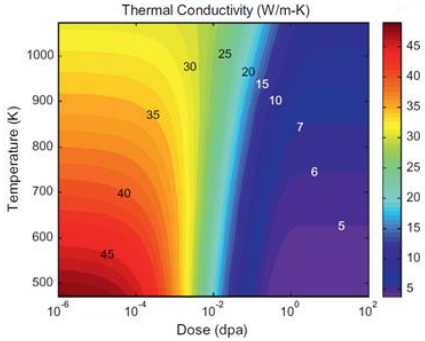
Reproduced from Figure 2 in: Terrani KA. Accident tolerant fuel cladding development: Promise, status, and challenges. J Nucl Mater. 2018;501:13–30.

Impact Upon Fuel Performance

Reproduced from Figures 1&2 in: Ben-Belgacem M, Richet V, Terrani KA, Katoh Y, Snead LL. Thermo-mechanical analysis of LWR SiC/SiC composite cladding. J Nucl Mater. 2014;447:125–42.

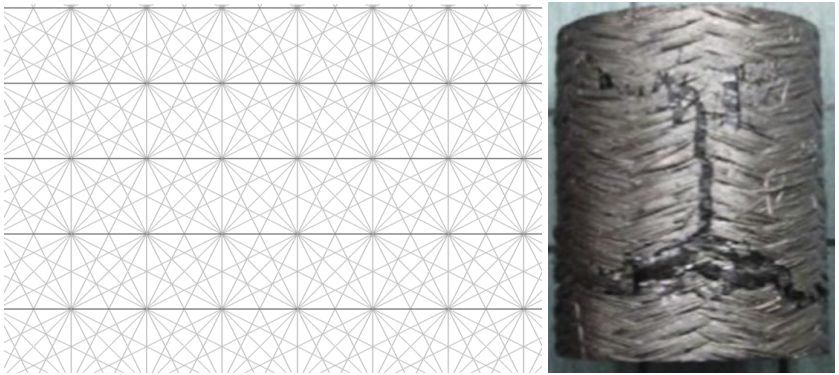
- Lower Thermal Conductivity:
  - This will give rise to larger temperature changes across the cladding and potentially higher fuel temperatures.
- Reduced Creep Rate
  - Normally, zirconium-based claddings creep onto the fuel over a number of years, reducing the fuel temperature and fission gas release.
- Increased Thermal Expansion:
  - This is likely to give rise to stresses within the cladding.
- Increased Swelling:
  - This is likely to give rise to stresses within the cladding.





Why Apply Peridynamics to SiC/SiC Cladding

- Complicated loading.
- Analogy between bonds and fibres.
- Ability to model anisotropy.
- Ability to model complicated architectures.

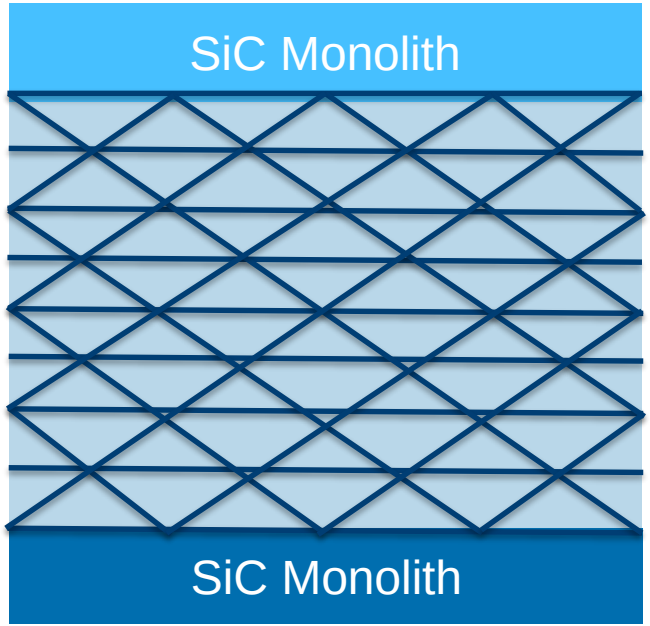


Reproduced from Figure 2 in: Jacobsen GM, Stone JD, Khalifa HE, Deck CP, Back CA. Investigation of the C-ring test for measuring hoop tensile strength of nuclear grade ceramic composites. J Nucl Mater. 2014;452:125–32.

Methodology – Architectures Studied

SiC Fibres

SiC Matrix

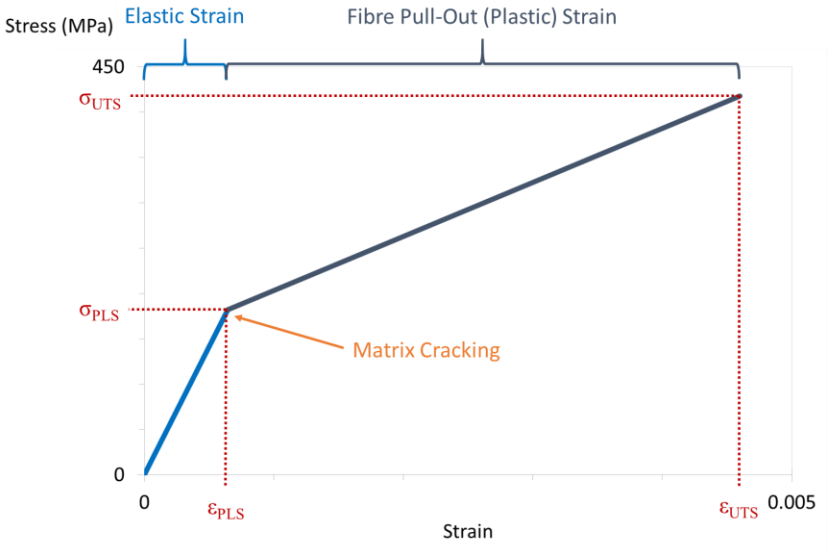


Outer Surface

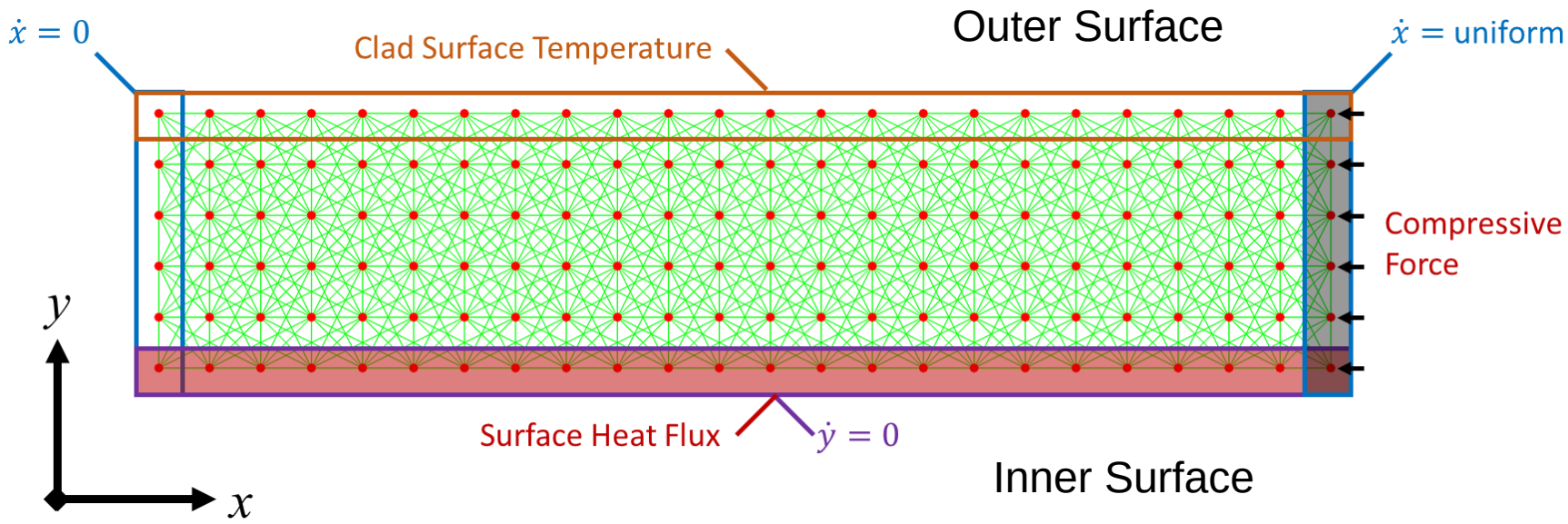
Inner Surface

Methodology – Smeared Fibre Response

- Initially, the material has been assumed to be isotropic.
- Fracture data was taken from Jacobsen et al. (JNM vol. 452).
- Matrix cracking was assumed to occur at the proportional limit strain.
- Fibre pull-out then occurs until the ultimate tensile stress.
- Fibre pull-out is modelled by plastic strain, referred to here as ‘pull-out strain’.

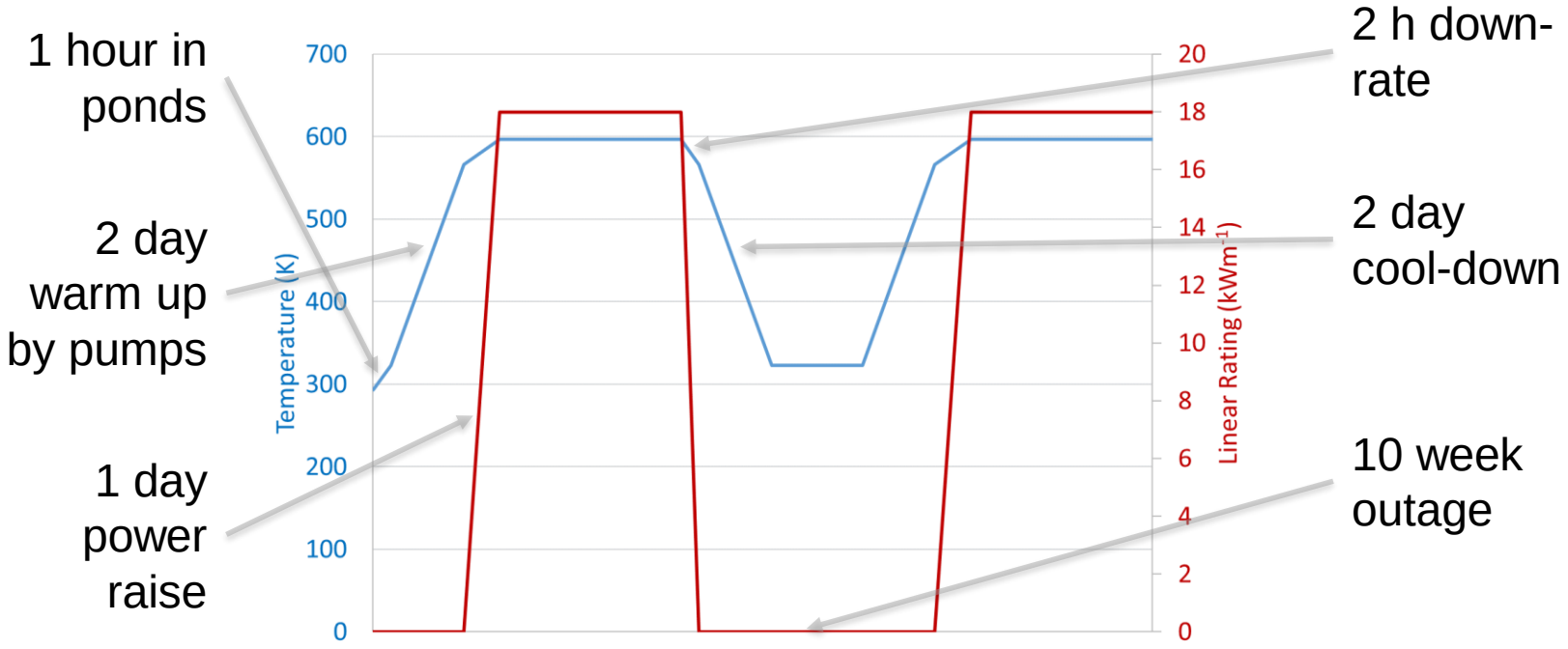


Methodology – Geometry, Loads & Boundary Conditions

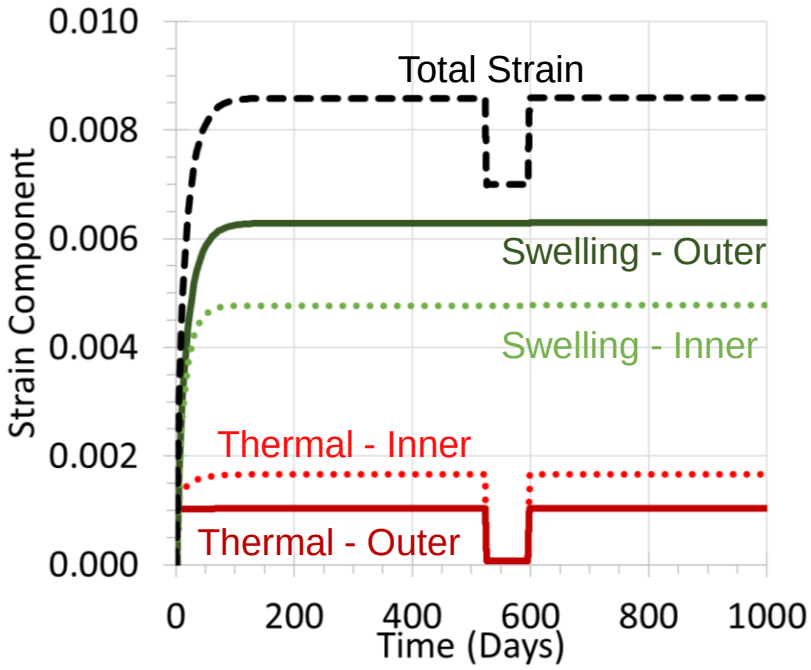


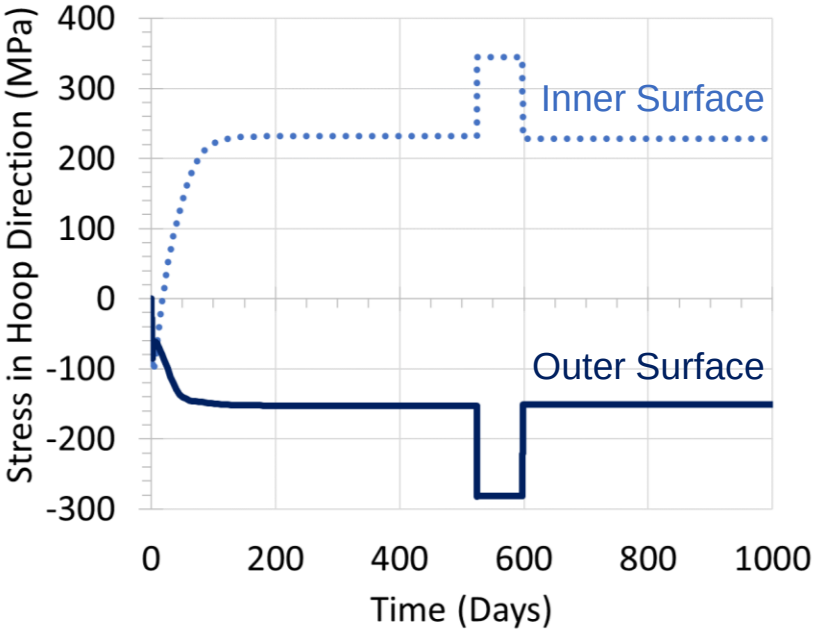
Straightened 1/8th segment of cladding

Methodology – Test Simulation

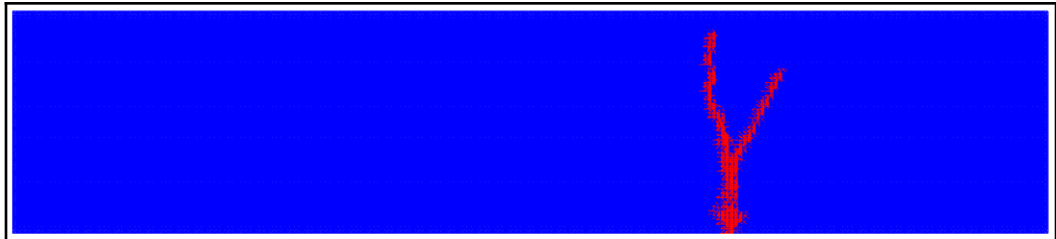
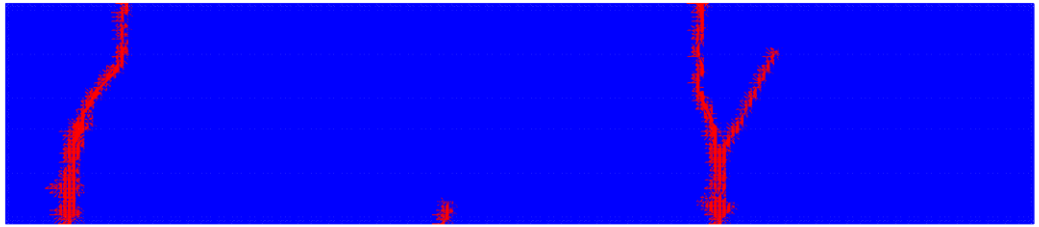
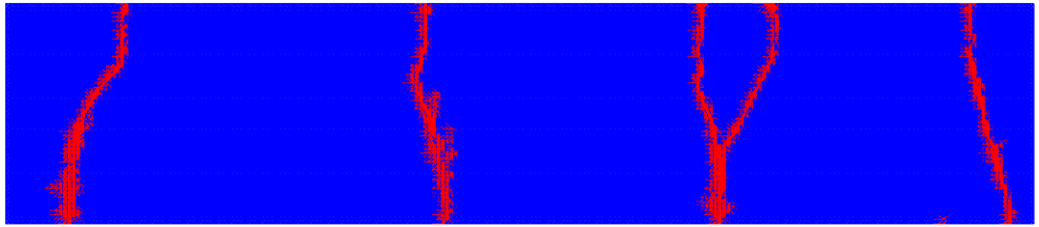


Stress State in the Cladding

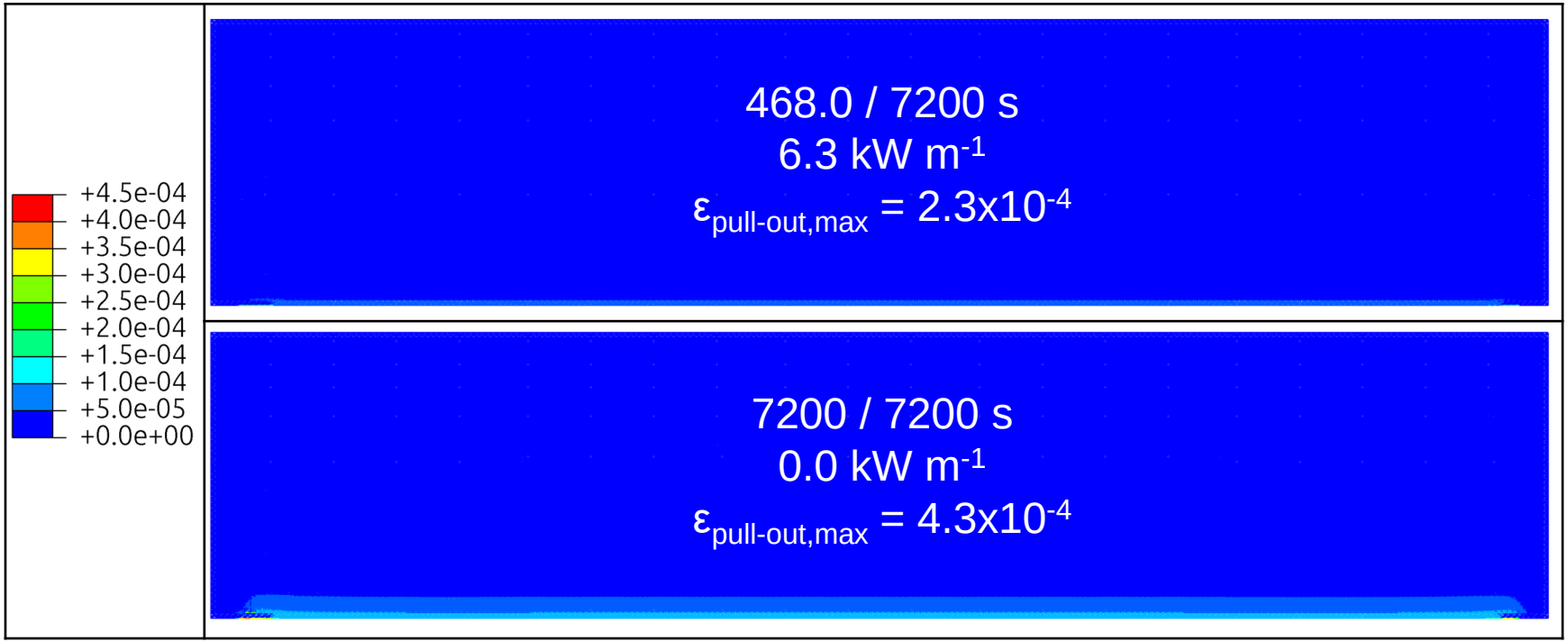




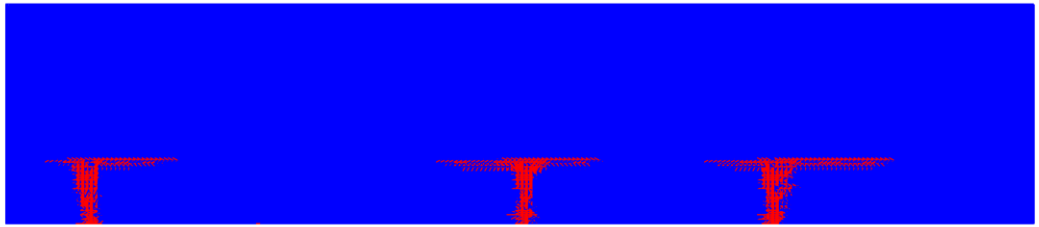
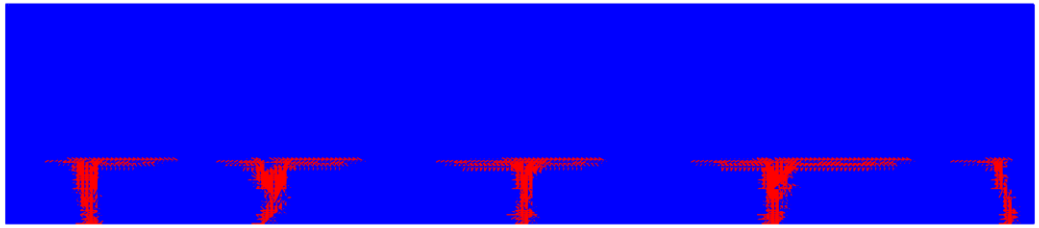
No Fibre Pull-Out – Cracking During Down-Rate

	Increment 300 405.7 / 7200 s Linear Rating = 17.0 kW m^{-1} Clad Surface Temperature = 595 K
	Increment 400 405.7 / 7200 s Linear Rating = 17.0 kW m^{-1} Clad Surface Temperature = 595 K
	Increment 600 405.7 / 7200 s Linear Rating = 17.0 kW m^{-1} Clad Surface Temperature = 595 K

With Fibre Pull-Out – Damage During Down-Rate

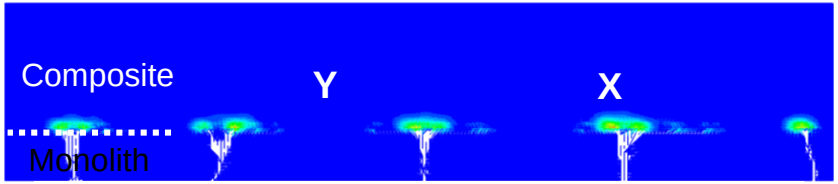


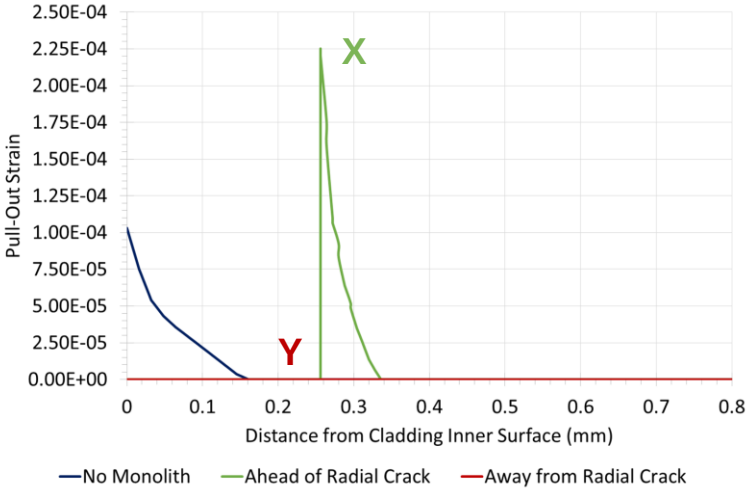
With Inner Monolith – Cracks in the Monolith

	Increment 200 413.6 / 7200 s Linear Rating = 17.0 kW m^{-1} Clad Surface Temperature = 595 K
	Increment 300 413.6 / 7200 s Linear Rating = 17.0 kW m^{-1} Clad Surface Temperature = 595 K
	Increment 500 413.6 / 7200 s Linear Rating = 17.0 kW m^{-1} Clad Surface Temperature = 595 K

With Inner Monolith – Strain Concentration in Composite

- When the inner monolith is modelled, strain concentration is observed in the fibre region (X).
- No pull-out strain is predicted away from the monolith cracks (Y).
- The maximum fibre pull-out strain predicted is doubled by the use of an internal monolith.





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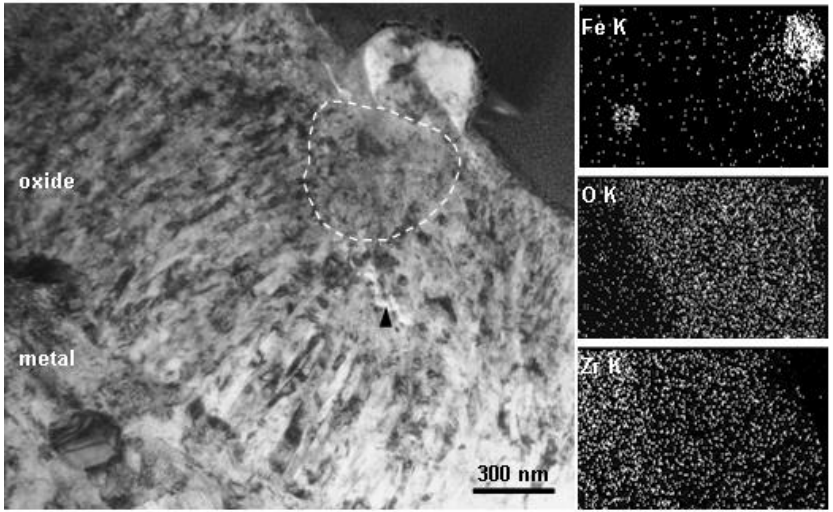
Secondary Phase Precipitates in Zirconium Alloys

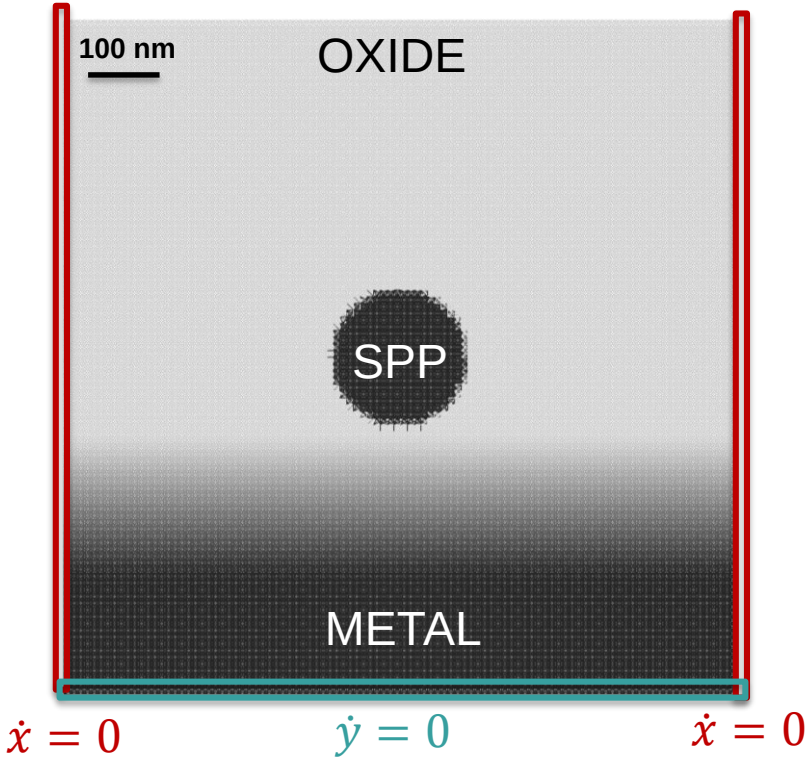
- SPPs (70-400 nm) are formed in claddings because alloying elements are above their solubility in zirconium.
  - In Zirc-2, Zr(Ni,Fe).
  - In Zirc-4, $Zr(Fe,Cr)_2$.
- When the oxidation front reaches an SPP, the SPP does not oxidise immediately and is left as a hard deformable island in a sea of brittle oxide.
- Some evidence that cracks in the protective oxide are associated with SPPs.



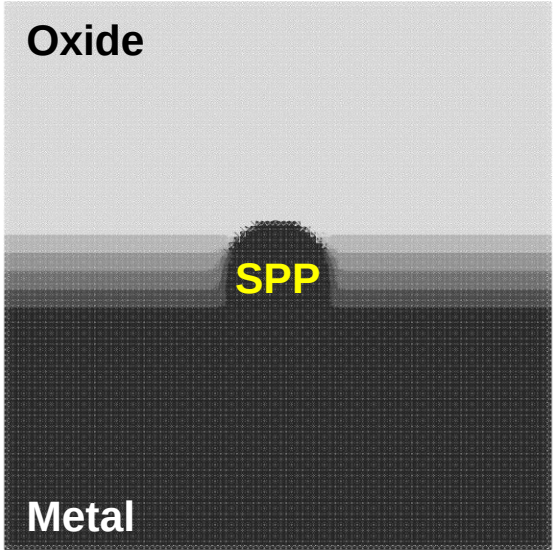
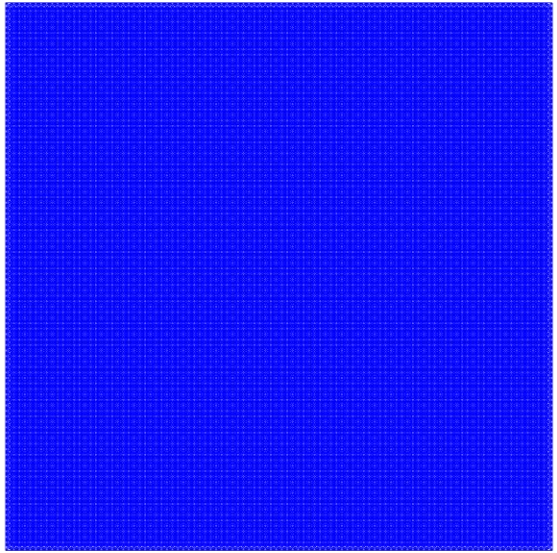
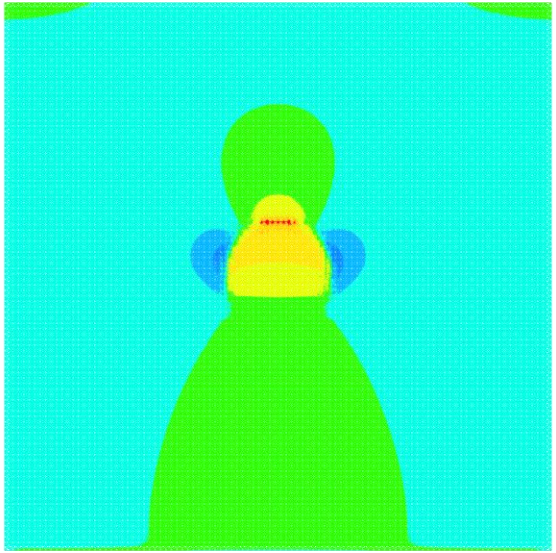
Reproduced from Figure 65 in: Proff, C., Aspects microstructuraux de l´oxydation d´alliages de zirconium. PhD Thesis, Universite de Grenoble, 2006

Modelling A Secondary Phase Precipitate

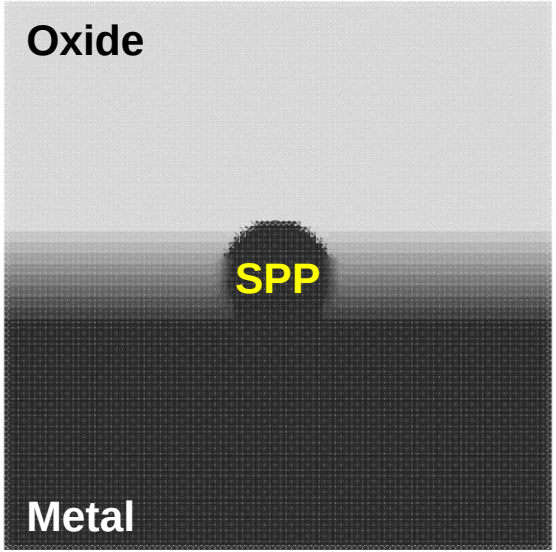
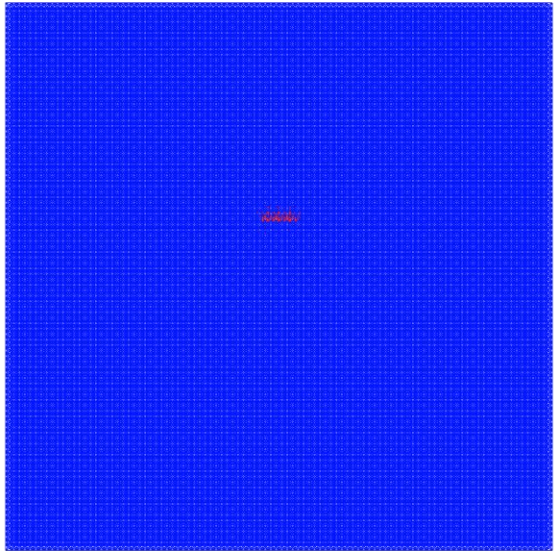
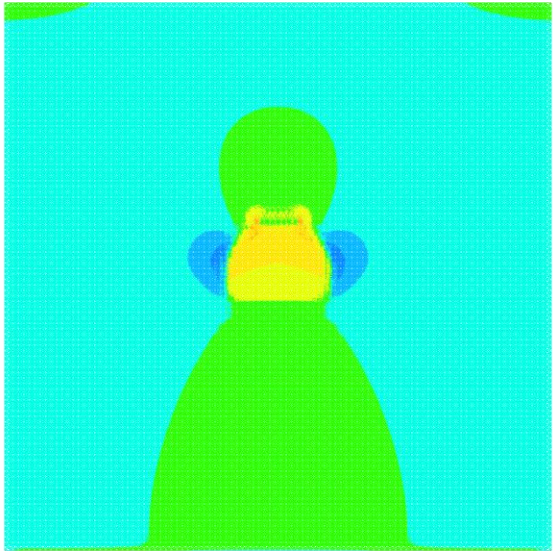
- SPP Radius = 100 nm
- Box = 1 µm
- 200 nm Metal-Oxide Transition
- Anisotropic Expansion:
  - $\varepsilon_x = 0.005$
  - $\varepsilon_y = 0.54$
- Elastic Moduli:
  - Metal 76 GPa
  - Zirconia 253 GPa
  - SPP 180 GPa



Crack Development Surrounding A SPP

Oxide Front	Crack Pattern	Bond Stress (MPa)
		

Crack Development Surrounding A SPP

Oxide Front	Crack Pattern	Bond Stress (MPa)
		

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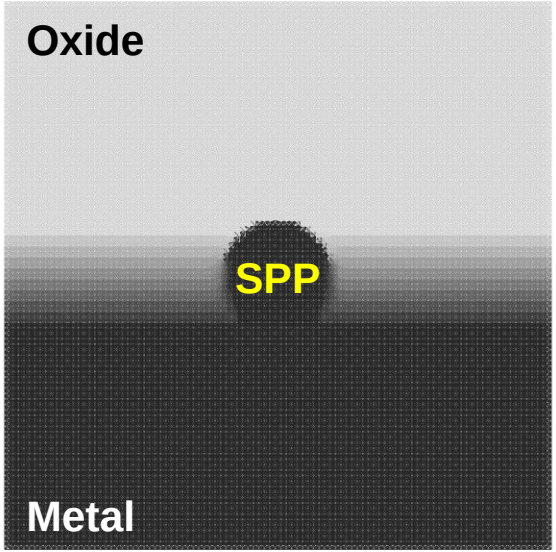	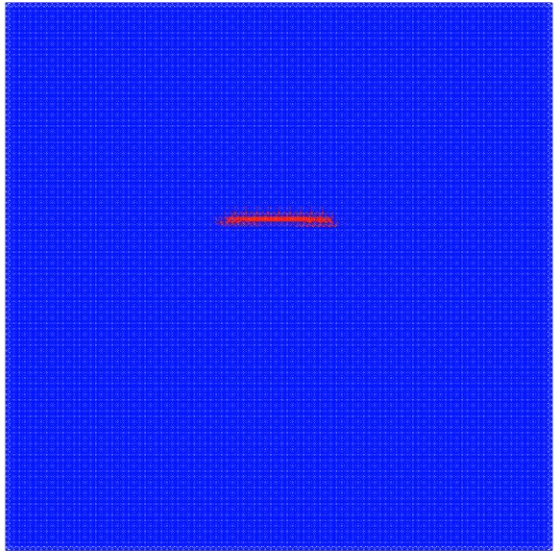	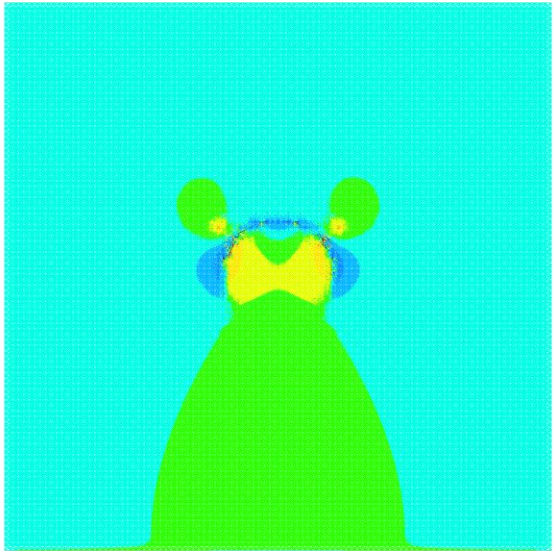

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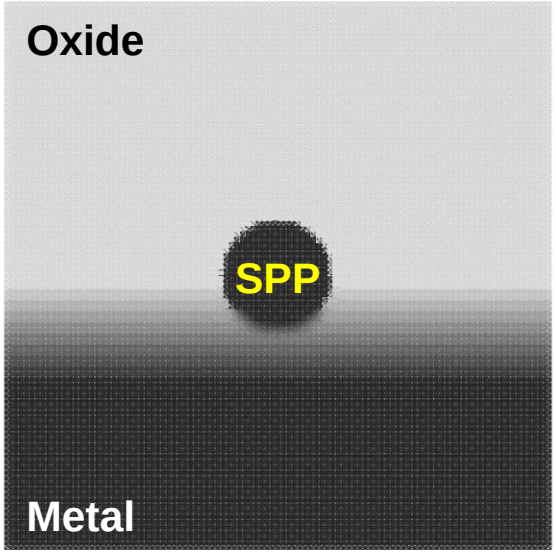	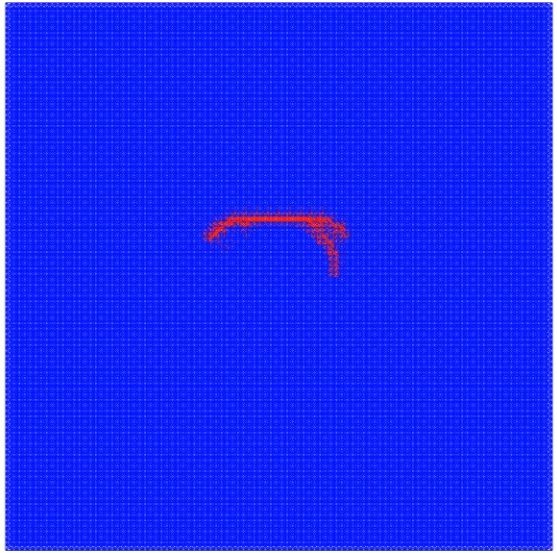	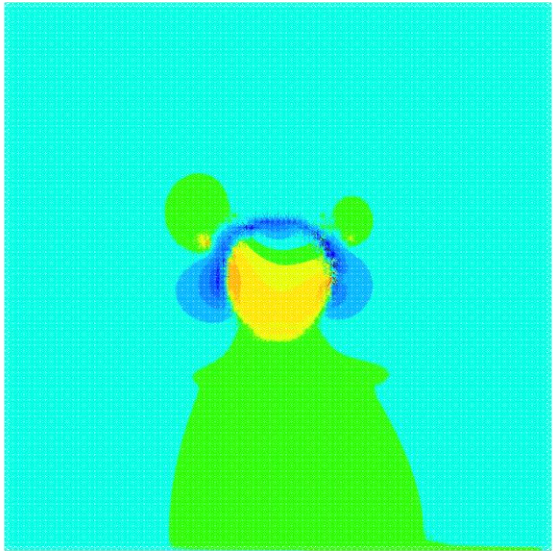

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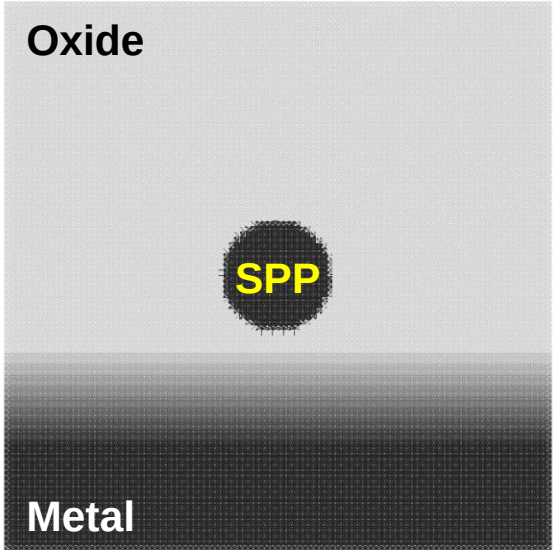
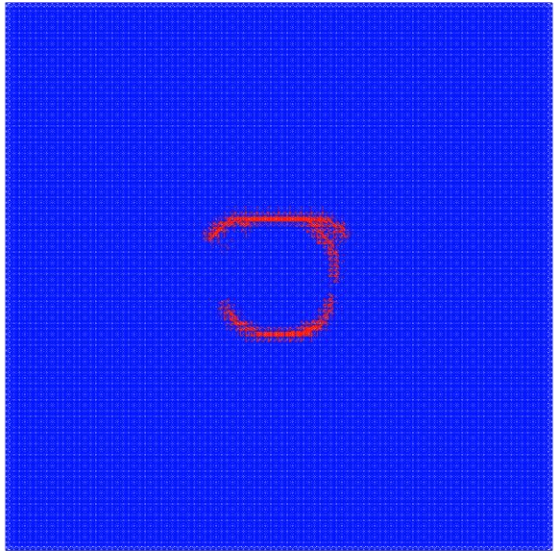
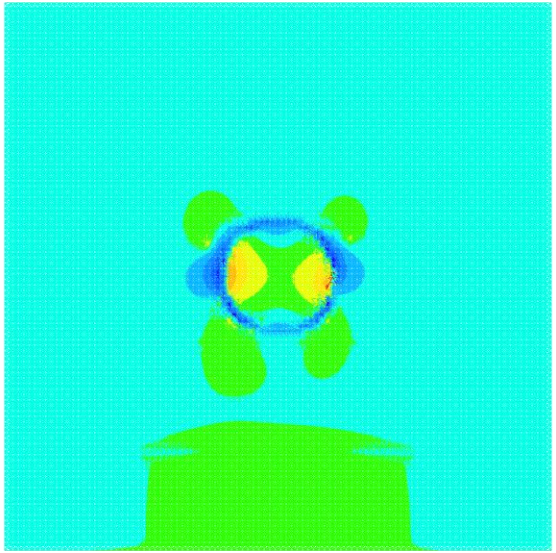
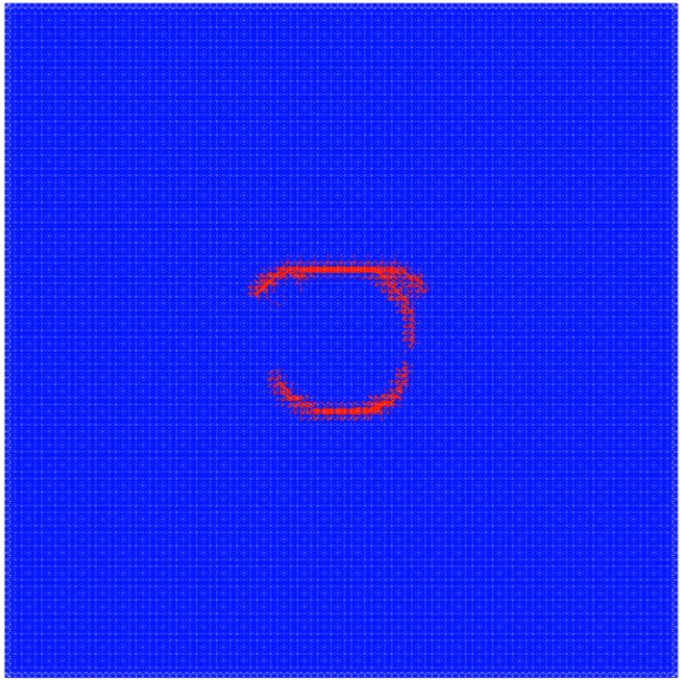
		

Next Steps

- Investigate Key Parameters:
  - SPP radius.
  - SPP ovality.
  - Oxide front width.
  - Level of oxide anisotropy.
- When might the cracks extend parallel to the oxide front?
- Possible Future Work:
  - Multiple SPPs.
  - Impact of orientation.
  - Impact of cladding microstructure.



Summary

- Peridynamics is an exciting technique which can be readily applied to nuclear materials.
- It has the ability to predict the crack pattern observed in fuel pellets.
- In SiC/SiC cladding, it is able to model the formation of cracks in the internal monolith and stress concentration in the composite above these.
- It is able to model crack formation surrounding SPPs in the protective oxide on zirconium based claddings.

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Peridynamic Modelling of Nuclear Materials

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MIDAS

EPSRC Engineering and Physical Sciences Research Council

NATIONAL NUCLEAR LABORATORY

Department for Business, Energy & Industrial Strategy