Peridynamic Modelling of Nuclear Materials

Thomas A. Haynes, Lloyd D. Jones, Mark R. Wenman

tah12@imperial.ac.uk
https://www.wenmannucleargroup.co.uk/
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.
Introduction to peridynamics:
- What is it?
- What are the advantages over FE?
- How do we do it?

- $\text{UO}_2$ fuel pellets.
- SiC/SiC accident-tolerant fuel.
- $\text{ZrO}_2$ cracking and Zr cladding oxidation.
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.


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.

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.
Contents

• Introduction to peridynamics:
  – What is it?
  – What are the advantages over FE?
  – How do we do it?
• $\text{UO}_2$ fuel pellets.
• SiC/SiC accident-tolerant fuel.
• $\text{ZrO}_2$ cracking and Zr cladding oxidation.
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:
UO₂ 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
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
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, $\lambda$, was used, corresponding to fracture stress of 112.5 MPa.
- A range of Weibull moduli, $k$ were used.

Current Work on Modelling LWR Fuel Pellets
<table>
<thead>
<tr>
<th>Weibull Modulus</th>
<th>Image 1</th>
<th>Image 2</th>
<th>Image 3</th>
<th>Image 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.0</td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.0</td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8.0</td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Infinite</td>
<td><img src="image9.png" alt="Image" /></td>
<td><img src="image10.png" alt="Image" /></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Weibull Modulus</td>
<td><img src="image11.png" alt="Image" /></td>
<td><img src="image12.png" alt="Image" /></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Varying the Weibull Modulus (Early Work)
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.
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.
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:
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 SiO₂.
  - SiO₂ 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

- 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.

Methodology – Architectures Studied

SiC Fibres

SiC Matrix

SiC Monolith

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 $1/8^{th}$ segment of cladding
Methodology – Test Simulation

1 hour in ponds

2 day warm up by pumps

1 day power raise

2 h down-rate

2 day cool-down

10 week outage
Stress State in the Cladding

- Total Strain
- Swelling - Outer
- Swelling - Inner
- Thermal - Inner
- Thermal - Outer

Strain Component

- Inner Surface
- Outer Surface

Stress in Hoop Direction (MPa)
### No Fibre Pull-Out – Cracking During Down-Rate

<table>
<thead>
<tr>
<th>Increment</th>
<th>Linear Rating</th>
<th>Clad Surface Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>405.7 / 7200 s</td>
<td>17.0 kW m$^{-1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>595 K</td>
</tr>
<tr>
<td>400</td>
<td>405.7 / 7200 s</td>
<td>17.0 kW m$^{-1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>595 K</td>
</tr>
<tr>
<td>600</td>
<td>405.7 / 7200 s</td>
<td>17.0 kW m$^{-1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>595 K</td>
</tr>
</tbody>
</table>
With Fibre Pull-Out – Damage During Down-Rate

468.0 / 7200 s
6.3 kW m\(^{-1}\)
\(\varepsilon_{\text{pull-out, max}} = 2.3 \times 10^{-4}\)

7200 / 7200 s
0.0 kW m\(^{-1}\)
\(\varepsilon_{\text{pull-out, max}} = 4.3 \times 10^{-4}\)
### With Inner Monolith – Cracks in the Monolith

| Composite containing fibres | Increment 200  
413.6 / 7200 s  
Linear Rating = 17.0 kW m\(^{-1}\)  
Clad Surface Temperature = 595 K |
|-----------------------------|---------------------------------------------------------------|
| Monolith                    | 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.
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.
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.

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

[Diagram showing the modeling of a secondary phase precipitate with SPP radius, box size, and metal-oxide transition.]
<table>
<thead>
<tr>
<th>Oxide Front</th>
<th>Crack Pattern</th>
<th>Bond Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Oxide</strong></td>
<td><img src="image1.png" alt="Crack Pattern" /></td>
<td><img src="image2.png" alt="Bond Stress" /></td>
</tr>
<tr>
<td><strong>Metal</strong></td>
<td><img src="image3.png" alt="Crack Pattern" /></td>
<td><img src="image4.png" alt="Bond Stress" /></td>
</tr>
</tbody>
</table>

**Crack Development Surrounding A SPP**
# Crack Development Surrounding A SPP

<table>
<thead>
<tr>
<th>Oxide Front</th>
<th>Crack Pattern</th>
<th>Bond Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxide</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Metal</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

![Oxide Front](image1.png)

![Crack Pattern](image2.png)

![Bond Stress](image3.png)
Crack Development Surrounding A SPP

<table>
<thead>
<tr>
<th>Oxide Front</th>
<th>Crack Pattern</th>
<th>Bond Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxide</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>SPP</td>
<td></td>
</tr>
<tr>
<td>Metal</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
# Crack Development Surrounding A SPP

<table>
<thead>
<tr>
<th>Oxide Front</th>
<th>Crack Pattern</th>
<th>Bond Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Oxide</em></td>
<td><em>Crack Pattern</em></td>
<td><em>Bond Stress (MPa)</em></td>
</tr>
</tbody>
</table>

![Oxide Front](image1.png)

![Crack Pattern](image2.png)

![Bond Stress](image3.png)
## Crack Development Surrounding A SPP

<table>
<thead>
<tr>
<th>Oxide Front</th>
<th>Crack Pattern</th>
<th>Bond Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxide</td>
<td>Crack Pattern</td>
<td>Bond Stress (MPa)</td>
</tr>
<tr>
<td>Metal</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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.
Peridynamic Modelling of Nuclear Materials

Thomas A. Haynes, Lloyd D. Jones, Mark R. Wenman

tah12@imperial.ac.uk
https://www.wenmannucleargroup.co.uk/