INL/MIS-20-59029-Revision-0

Coupling of Spark Plasma Sintering with Advanced Modeling to Enable Process Scale-Up: Presentation to DOE-NE

July 2020

Stephanie A Pitts, Troy Benton Holland, Larry K Aagesen Jr, Casey T Icenhour, Derek R Gaston, Albert Casagranda, Nathan D Jerred, Daniel Schwen, Dennis Stephen Tucker

Changing the World's Energy Future

Idaho National Laboratory

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Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Coupling of Spark Plasma Sintering with Advanced Modeling to Enable Process Scale-Up

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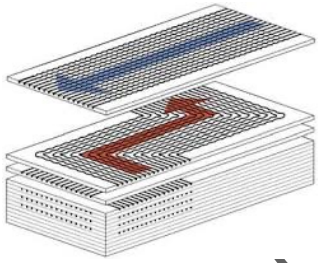
Swift Production of Specialized Parts

- Industrial scale Spark Plasma Sintering (SPS) has the potential to deliver rapid manufacture of consistent, high-performance parts

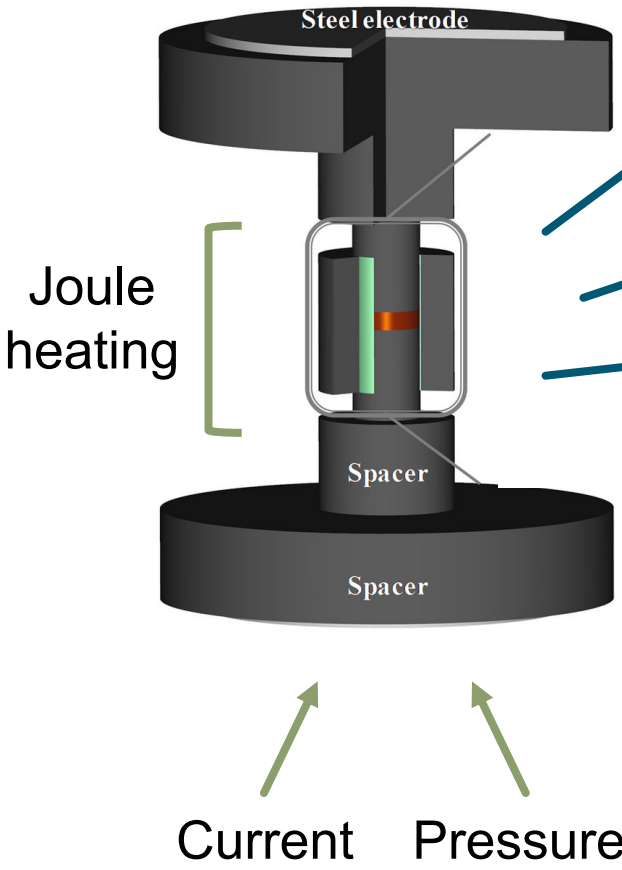


Gap: Inability to **predict** how SPS manufacturing **process parameters variations** affect the microstructure evolution of the part

Part microstructure **determines part performance**

Chanthapan et al., Advanced Materials and Processes (2011),
Le Pierres et al., Proceedings of SCO2 Power Cycle Symposium (2011), Chen et al., Applied Thermal Engineering 108 (2016)1409

Spark Plasma Sintering Applications Exist Throughout a Nuclear Reactor Power Plant



Fuel: Multicomponent and complex shapes (conductive ceramics)

First Wall: ITER heat shield (refractory metals)

Printed Circuit Heat Exchanger: Molten salt reactor power generation (refractory metals)

Advantages of SPS Manufacturing

- Reduced temperature and pressure requirements lows energy usage
- Near net shape parts
- Rapid heating rate enables better microstructure control

Manière et al. J. American Ceramic Society (2018) 16046

Leverage Modeling to Fine-Tune Manufacturing

- SPS is an effective technology to develop bulk nanostructured parts
- Viewed by industry as low volume, performance-tailored materials

Coarse Input Process Parameters

Desired Output:
- Consistent microstructure
- Reliable part performance
- Increased production

- Develop a modeling and simulation tool to add fine-tuned control of the SPS manufacturing process and scale-up
  - Increased output with 5-10x manufacturing speed-up
  - Reduction of energy use requirements by 70-80%

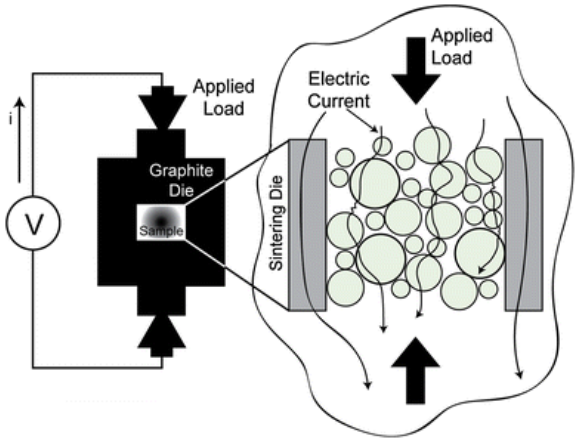
Kelly and Graeve, JOM 67 (2015) 1, Anselmi-Tamburini and Groze, Materials Science and Technology 22 (2017) 16
Etcha. The Taj Mahal, complete with ripples in the reflection (2007), Manière et al. J. American Ceramic Society (2018) 16046

Novel Multi-physics Multi-scale Approach

- A **high-fidelity and validated modeling** and simulation code application **advances** manufacturing for nuclear energy by
  - enabling process-informed manufacturing design
  - increasing **process scale-up**, microstructure consistency, and part performance.

Engineering scale model

acts as the framework for thermo-mechanical - electrical coupling

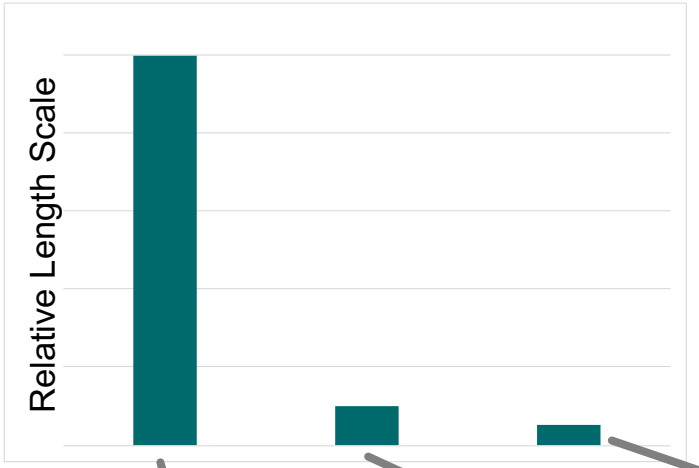


High fidelity information provided by local microstructure models

Deliberate validation experiments conducted at each length scale

Kelly and Graeve, JOM, 67 (2015) 1

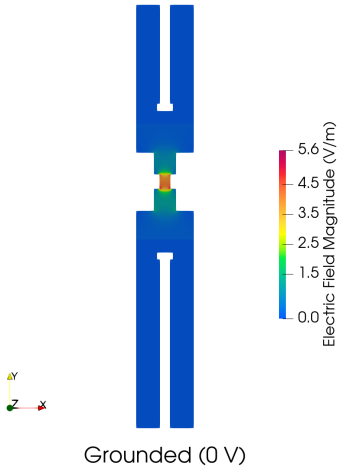
Proof of Principle: Capture Key Physics First



- Yttrium oxide selected as model material:
  - Simple crystal cubic structure
  - Does not form a space charge layer
  - Available in both micro- and nano-sized powders
  - Stable conductive ceramic can represent both metals and ceramics

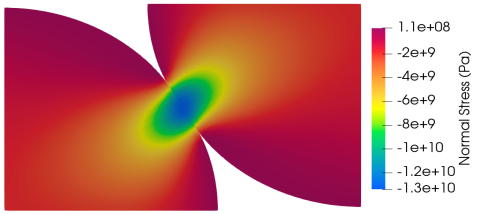
Engineering Scale

Applied Potential = 0.68 V

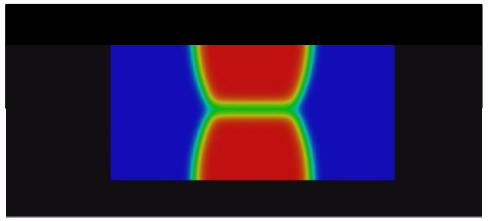


Grounded (0 V)

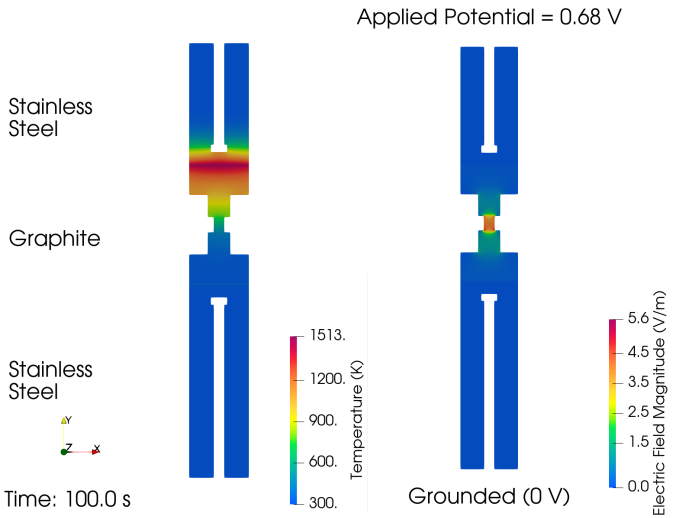
Multi-Particle Contact Model

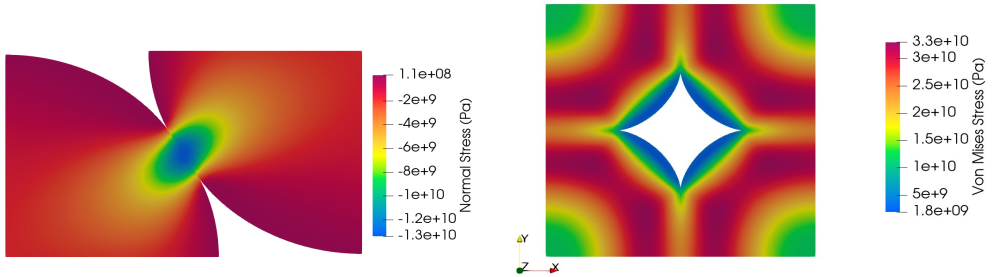


Microscale Particle Coalescence



Proof of Principle: Modeling on Multiple Scales





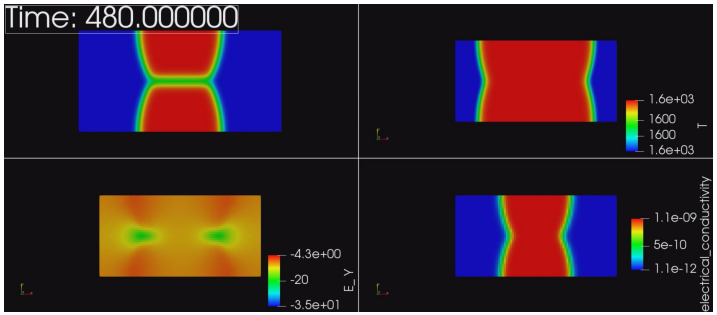
Multi-Particle Scale Contact Model:

Densification resulting from friction, sliding, and local particle deformation

Engineering Scale Die Model:

Thermodynamics and electrical field simulation as multiscale framework

Milestone: code repository established



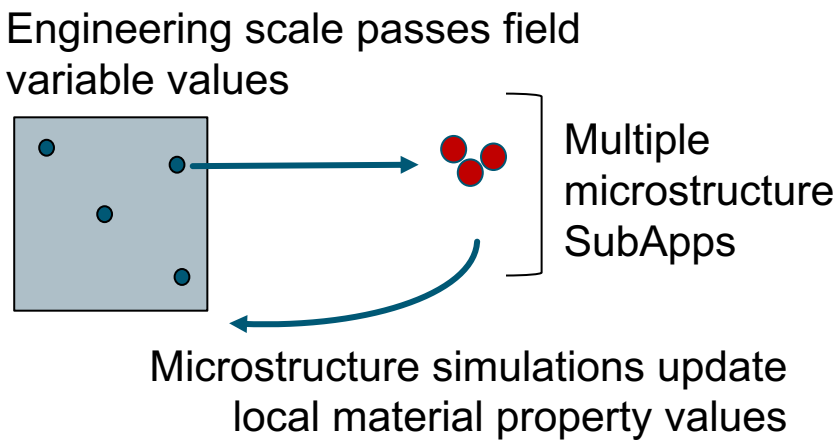
Microstructure Phase Field Model:

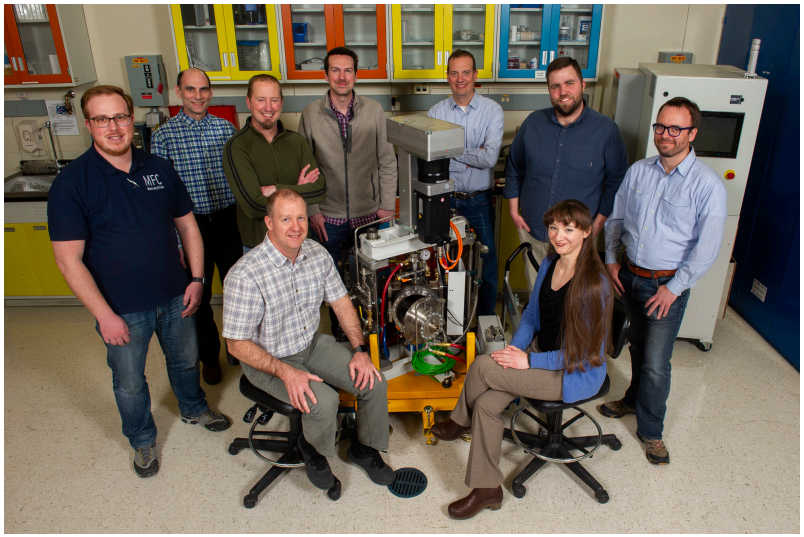
Particle coalescence causes local microscale property evolution

Key Finding: Local Joule heating does not significantly contribute to temperature increase for yttrium oxide

Multi-Disciplinary and Multi-scale Strengths

Multiphysics M&S code utilizes MOOSE's native MultiApp capability for parallel, coupled solves among scales





Modeling and Simulation Developers: Domain experts incorporate multiple physics at each length scale

Experimental Experts: Carefully design experiments to validate both individual length scales and multiscale models

Permann et al. SoftwareX 11 (2020) 100430

Delivering on the Initiative

- **Predictive modeling and simulation capabilities** being developed through FY21 will reduce manufacturing time and cost
  - **Shorten development time** for producing advanced materials
  - Extend code to additional advanced manufacturing techniques
- Many potential applications within nuclear power plants and wider energy sector for industrial scale advanced manufacturing

Enabling Process Scale-Up

from laboratory bench to industry setting

Idaho National Laboratory