INL/MIS-21-64076-Revision-0

Coupling of Spark Plasma Sintering with Advanced Modeling to Enable Process Scale-Up: LDRD Final Project Poster

August 2021

Stephanie A Pitts, Larry K Aagesen Jr, Casey T Icenhour, R. Edwin Garcia, Dennis Stephen Tucker, Jorgen Fredrick Rufner, Spencer T Doran, Lynn Brendon Munday, Al Casagranda, Troy B. Holland

Changing the World's Energy Future

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Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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

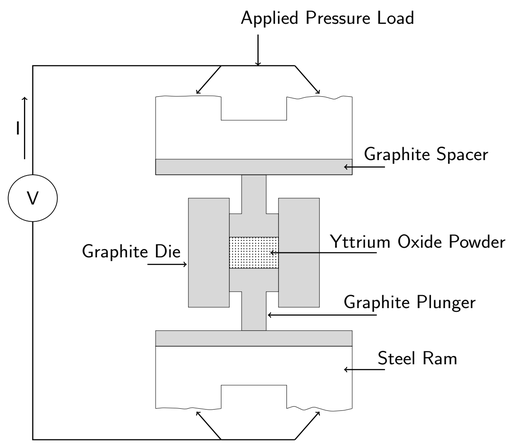
ADM Initiative: Innovative Modeling and Simulation (M&S) of Materials under Extreme Environments (3.2)

PI: Stephanie Pitts, **Co-PIs:** Larry Aagesen, Casey Icenhour (INL Graduate Fellow), **Collaborators:** Edwin García (Purdue University), Dennis Tucker, Jorgen Rufner, Luke Robinson (graduate student), Spencer Doran (INL intern), Lynn Munday, Al Casagranda, Troy Holland

Modeling Capabilities Developed to Predict Sintered Microstructure from Manufacturing Process Parameters

- Electric-field assisted sintering (EFAS) manufacturing techniques reduce energy usage requirements, fabricate near-net-shape parts, and produce bulk nanostructured materials through rapid heating and cooling rates achievable through Joule heating.
- Process parameters of pulsed DC voltage and constant pressure are applied through stainless steel rams and graphite tooling to the ceramic yttrium oxide powder to be sintered.

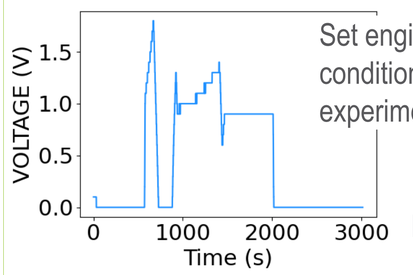
Our high-fidelity modeling code application advances manufacturing for extreme environments by enabling process-informed design and improving microstructure consistency through multiphysics, multiscale process-structure-property-performance correlation simulations. This code application is built on INL's Multiphysics Object-Oriented Simulation Environment (MOOSE) framework.



Schematic of EFAS technique rams, tooling, and powder

Concurrent Multiscale Electro-Thermal Simulations

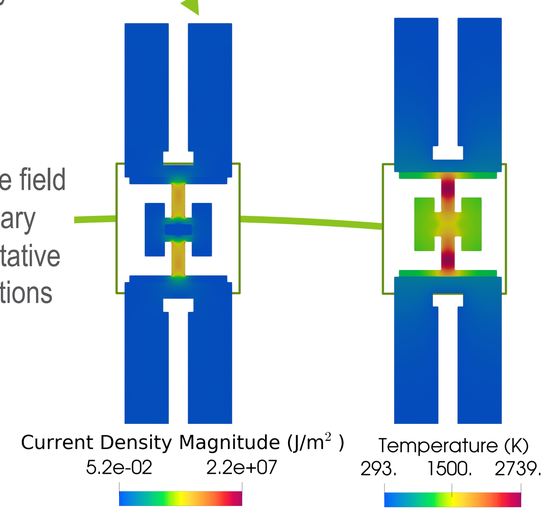
Applying advanced modeling capabilities to the inherently multiscale multiphysics EFAS technique, solve concurrently for coupled electric potential and temperature fields on multiple length scales throughout the entire simulation:



Applied voltage from actual run using the CAES "Dr. Sinter'" EFAS machine

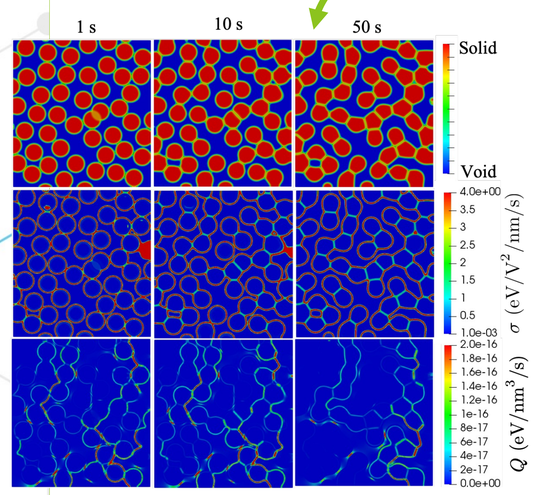
Set engineering scale boundary conditions from collected experimental data

Local engineering-scale field values set as boundary conditions to representative microstructure simulations



Standalone engineering-scale simulation after 10 minutes of applied electric potential and temperature evolution

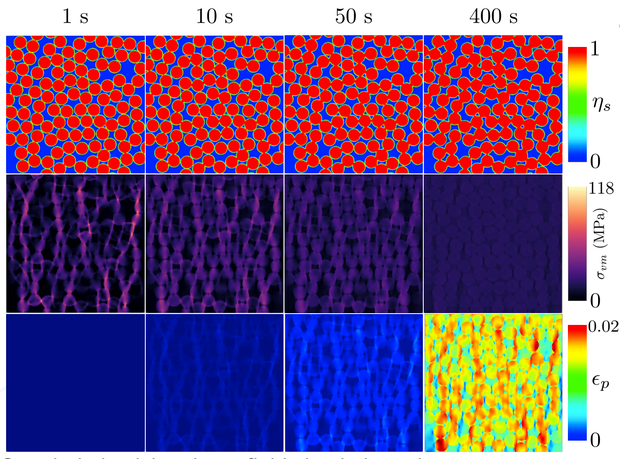
Pending two-way coupled calculation of the effective microstructure properties and heat generation for use in engineering-scale simulation



Electro-thermal phase field simulation results at 1600 K. Top row: microstructure, middle: electrical conductivity, bottom: heat generation.

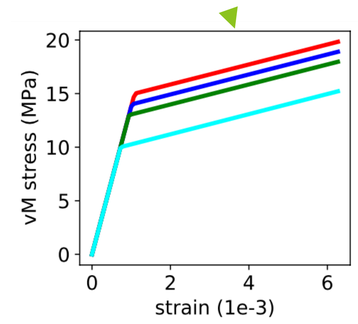
Lagged Electro-Thermal-Mechanical Simulations Focus on Powder Microstructure Evolution

Perform subsequent simulations focused solely on the powder to investigate the combination of mechanics and electro-thermal fields on sintering



Coupled plasticity-phase field simulations demonstrate the key role of stress in driving diffusion processes in sintering. Top row: microstructure, middle: effective stress, bottom: effective plastic strain.

Upscale microstructure evolution to the engineering scale



Engineering-scale stress-strain response with temperature dependent yield stress; the cyan curve is highest temperature and red is the lowest.

Connecting Microstructure Evolution to Manufacturing Process Parameters Across Time and Length Scales

- Developed a phase-field model of sintering that accounts for charged vacancies and effect of electric field on vacancy transport.
- Developed a coupled phase-field-mechanics model to simulate the effect of applied stress, power law plasticity, and large deformation mechanics on the densification of a sintering particle powder compact.
- Improved the electro-thermo-mechanical engineering-scale model parameters for temperature and electrical conductivity through in-progress coupling with subApp phase-field simulations of particle sintering. Future work will use the multiApp system to weakly couple the physics at the macroscale to improve the convergence behavior.
- Enhanced MOOSE electromagnetic and heat conduction capabilities for electrostatic and thermal contact for domain interfaces without gaps.
- Employed stepped plungers for a constant electric potential drop during EFAS runs.
- Insulated yttrium oxide from graphite with tungsten carbide spacers to mitigate reduction of the oxide to metallic phase.

Research Outcomes Contribute to M&S Capabilities

- Contributions to MOOSE Electromagnetic Module for enhancement of interface models and multiphysics verification and validation. Copyright approved and introduction to public open-source framework pending.
- S.A. Pitts, S. Biswas, D. Yushu, A.D. Lindsay, W. Jiang, L.K. Aagesen, Modeling and Simulation of Advanced Manufacturing Techniques using MOOSE and MALAMUTE. Risk-Informed Methods and Application in Nuclear and Energy Engineering (submitted)
- L. K. Aagesen, L. D. Robinson, R. E. García. "An electrochemical phase-field model of sintering and application to SPS." In preparation.
- L. D. Robinson, L. K. Aagesen, R. E. García. "Large Deformation Mechanics and Sintering Mechanisms in SPS." In preparation.
- C. Icenhour, Development and Validation of Open Source Software for Electromagnetics Simulation and Multiphysics Coupling. PhD Dissertation, NC State Univ. In preparation.
- Contributions to the MOOSE Application Library for Advanced Manufacturing UTilitiEs (MALAMUTE) modeling and simulation tool, copyright application in process.

Capabilities developed through this project will be used in future projects to explore the influence of die geometries, powder materials and characteristics, and die materials on the final microstructure and the sintered material performance.

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