CANFSA

Center for Advanced Non-Ferrous Structural Alloys

An Industry/University Cooperative Research Center

Project 44-L: Characterization of Particulate Materials Simulating High Explosives

Semi-annual Spring Meeting

April 2022

Student: Summer Camerlo (Mines)

Faculty: Dr. Kester Clarke, Dr. Amy Clarke (Mines)

Industrial Mentors: Dr. Alexandra Burch (LANL), Dr. Brian Patterson (LANL)

National Nuclear Security Administration

Center for Micromorphic Multiphysics Porous and Particulate Materials Simulations with Exascale Computing Workflows, US DOE National Nuclear Security Administration (DOE/NNSA) Predictive Science Academic Alliance Program (PSAAP) III, NNSA Office of Advanced Simulation and Computing (ASC), in collaboration with Lawrence Livermore National Laboratory, Los Alamos National Laboratory, and Sandia National Laboratories

COLORADO SCHOOL OF MINES | NSF | IOWA STATE UNIVERSITY

Project 44-L: Characterization of Particulate Materials Simulating High Explosives

- Student: Summer Camerlo (Mines)
- Advisor(s): Amy Clarke, Kester Clarke (Mines)

Project Duration
MS: September 2020 - September 2022

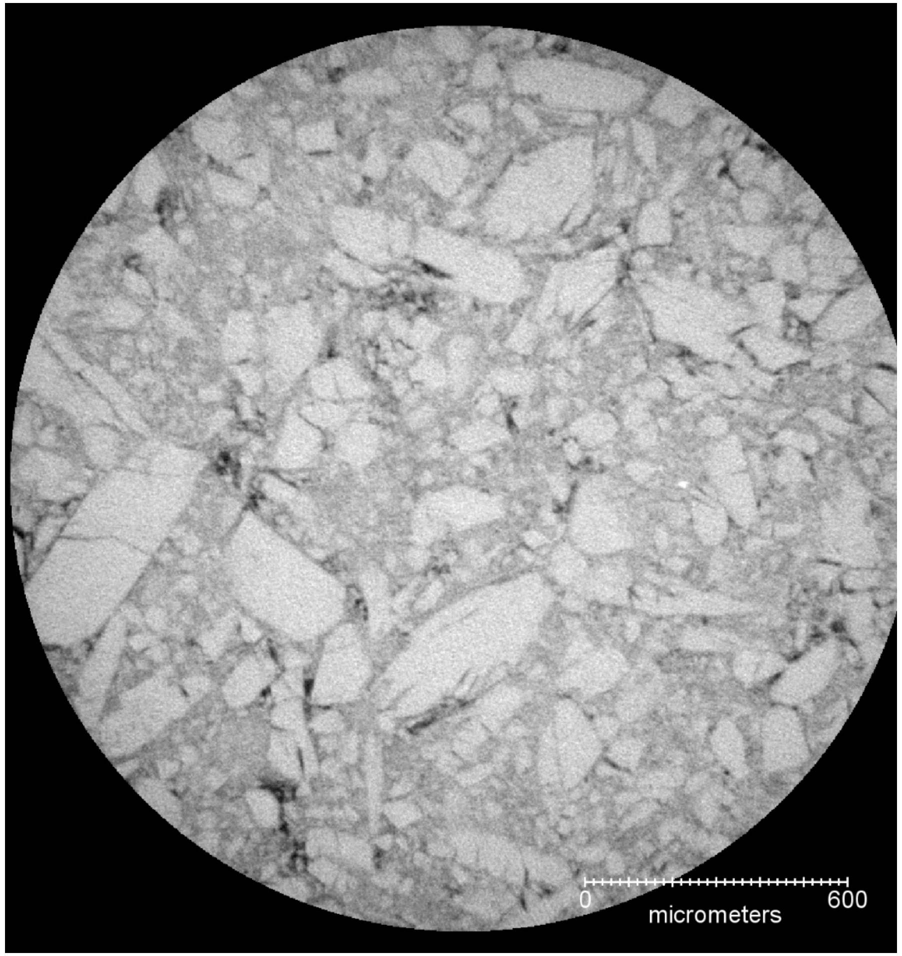
- Problem: Mock high explosive (HE) deformation characteristics are relatively unknown in the pristine and recycled states.
- Objective: Perform processing and multiscale experiments on the quasi-static to dynamic mechanical response of mock HE to support a 5-year, multi-university exascale computing effort lead by CU Boulder.
- Benefit: Experimental data sets for a range of particulate material responses that will be used for model calibration, verification and validation.

Recent Progress

- Completed internship at LANL. Formulated IDOX as well as new surrogate materials for testing at Mines
- Fabricated samples for distribution within research group for extensive testing at APS, SNL, UT Dallas, and CU Boulder
- Began investigation of CT hardening across different materials and binder types

Metrics		
Description	**% Complete**	**Status**
1. Literature review	75%	●
2. Creation of model samples for CT imaging for calibration	100%	●
3. Processing of recycled mock HE and making samples	100%	●
4. CT imaging of pristine and recycled mock HE	75%	●
5. Mechanical properties and characterization of pristine and recycled mock HE and surrogate mocks	50%	●

What are Mock High Explosives?



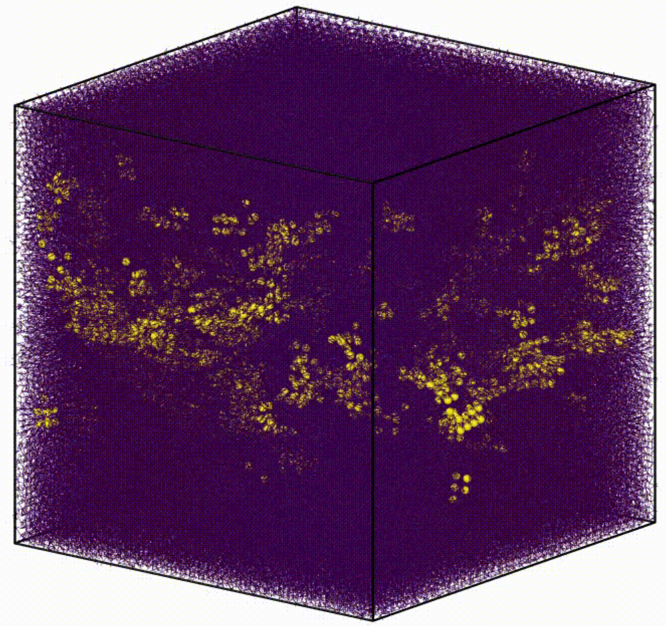
J.D. Yeager et al., J. Energ. Mater. 36 (2018) 253–265.

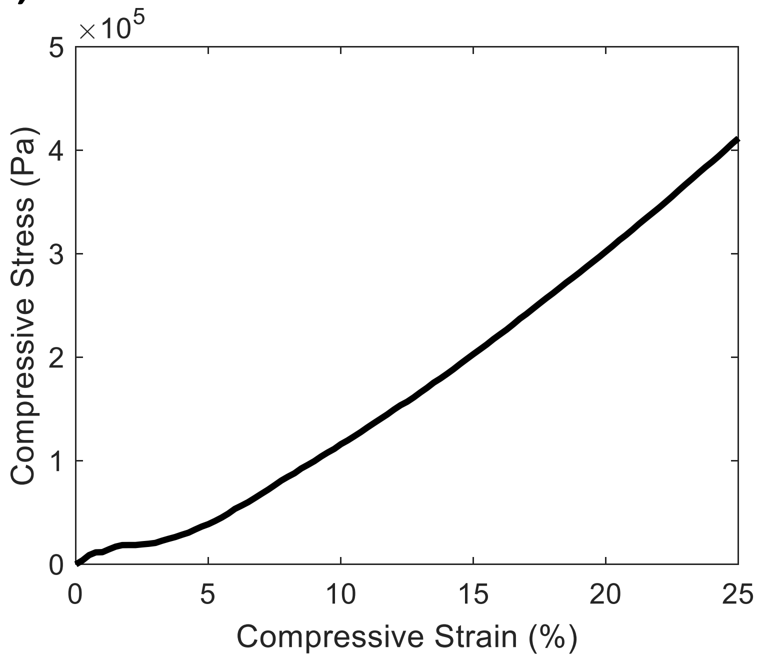
- High explosives (HE) replaced with mock HE during mechanical testing for safety
- Better mock = more experiments that can be done
- Cyclotetramethylene-tetranitramine (HMX) in particular is very difficult to manufacture
- 5-Iodo-2'-deoxyuridine (IDOX) crystals identified as best surrogate for HMX

Mock HE = mix of 10-600 micrometer diameter particles of idoxuridine (IDOX) with polymeric binder (Estane)

PSAAP Objective

- Mock HE's are cheaper and safer
- Ideally match multiple properties
- The best match for HMX, idoxuridine, is challenging
- By working up to modeling IDOX through F50 sand, can produce a robust computer modeling simulation for safer, cheaper, and more extensive testing of high explosives





Courtesy Samuel Lamont, CU Boulder 2022

Center Proprietary – Terms of CANFSA Membership Agreement Apply

Global Overview

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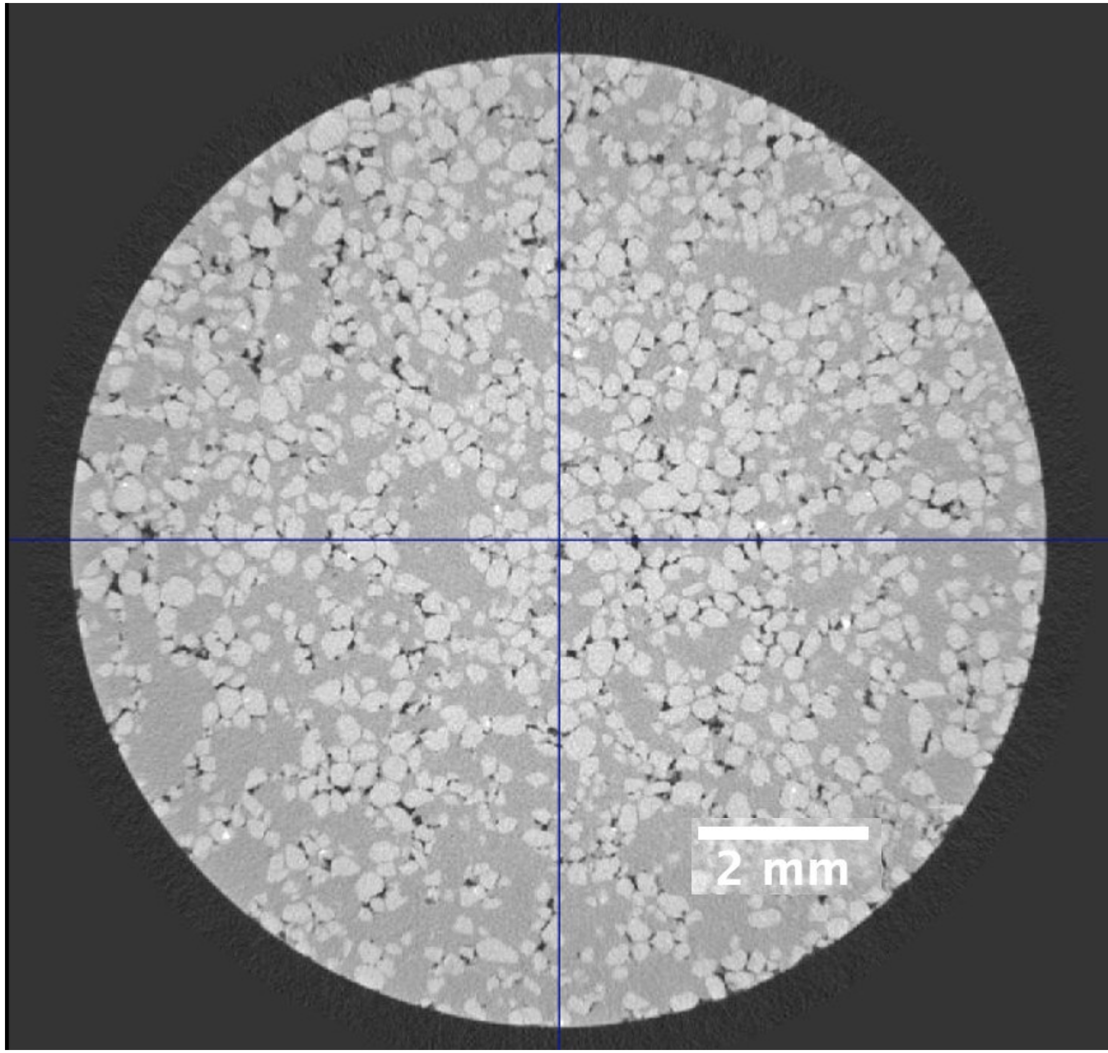
- Testing samples at quasi static, intermediate, and high strain rates
- Models need to account for variation in binders and materials
- Single particle experiments to test individual components

PSAAP III

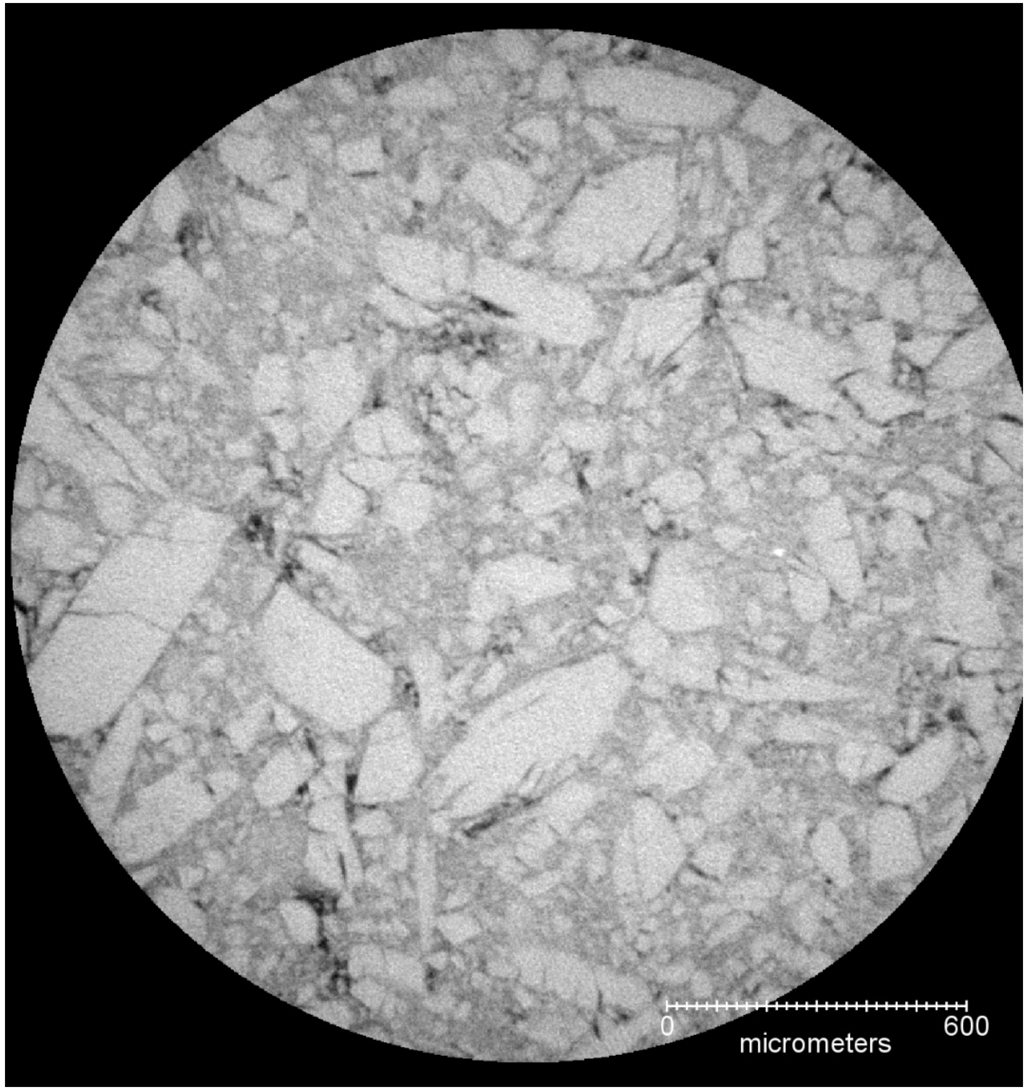
Surrogate Mock Materials

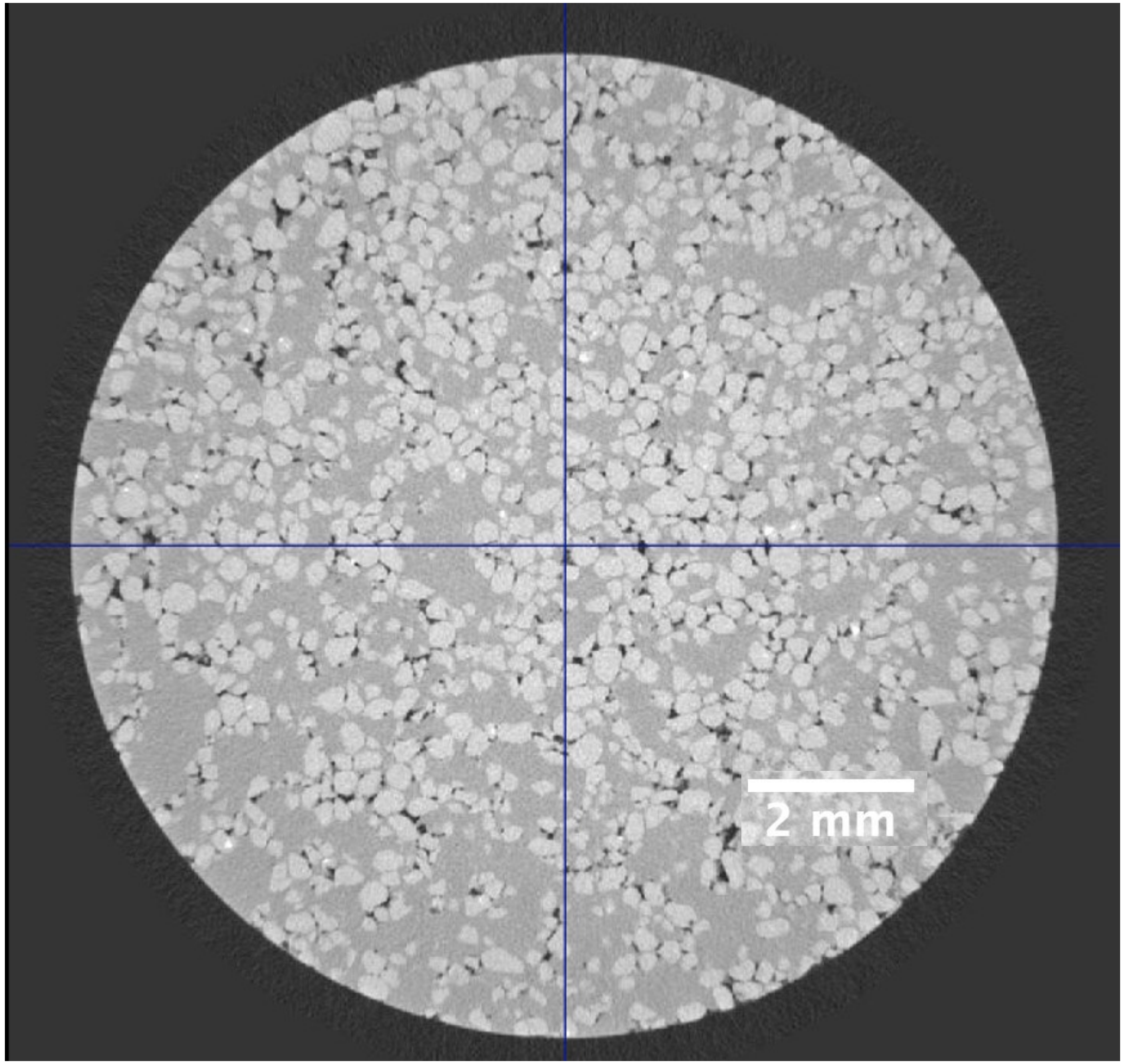
- IDOX is expensive and hard to model
- Main component, iodine, hard to CT image
- Creation of surrogate samples (F50 sand in FK-800 resin) allows for in depth preliminary testing and calibration of systems
- Recycled samples also investigated



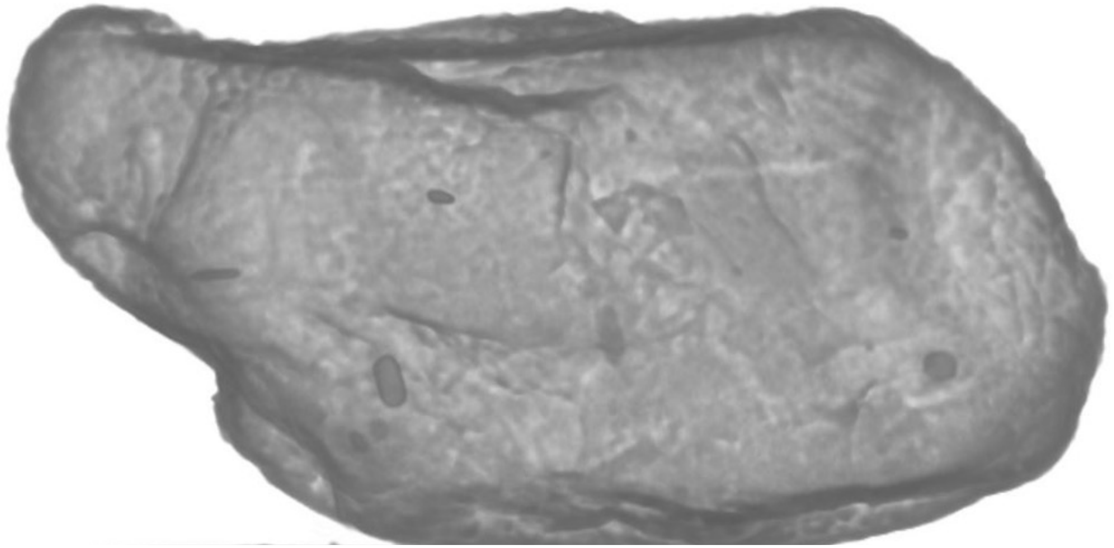
Looking down y axis CT of sand in resin

IDOX vs Sand



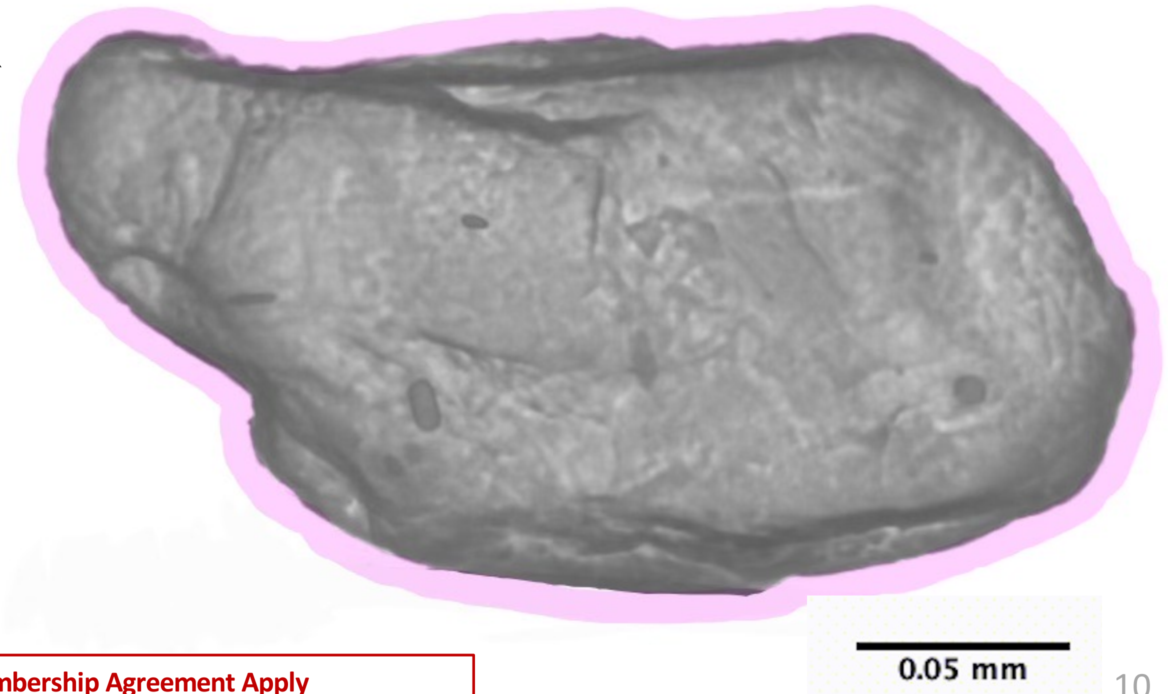


Processing and Formulation

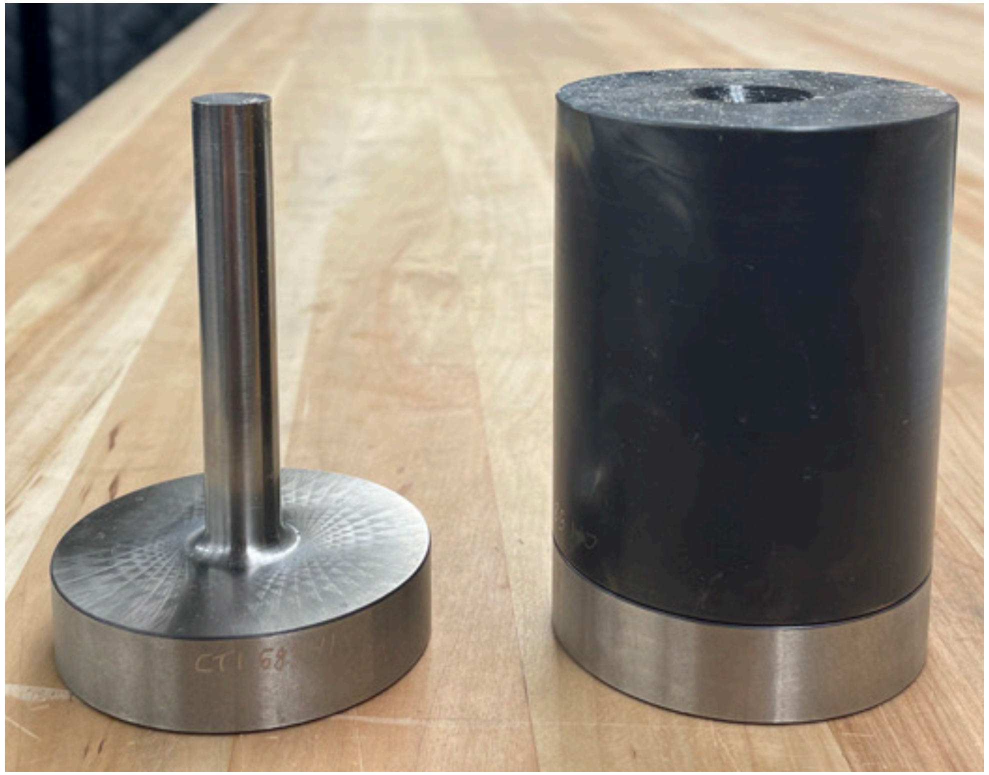


Single grain of sand scanned at 4x using Zeiss Versa µCT

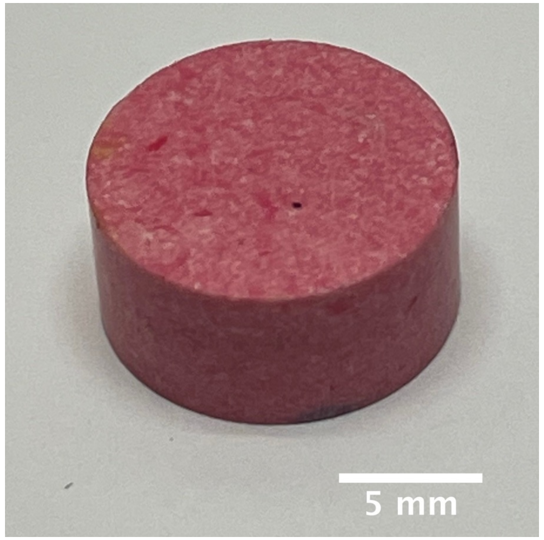
- A solvent/resin slurry is used to finely coat each grain
- The mixture dries
- Resultant powder pressed into shape



Pressing



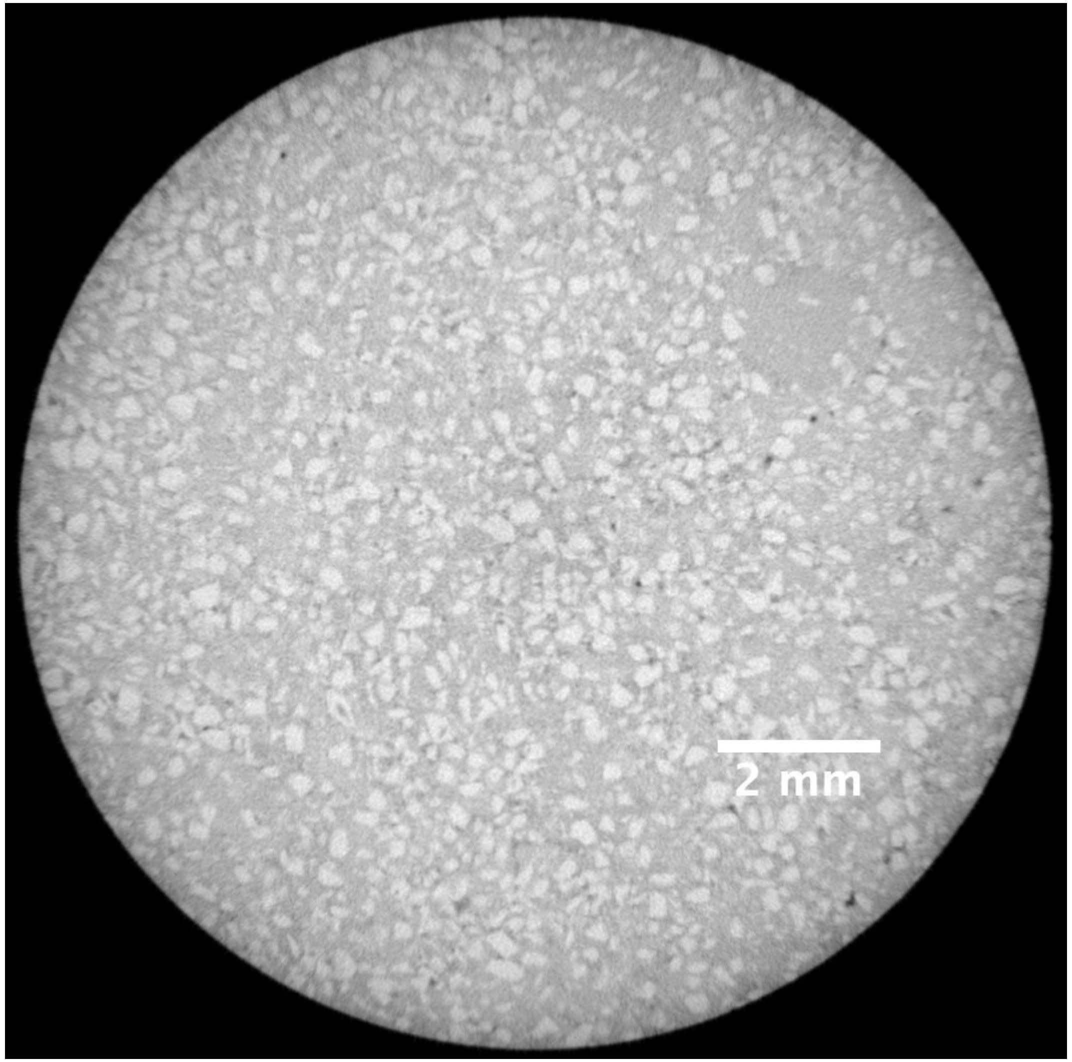
Half inch die



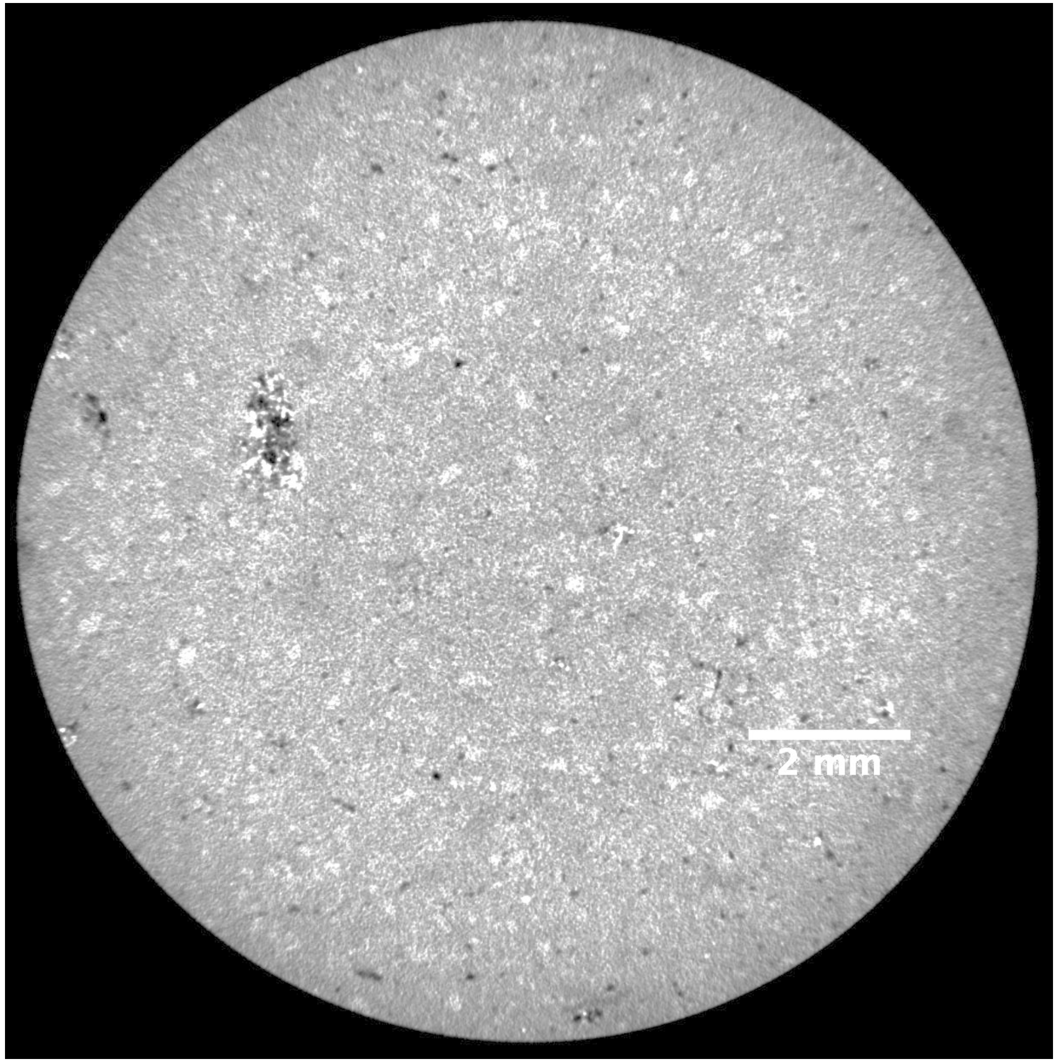
Final Pressed Sample

- Die is heated to glassy transition temperature range
- Material is preheated inside die
- Die loaded into hydraulic press and held at constant load

CT of IDOX+Estane Samples

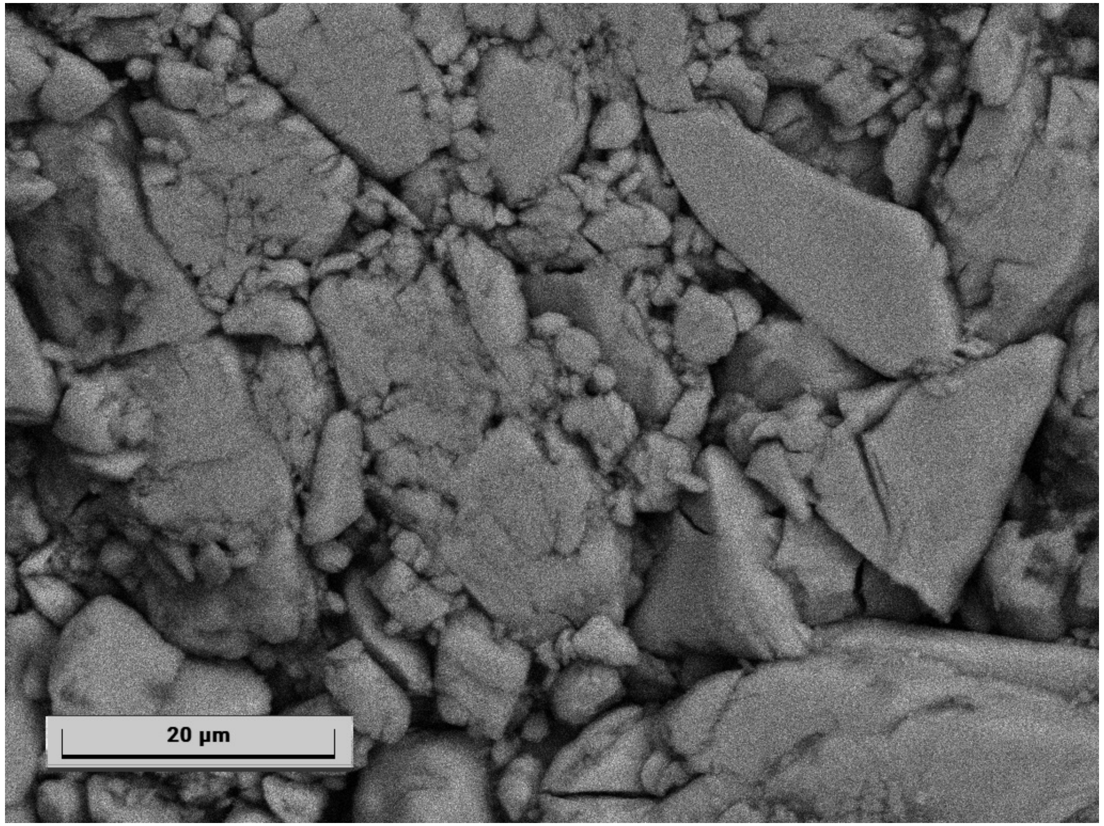


Pristine LANL Sample

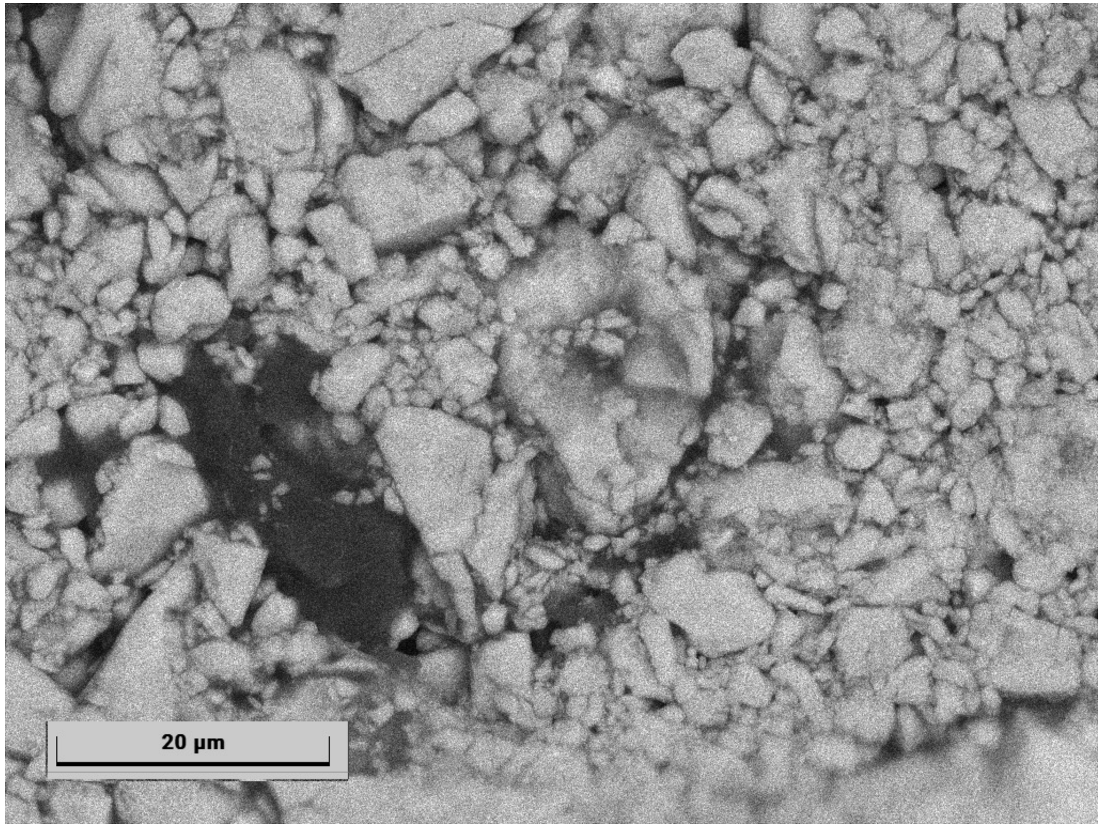


Pressed Recycled Sample

SEM: LANL vs. Recycled

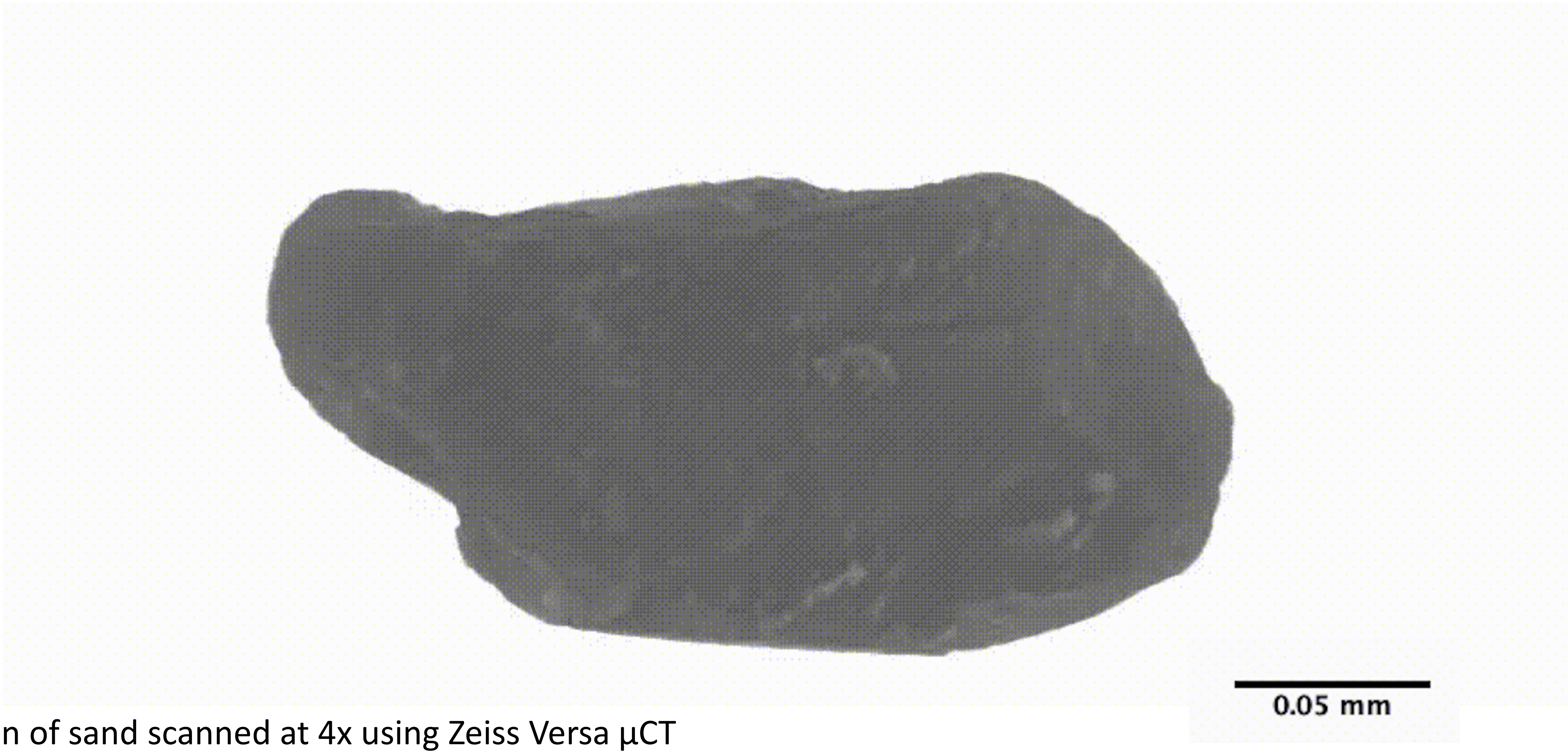


SEM, LANL Mock,
average crystal ~43.6 μm^2



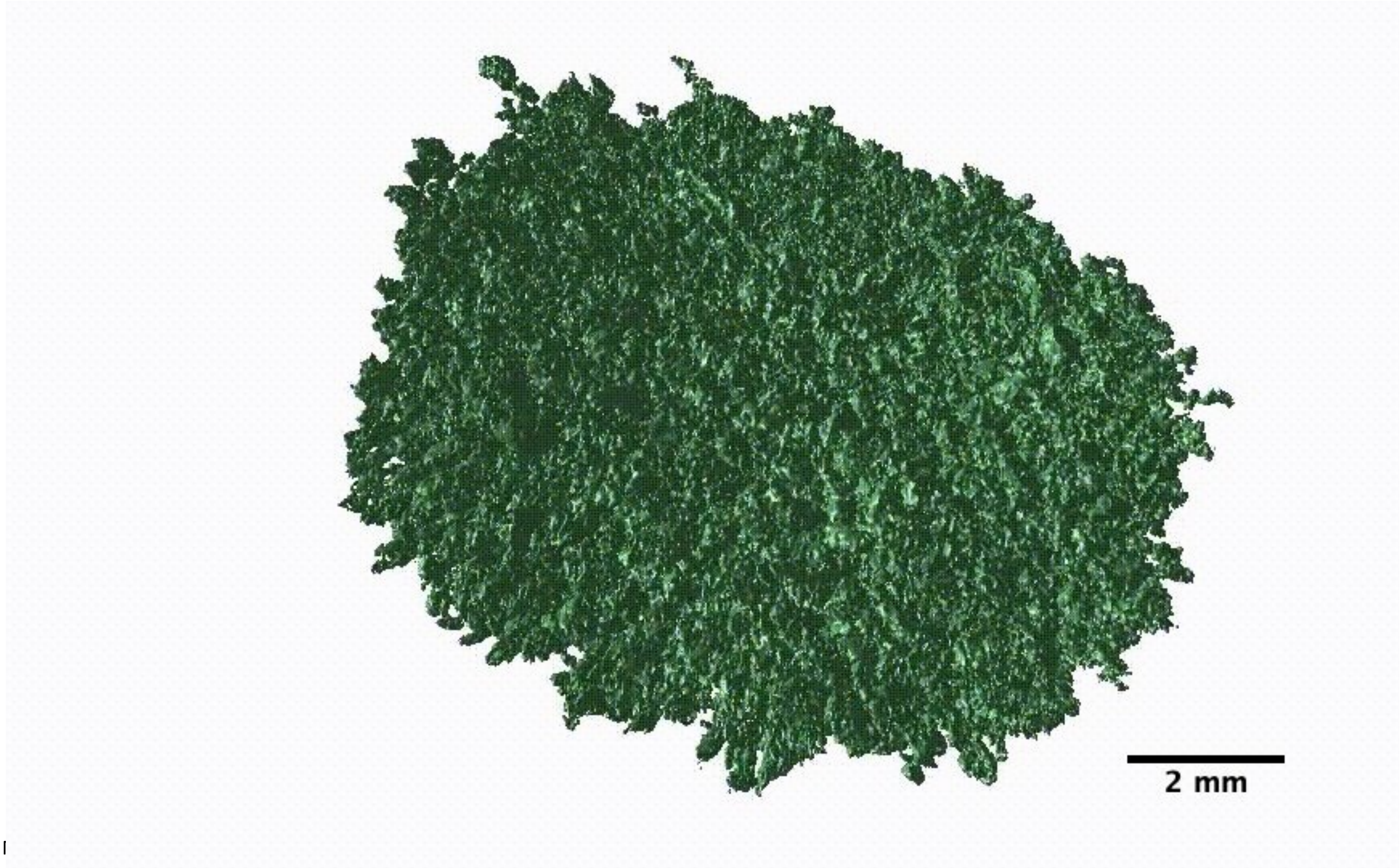
SEM, LANL Recycled,
average crystal ~29.7 μm^2

Single Grain of Sand

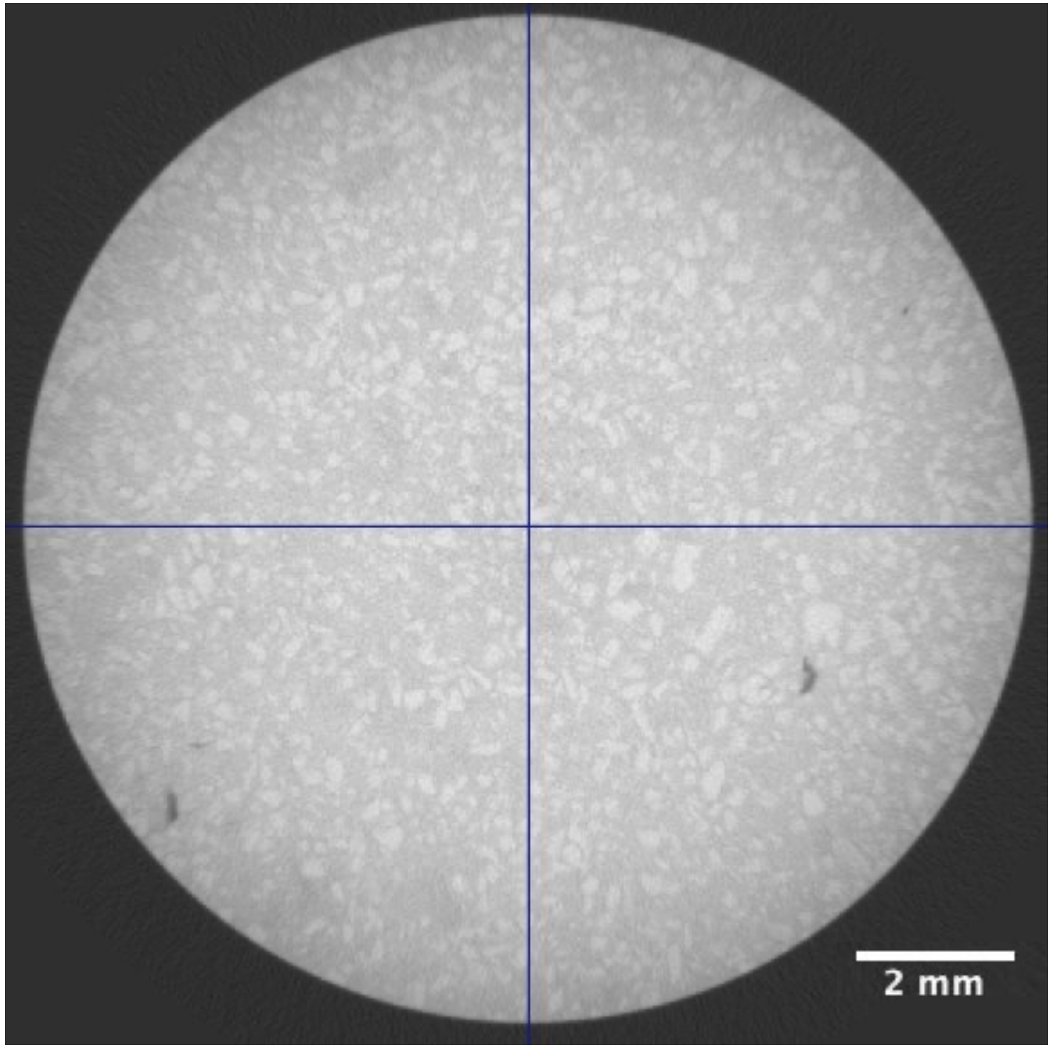


Single grain of sand scanned at 4x using Zeiss Versa µCT

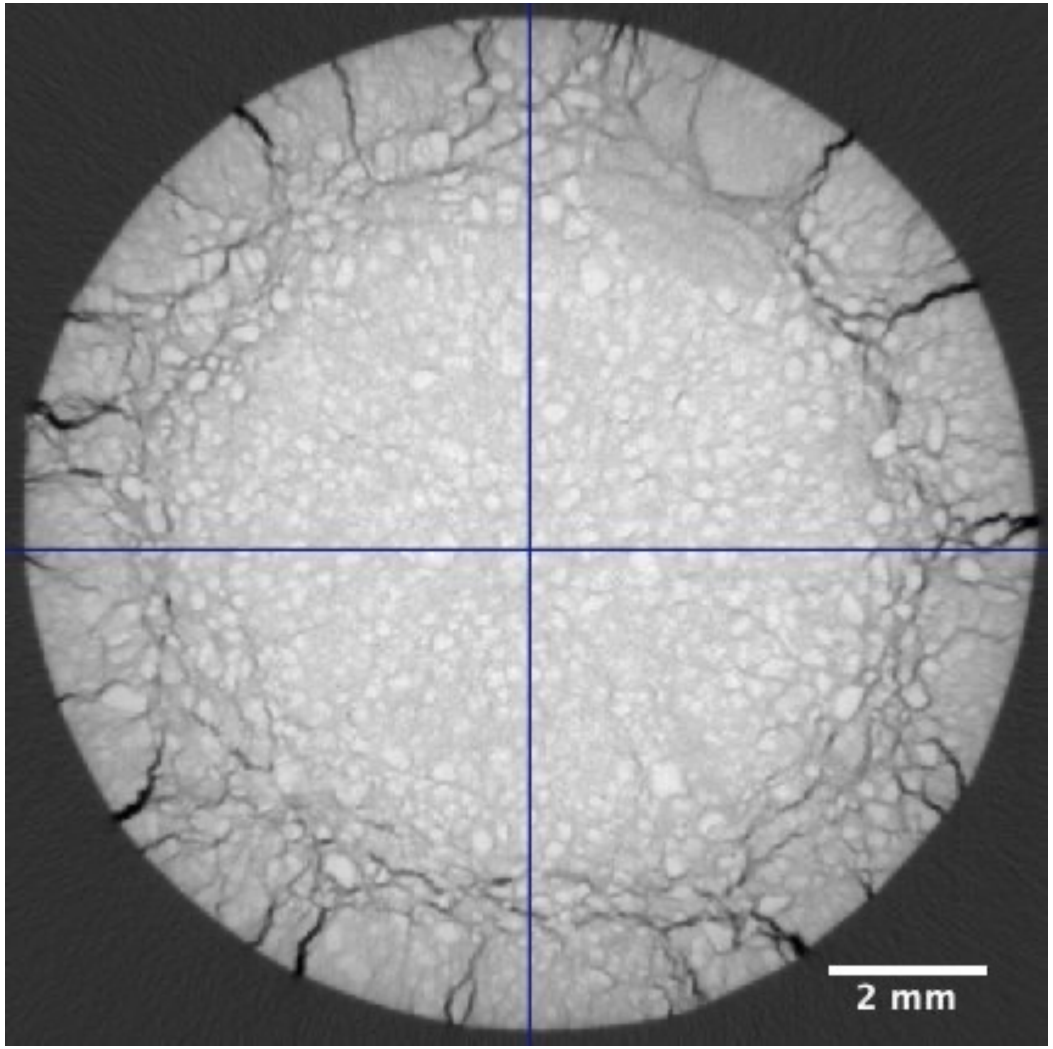
IDOX



In-situ CT Experiments

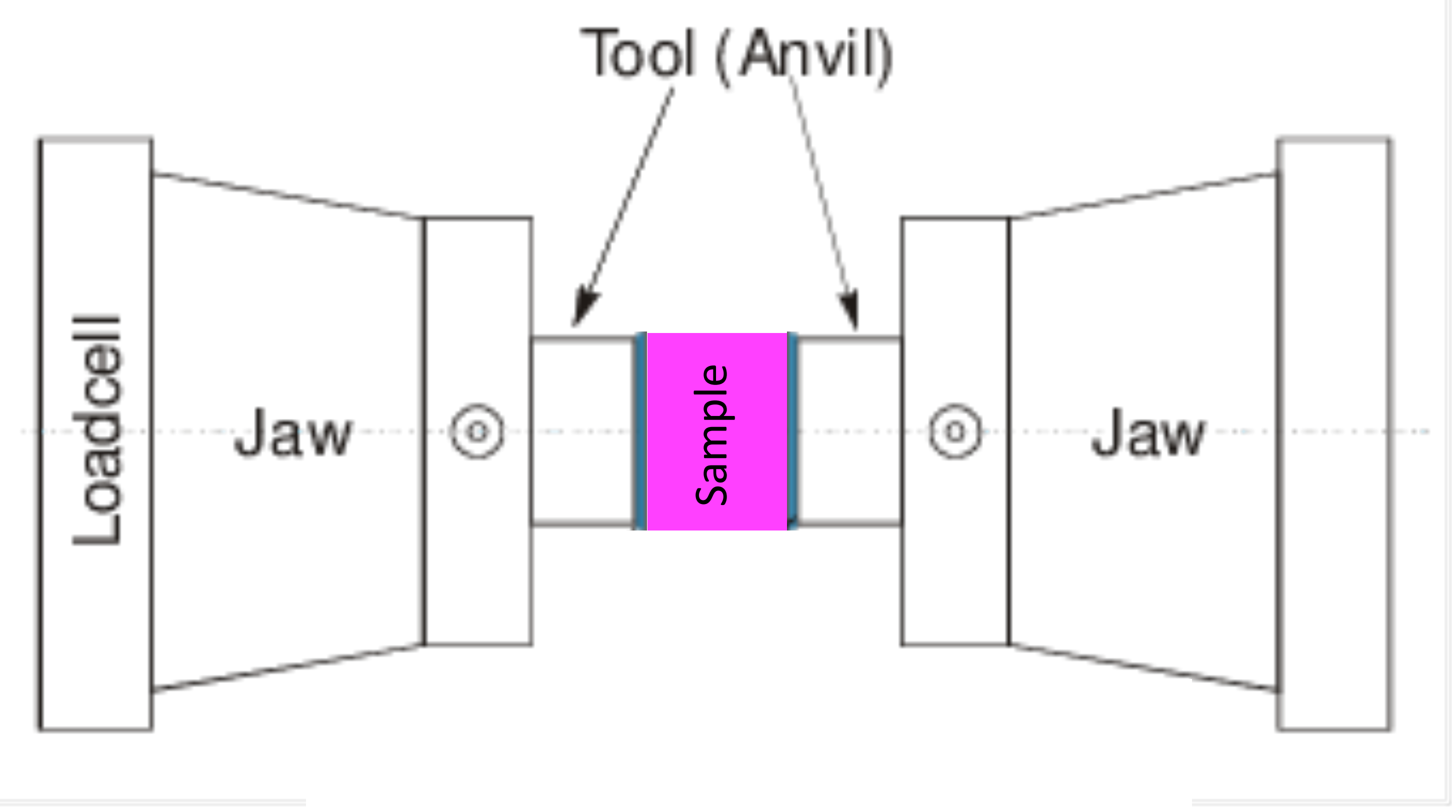


Pre compression IDOX



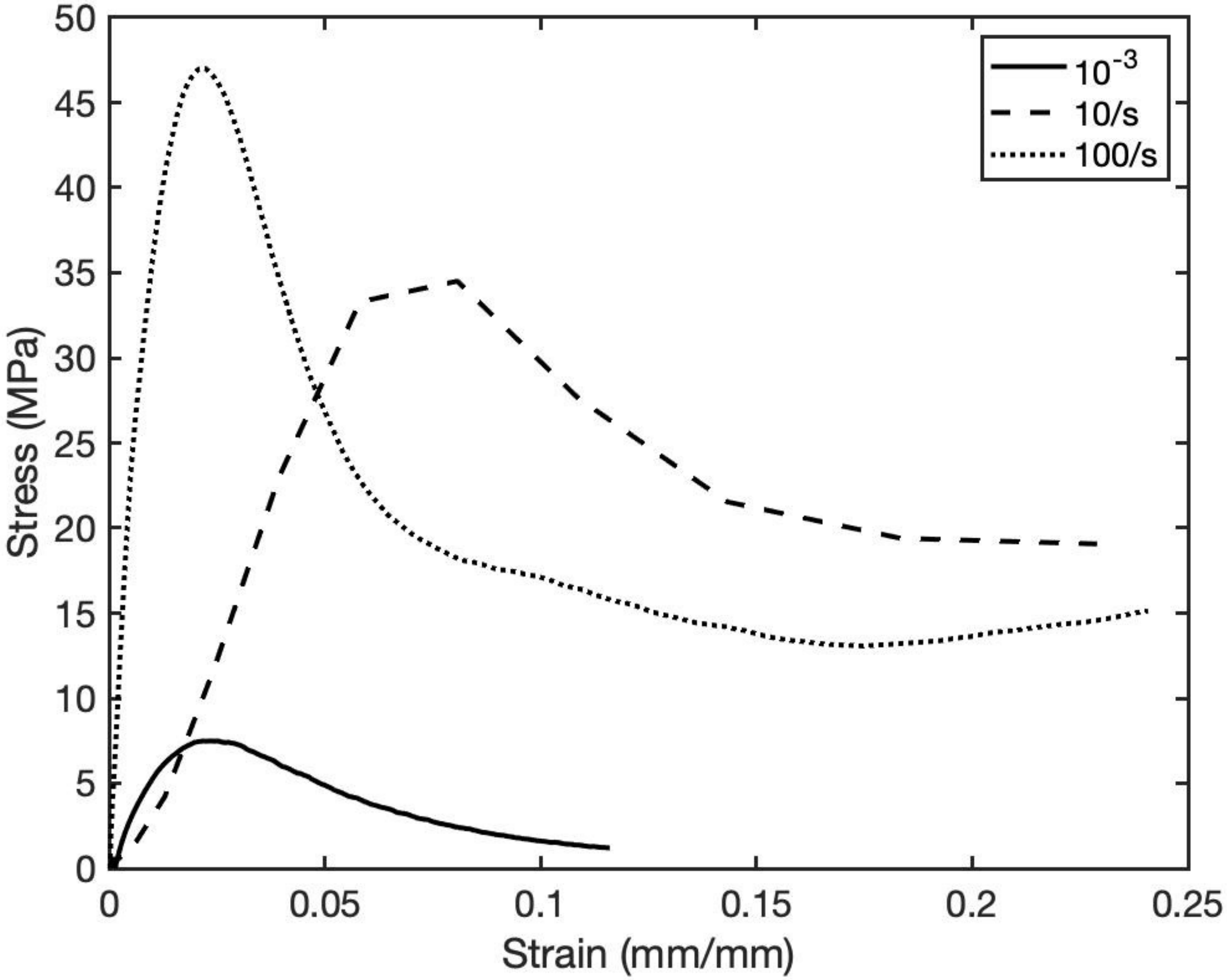
Post compression IDOX

Mechanical Testing



Gleeble Thermomechanical Load System Setup

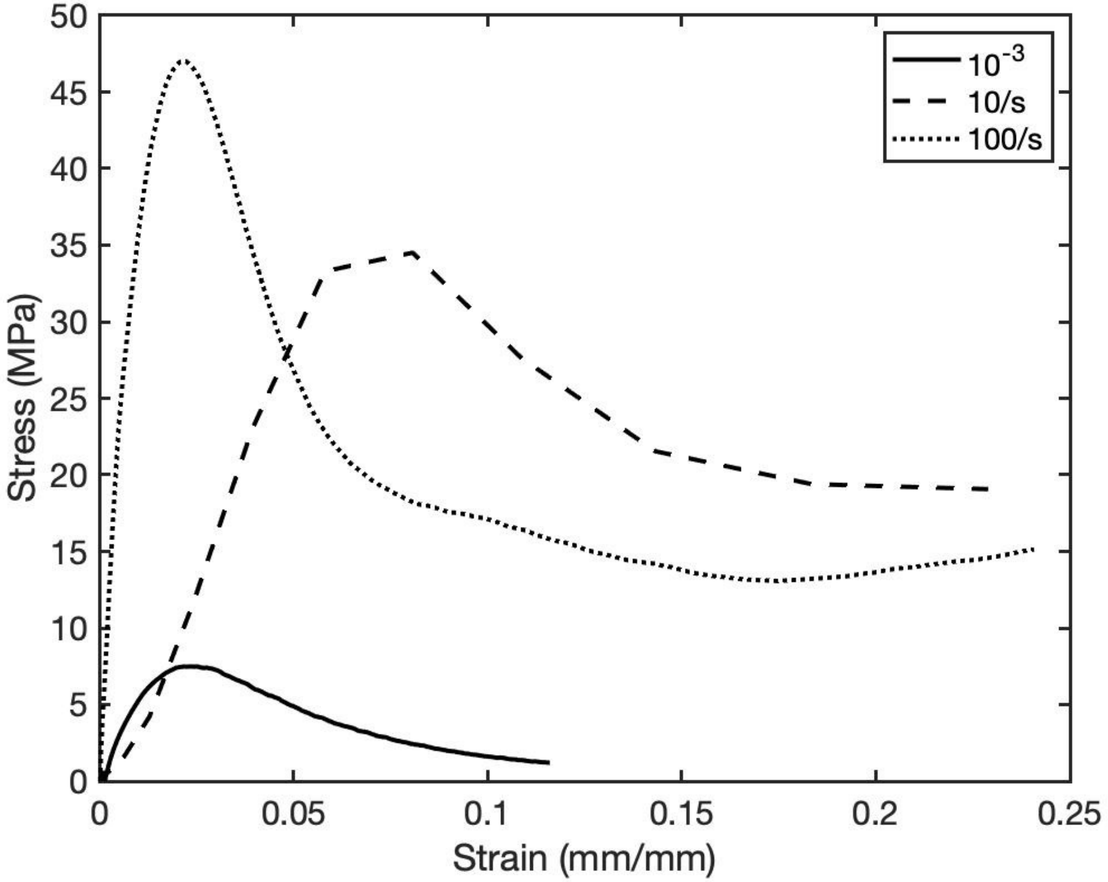
Intermediate Strain Rates

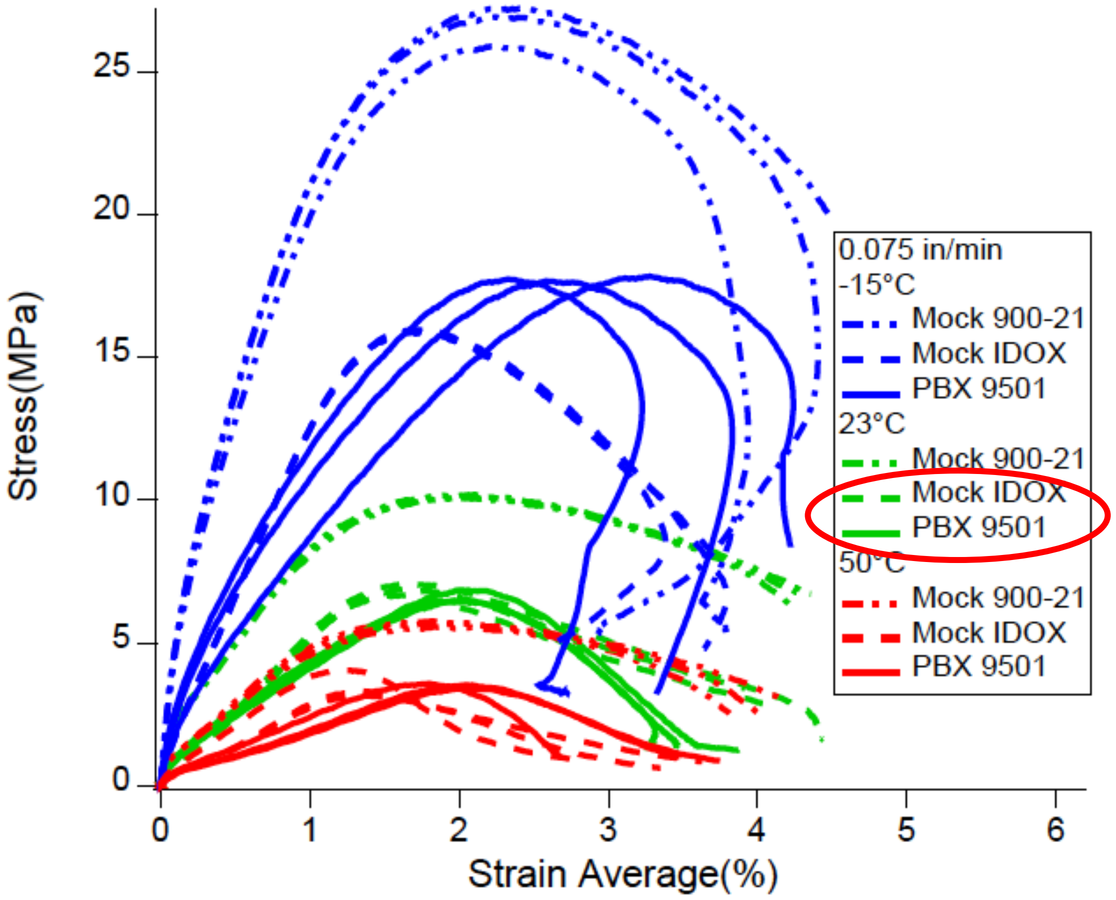


Stress vs strain for as-received LANL IDOX MHE samples

- Initial results very promising
- Able to achieve unusual 100/s intermediate strain rate

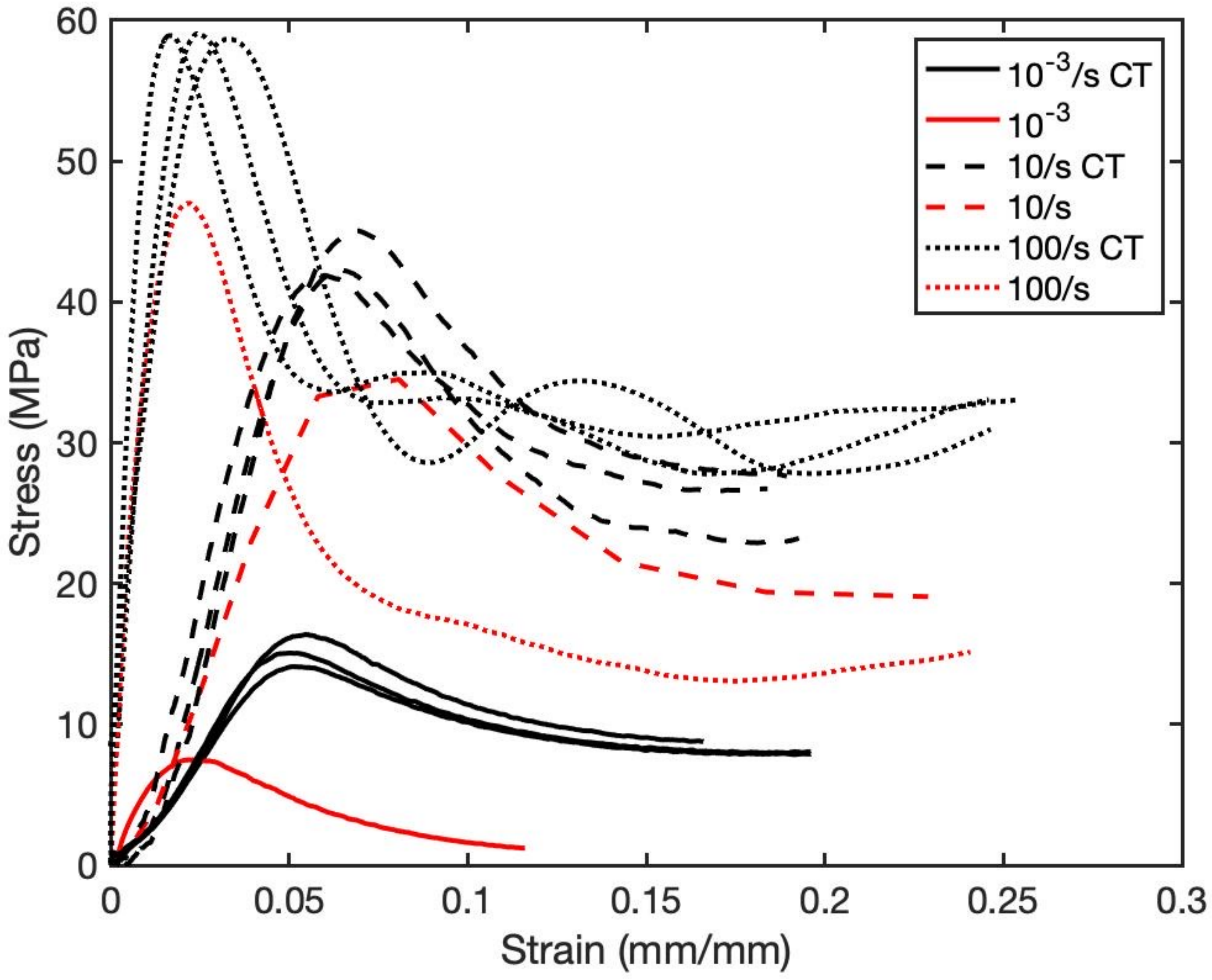
Comparison to existing results





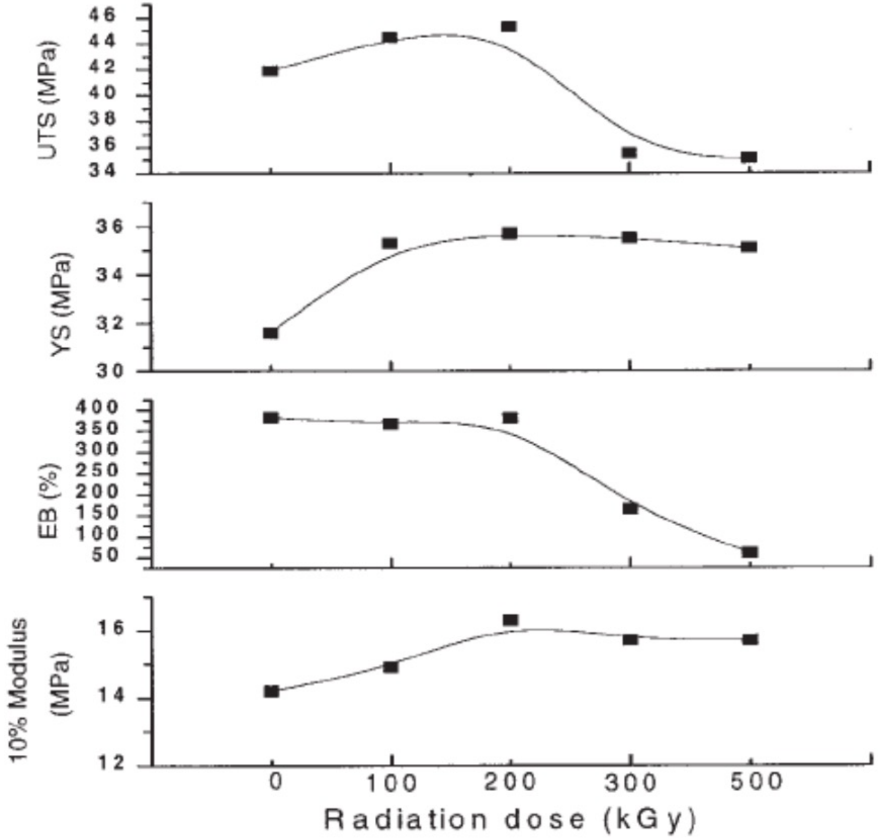
Yeager, John David, et al. *Development of a new density and mechanical mock for HMX*. No. LA-UR-18-25764. Los Alamos National Lab.(LANL), Los Alamos, NM (United States), 2020.

Mechanical Properties post-CT



- Post-CT values significantly higher
- No other processing differences

Strength Discrepancy



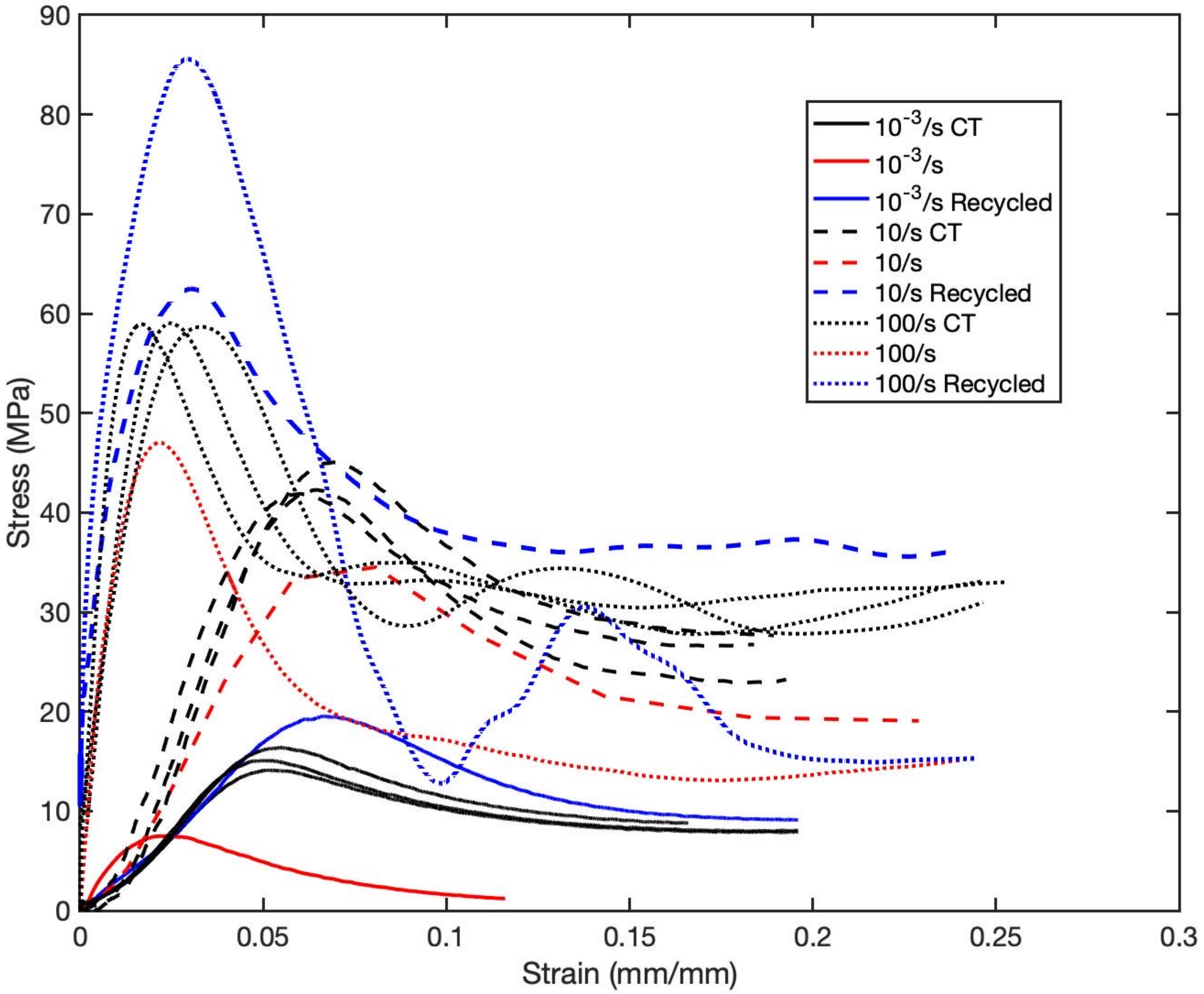
Variation in YS, UTS, EB and 10% modulus across varying radiation doses

R. Sengupta, S. Sabharwal, V.K. Tikku, A.K. Somani, T.K. Chaki, A.K. Bhowmick, Effect of ambient-temperature and high-temperature electron-beam radiation on the structural, thermal, mechanical, and dynamic mechanical properties of injection-molded polyamide-6,6]

Hypothesis: x-ray radiation from CT caused the increase in strength

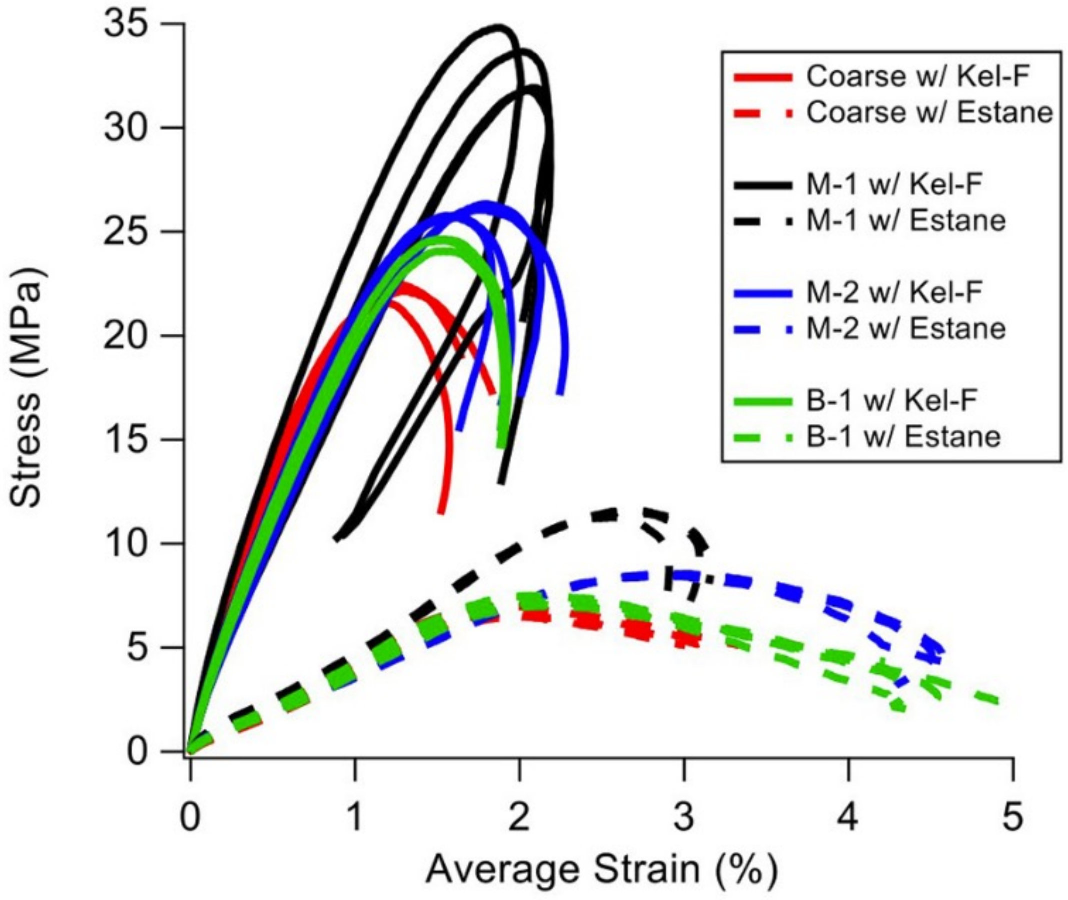
- Phenomenon is well documented for polymers (injection molded polyamide on right)
- Binder used in is a thermoplastic polyurethane with nitro-plasticizer
- Need to investigate whether radiation is affecting just polymeric binder or sample as a whole

Recycled vs Pristine



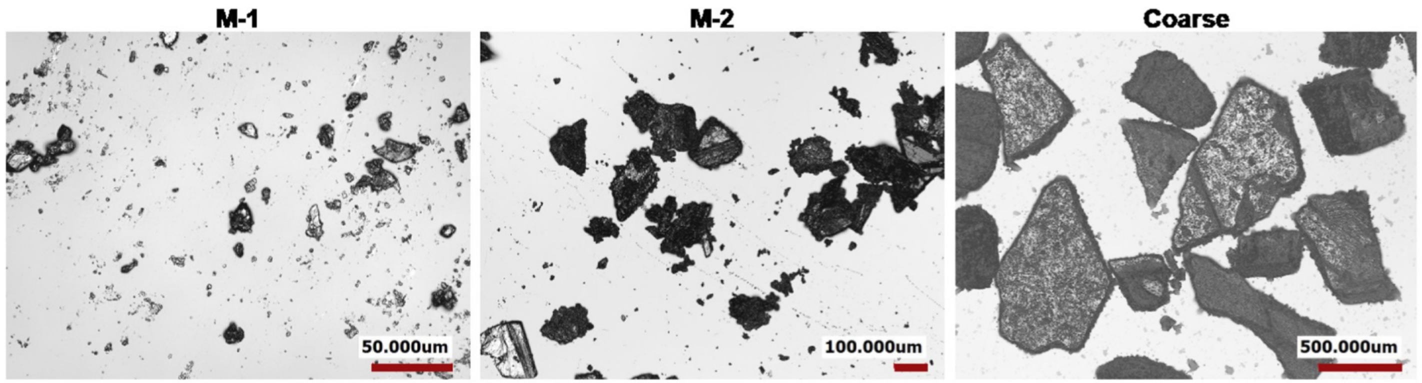
- Strength increase follows expected trend for decrease in particle size
- Particle size causes almost exponential increase compared to CT effects

Crystal Size and Binder Effects



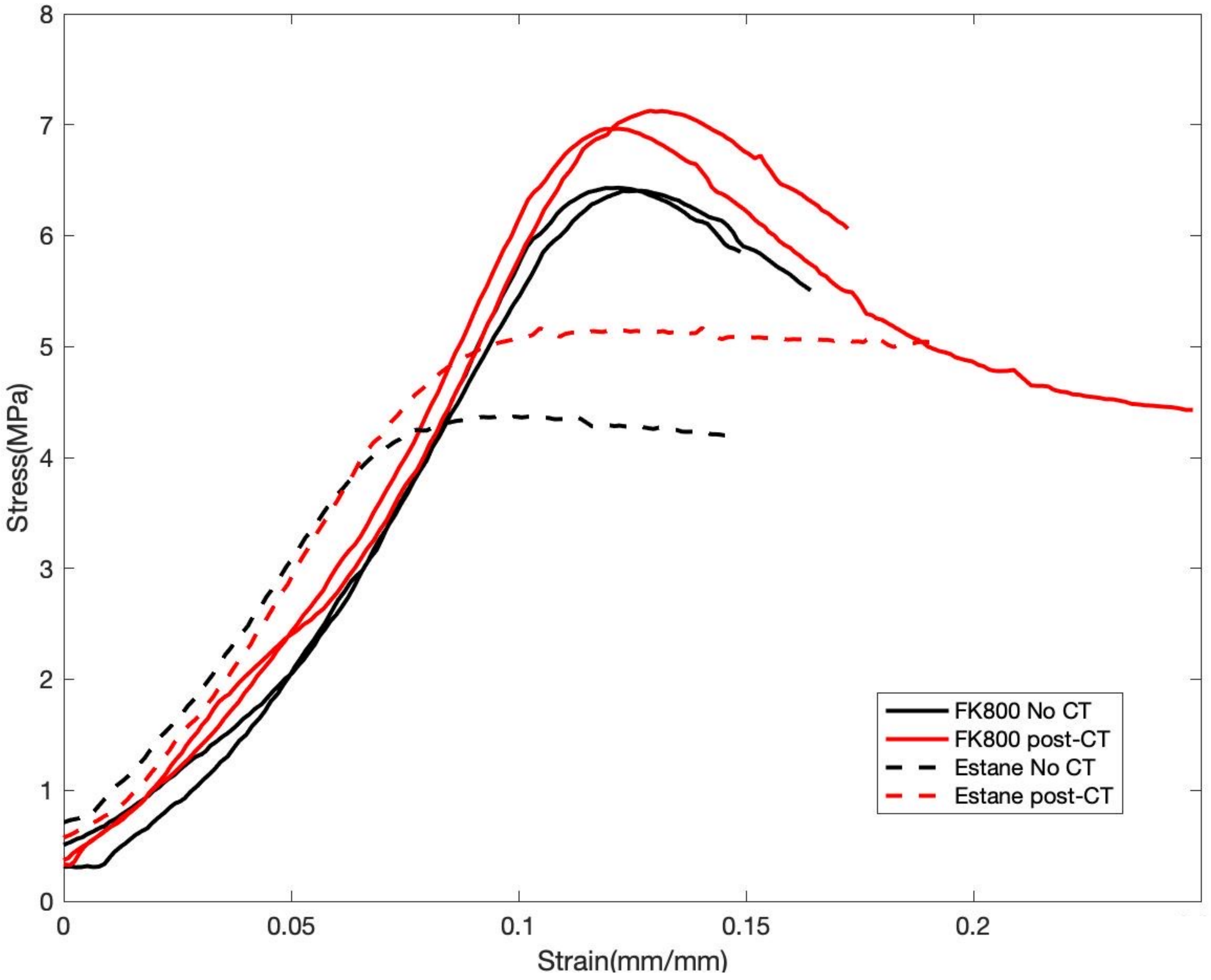
M.J. Herman, C.S. Woznick, S.J. Scott, J.T. Tisdale, J.D. Yeager, A.L. Duque, Composite binder, processing, and particle size effects on mechanical properties of non-hazardous high explosive surrogates, Powder Technol. 391 (2021) 442–449

- Clear inverse relation between particle size and YS
- Binder properties affect mechanical response even more strongly than particle size



Images of IDOX crystals with M-1 (< 75 um), M-2 (75<x<150um), and coarse (>150um) particle size distributions.

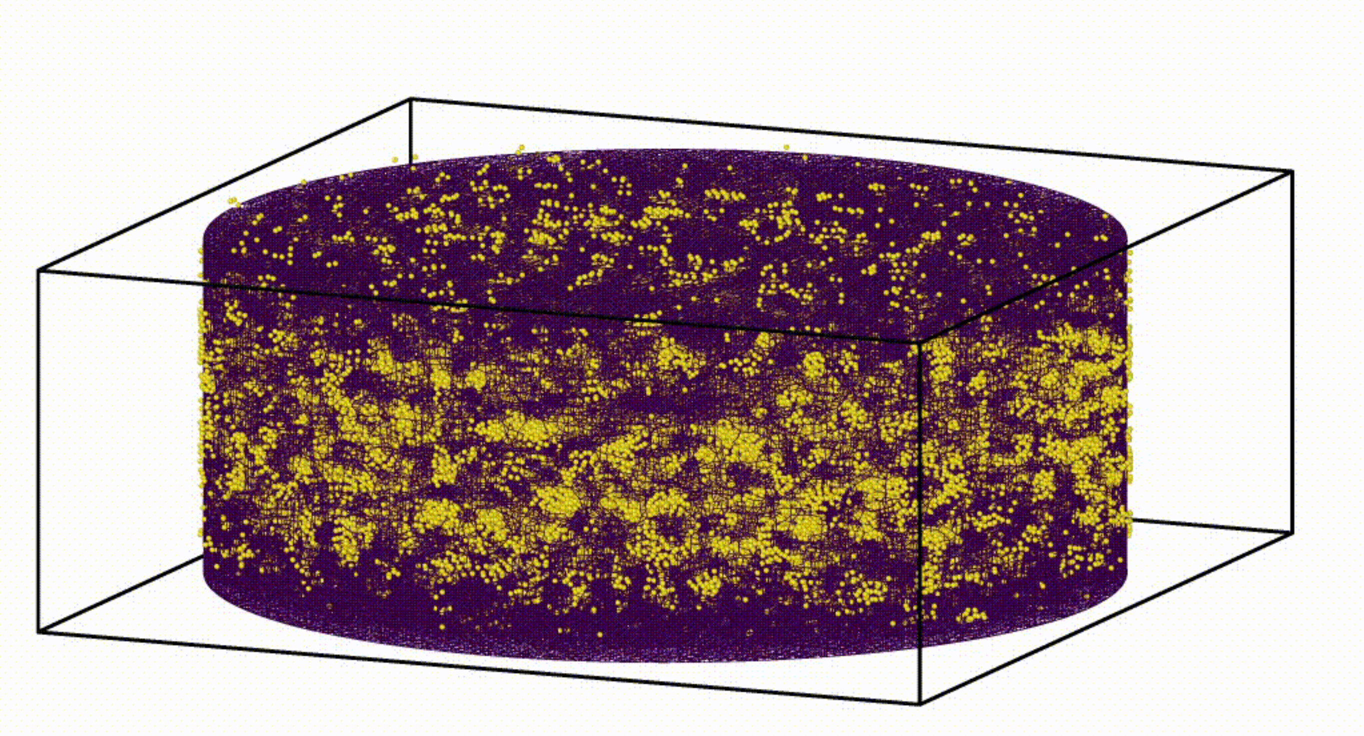
CT Hardening of $CaCO_3$ Samples



- Quasi-static strain rates
- Both binder types exhibit hardening
- Smaller increase, still significant

Future Work

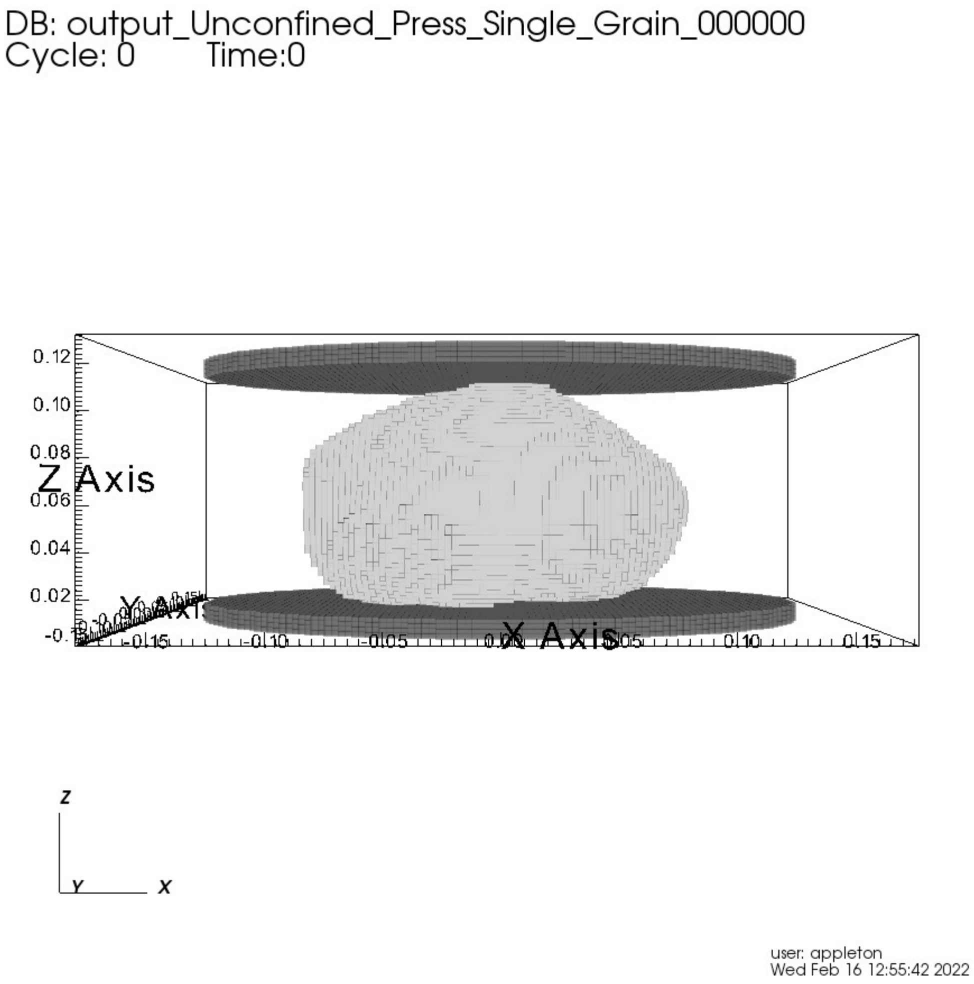
- Investigation of CT Hardening
- Improving segmentation and mesh creation for modeling
- Continuing intermediate strain rate testing of surrogate mocks



Courtesy Samuel Lamont, CU Boulder 2022

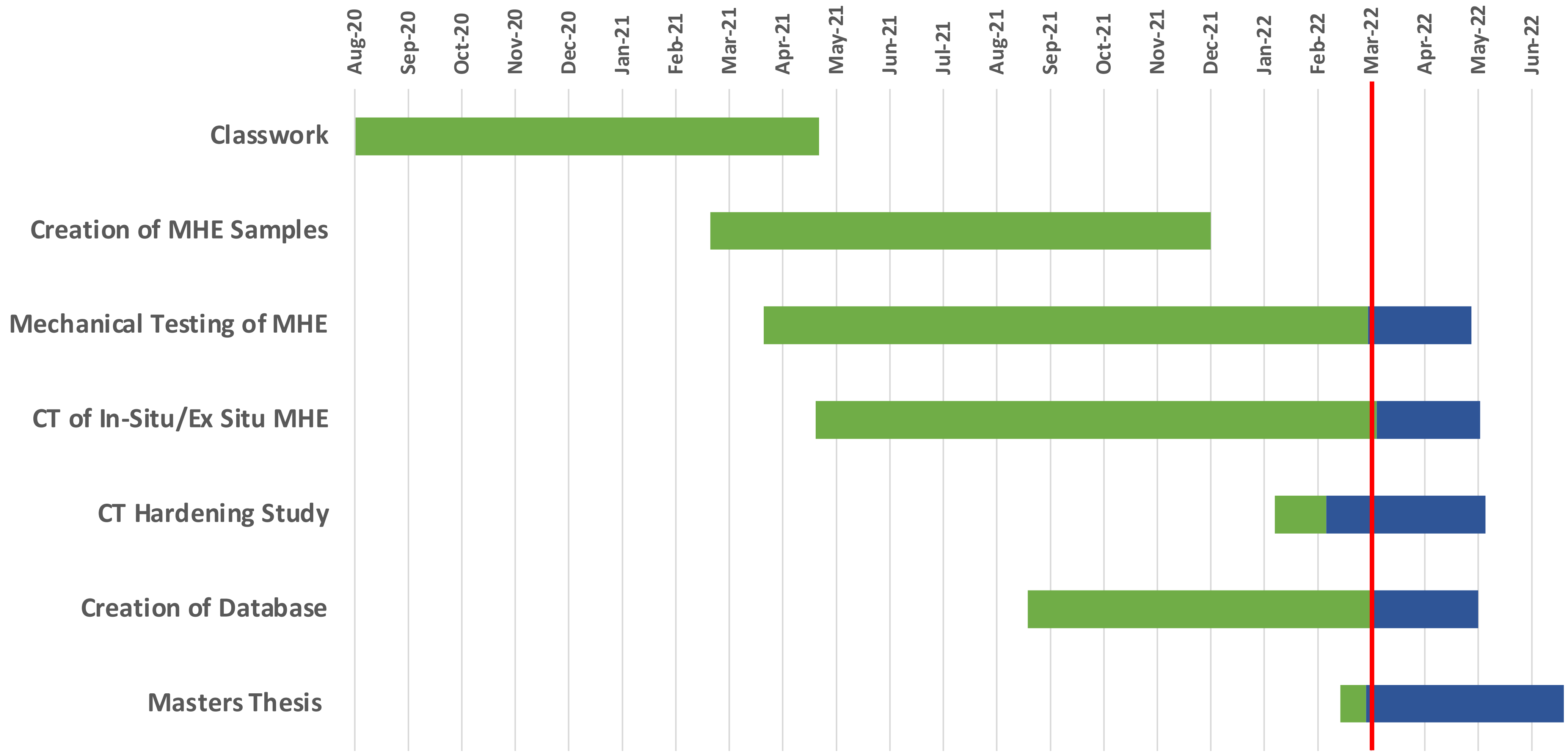
Conclusion

- Generate three-dimensional information about particle sizes, morphologies, distributions
- Obtain thermo-mechanical response to inform modeling of problems involving granular flows, large deformations, and fracture/fragmentation of unbonded and bonded particulate materials, emphasizing mock HE



Courtesy Jay Appleton, CU Boulder 2022

Gantt Chart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Classwork
Creation of MHE Samples
Mechanical Testing of MHE
CT of In-Situ/Ex Situ MHE
CT Hardening Study
Creation of Database
Masters Thesis

Challenges & Opportunities

- Zeiss Versa Often Under Maintenance
  - CT scans take several hours, many experiments are planned for this spring
  - New X-ray cabinet could be a solution

- Interdisciplinary studies beginning
  - New and different testing methods require innovation in sample preparation
  - Working with people from many different places

Thank you!

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- Thanks to Jay Appleton and Samuel Lamont for providing modeling animations and a big thank you to Dr. Alexandra Burch for teaching me everything I know about IDOX

References

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[4] H.M. Hsiao, I.M. Daniel, Strain rate behavior of composite materials, Compos. Part B Eng. 29 (1998) 521–533. https://doi.org/10.1016/S1359-8368(98)00008-0.

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