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

Semi-annual Fall Meeting

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National Nuclear Security Administration

PSAAP III

- Student: Summer Camerlo (Mines)
- Faculty: Dr. Amy. Clarke (Mines), Dr. Kester Clarke (Mines)
- Industrial Mentors: John Yeager (LANL), Brian Patterson (LANL)

COLORADO SCHOOL OF MINES. NSF IOWA STATE UNIVERSITY

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

CANFSA
CENTER FOR ADVANCED NON-FERROUS STRUCTURAL ALLOYS

- 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.

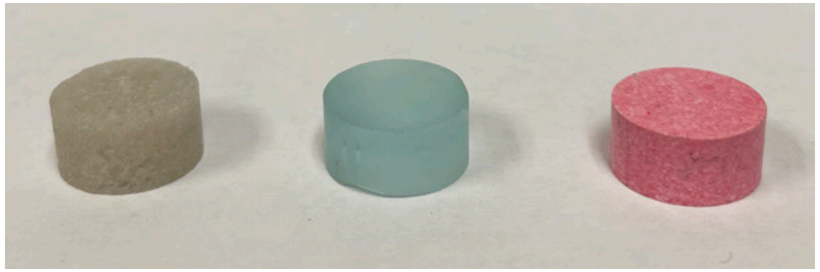
Recent Progress

- Completed mechanical testing (stress/strain relationships) and computed tomography of pristine samples received from LANL as part of a multi-university round robin
- Started internship at LANL with a focus on production and characterization of new mock HEs

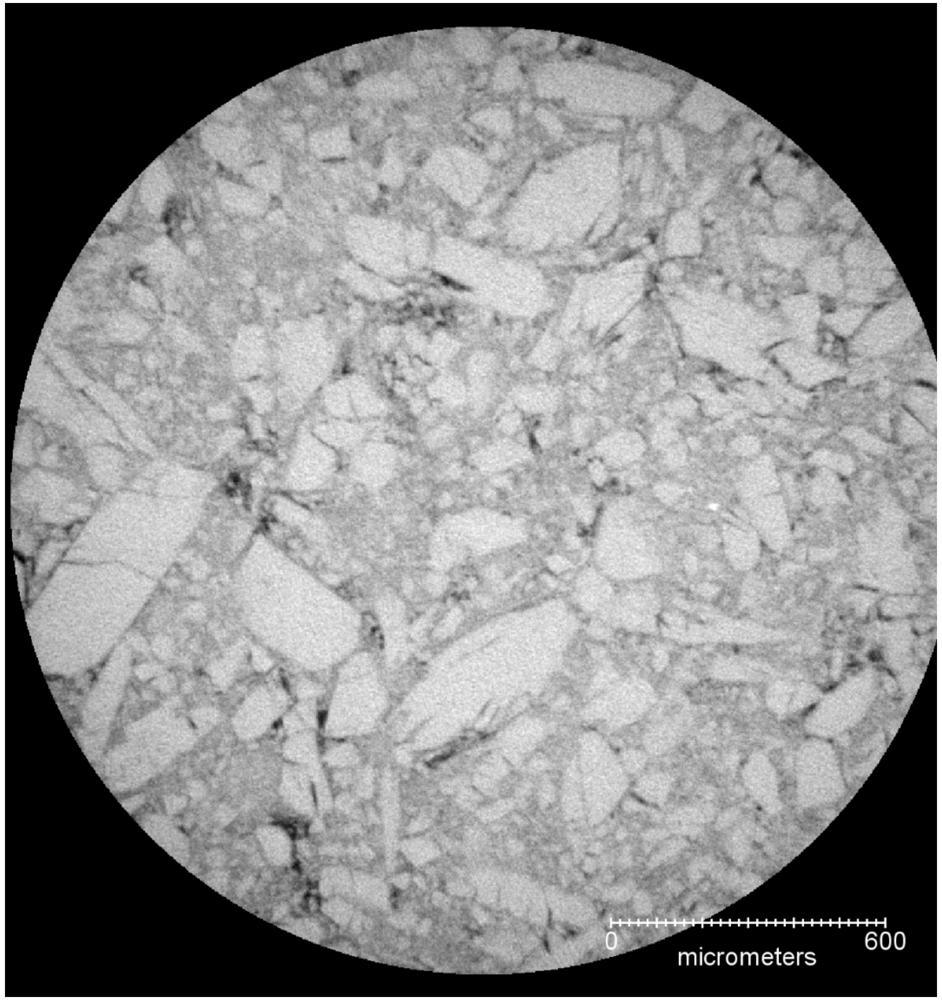
Metrics		
Description	**% Complete**	**Status**
1. Literature review	25%	●
2. Creation of model samples for CT imaging for calibration	75%	●
3. Processing of recycled mock HE and making samples	75%	●
4. CT imaging of pristine and recycled mock HE	75%	●
5. Mechanical properties and characterization of pristine and recycled mock HE	50%	●

Background

- Mock High Explosives are of great interest to the NNSA and other government agencies because they allow for safer and less expensive testing options [1]
- Idoxuridine (IDOX) is a relatively new mock surrogate that closely matches the properties of HMX [1] and the PSAAP project was developed to fully characterize its properties and build a robust database for computer simulations of IDOX [2]
- Other materials (sand and glass beads) will be used to create a baseline for calibration of the simulations

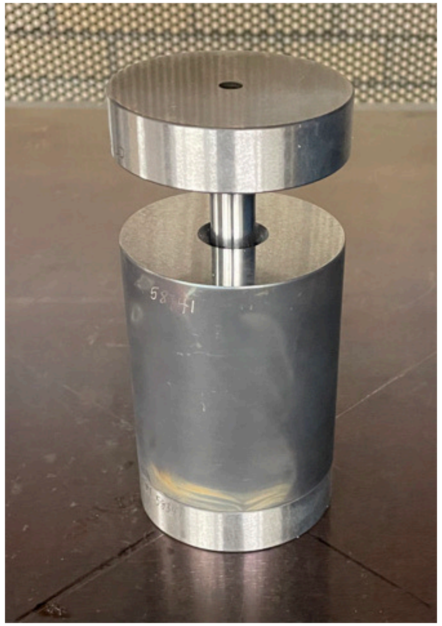


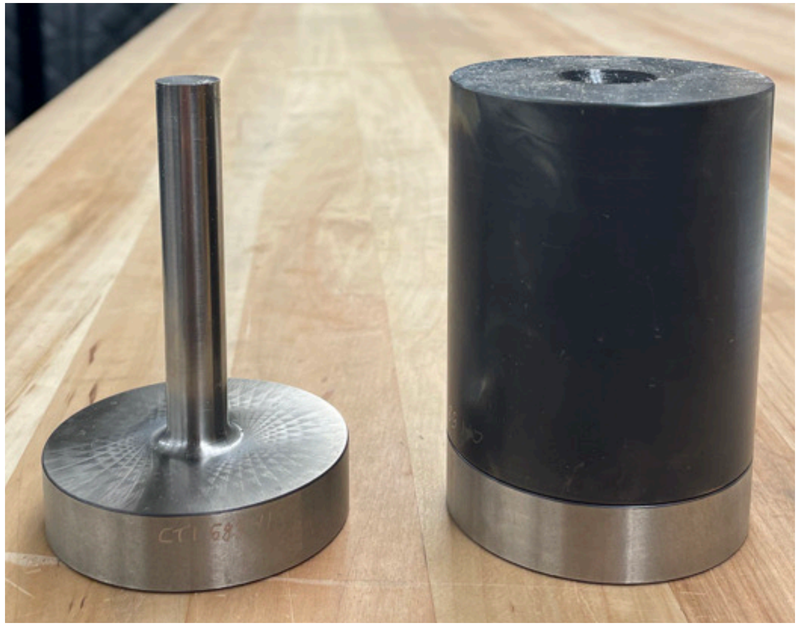
From left to right: Sand in FK-800 resin, plain epoxy, and recycled IDOX mock HE (half inch diameter)

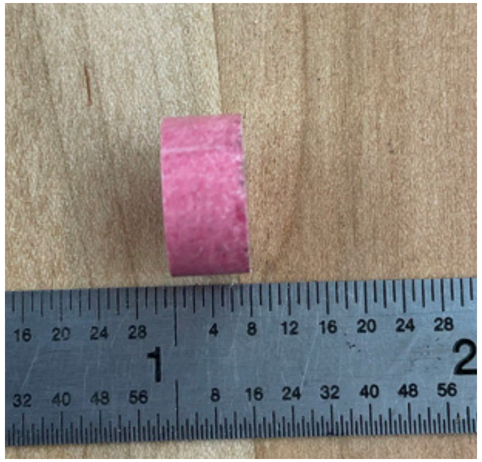


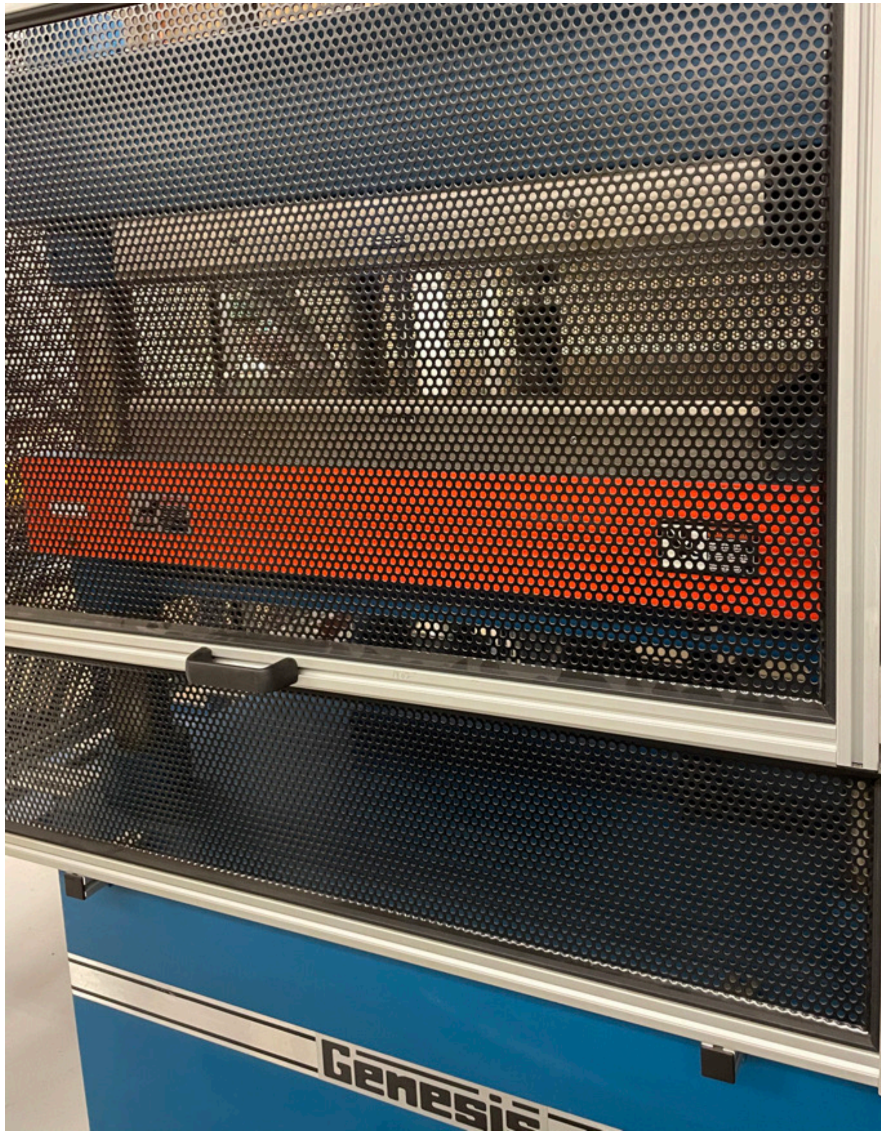
IDOX + Binder CT, XY slice
Courtesy: Brian Patterson and John Yeager, LANL

Pressing





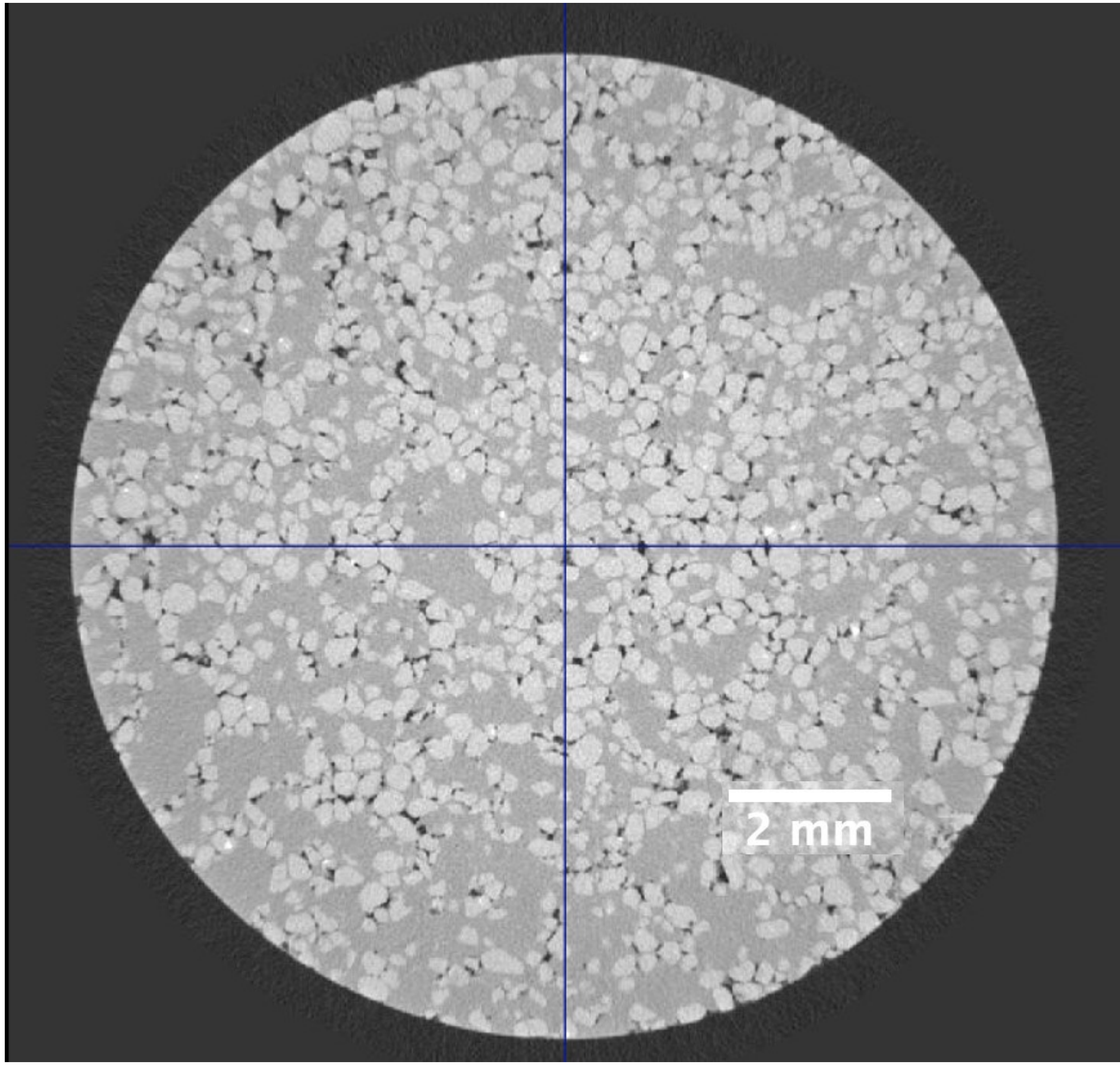




Half-inch die (top), recycled mock HE sample (bottom middle), Genesis Hydraulic Press (right)

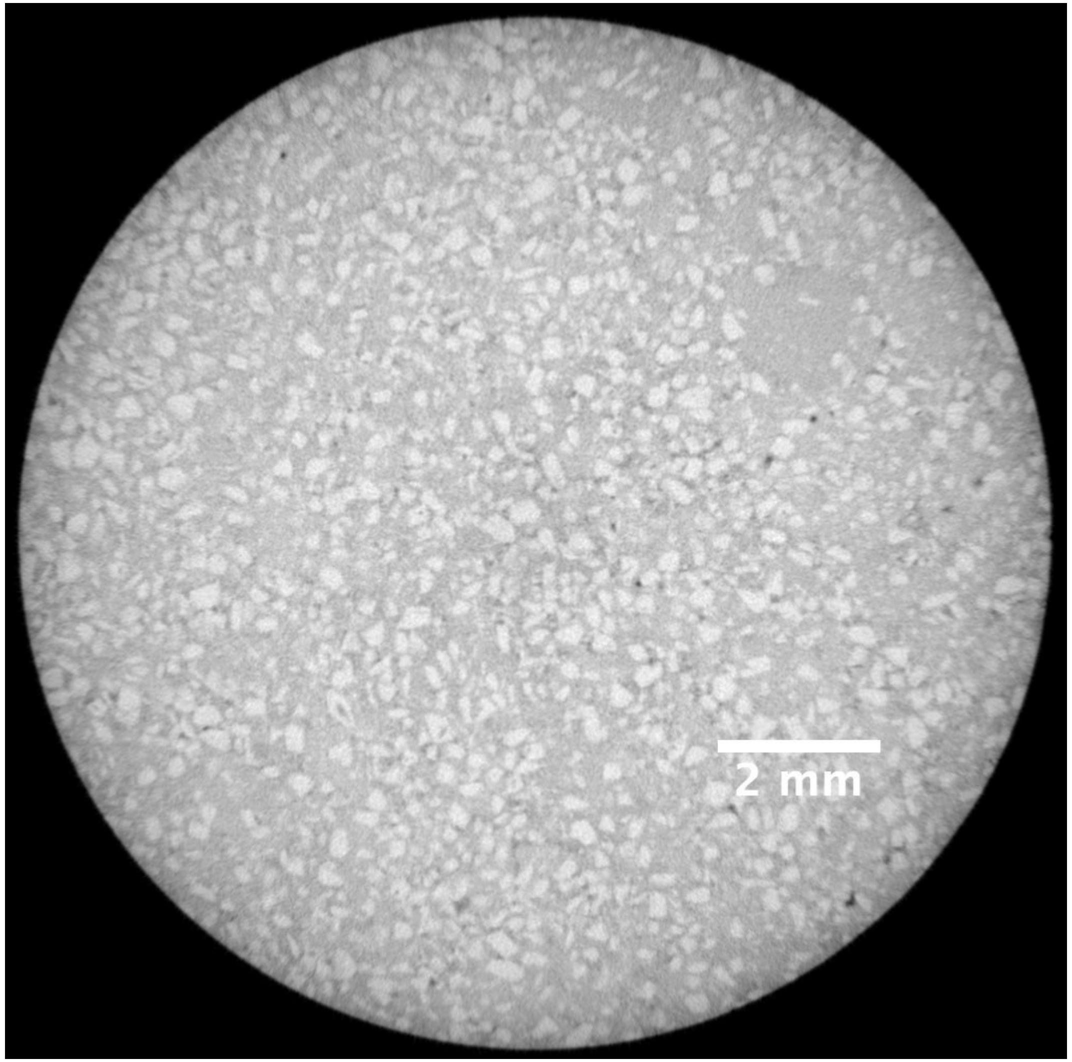
Current Progress

- Creation of surrogate samples (glass beads in epoxy, F50 sand in FK-800 resin) along with characterization (computed tomography [CT] and compression testing)
- Pressing of machining fines to produce recycled IDOX MHE samples
- CT of both pristine and recycled IDOX MHE samples
- In-situ computed tomography of epoxy embedded with glass beads and neat F50 sand

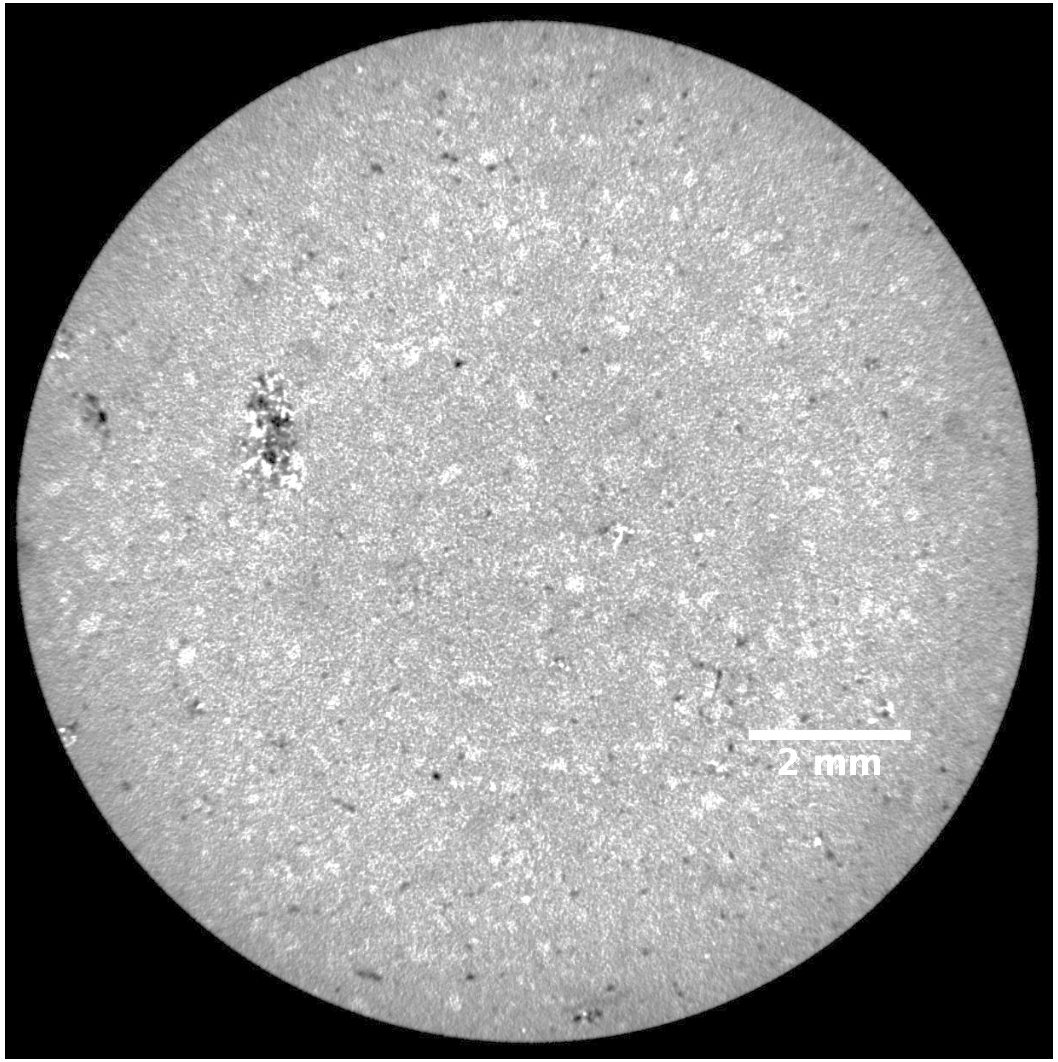


Top down CT of sand in resin

CT of IDOX+Estane Samples

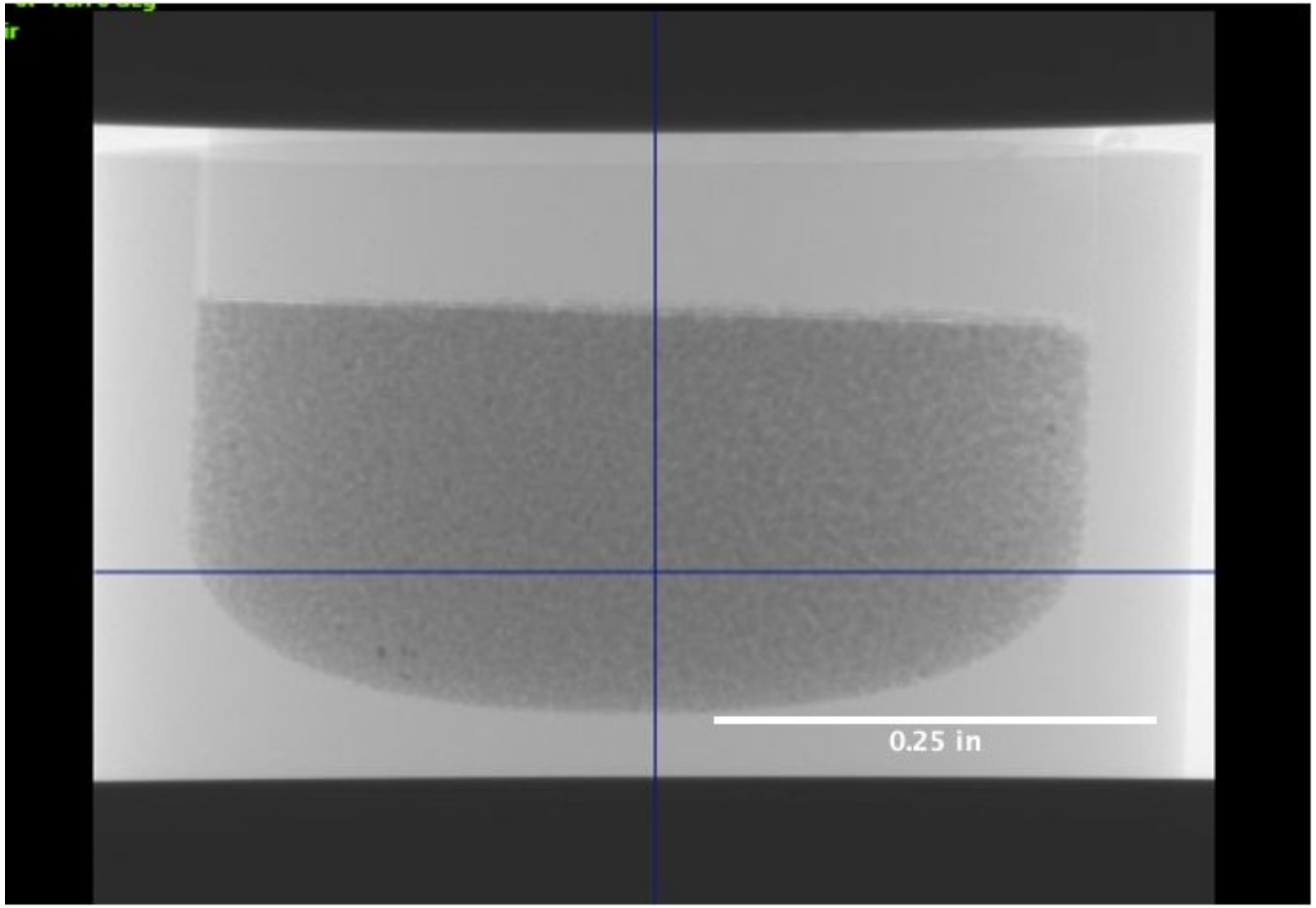


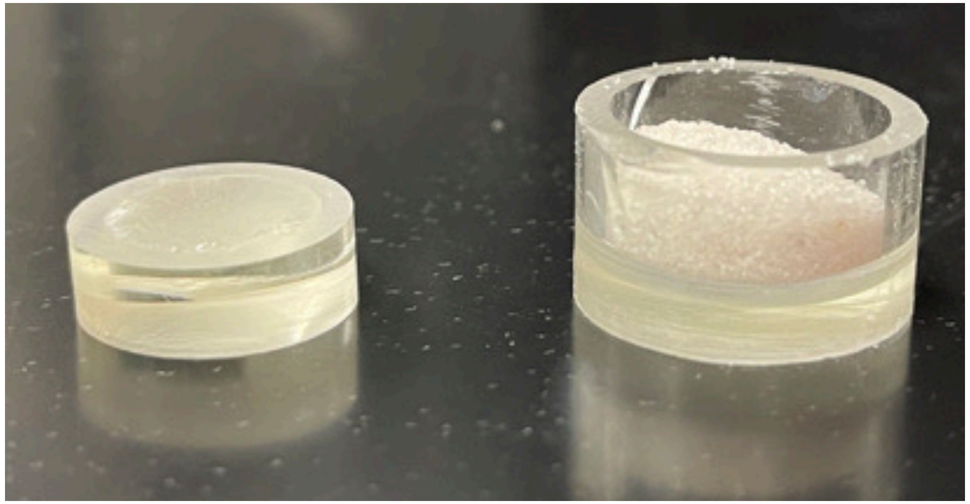
Pristine LANL Sample

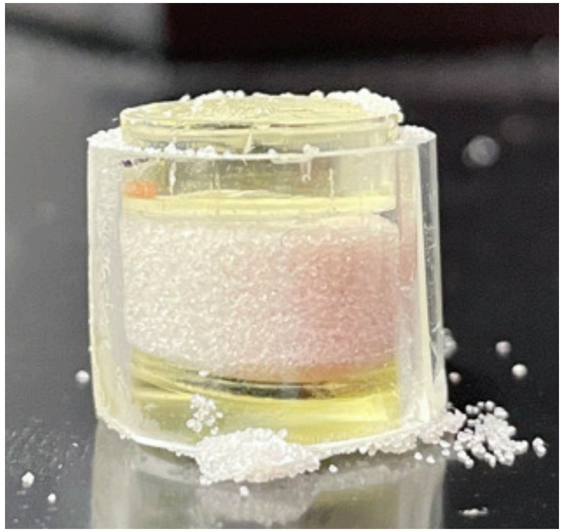


Pressed Recycled Sample

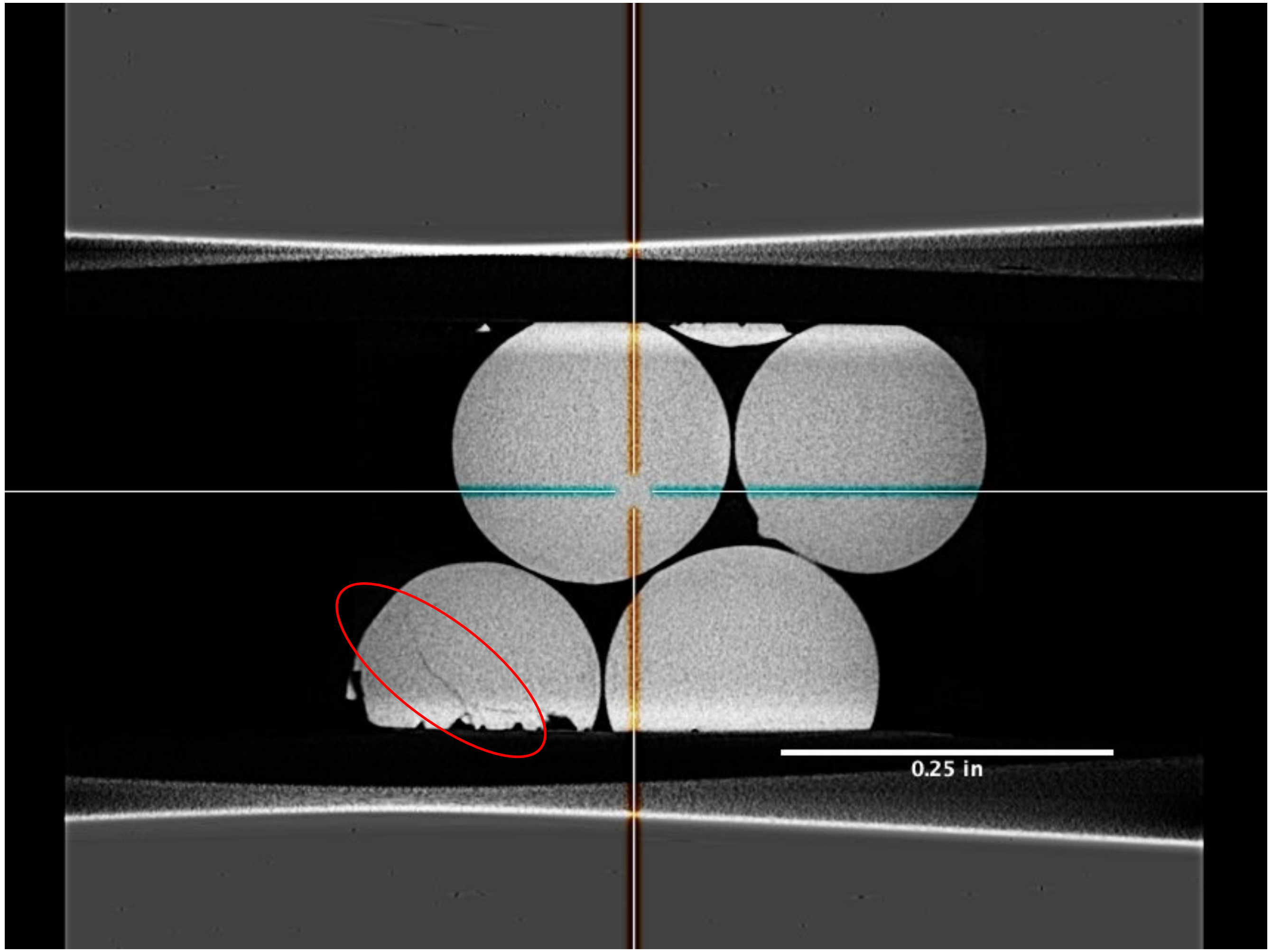
In-situ CT





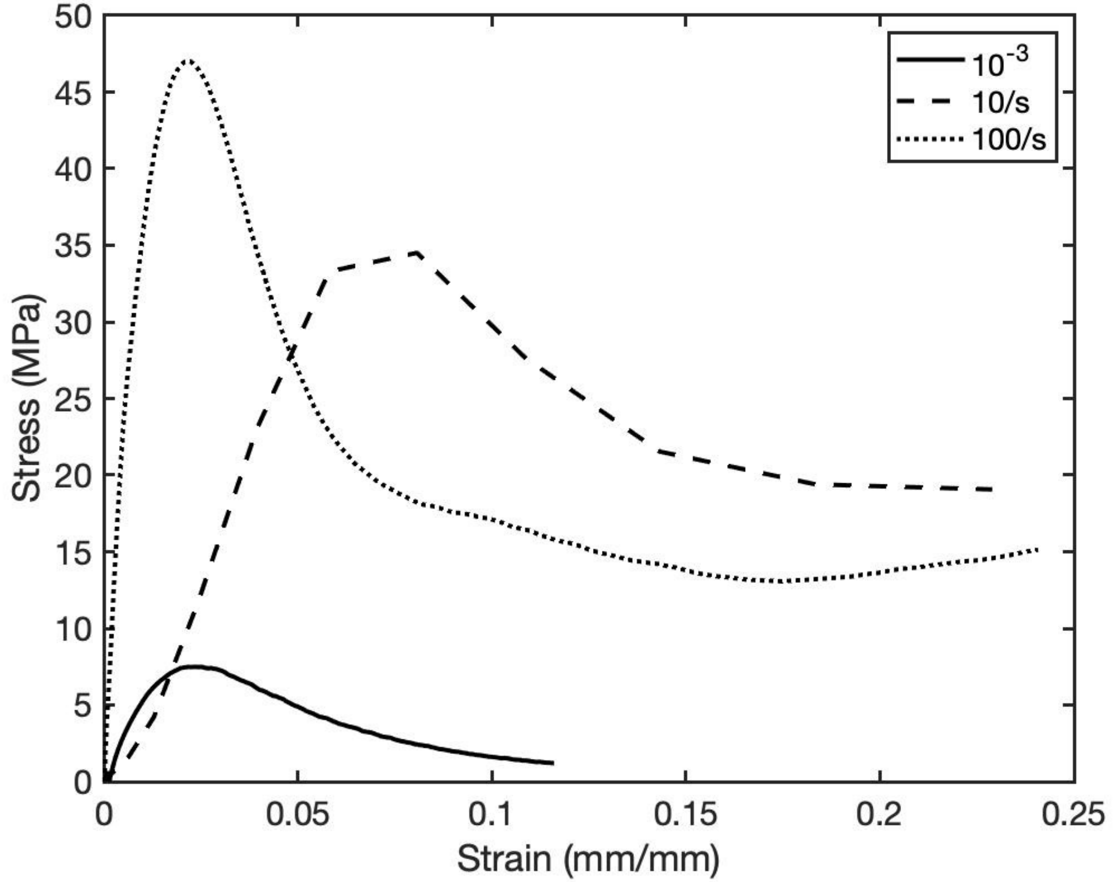


Acrylic die with F50 sand (neat)
for in-situ compression testing



Post compression glass bead with fracture denoted

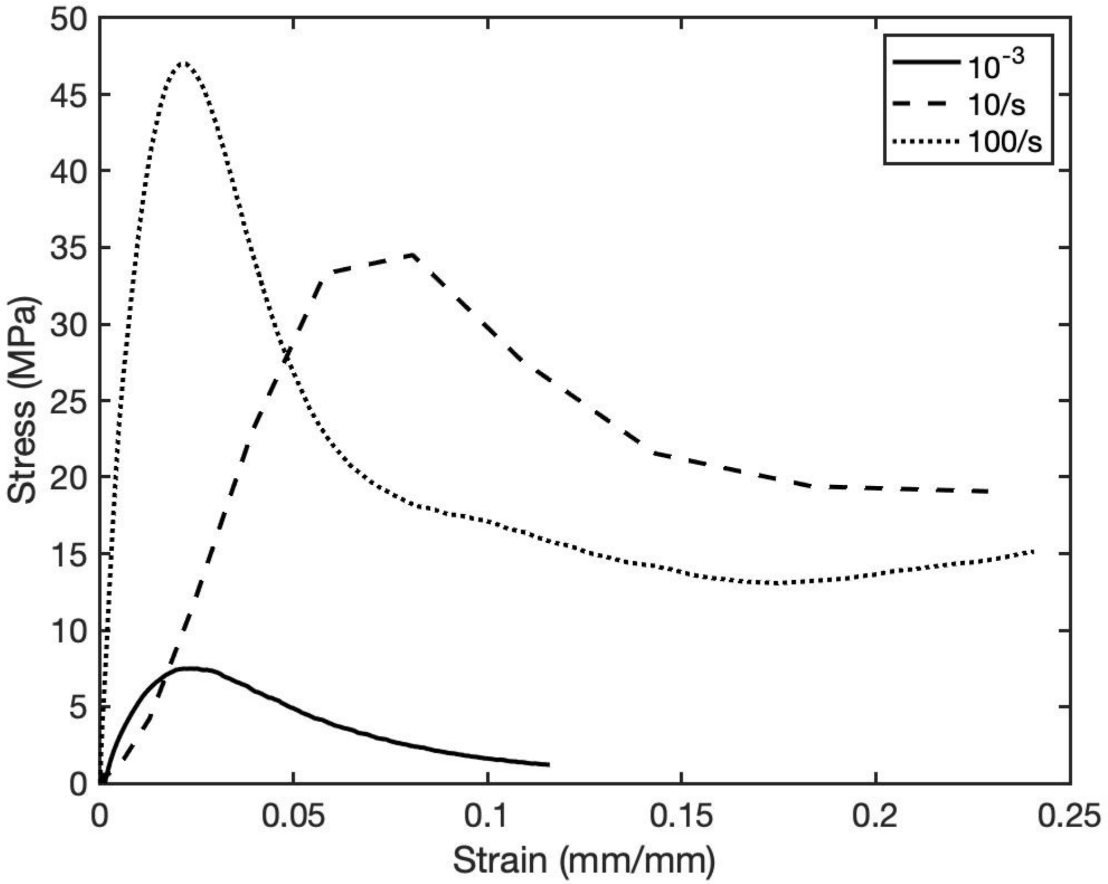
Mechanical Properties

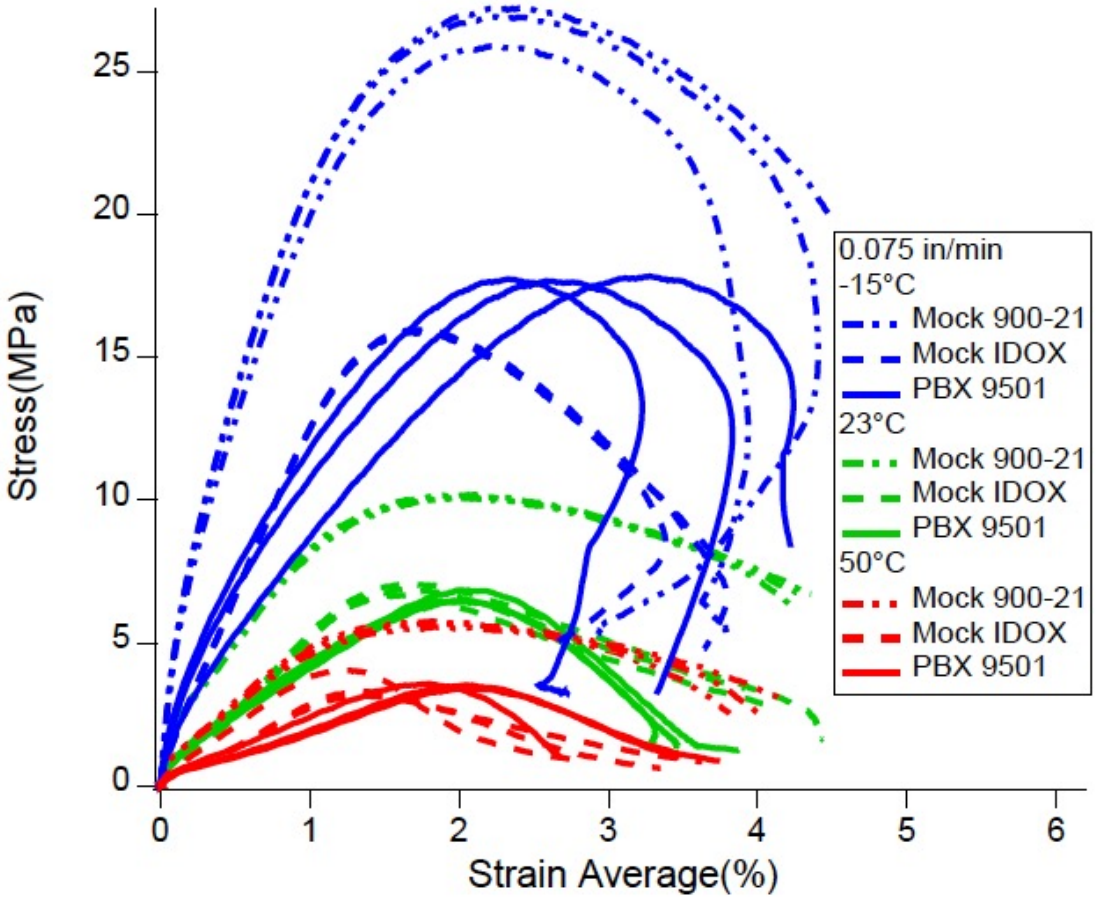


Stress vs strain for as-received LANL IDOX MHE samples

Gleeble thermomechanical load system

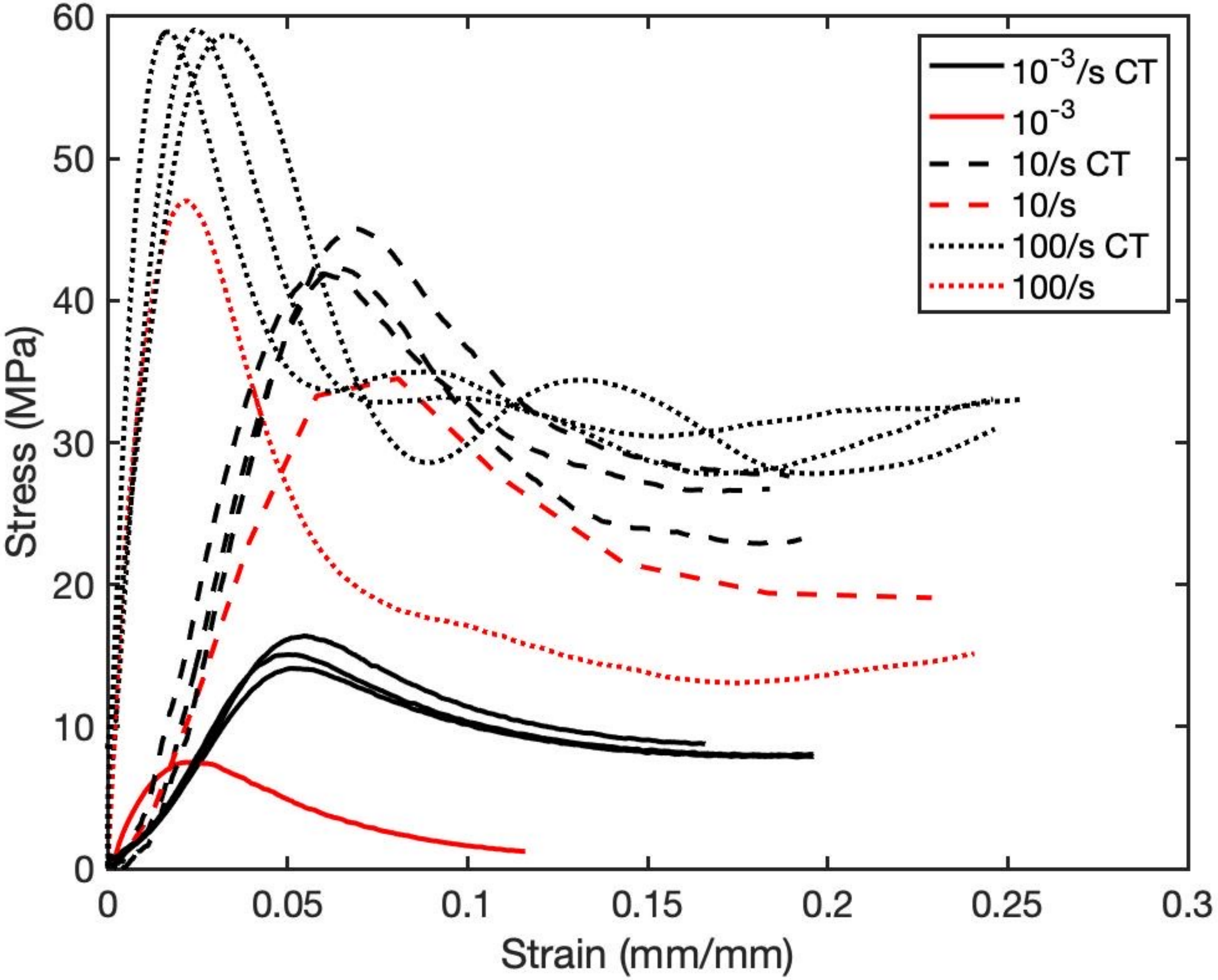
Mechanical Properties cont.





[1] 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.

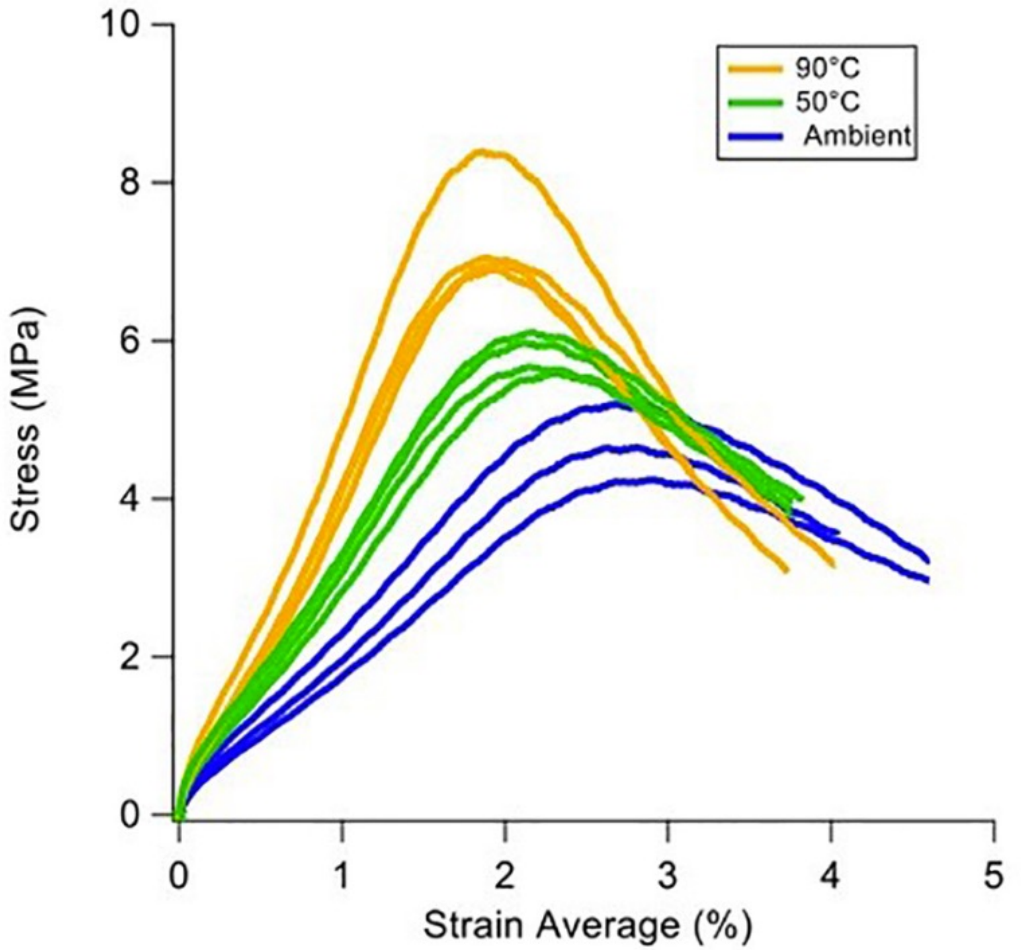
Mechanical Properties post-CT



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

Effect of Pressing Temperature

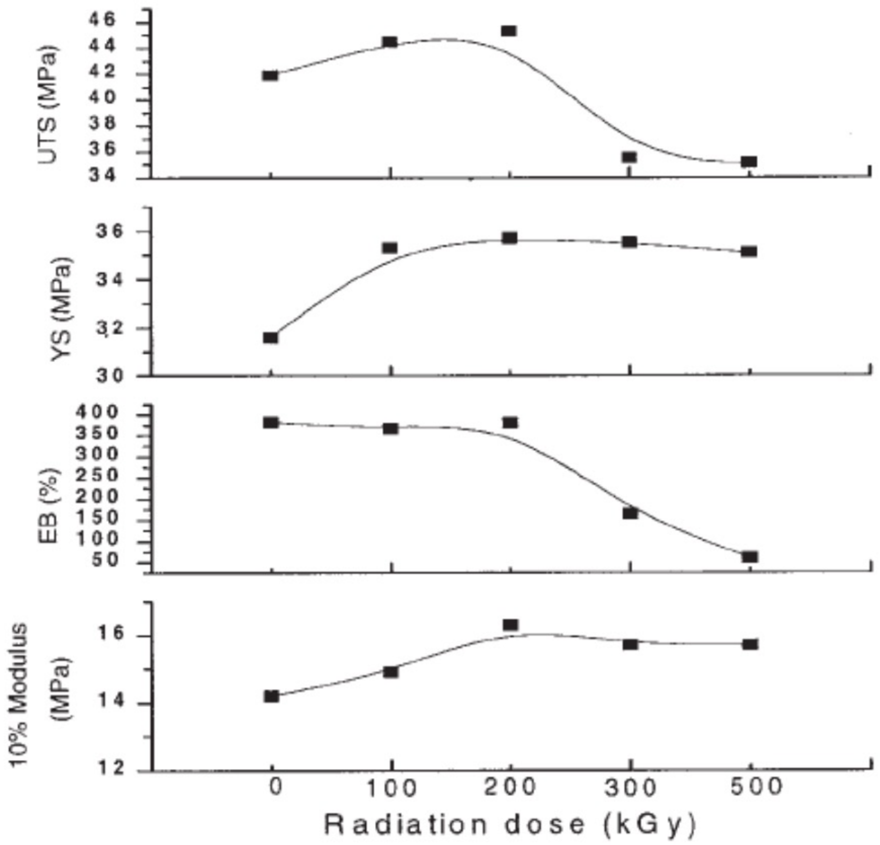
- Pressing temperature has a positive correlation to strength
- Negative relation to strain at UTS
- Does sample heat up during computed tomography?



Stress vs. strain for compression of B-1 IDOX mock pressed at ambient, 50° C, and 90° C

[3] 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

Strength Discrepancy



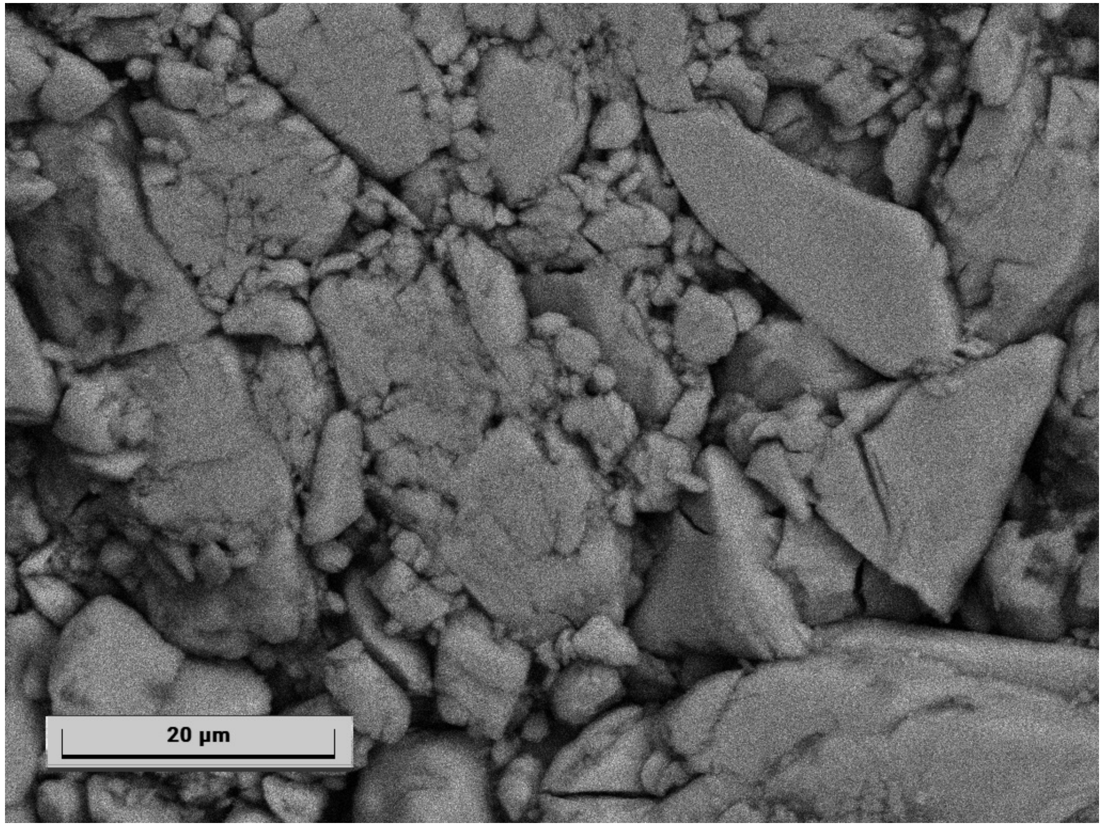
Variation in YS, UTS, EB and 10% modulus across varying radiation doses

[4] 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]

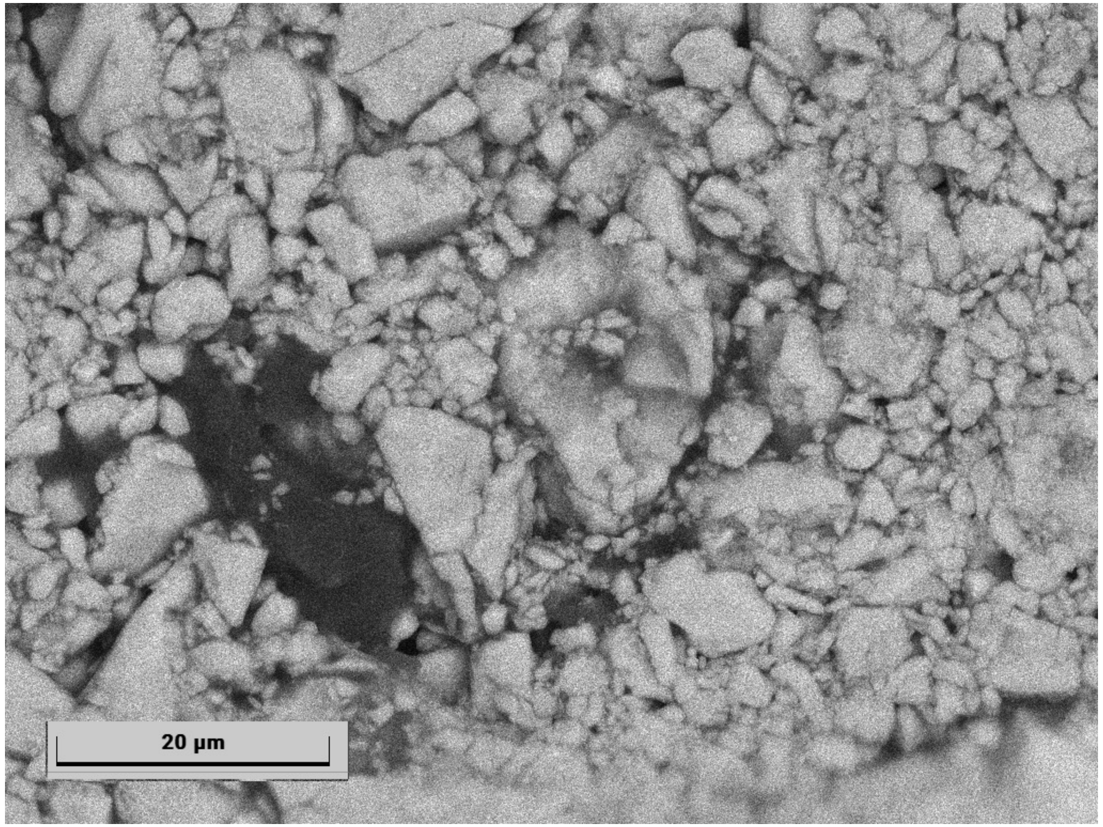
Theory: x-ray radiation from CT caused the increase in strength

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

Particle Size Comparison

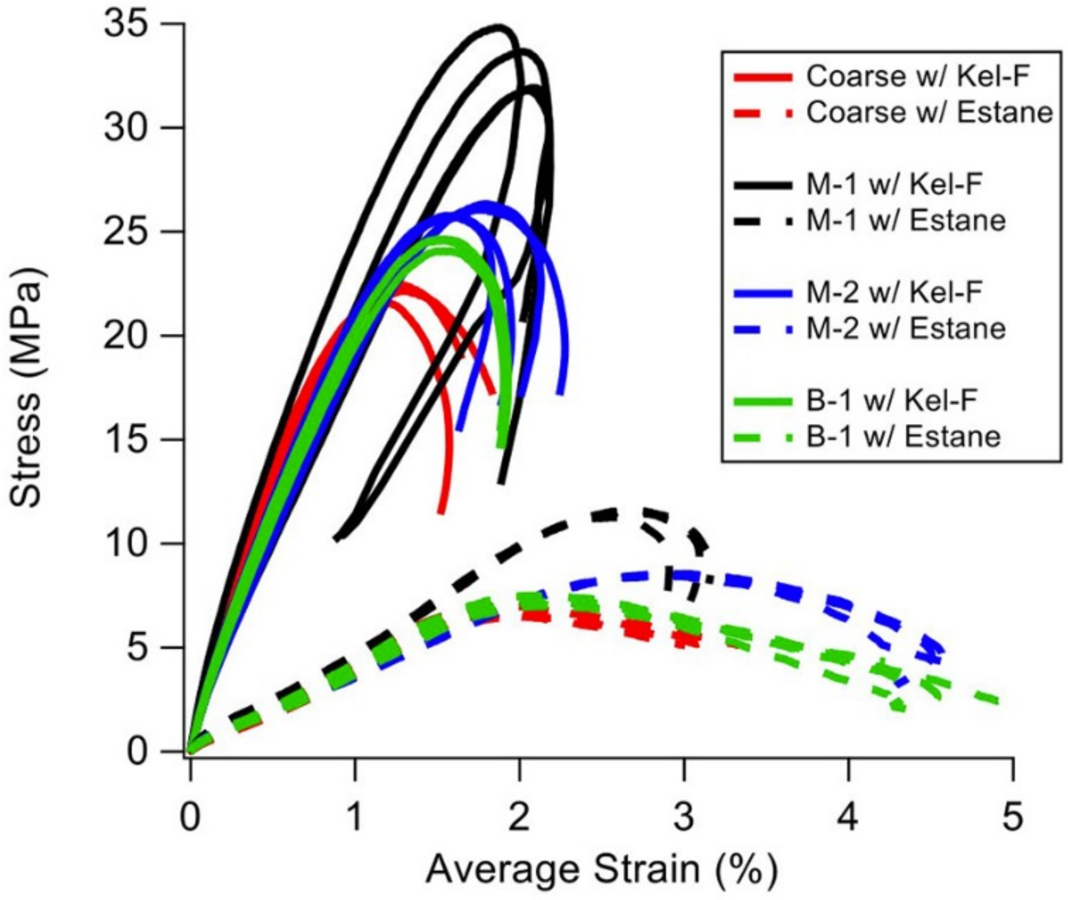


SEM, LANL Mock,
average crystal size ~43.6 µm²

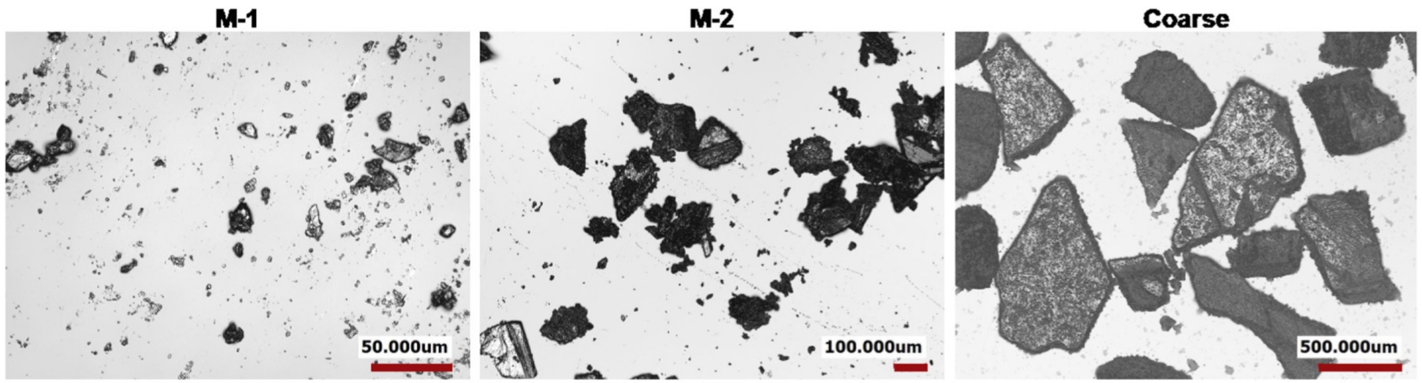


SEM, LANL Recycled,
average crystal size ~29.7 µm²

Crystal Size and Binder Effects



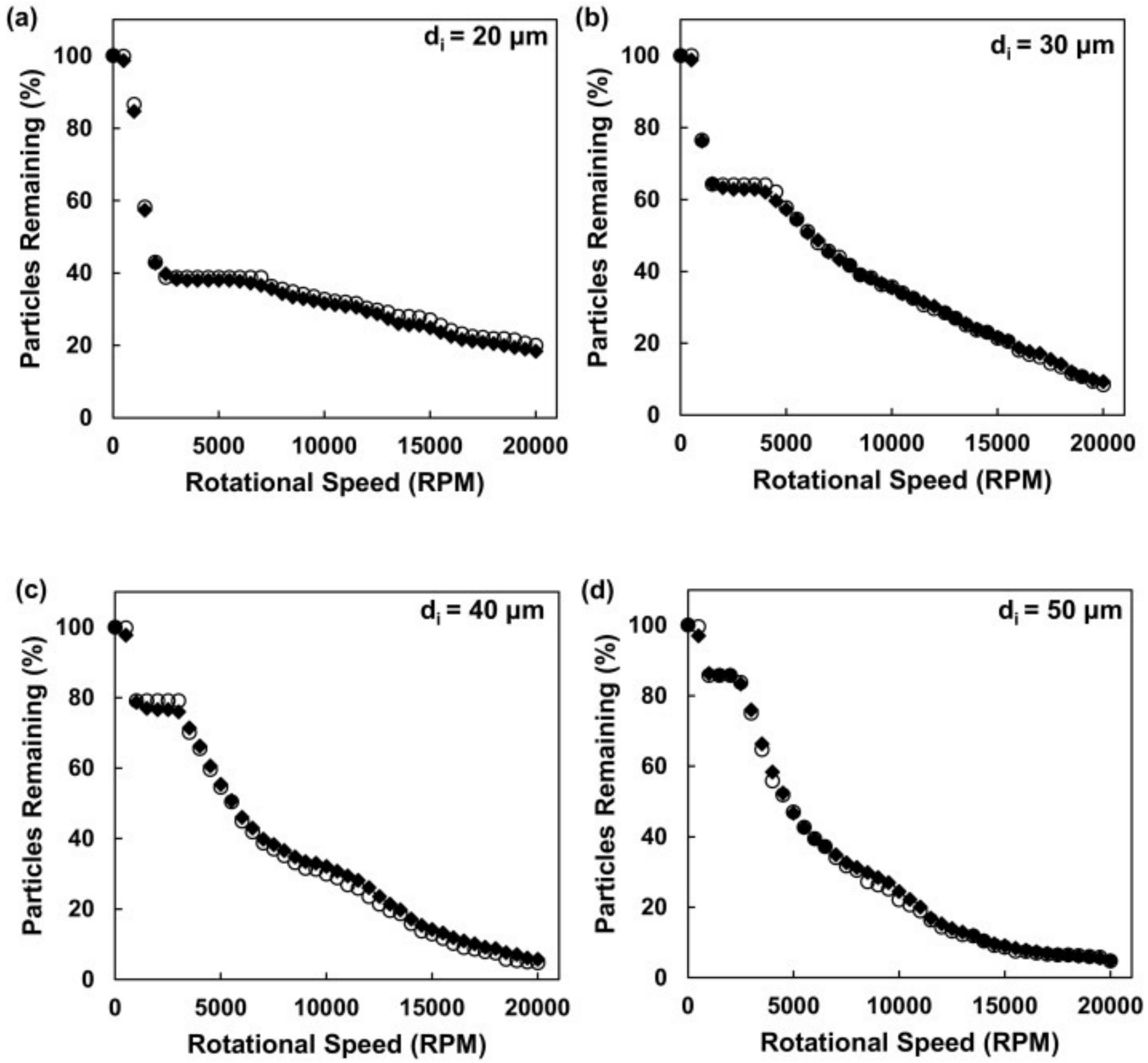
- Clear inverse relation between particle size and UTS
- Binder properties affect mechanical response even more strongly than particle size



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

[3] 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

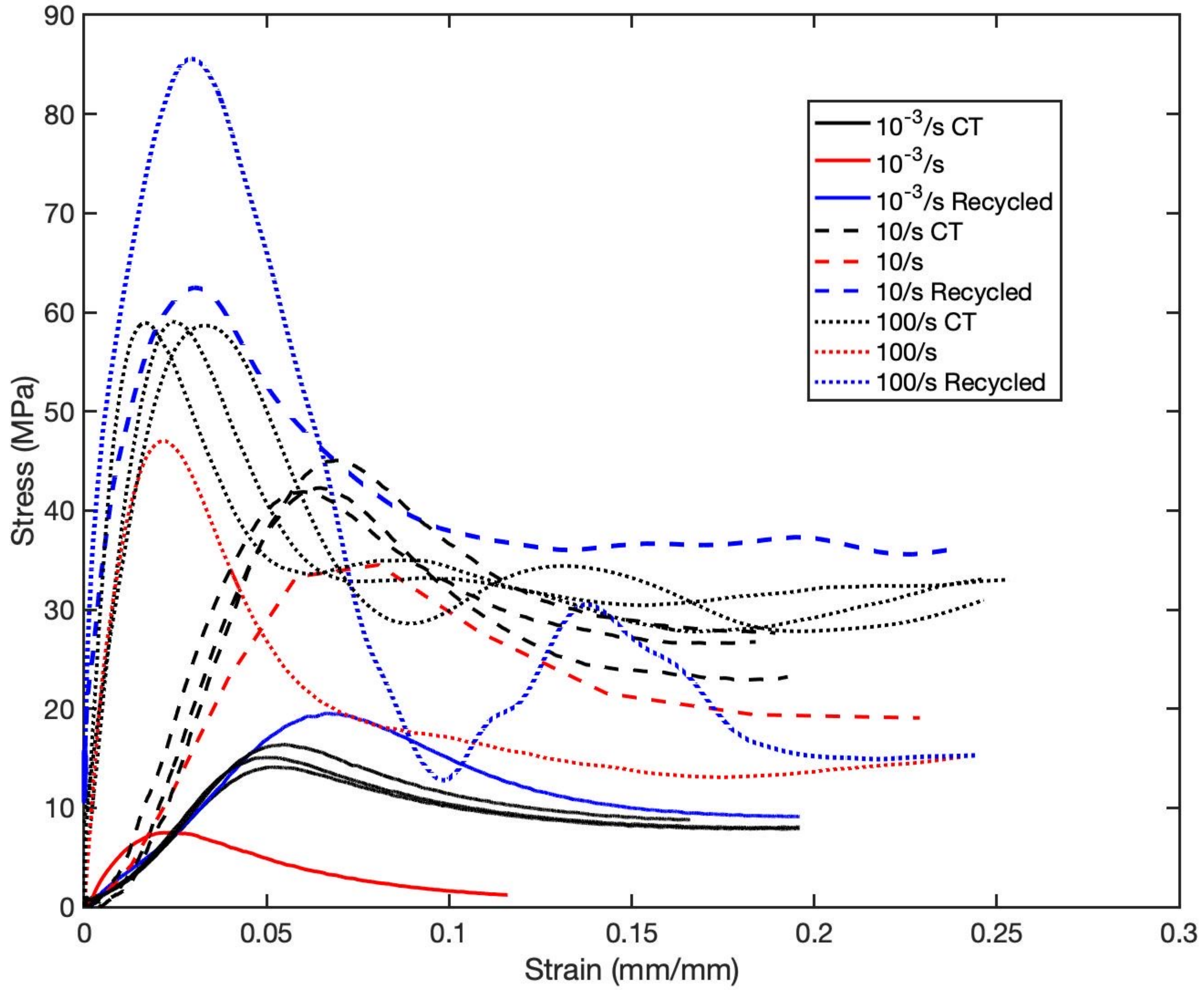
Particle Size cont.



- Centrifuge speed used to simulate increasing separation forces on silica powder of varying size
- Described through an effective Hamaker constant, which defines van der Waals body-body interactions
- Smaller particle size retained adhesion at higher RPMs
- By varying particle size intentionally, mocks can be tailored to better exhibit desired HE properties [4]

[5] C.A. Stevenson, M.C. Thomas, S.P. Beaudoin, An enhanced centrifuge-based approach to powder characterization: The interaction between particle roughness and particle-scale surface topography

Recycled vs Pristine

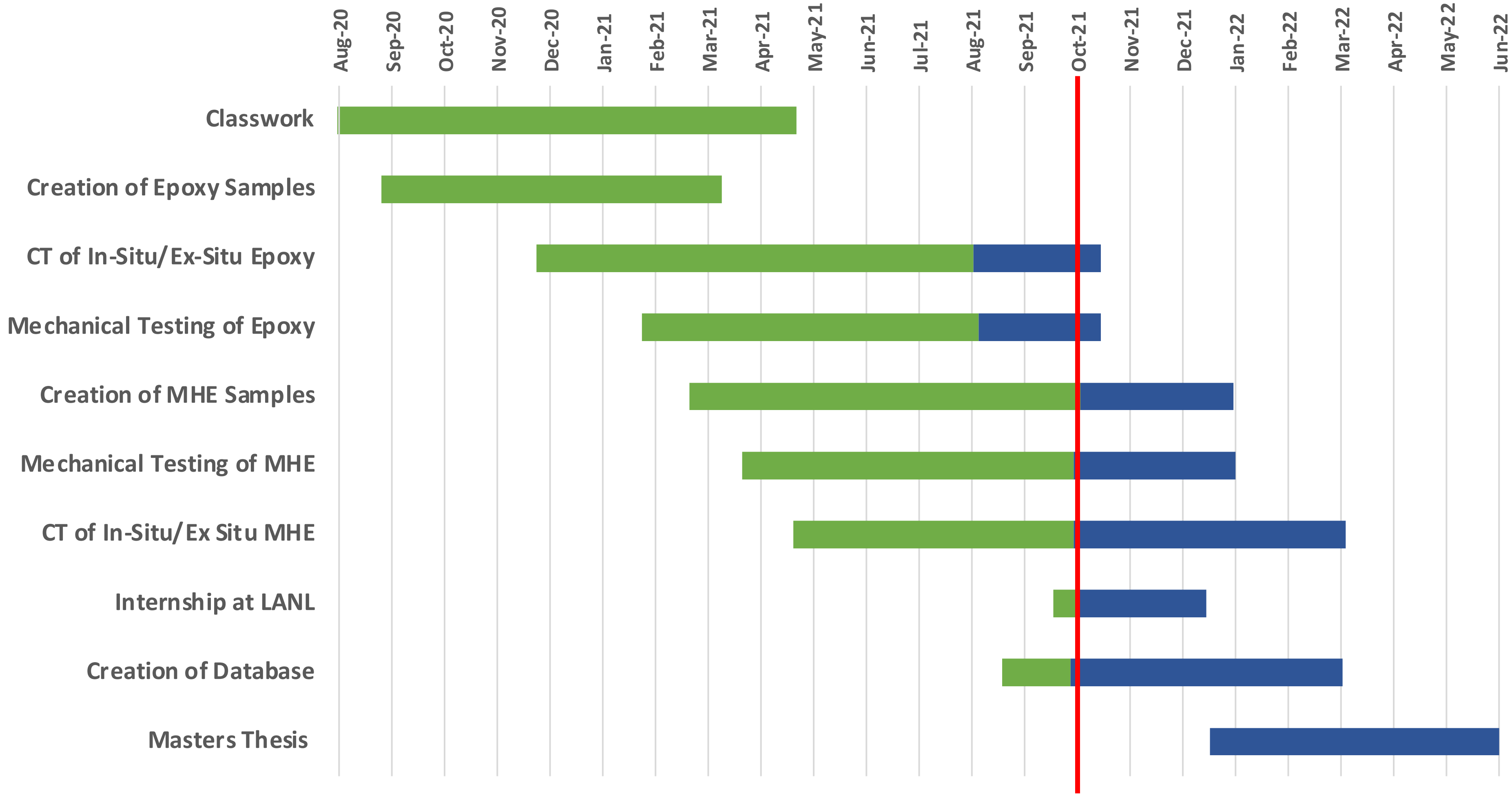


- Strength increase follows expected trend for decrease in particle size
- Particle size causes almost exponential increase compared to CT effects

Summary

- Higher strain rates lead to higher strength across sample conditions
- Probable radiation effects from computed tomography lead to increase in strength
  - Needs further investigation including between different binders
- Particle size has inverse relation to strength
  - Recycled samples have significantly smaller crystal sizes than pristine
- All of the above lead to a complicated material that will prove difficult to model with computer simulations, therefore it is necessary to collect as much data as possible to assist them in producing a robust simulation

Gantt Chart



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Classwork
Creation of Epoxy Samples
CT of In-Situ/Ex-Situ Epoxy
Mechanical Testing of Epoxy
Creation of MHE Samples
Mechanical Testing of MHE
CT of In-Situ/Ex Situ MHE
Internship at LANL
Creation of Database
Masters Thesis

Challenges & Opportunities

- More in-depth computed tomography
  - Iodine notoriously difficult to image with x-rays [6]
  - Beginning nano-CT and compression of IDOX crystals
  - Understanding effect of radiation on strength
  - Image segmentation of CT images

- Creation of new MHEs
  - Ideally, materials that are cheaper and easier to image than IDOX
  - Want to match as many properties as possible

New 1 inch die

Thank you!

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References

[1] J.D. Yeager, C.S. Woznick, D.G. Thompson, A.L.H. Duque, C. Liu, A.C. Burch, P.R. Bowden, M. Shorty, D.F. Bahr, Development of a new density and mechanical mock for HMX, Proc. 16th Int. Detonation Symp. (2018) 1631–1641.

[2] J. Brown, A.C. Co-director, PSAAP III Statement of Work (1) 4, (2020).

[3] 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. https://doi.org/10.1016/j.powtec.2021.06.009.

[4] 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, J. Appl. Polym. Sci. 99 (2006) 1633–1644. https://doi.org/10.1002/app.22689.

[5] C.A. Stevenson, M.C. Thomas, S.P. Beaudoin, An enhanced centrifuge-based approach to powder characterization: The interaction between particle roughness and particle-scale surface topography described by a size-dependent ‘effective’ Hamaker constant, Powder Technol. 391 (2021) 198–205. https://doi.org/10.1016/j.powtec.2021.06.006.

[6] A. Murphy, I. Bickle, Iodinated contrast media, (2016).