Understanding Complex Dynamic Response Through New Diagnostic and Analysis Methods

3rd DyCoMax Workshop
15 January 2021

Minta C. Akin, LLNL
Acknowledgments

- Staff at DCS/APS, GSECARS/APS, Sector 1/APS, Sector 32/APS, CHESS, ALS, ESRF
- LLNL LDRD program 16-ERD-010
- DyCoMax Organizers

“Complex Dynamic Response” is all the messy and complicated physics we don’t have great models for (yet)

- Standards in the field show where our strengths lie:
  - Al, Cu, Ta

- Easy to
  - Machine
  - Measure/characterize
  - Describe with conservation equations and bulk variables

- Contrast: all the fun, cool stuff we don’t understand
  - Chemistry, Kinetics, Temp.
  - Heterogeneous materials
    - Grains, additive manufacture
  - Strength, shear, failure

- Probing these topics means we need inside knowledge

Most models are built around idealized, bulk materials. Most materials are not ideal. Beam lines are great tools for improving our understanding!
Granular systems are a special case of heterogeneous media

- Metamaterials
  - Additive manufacturing
- Foams
- Aggregates
  - concrete, raisin bran, most rocks
- Fibers
  - Felts, fiberglass, woven materials

Knowledge of bulk material does not mean we can predict its discontinuous forms’ response
Granular response is complex; current models are inadequate

Small changes in initial properties lead to large changes in response

Perry et al, 2015

Ta$_2$O$_5$ Hugoniot results from the P-λ model (dashed lines) compared to experimental results for granular and consolidated Ta$_2$O$_5$.

Ko = Er$_3$($\frac{1}{2}$n)($\frac{1}{2}$n)($\frac{1}{2}$)

and assuming a value of 0.2 for n, which is a reasonable assumption for most ceramics, we find a value of 86.8 GPa for the bulk modulus Ko. From this, a value for the bulk sound speed of 3.3 km/s is obtained. This is used in the common linear $U_s$–$U_p$ relationship of $U_s$ = $c_0$ + $U_p$.

Although $c_0$ is not, in general, equal to the bulk sound speed, it is often very close to that value making it a reasonable assumption here. It is necessary to specify the thermal behavior of the material; here, that is done through the Grüneisen parameter G, which is assumed to have the form $G(P) = G_{oe}(\frac{P}{K_0})^n + G_e(\frac{P}{K_0})^n$.

Values of 1.15 and 0.5 are assumed for $G_{oe}$ and $G_e$, respectively, and a value of unity is used for n. This gives a gradual decay of G from 1.15 at ambient conditions to 0.5 at high pressures, the latter based upon the limiting case for very high pressures. As can be seen in Fig. 15, the model constructed in this manner fits the data quite well. The model results shown are not quite "blind" in that the value of G was adjusted slightly to fit the data, but in some cases the ambient value might be available. If it were not, an assumption of $G_{oe} = 1$ would be reasonable and, in this case, not much different from the results shown.

While the P-λ results agree well with the Z and 2-stage results, there are additional data for Ta$_2$O$_5$ aerogel from the OMEGA laser facility [Miller et al., 2007]. These experiments were done for material with initial density $\rho_{\infty}$.

Grain scale data are missing, and we need them to advance predictive ability.

Vogler et al., SAND2011-6770
Key questions about heterogeneous materials remain

- Scatter sources?
- When are data good/trusted enough?
- What’s going on inside?
- Can we avoid measuring every single form?

We need data to build internal micromechanical models to combine with bulk material models.
Vertical and radial packing variation violate assumptions made in bulk measurements

- Not uniform
- How thick is a boundary? How big does a sample need to be to not be dominated by boundary effects?
- If the sample is small enough, it will be all boundary and more uniform. Is this preferable? Sometimes...

GSECARS computed tomography
Vertical and radial packing variation violate assumptions made in bulk measurements

- Not uniform
- How thick is a boundary? How big does a sample need to be to not be dominated by boundary effects?
- If the sample is small enough, it will be all boundary and more uniform. Is this preferable? Sometimes...

We need to look at this variation in larger, more representative samples.
Larger samples also show lots of variation. We need to determine how much packing variation is present.

In this measurement, crack volume can be up to 7%.
Combined Topology and Stress Analysis gives a rich data set

X-Ray Radiographs

Far Field Diffraction Data

-116N

Micro Computed Tomography

Grain Position, Lattice Orientation, and Lattice Strain Analysis

P (MPa)

0 350

CHESS (Cornell U.)
Imaging and diffraction setups constrain experimental design

DCS setups
Dynamic imaging experiments are designed to be close to 1D.

IMPULSE imaging setup at DCS

Crum et al., J. Appl. Phys. 125, 025902 (2019); https://doi.org/10.1063/1.5057713
Detailed data are extracted to improve models and analysis

- Reconstructed CT of sample
- Segmented to find sample properties
  - particle size distribution
  - thickness averaged attenuation of the sample.
- Used to inform models and calculations
Fracture and compaction response differ in wet vs. dry media

- X-ray phase contrast imaging of shocked glass spheres
- Deformation mechanisms of dry and water-saturated samples are not the same — consistent with shock recovered samples
- We update our models using these data
Packing variation seeds variation in compaction front in sand

465 m/s impactor

Middle region = between black bands

Mean density profiles of middle region; red = density compaction front

Compaction front (cyan)

Sample-polymer interface (blue)

Length scale of variation depends on analysis method. Density variation finds a length scale of ~30 grains. Local filtering reduces this to a few grains.
Simulation results qualitatively agree but can be improved.

Simulation results showing thickness-averaged density in the $x$ - $y$ plane for the granular material impacted at 465 ms$^{-1}$. 

Packing variation seeds variation in compaction front.
Identifying shock boundaries and densities can be done with machine learning (ML)

- As throughput increases, analysis becomes more time consuming
- Identifying shock boundaries in images is a challenge
  - Want to avoid subjective assignment
  - Can be slow

Machine learning can be challenged to determine if X is ball or table

Lund et al in press
We apply the ML algorithm to train each image and find boundaries.
We apply the ML algorithm to train each image and find boundaries

Original Image

Training regions

Assigned regions

Lund et al in press
Repeating for each image, we can find the boundary evolution.
Out-of-plate deformation must be accounted for; we built new models to do so.
Conclusions

- We need to understand/characterize samples at detailed level
  - Not just bulk EOS/strength, but also local variations in density and network
  - Local structures may imprint
  - Wetting (water or container) changes both contact type and friction

- Analysis methods can give different results
  - When are we over-filtering?

- Multiple length, pressure, and time scales apply
  - At grain/grain or grain/liquid contact
  - Within grain
  - Between grains/ across network
  - At boundaries

- Improving model capabilities for packing, local stress-strain, friction, and strength has led to better models that can capture some of the response