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National Nuclear Security Administration

## HARD Solids
# Micro-Scale Measurements

*PL14-V-HARD solids-PD3WA*
*Thomas J. Kulp, Charles LaCasse IV, Thomas A. Reichardt, and Julia Craven-Jones*
*Sandia National Laboratories, Livermore, CA*

## Goals and Objectives

- Construct ideal material systems having well-characterized properties (e.g., complex refractive index – n(λ) and k(λ), particle size and shape distribution, packing density)
- Measure their reflectance spectra for use in radiative-transport model validation
- Measure the dependence of spectroscopy on specific ideal-system material parameters, serving to:
  - prioritize the importance of various parameters
  - stimulate development of new modeling approaches

## Introduction

- Reflectance spectra of particulate solids are determined by radiative transport among its grains
- Radiative transport depends on n(λ) and k(λ) and the morphology (PSD, packing density, particle shape) of the solid material
- The refractive indices of materials of interest (MOIs) are not known and their morphologies are usually very complicated
- Numerical models often assume a simplified morphology (e.g., spherical particles)
- Measurements on ideal systems allow testing of solids having known refractive indices in tailored geometries (simple → complex)

## Methods

### *Spectral measurements*

- Spectral measurements made using conventional spectrometers (LWIR→VIS) equipped with integrating spheres (total/diffuse)
- Polarimetric/directional reflectance capabilities are being developed

### *Morphological characterization*

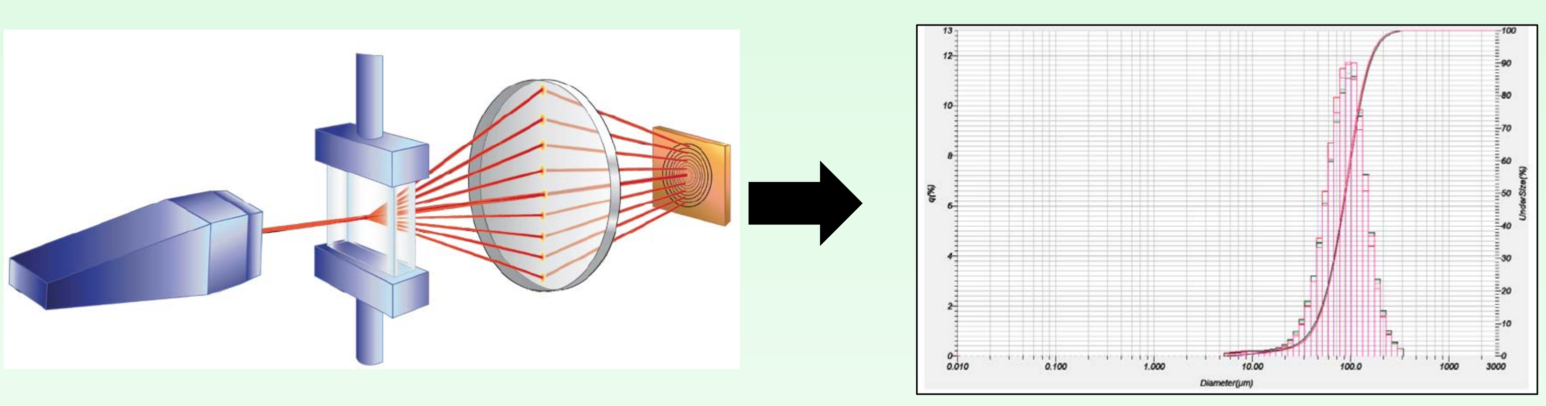
The morphology of a packed granular solid is being characterized by:

A. Measuring detailed size and shape distribution for constituent particles; assuming that they pack with some density;

B. Directly measuring the three dimensional properties of the full (packed) solid, after which its spatial properties can be described.

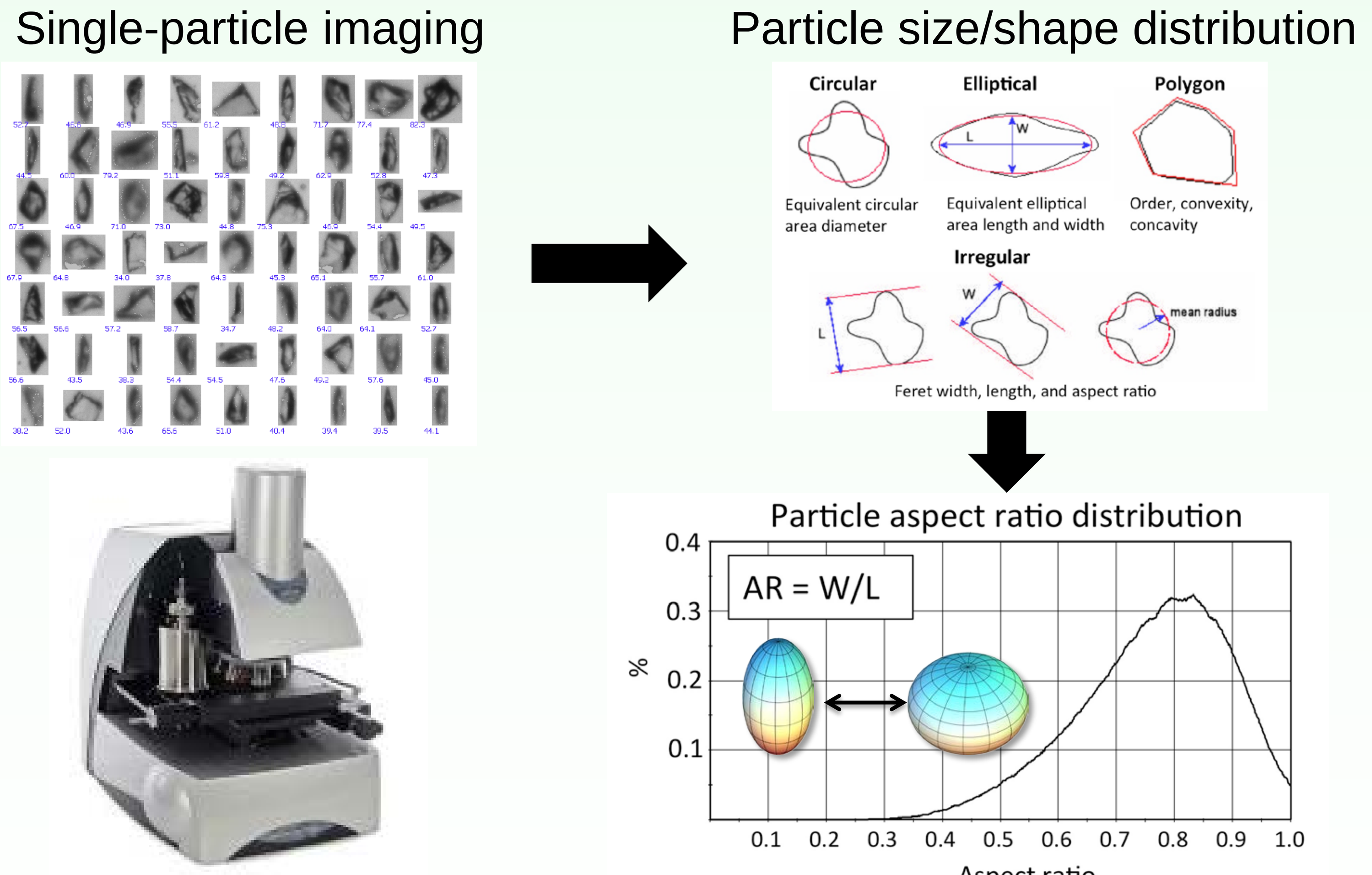
A. Detailed distribution measurements

Diffraction measurement | Particle size distribution



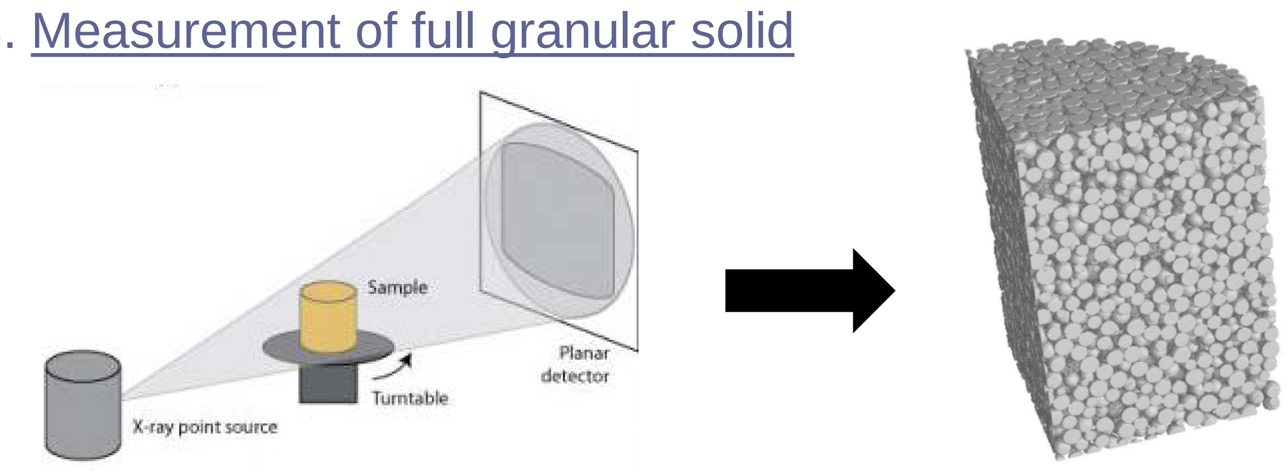
Optical scattering from many (1000's) particles is measured and fit (Mie theory) using a commercial instrument (Micromeritics Saturn 5205)

Single-particle imaging | Particle size/shape distribution




Optical images of many (10,000's) single particles are recorded and analyzed to determine size/morphology (Malvern MorphologiG3)

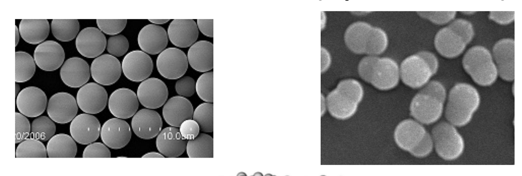
B. Measurement of full granular solid

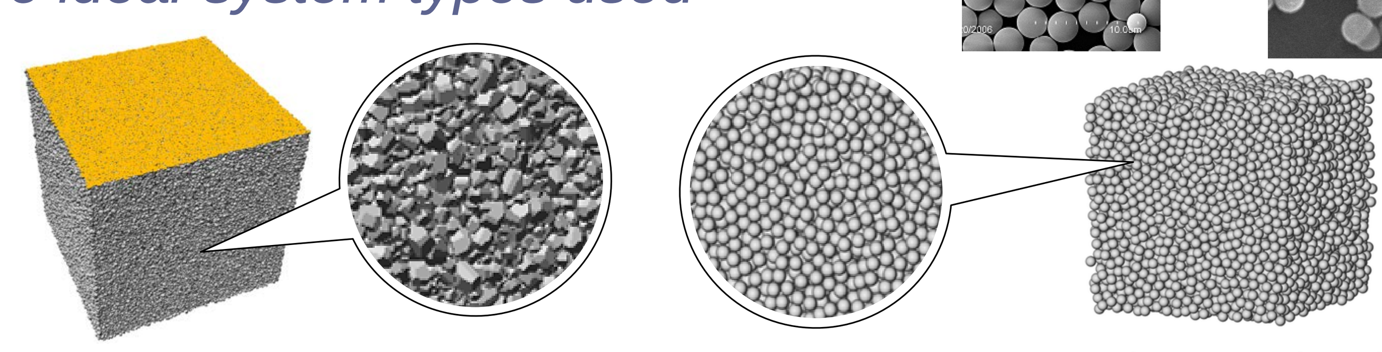



X-ray tomography is used to digitize the full structure of the solid; this can be input into the model directly or through extracted parameters (e.g. pair correlation function, Fourier parameters)

## Results / Major Findings

### *Two ideal-system types used*

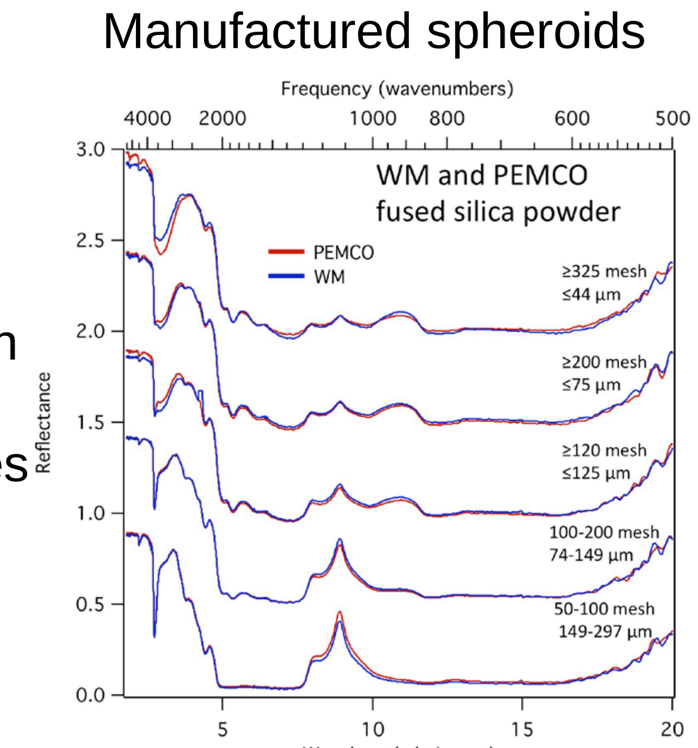


Crushed, sieved powders | Manufactured spheroids

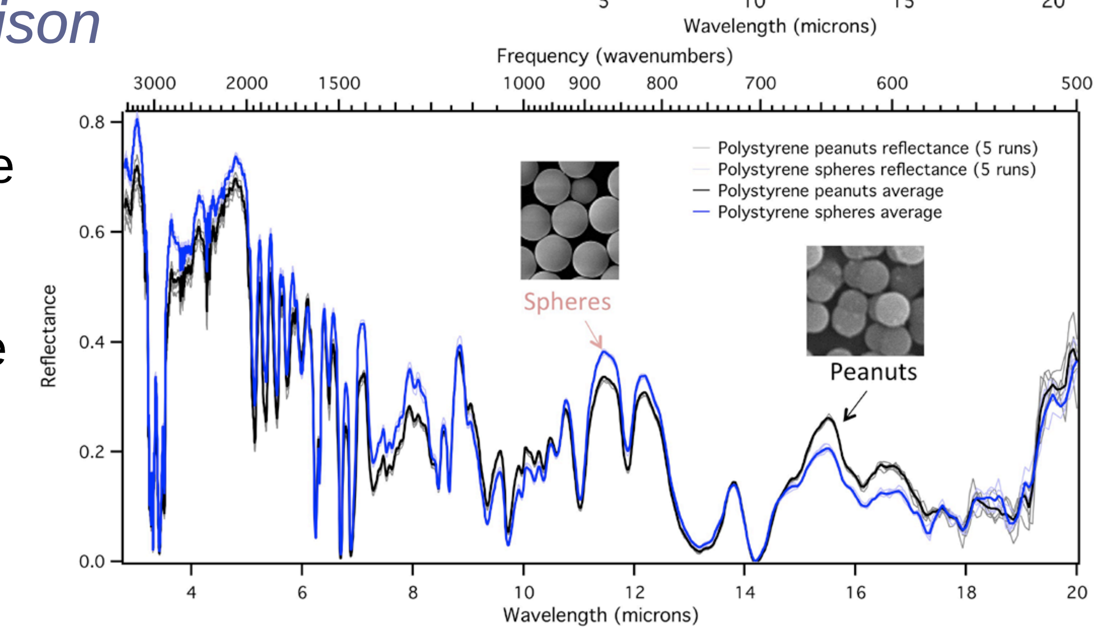
### *First model validation set provided*

- Crushed, sieved fused silica
- Known n, k
- Complete morphological characterization of 5 size fractions
- Excellent agreement, 2 materials sources
- Microscale model replicates data (see Inverse Microscale Model poster

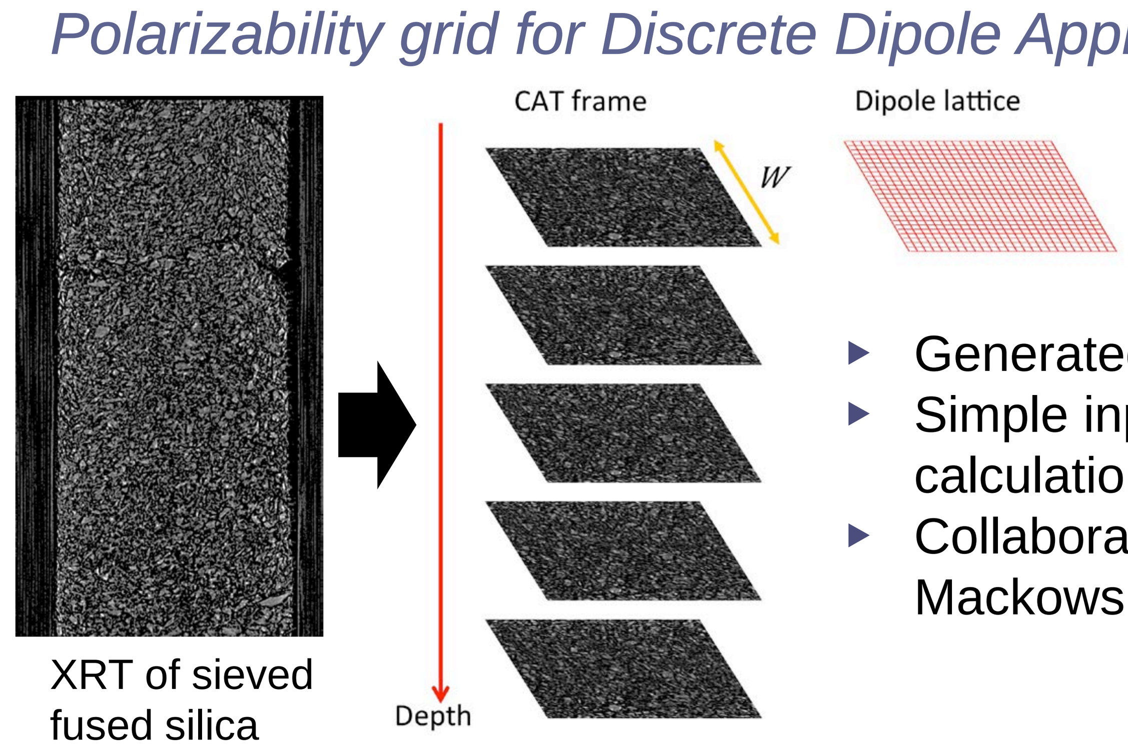



### *Particle shape comparison*

- Latex particles
- Unknown n, k, but same for both
- Coordinated with Spheroid modeling (see Inverse Microscale Model poster)




### *Polarizability grid for Discrete Dipole Approximation (DDA)*




- Generated by XRT
- Simple input for efficient EM calculation of reflectance
- Collaboration with Dan Mackowski of Auburn University

## Conclusion, Next Steps, and Relevance to Program Objectives

- The ideal system measurements provide data to verify models and stimulate new model generation (e.g., for spheroids and for DDA)
- Next steps include:
  - Comparison of spheroid measurement and model
  - Implement and test XRT→DDA with Auburn
  - Advance from optically thick → arbitrarily thick solids (next "spiral" in HARD Solids advancement)
  - Implement polarimetric / directional reflectance
- This tasks contributes to the overall HARD Solids objective of generating new physical models to support the remote sensing of solids

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**CONTACT**
Thomas Kulp
Phone: 925.294.3676
tjkulp@sandia.gov