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HARD Solids
Micro-Scale Spectral Modeling

PL14-V-HARD solids-PD3WA

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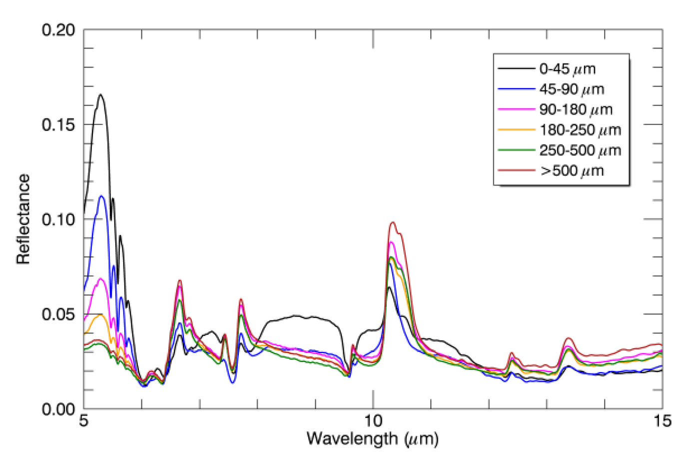
Goals and Objectives

- Develop physics-based models to compute spectra of complex solid materials
  - for use in algorithms leveraging these model and in spectral signature libraries
  - and supported by measurements that provide input data for models, validate models, and enable new models
- Model will incorporate fundamental physical properties (n,k) and account for morphological characteristics – particle size, shape, packing density, surface roughness, deposit thickness.

Introduction

Reflectance spectra of particulate media can exhibit strong dependence on morphology.

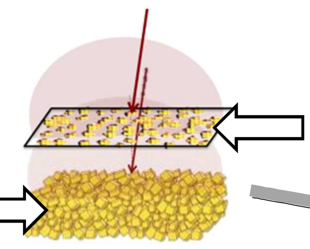


Varying the particle size, shape, packing density, surface roughness, and deposit thickness over entire parameter space is to be accomplished via modeling the interaction of incident radiation with the chemical deposit.

Micro-scale spectral modeling effort encompasses both forward and inverse modeling.

- Forward modeling considers the physics of incident radiation interacting with the chemical deposit (e.g., via numerical simulation).
- Inverse modeling parameterizes the forward model(s), and then varies these parameters to achieve optimum agreement with experimental data.

Baseline model combines 1-D radiative transfer (RT) within the particulate medium…



… with the Fresnel equation for 1st-surface reflection

The resulting reflectance for the baseline model is the sum of the *2 contributions*:

$R = F_{Fresnel} \times R_{Fresnel} + (1 - F_{Fresnel} \times R_{Fresnel}) \times R_{medium}$,

where

$F_{Fresnel}$ is the fractional area of the Fresnel reflectance ($0 \leq F_{Fresnel} \leq 1$)

R_{medium} is the 1-D radiative transfer solution

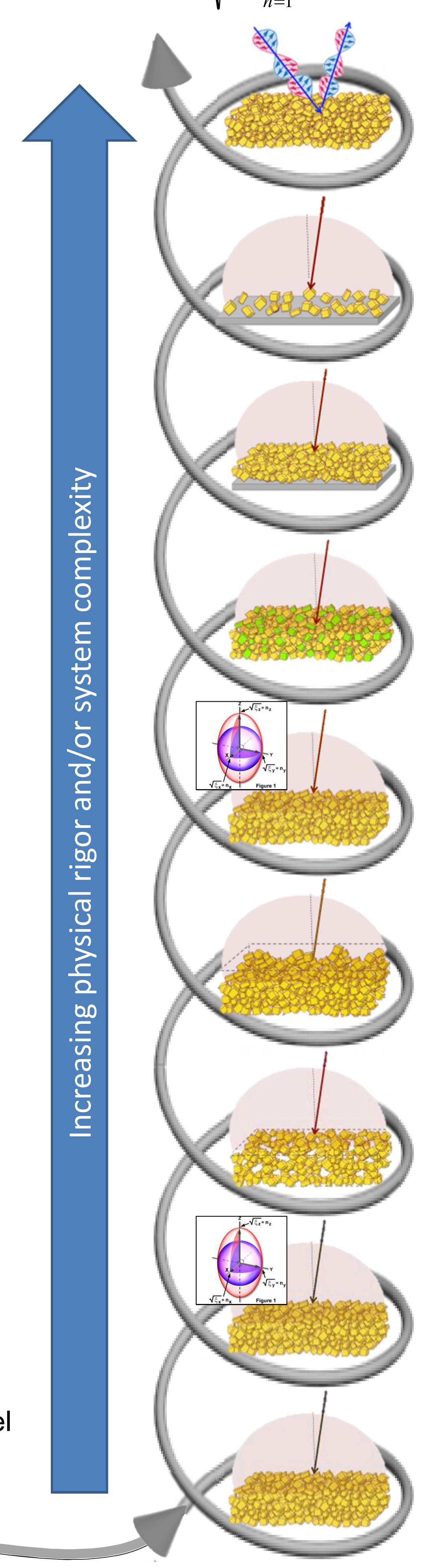
$R_{Fresnel}$ is the Fresnel reflectance of the medium → $R_{Fresnel} = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$

Currently assessing approximation via ray-tracing

Methods

Increasing physical rigor and/or system complexity considered when achieving reflectance-*RMSE*<0.03 over *N* spectral channels, where

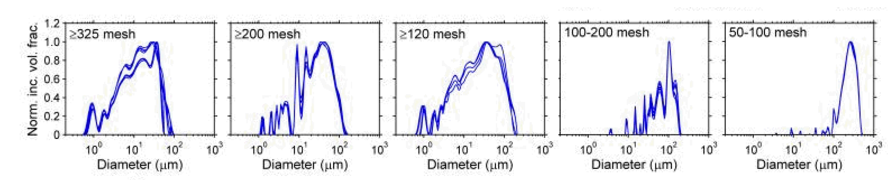
$$RMSE = \sqrt{\frac{1}{N}\sum_{n=1}^{N}\left|R_{model,n} - R_{measured,n}\right|^2}$$

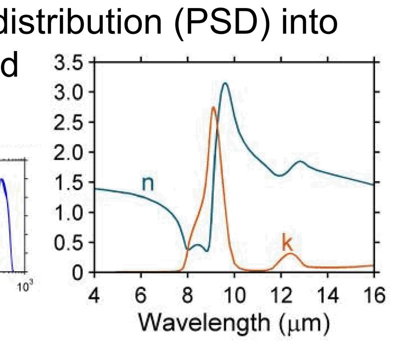


9. Polarimetric and angularly resolved measurements
8. Dispersed particles (sub-monolayer)
7. Optically thin deposits
6. Mixed materials
5. Strongly birefringent material
4. Variable surface roughness
3. Optically thick, variable packing density
2. Mildly birefringent material
1. Optically thick, single packing density

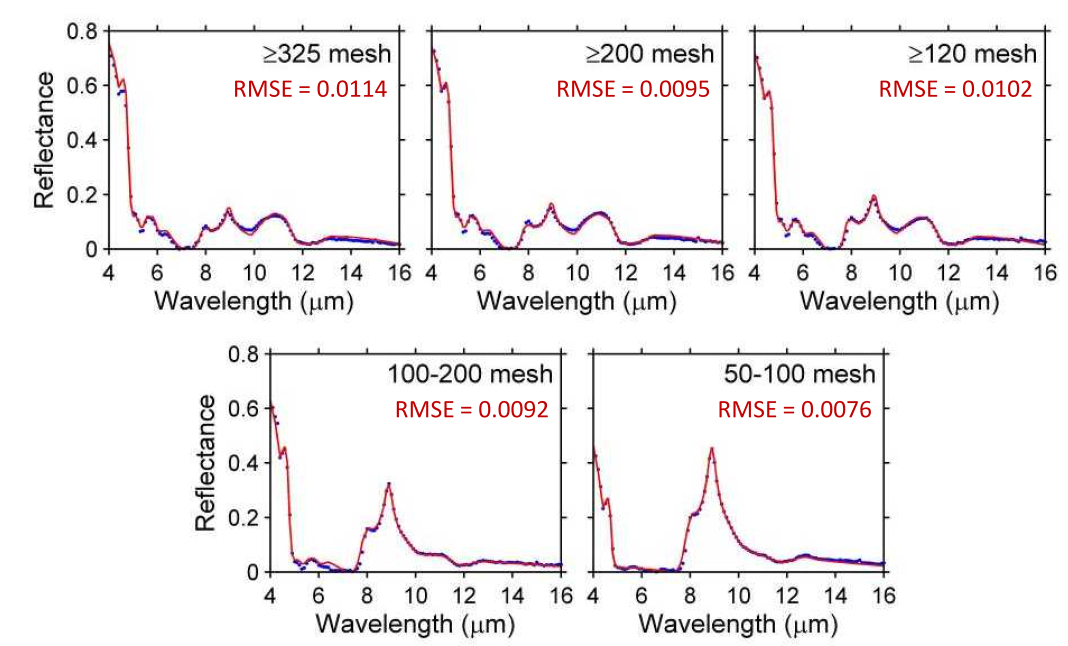
Results / Major Findings

The baseline model divides measured particle size distribution (PSD) into size bins, and averages the calculated scattering and extinction properties over the PSD.





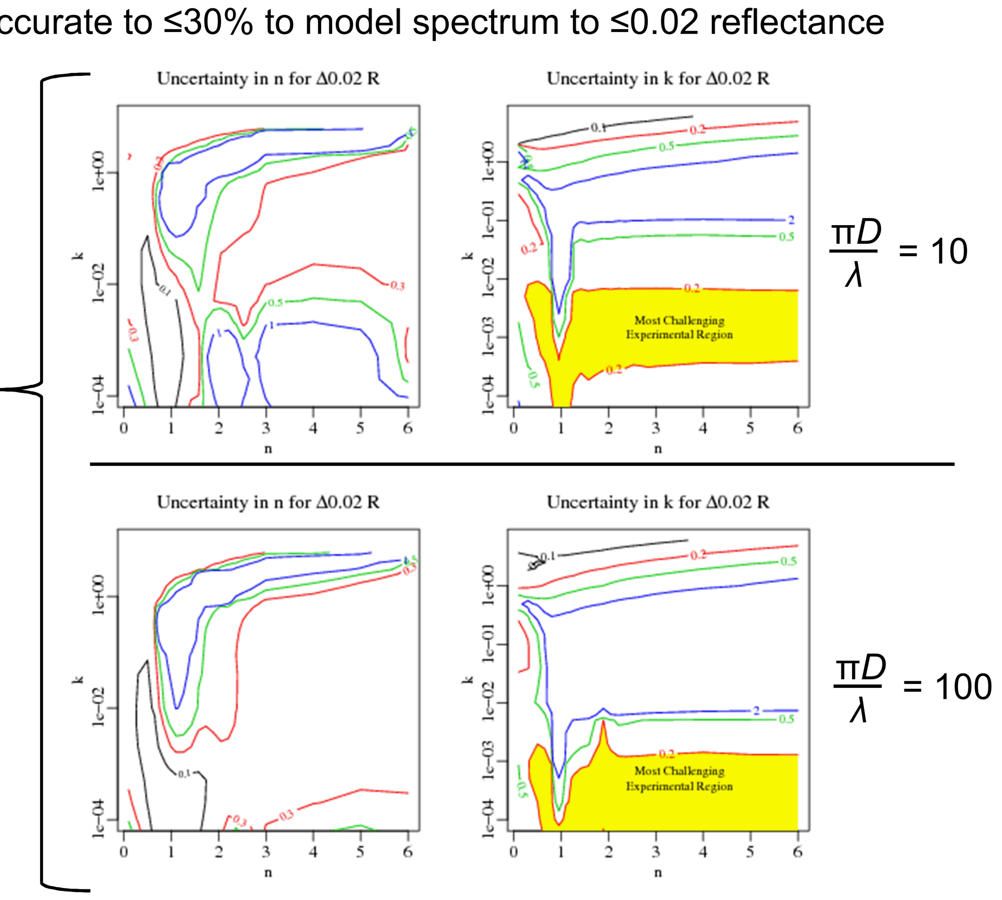
The baseline modeling results (red lines) demonstrate ~0.01-reflectance RMSE agreement with measurements (blue points) of size-selected fused silica powders.

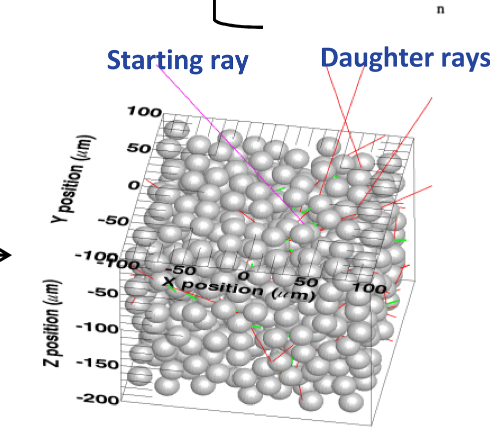


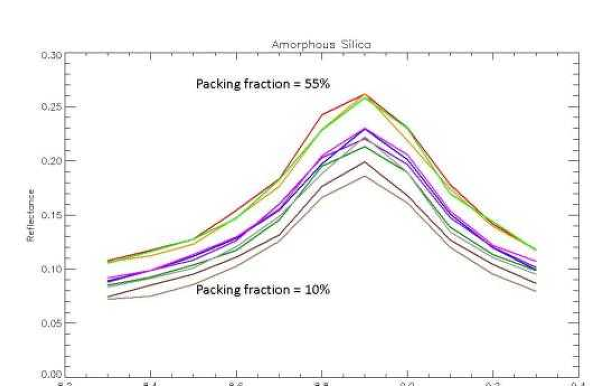
The baseline model is used to assess required accuracy of n/k measurements.

- Need n/k accurate to ≤30% to model spectrum to ≤0.02 reflectance

1-D RT: Ambartsumian invariant imbedding solution for an optically thick layer

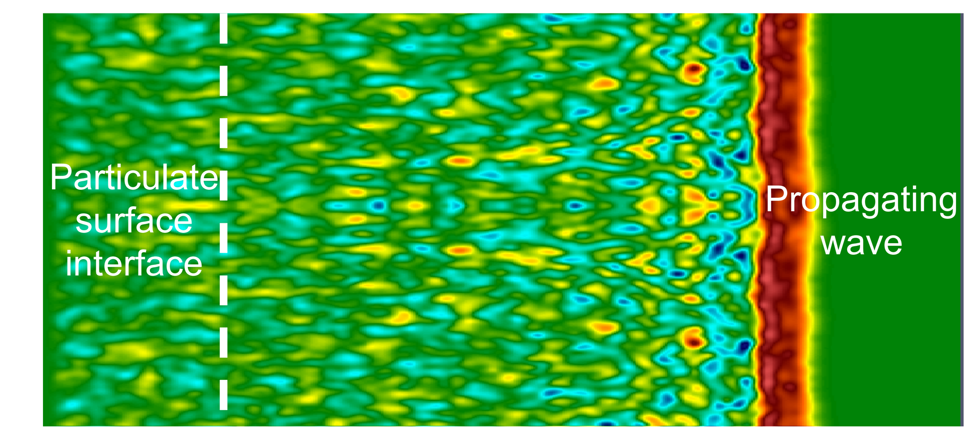






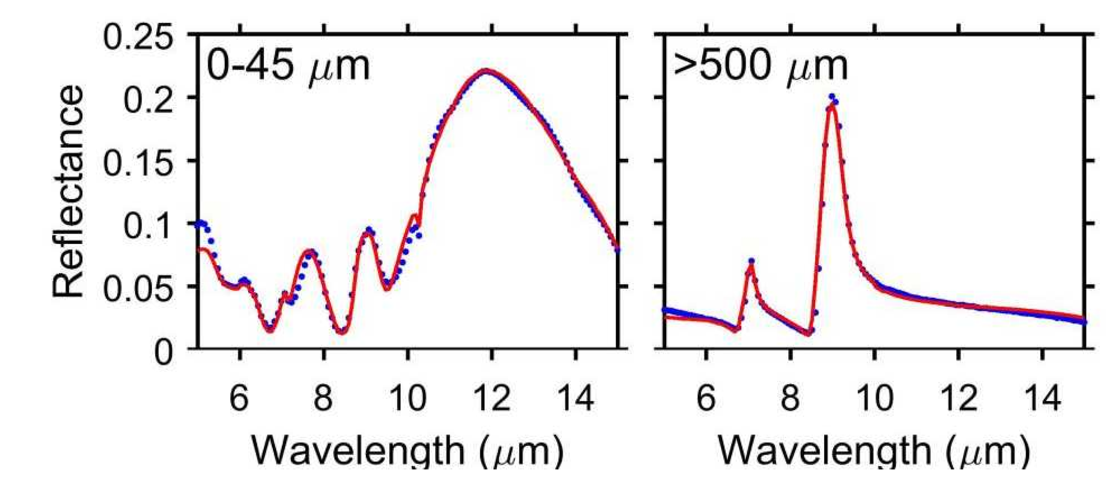
Discussion / Next Steps

We are performing quantitative assessment of the 1st-surface reflection contribution via finite difference time domain (FDTD) simulations.



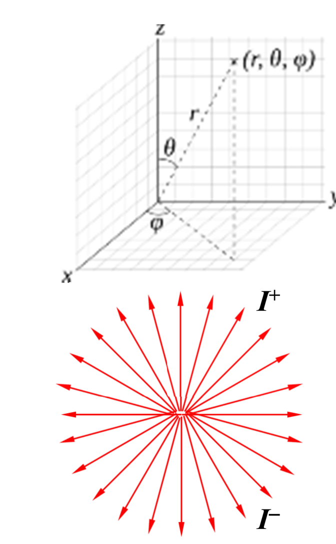
FDTD calculations provide time-dependent simulations of radiation propagating within the particulate medium.

We are demonstrating end-to-end capability to model particulate spectra using pellet-measured *n/k*.



DISORT: **DIS**crete **O**rdinates **R**adiative **T**ransfer

- Application: Transfer of monochromatic radiation in a scattering, absorbing, and emitting plane-parallel, vertically inhomogeneous medium with a specified BRDF at the lower boundary
- DISORT is a "standard" code and well-known by the RT community.
- It is well-documented, versatile, and freely available.
- DISORT can handle *optically thin deposits.*
- We have verified it against the Ambartsumian solution for the limiting case of an optically thick layer.
- We will also be comparing to adding-doubling solution.



Conclusion and Relevance to Program Objectives

- Our baseline model for the reflectance of an optically thick deposit provides the means to account for particle size effects in the reflectance spectra of particulate media.
  - Based on fundamental material properties (n,k) and measured morphology
- Modeling results demonstrate excellent agreement with data acquired on fused silica and ammonium sulfate
- But 1st-surface reflection is currently phenomenologically approximated as Fresnel reflectance
  - Both ray-tracing and FDTD calculations are being pursued to define dependence on particle size and packing density.
- Moving up the spiral: Mixed materials, optically thin deposits, etc.

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