

***Calculating optical properties of
irregular grains
(and perhaps regoliths...)***

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Tadashi Mukai led the way...

- Mukai, S, & **Mukai, T.** 1990, “Analysis of photopolarimetric data of comets at small phase angles by rough surface scattering”, *Icarus*, 86, 257
- Mukai, S., & **Mukai, T.** 1991, “Scattering Properties of Cometary Dust Based on Polarimetric Data”, *ASSL*, 173, 249
- Kozasa, H., Blum, J., & **Mukai, T.** 1992, “Optical Properties of Dust Aggregates I. Wavelength Dependence”, *A&A* 263, 423
- Kozasa, T., Blum, J., Okamoto, H, & **Mukai, T.** 1993, “Optical Properties of Dust Aggregates II. Angular Dependence of Scattered Light”, *A&A* 276, 278
- Kimura, H., Okamura, H., & **Mukai, T.** 2002, “Radiation Pressure and the Poynting-Robertson Effect for Fluffy Dust Grains”, *Icarus* 157, 349
- **Mukai, T.**, Nakamura, A. M., & Sakai, T. 2006, “Asteroidal surface studies by laboratory light scattering and LIDAR on HAYABUSA”, *Adv. Sp. Res.*, 37, 138
- Levasseur-Regourd, A. C., **Mukai, T.**, Lasue, J., & Okada, Y. 2007, “Physical Properties of Cometary and Interplanetary Dust”, *Plan. Sp. Sci.* 55, 1010

Plan

- What is the geometry of interstellar or interplanetary grains?
- Ballistic Agglomerates as candidates for irregular aggregates.
 - *Two new classes: BAM1 and BAM2*
 - *How to measure size and porosity for a random aggregate?*
- How to calculate scattering and absorption for irregular geometries?
- The discrete dipole approximation
- Some scattering properties of ballistic aggregates
- Moderate-porosity candidates for dust in a debris disk
- Moderate-porosity candidates for cometary dust.
- Future: applying DDA to dust layers.

Grain Geometry?

- Modeling usually assumes spherical grains (because calculations are easy).
- Polarization of starlight and polarization of infrared emission: real grains are NOT spherical.
- What is *actual* grain geometry?

Dust Grain Geometry

- Interplanetary Dust Particles (IDPs)

228 John Bradley

Bradley, J. P. 2003, *Treatise on Geochemistry*, vol.1, 689-711

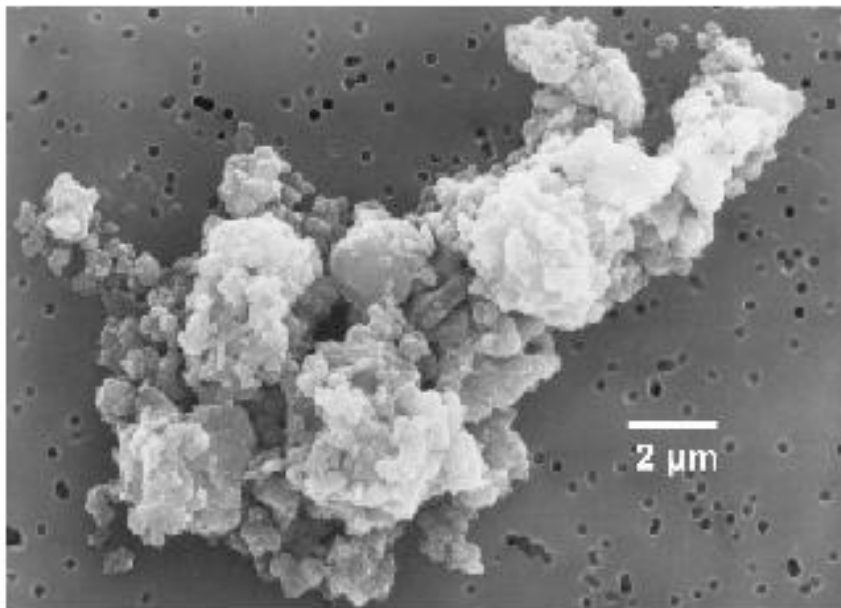


Fig. 1. Secondary electron image of chondritic porous (CP) interplanetary dust particle (IDP) U230B43.

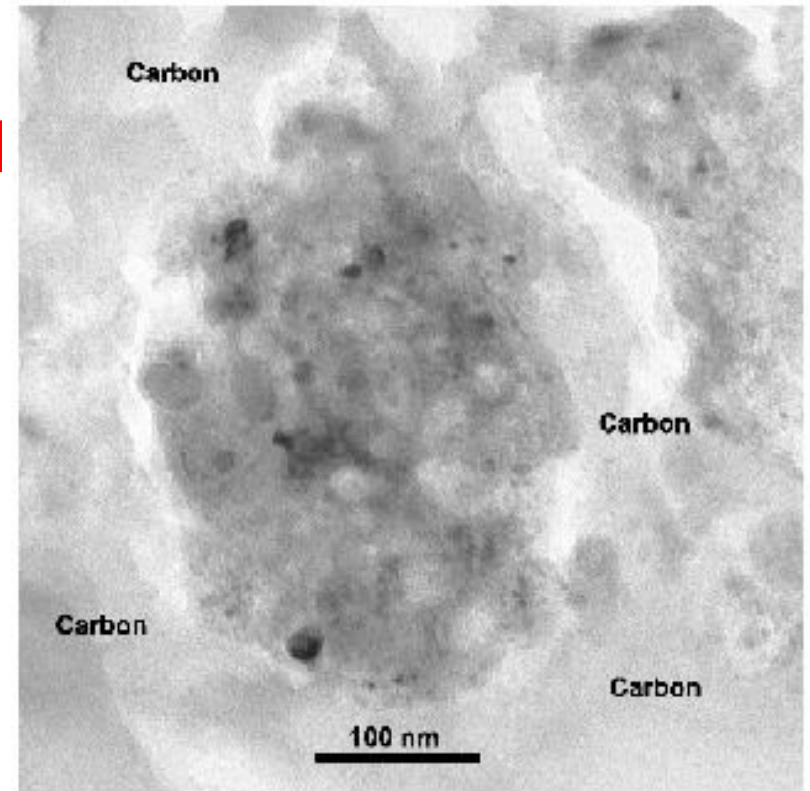
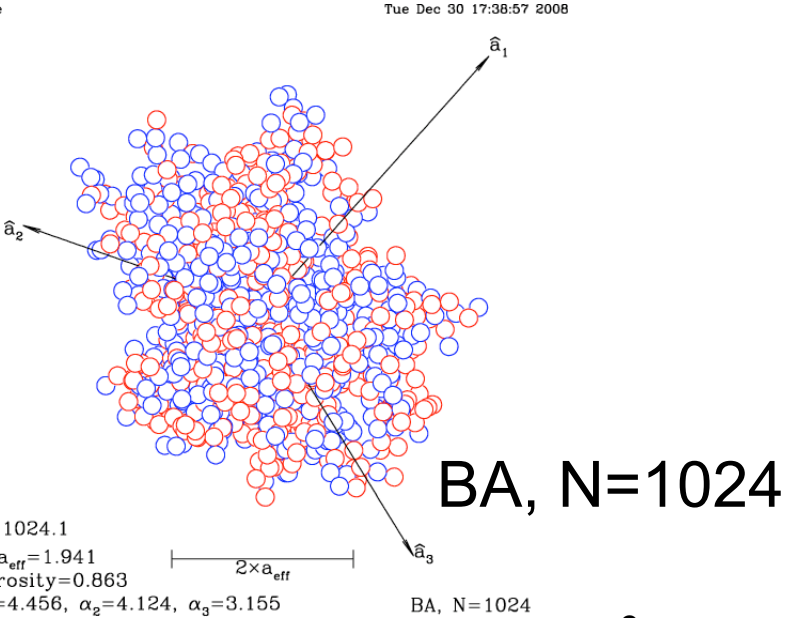
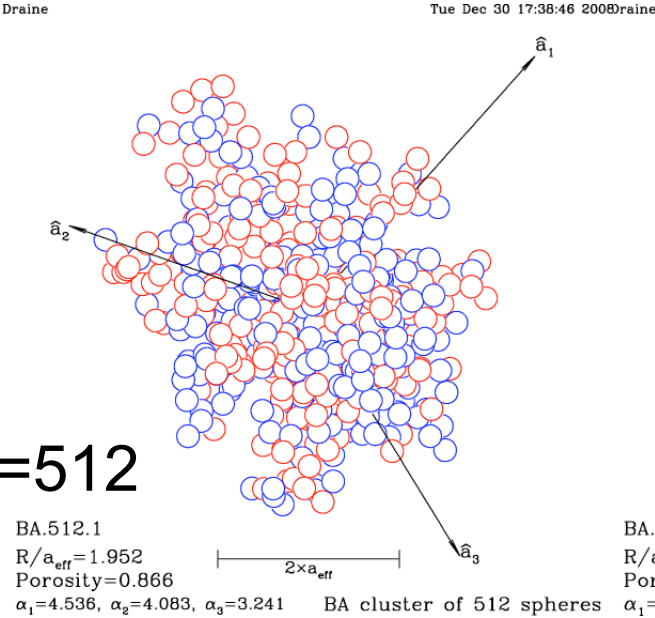
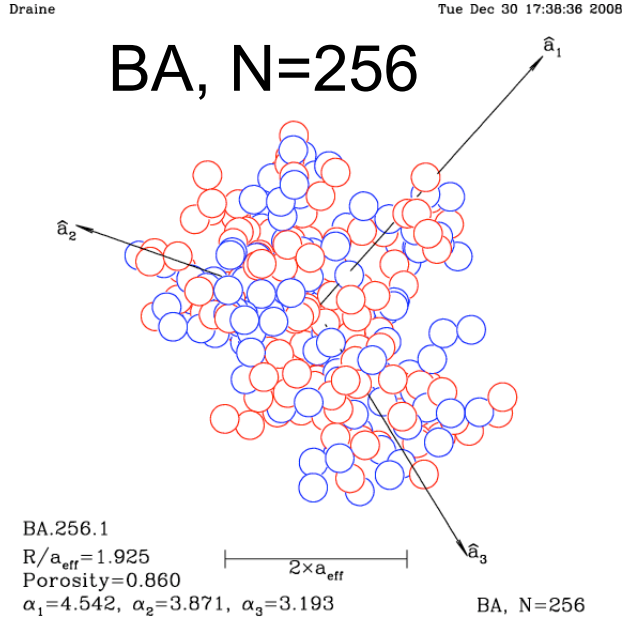
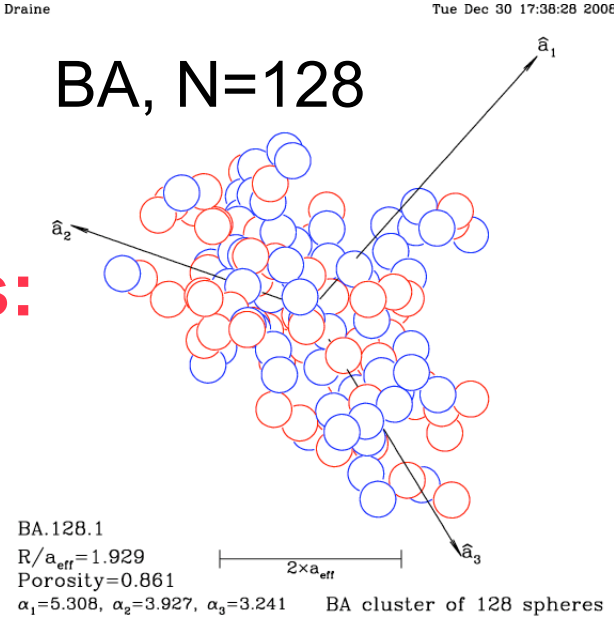


Fig. 8. Brightfield transmission electron micrograph of a GEMS embedded in amorphous carbon material in IDP L2011R11. The remnants of a deeply eroded relict grain with "swiss cheese" microstructure can be seen towards the center of the grain.

**BA clusters
≡ BPCA clusters:
monomers arrive
on random traject.
and stick at point
of first contact**



Two New Classes of Random Aggregates: BAM1 and BAM2

BA growth process →

- very low filling factor (≈ 0.14)
- high “porosity” (≈ 0.86)
- very fragile

Real IDPs appear to be more robust than BA aggregates.

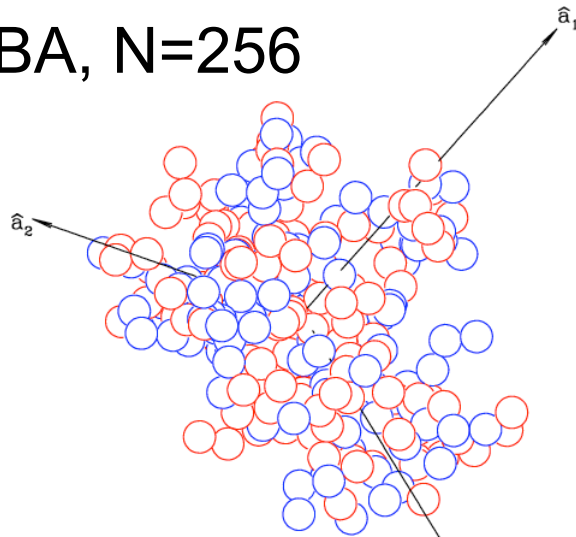
Would like to have aggregates that are random but somewhat more dense than BA clusters. Consider two new classes of random agglomerates: **BAM1** and **BAM2**.

Monomers arrive on random trajectories, just as for BA.

- **BAM1**: At first contact, roll to make contact with a second monomer, then stop.
BAM1 more dense than BA.
- **BAM2**: At first contact, roll to make contact with second monomer, then roll again to make contact with third monomer, then stop.
BAM2 more dense than **BAM1**.

Algorithms are not difficult to implement for spherical monomers.

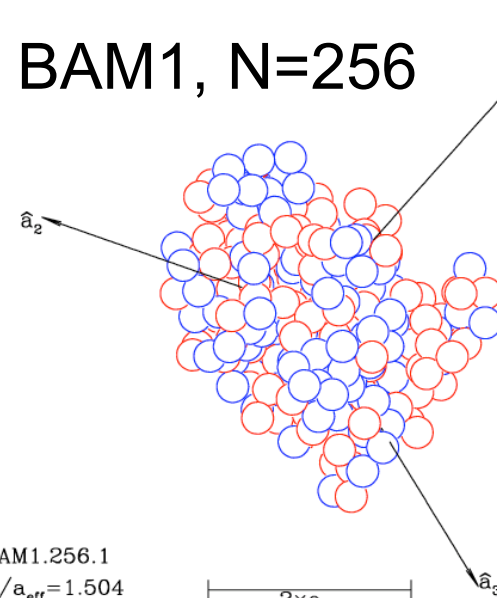
BA, N=256



BA.256.1
 $R/a_{eff} = 1.925$
 Porosity = 0.860
 $\alpha_1 = 4.542, \alpha_2 = 3.871, \alpha_3 = 3.193$

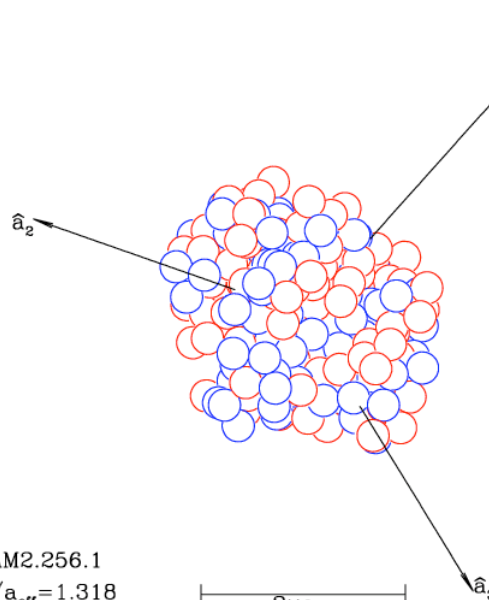
BA, N=256
 Draine

BAM1, N=256



BAM1.256.1
 $R/a_{eff} = 1.504$
 Porosity = 0.706
 $\alpha_1 = 2.846, \alpha_2 = 2.501, \alpha_3 = 1.851$

BAM1, N=256



BAM2, N=256

BAM2.256.1
 $R/a_{eff} = 1.318$
 Porosity = 0.563
 $\alpha_1 = 2.083, \alpha_2 = 1.685, \alpha_3 = 1.608$

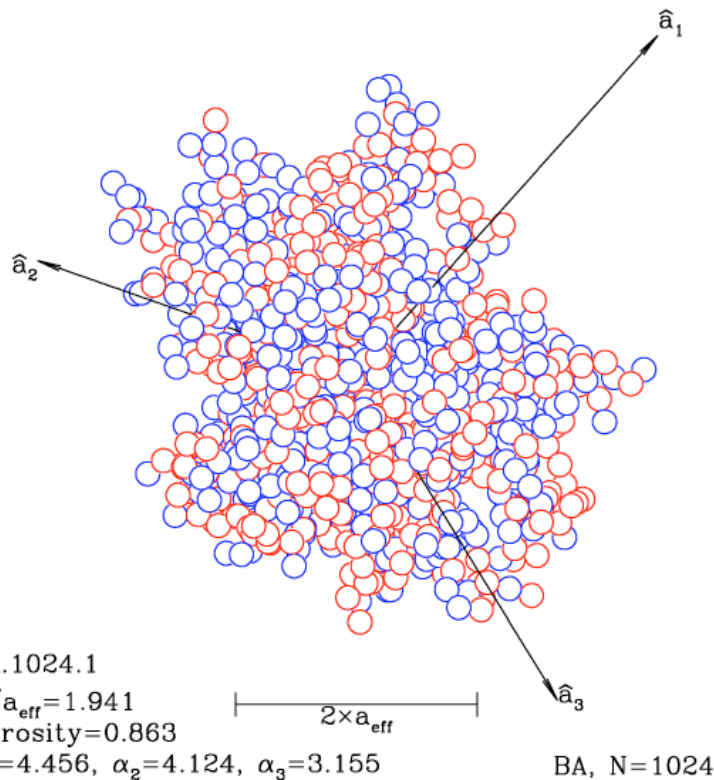
BAM2, N=256

Shen, Draine & Johnson 2008, ApJ, 689, 260

How to measure “porosity”?

Draine

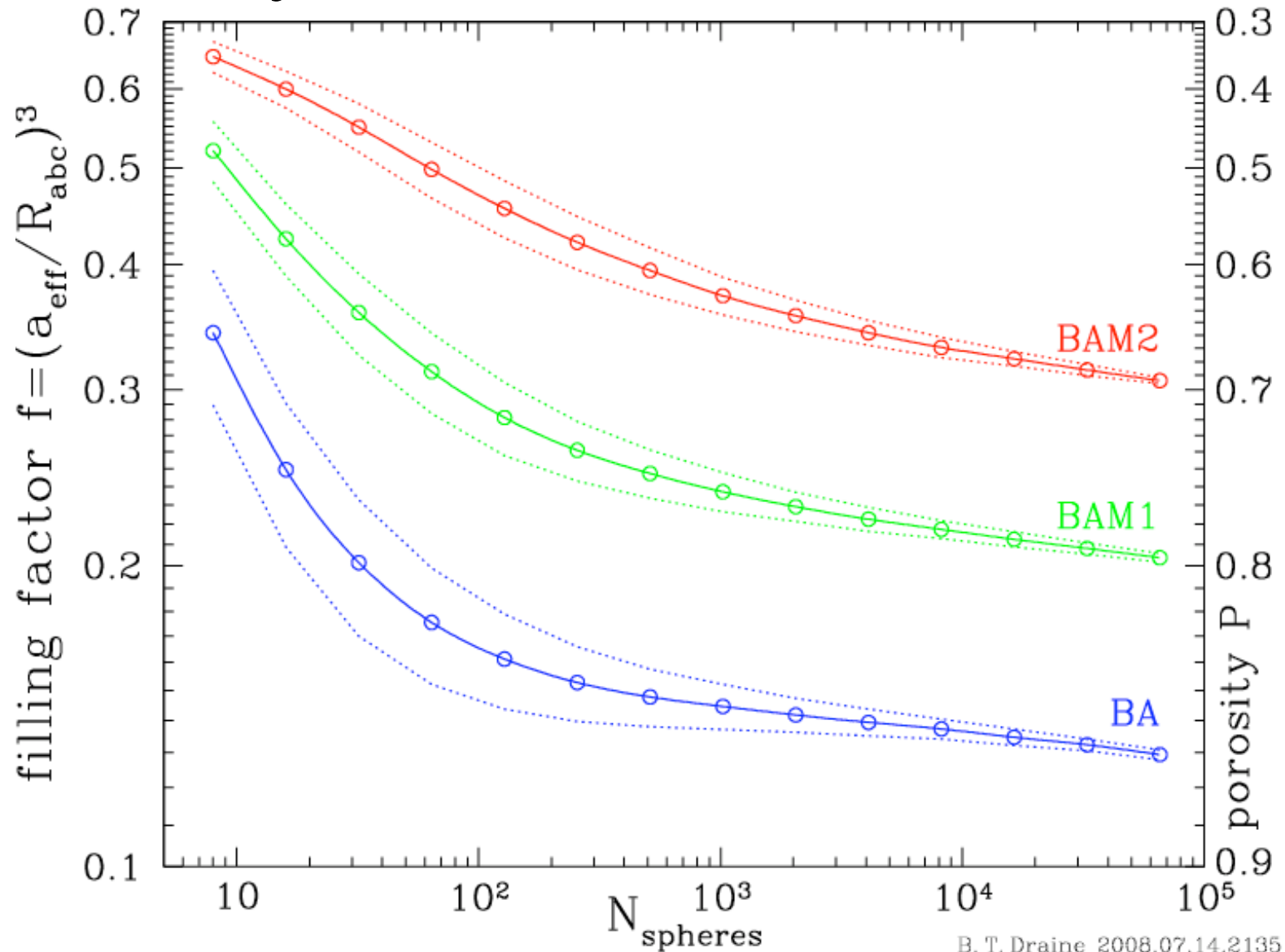
Tue Dec 30 17:38:57 2008



Shen, Draine & Johnson 2008, ApJ, 689, 260

- For extended material, \mathcal{P} = fraction of total volume that is unoccupied.
- For cluster, how to define “total volume”?
- Consider ellipsoid with semi-axes a, b, c and density $(1 - \mathcal{P})\rho$, with a, b, c, \mathcal{P} such that total mass M and moment of inertia tensor I_{ij} are same as for cluster. This serves to define a, b, c and \mathcal{P} . This is porosity definition of Shen, Draine & Johnson (2008)
- 3×3 moment of inertia tensor I_{ij} easy to calculate and to find eigenvalues. \mathcal{P} is easily calculated from eigenvalues.
- Equivalent porous ellipsoid has semiaxes a, b, c
 - $b/a, c/b, c/a$ characterize asymmetry
 - Define **characteristic size** $R_{abc} \equiv (abc)^{1/3}$
 - Size parameter $x = 2\pi R_{abc}/\lambda$

Porosity vs. N for BA, BAM1, BAM2



B. T. Draine 2008.07.14.2135

Asymmetry of BA, BAM1, BAM2 clusters

Equivalent ellipsoid with semi-axes a, b, c

Asymmetry *decreases*

as

BA \Rightarrow BAM1 \Rightarrow BAM2

Asymmetry *decreases*

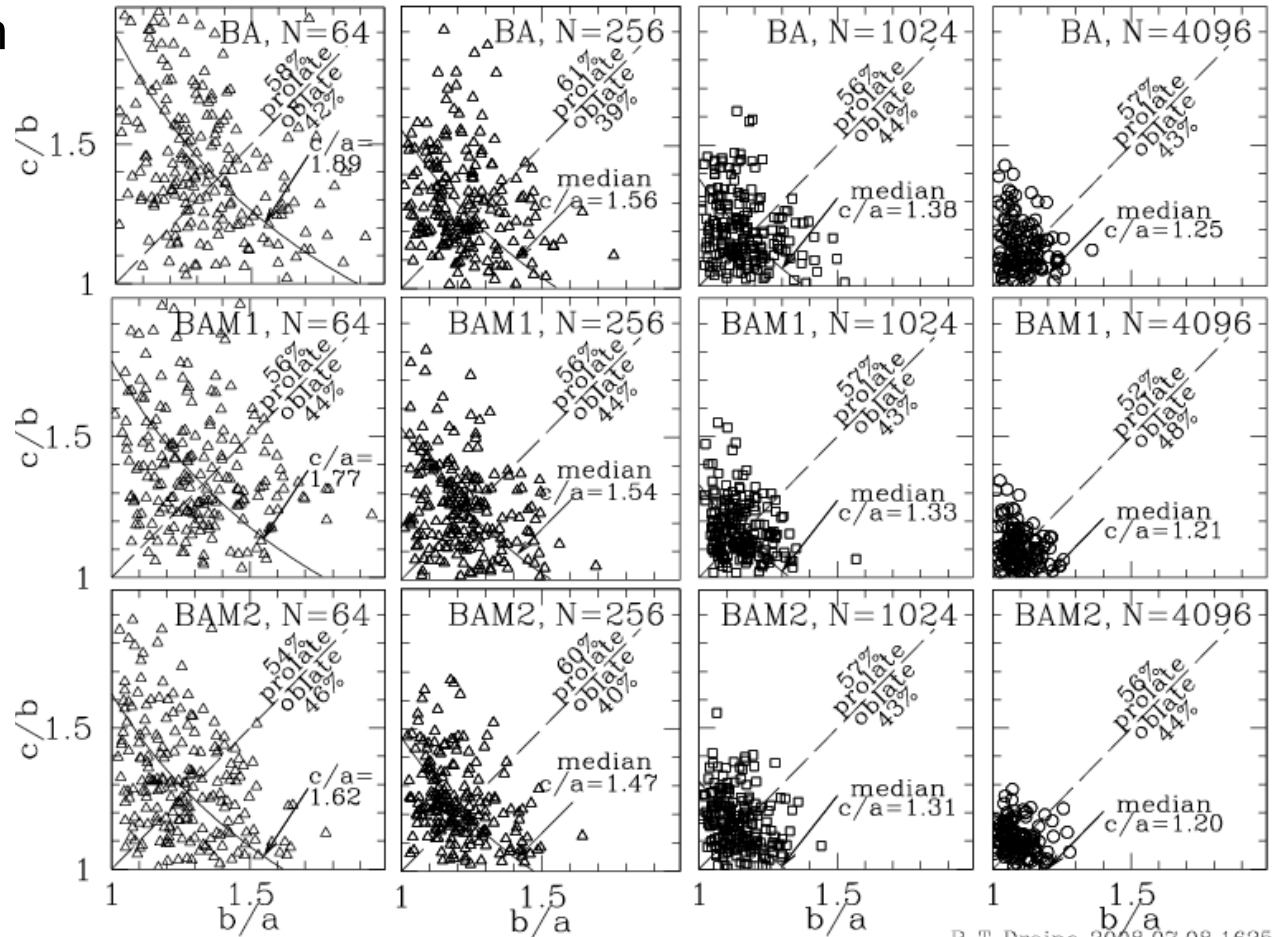
as N increases

$N=256$: median $c/a =$

1.56 for BA

1.54 for BAM1

1.47 for BAM2



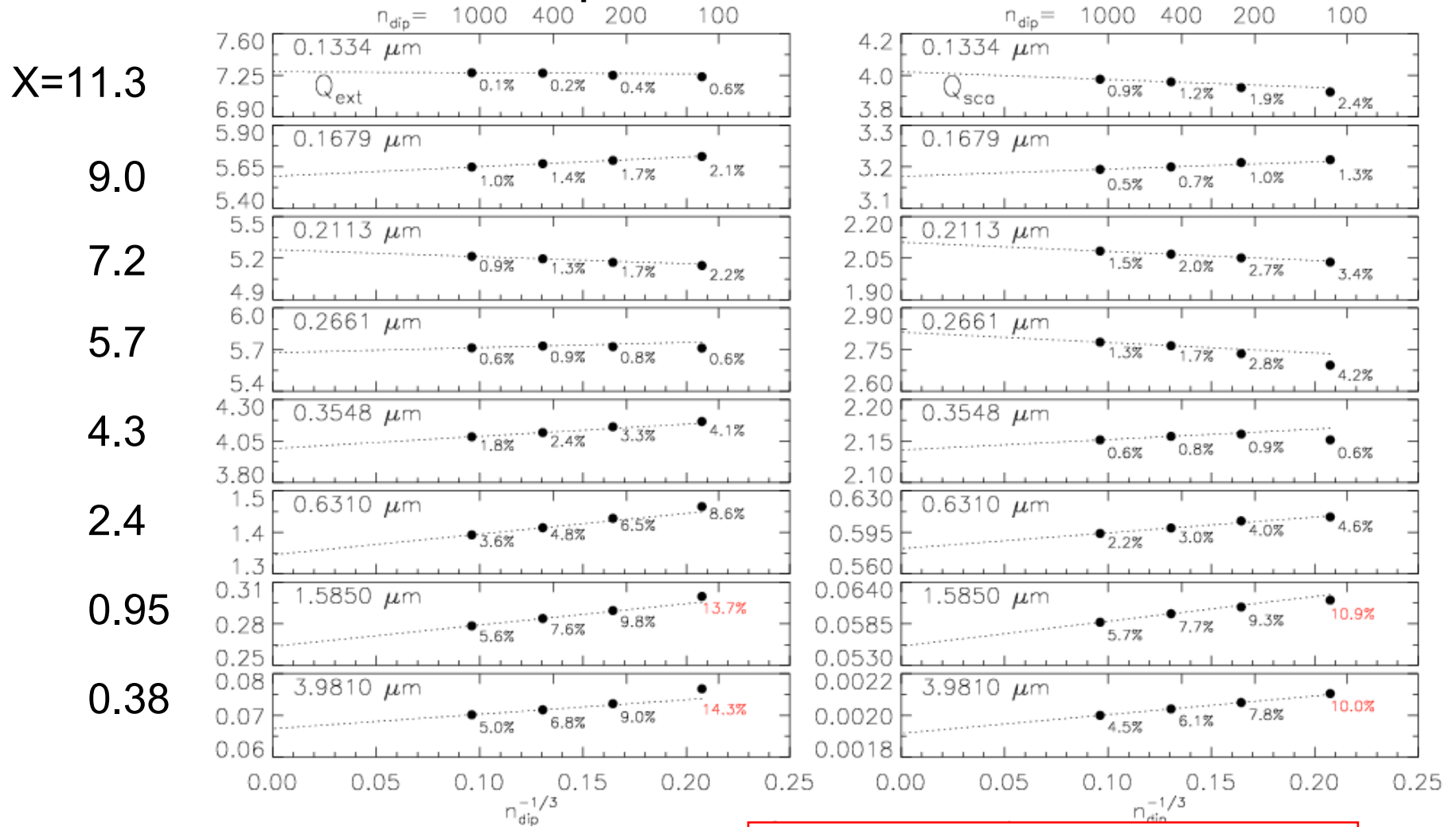
B. T. Draine 2008.07.08.1625

Shen, Draine & Johnson 2008, ApJ, 689, 260

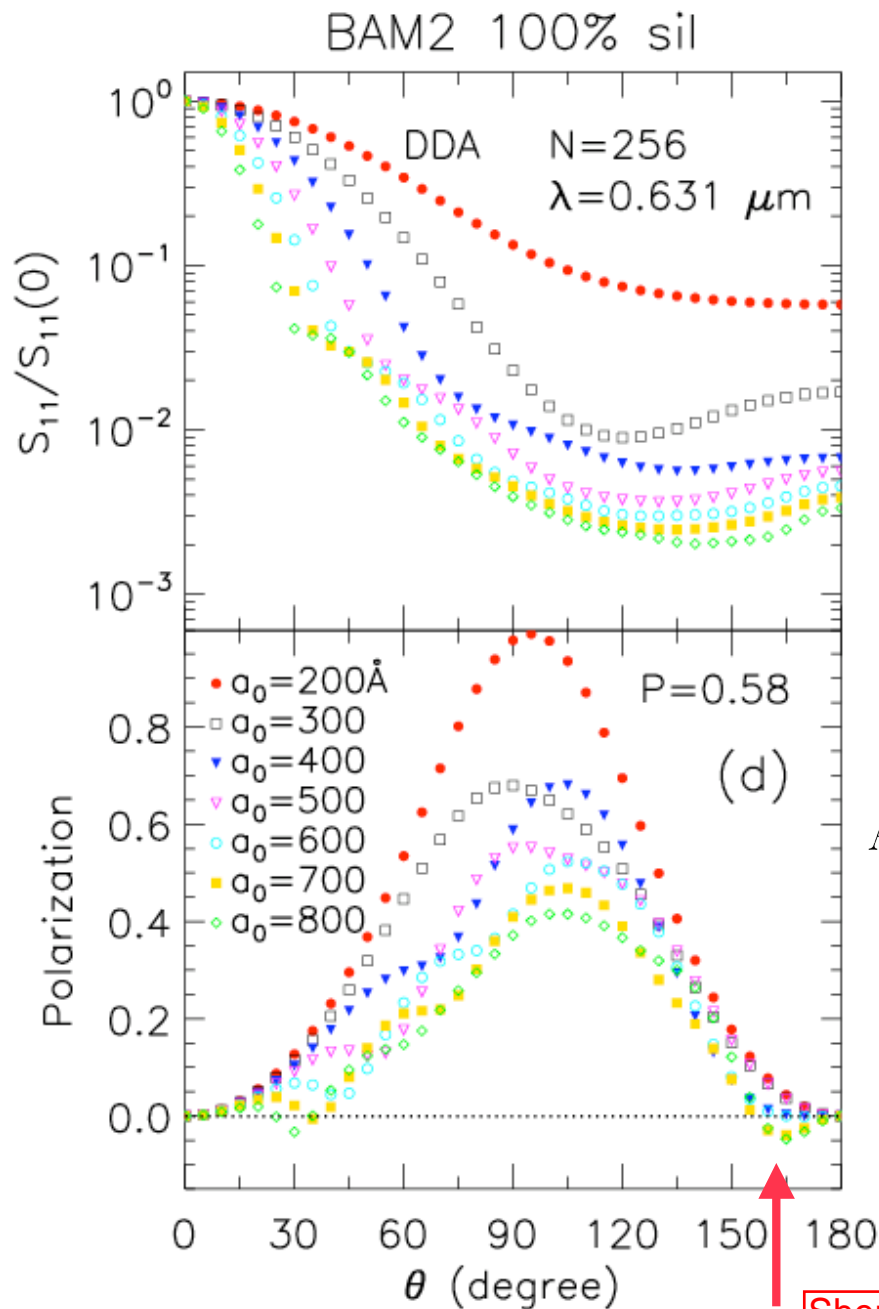
How to calculate absorption and scattering properties of irregular clusters?

1. Effective Medium Theory + Mie Theory
 - Fast
 - Moderate accuracy for total cross sections
 - Not accurate for scattering and polarization
2. “Exact”: Generalized Multisphere Mie for clusters of spheres (Mackowski 1991; Xu 1997)
 - For each sphere, use $L \times (L + 1)$ multipoles $Y_{\ell m}$.
 - Computationally demanding
(must solve $3N \times L \times (L + 1)$ coupled equations).
 - Does not apply to anisotropic materials (e.g., graphite).
3. Discrete Dipole Approximation (DDA):
 - Represent target by array of dipoles with interdipole spacing d
 - If $d \ll \lambda$ and $d \ll$ structural scales in target, then DDA is accurate
(error $\rightarrow 0$ as $d/\lambda \rightarrow 0$ and $d/R \rightarrow 0$)
 - Can treat any geometry
 - Can treat general anisotropic materials.
 - Computationally demanding (feasible up to $2\pi R/\lambda \sim 15$)
 - Public domain Fortran 90 code (DDSCAT 7.0).

DDA Accuracy for
 $N=256$ BA cluster, 50% graphite+50% silicate
 $a_{\text{eff}}=0.127\mu\text{m}$, $P=0.853 \Rightarrow R=0.241\mu\text{m}$
 $n_{\text{dip}} = \#$ dipoles in one sphere



Shen, Draine & Johnson 2008, ApJ, 689, 260



Effect of varying cluster size R

$N = 256$ BAM2 ($P = 0.58$):

a_0

$$200 \text{ \AA} \leftrightarrow R = 0.17 \mu\text{m}$$

$$2\pi R/\lambda = 1.68$$

$$800 \text{ \AA} \leftrightarrow R = 0.68 \mu\text{m}$$

$$2\pi R/\lambda = 6.75$$

As R/λ increases:

- Increasing forward/backward asymmetry
- decreasing polarization
- **appearance of negative polarization at $\theta \approx 160^\circ - 180^\circ$ for $2\pi R/\lambda \gtrsim 5$ ($\alpha \approx 20^\circ - 0^\circ$)**

Shen, Draine & Johnson 2009 (to be accepted in ApJ)

Dependence of polarization on wavelength

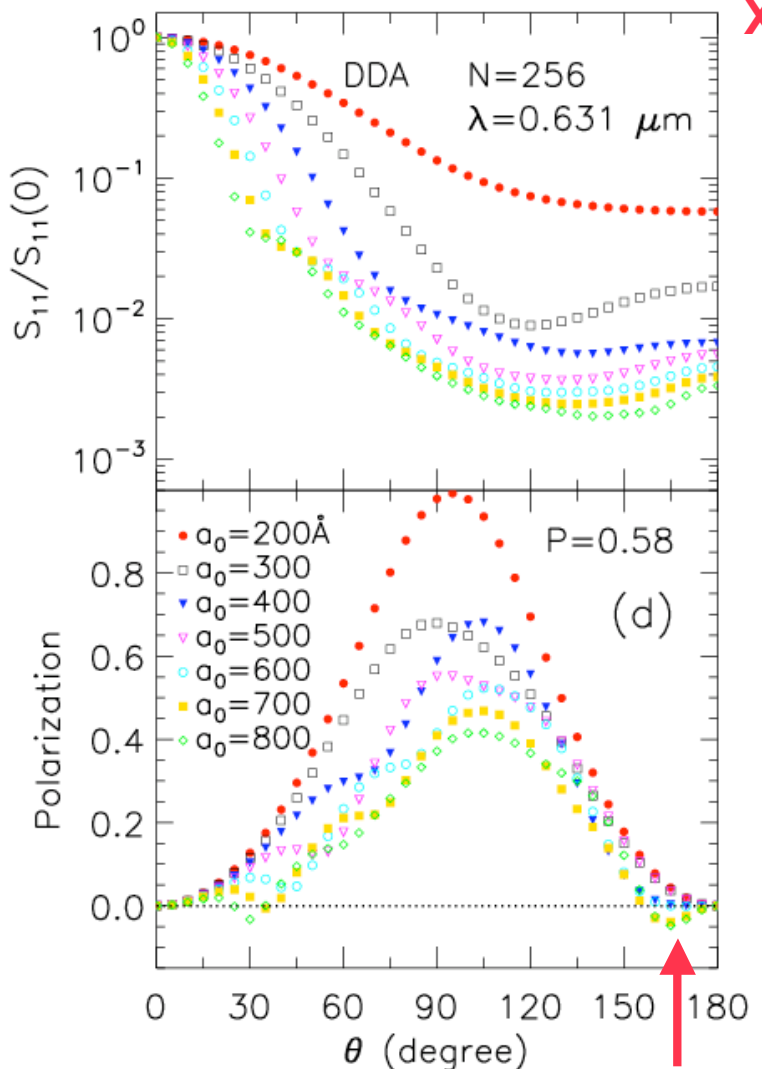
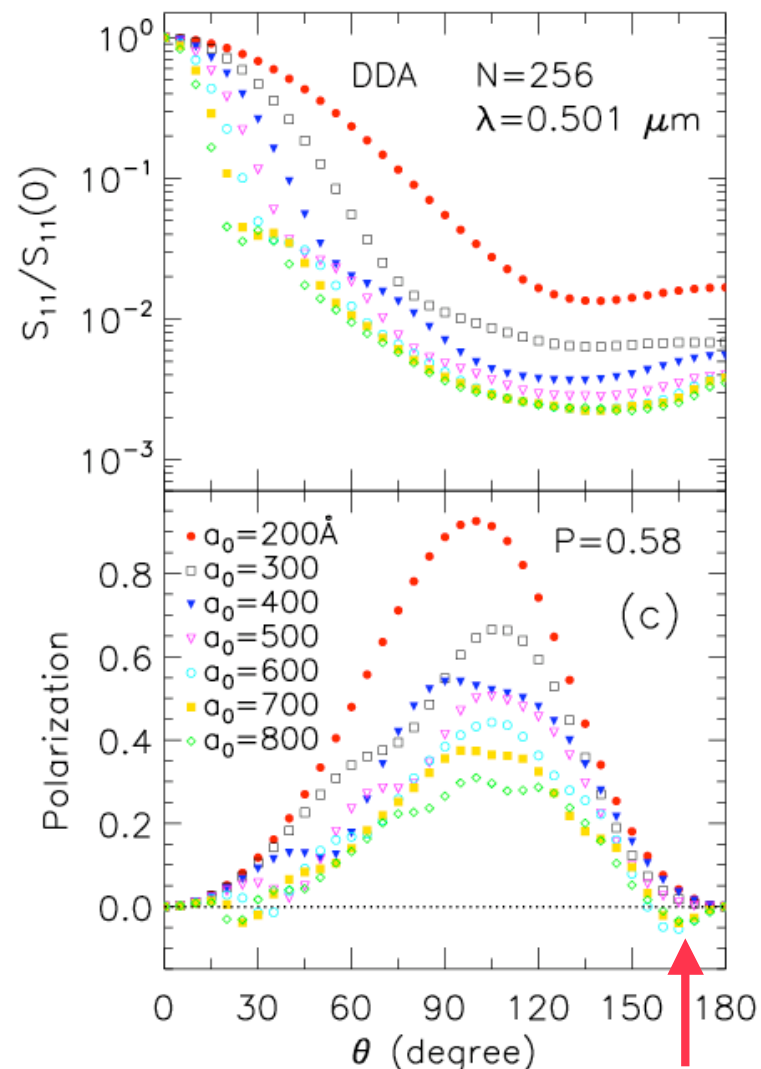
$\lambda=0.501\mu\text{m}$

BAM2 100% sil

$\lambda=0.631\mu\text{m}$

BAM2 100% sil

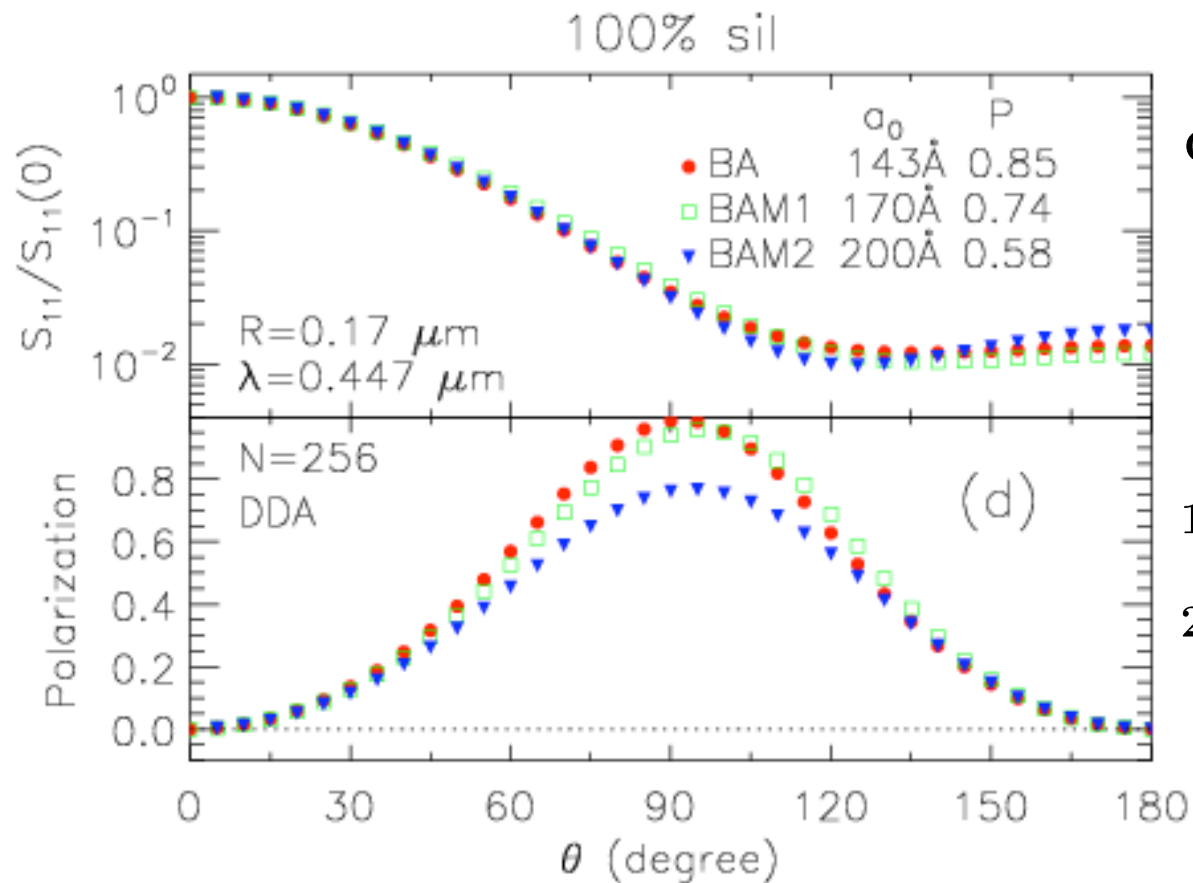
$a_0=0.02\rightarrow 0.08\mu\text{m}$
 $R=0.17\rightarrow 0.68\mu\text{m}$
 $X=2.1\rightarrow 8.5$
 (for $\lambda=0.50\mu\text{m}$)



$P(0.63\mu\text{m})$
 $>P(0.50\mu\text{m})$

pol<0

Effect of Varying Porosity P



Compare clusters with

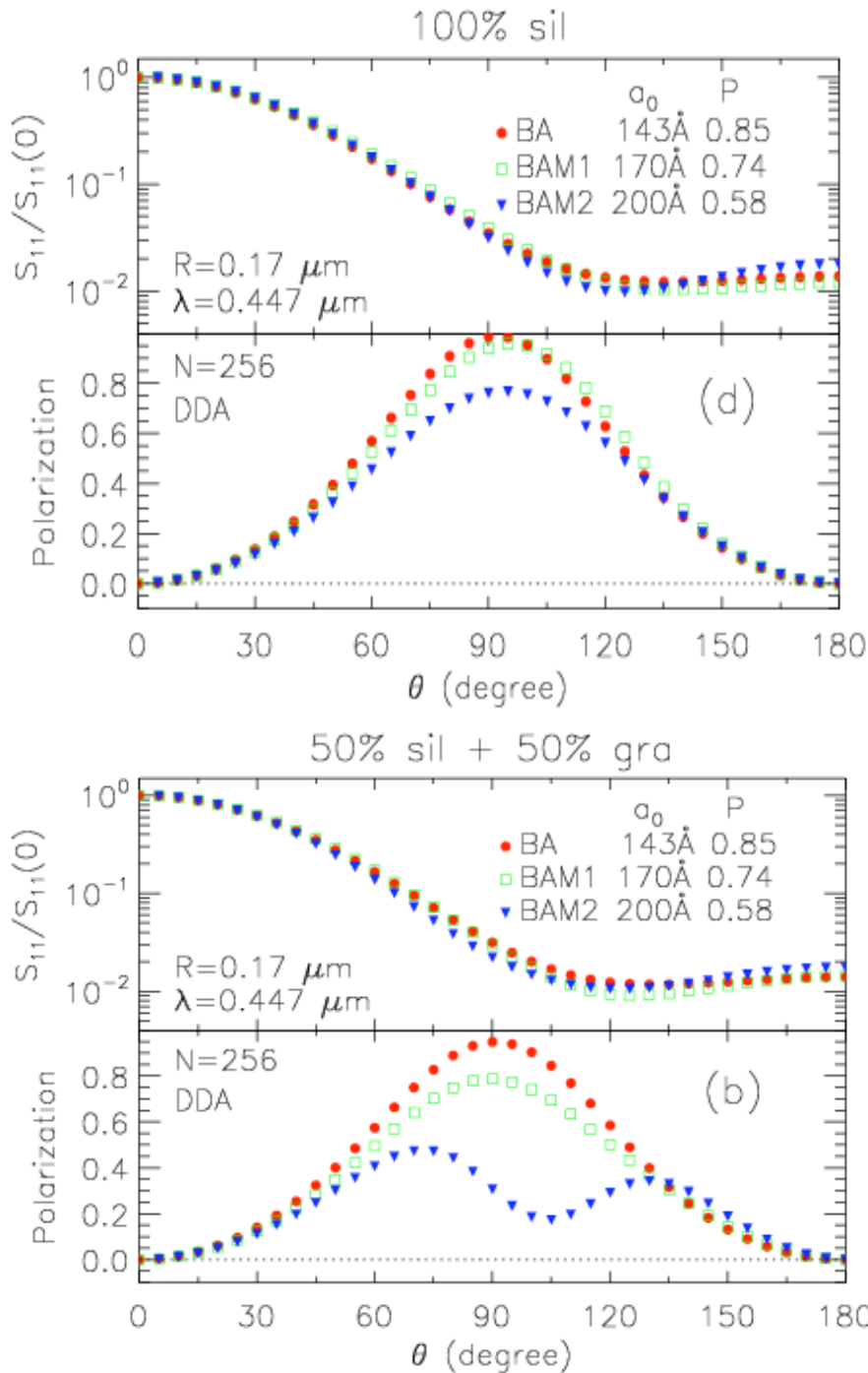
- same composition (silicate)
- same size $R = 0.17 \mu\text{m}$
($2\pi R/\lambda \approx 2.4$)
- varying porosity
 $P = 0.58 - 0.85$.

1. P has minimal effect on shape of phase function.
2. **Lower P**
→ **lower polarization.**

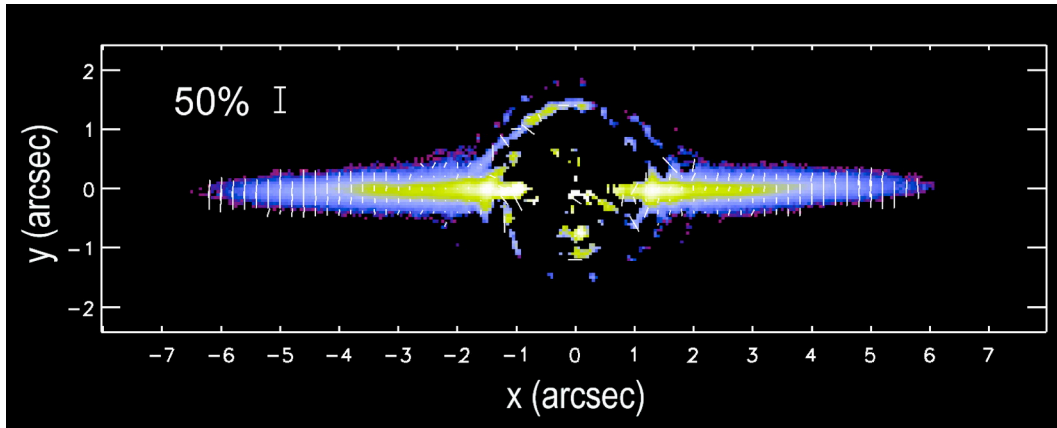
Shen, Draine & Johnson 2009 (to be accepted in ApJ)

Effect of Varying Composition

$N = 256$ BA, BAM1, BAM2 clusters
 $R = 0.17 \mu\text{m}$, $2\pi R/\lambda \approx 2.4$



1. 100% silicate
 2. 50% silicate+50% graphite (random)
 - increased absorption
- composition has relatively small effect on shape of phase function
 - composition has larger effect on polarization:
 - increased absorption
 - reduced polarization



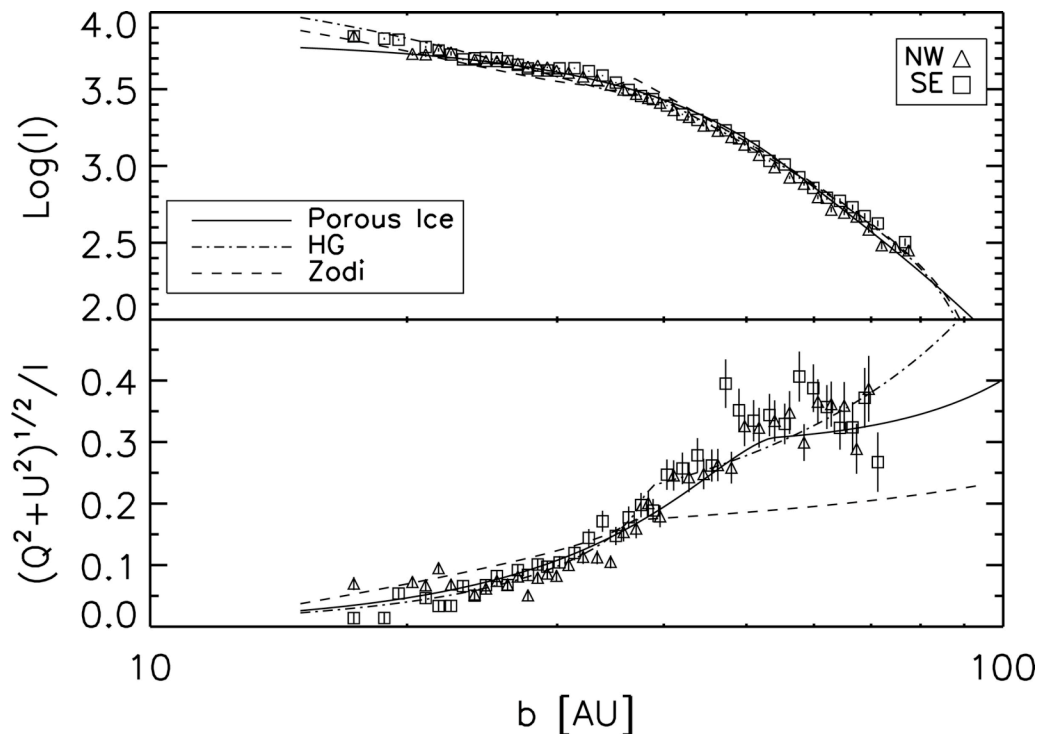
Debris Disk Around AU Mic (M1 dwarf, d=9.9pc)

Graham et al (2007) used HST ACS to obtain polarization map at $\lambda=0.61\mu\text{m}$

Model to reproduce $I(b)$ and $\text{pol}(b)$

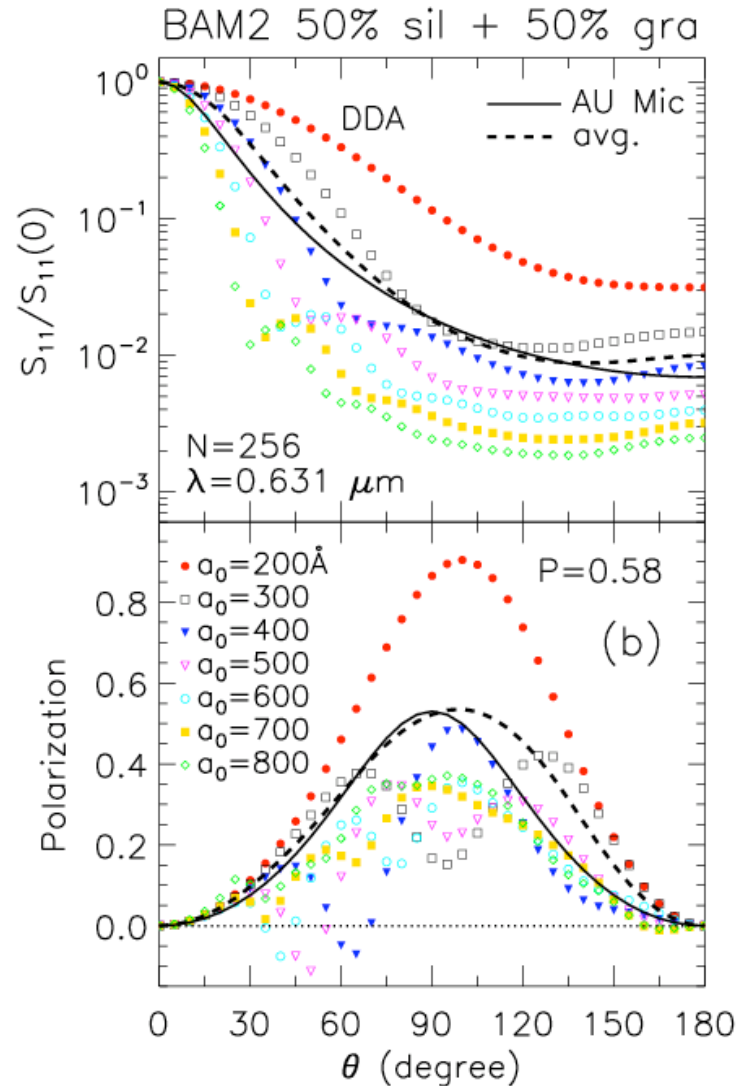
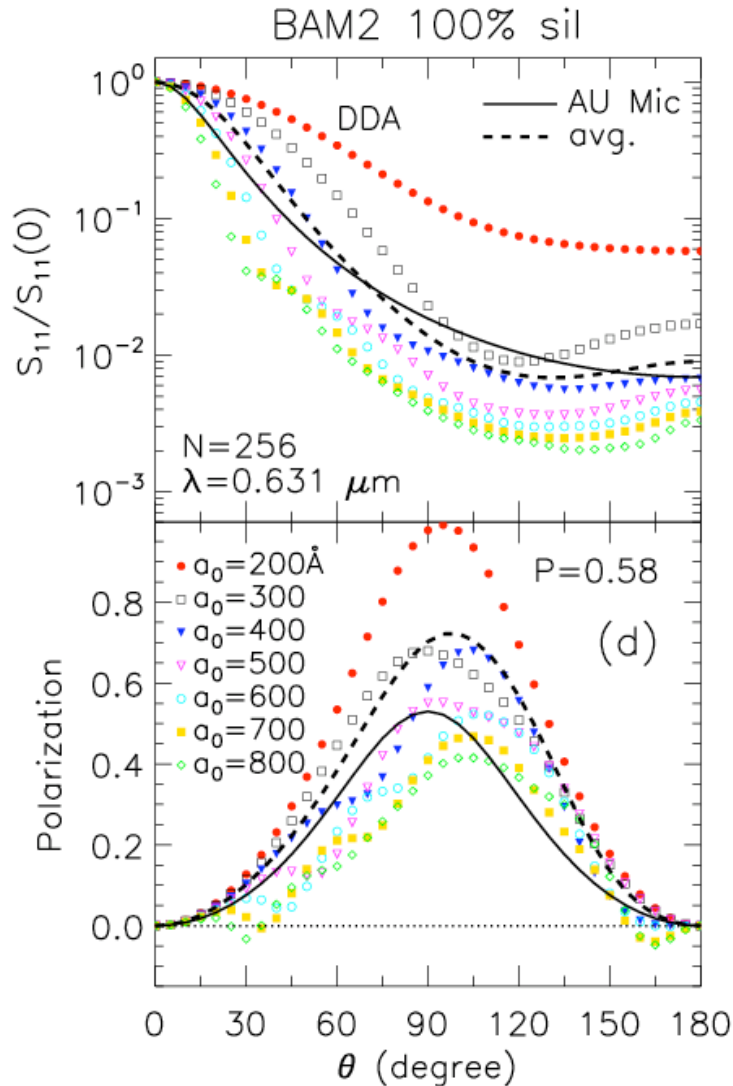
Based on EMT-Mie theory, Graham et al. claim water-ice model with porosity $P=0.91\pm 0.09$ fits data.

Are lower porosity clusters also able to reproduce observations?



BAM2 $N=256$ clusters, $P=0.58$

$a_0=0.02 \rightarrow 0.08 \mu\text{m}$
 $R=0.17 \rightarrow 0.68 \mu\text{m}$
 $X=1.7 \rightarrow 6.8$



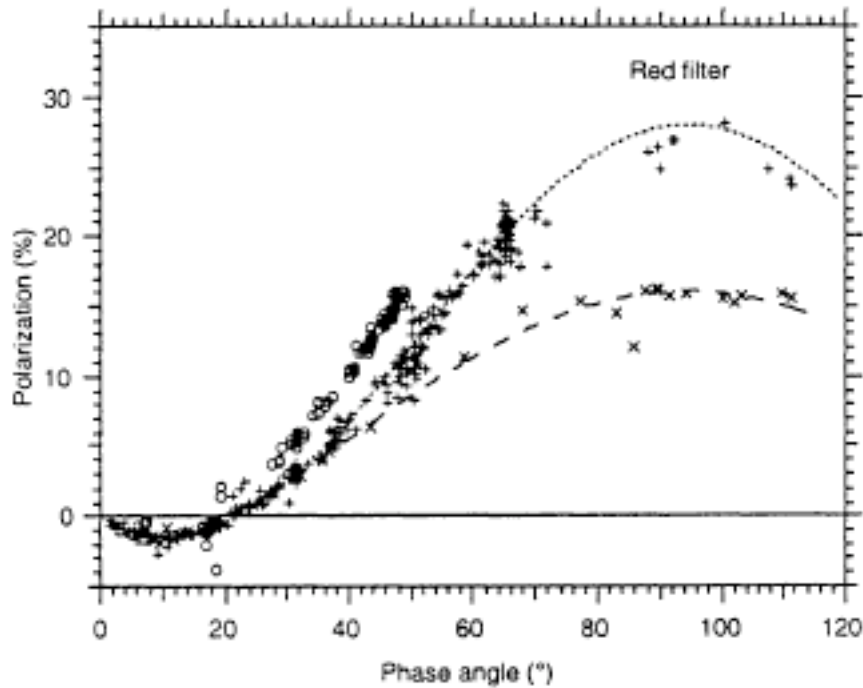
solid line: “HG”
 param. inferred by
 Graham et al

dashed: average
 for $dn/dR \propto R^{-3.5}$ for
 $0.13 < R < 0.55 \mu\text{m}$

good fit obtained for
 50%sil+50%graph.
 with $P=0.58$
 ($\ll 0.91$)

Shen, Draine & Johnson 2009 (to be accepted in ApJ)

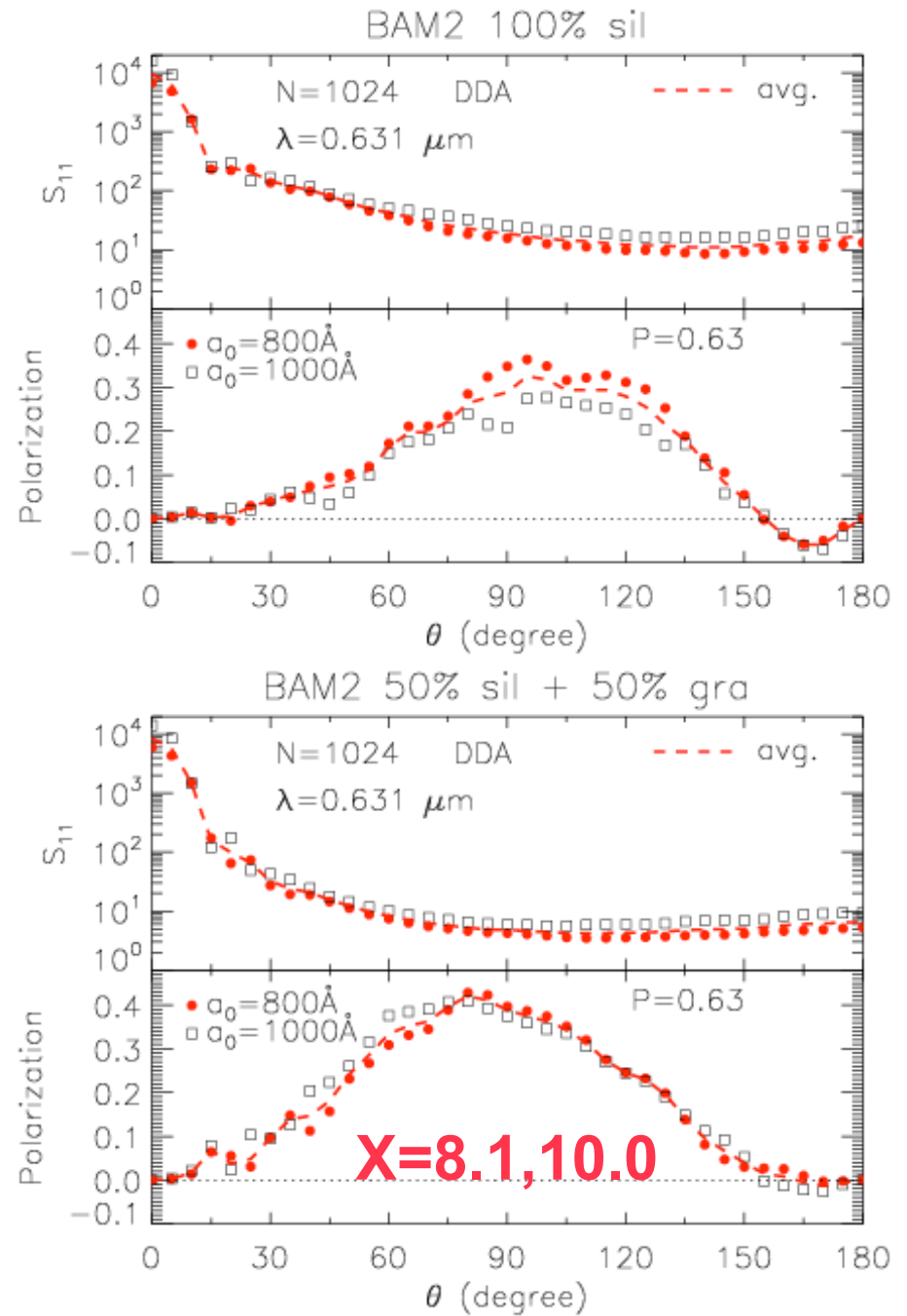
Cometary dust



Levasseur-Regourd & Hadamcik 2001, ESASP.495,587L

**BAM2 clusters with $P \approx 0.63$
and $R \approx 1.25 \mu\text{m}$ appear to reproduce
High-polarization comets.
Mix of 100% sil + 50/50 sil/gra clusters
would reproduce neg. pol. branch.
Might need even larger R ...**

CPS School, Kobe
2009.01.09



Shen, Draine & Johnson 2009 (to be accepted in ApJ)

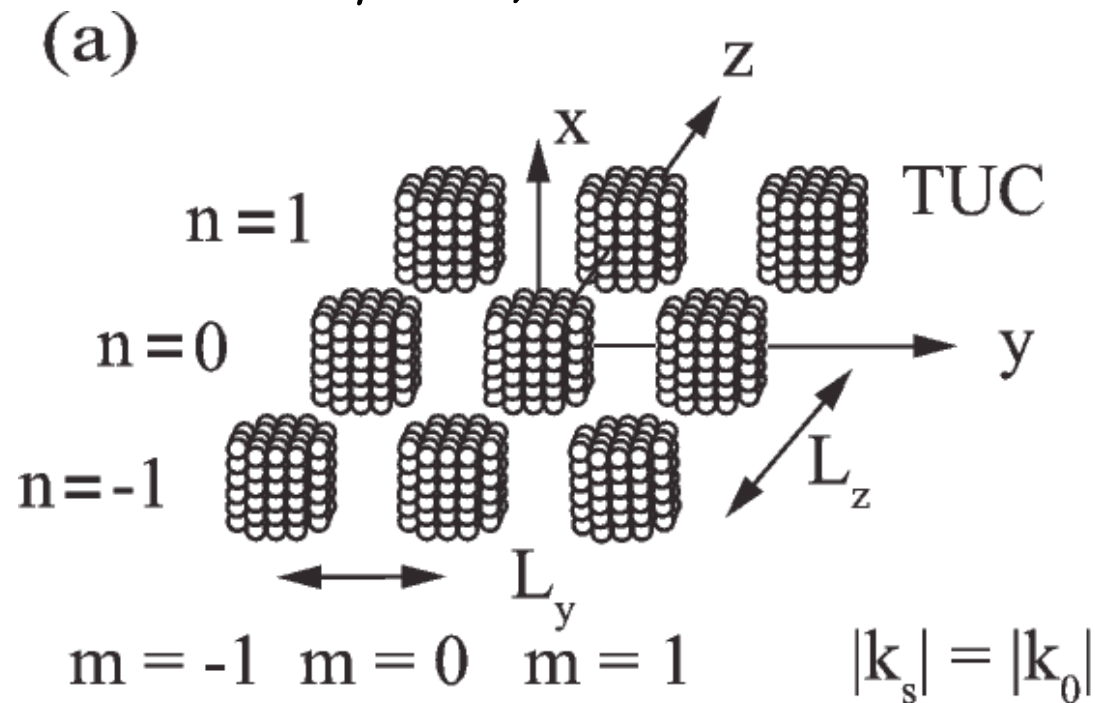
Can DDA be used to model dust layer = nano-regolith?

DDA can be used for periodic array of "Target Unit Cells" (TUCs) (Draine & Flatau 2008, JOSA A25, 2693).

TUC could be an irregular aggregate.

Near-field interactions/multiple scattering are taken into account.

DDSCAT 7.0 includes this capability.



Summary

- New definition of porosity P (and size R) for finite structures.
- 2 new classes of random ballistic agglomerates, BAM1 and BAM2. Library of cluster realizations is available on-line.
- BA, BAM1, BAM2 allow variation of P .
- Porosity: at fixed R , λ , and composition
 - porosity has only small effect on shape of phase function
 - reduced porosity \rightarrow reduced polarization at $\theta \approx 90^\circ$
- Size: at fixed P and composition
 - increased $R/\lambda \rightarrow$ increased forward/backward asymmetry
 - increased $R/\lambda \rightarrow$ reduced peak polarization
- **AU Mic debris disk:** BAM2 aggregates with $P \approx 0.6$ and size dist. extending up to $R \approx 0.55 \mu\text{m}$ gives good fit.
- **Cometary dust:** BAM2 aggregates with $P \approx 0.6$ and $R \approx 1.25 \mu\text{m}$ are consistent with “high polarization” comets.
- **Moderate porosity aggregates should be considered as candidates for dust in debris disk and comets.**
- **DDA can be applied to dust layers.**

Visible + Infrared

Thank You

Visible

Infrared

Sombrero Galaxy/Messier 104

Spitzer Space Telescope • IRAC

Visible: Hubble Space Telescope/Hubble Heritage Team

NASA / JPL-Caltech / R. Kennicutt [University of Arizona], and the SINGS Team

ssc2005-11a

References

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URL: <http://www.astro.princeton.edu/~draine/agglom.html>
- Shen, Draine & Johnson, (to be accepted in ApJ, 2009)
arXiv0901.2177
URL: <http://www.astro.princeton.edu/~draine/SDJ2009.html>
- Levasseur-Regourd & Hadamcik, ESASP 495, 587L (2001)
- Draine & Flatau, JOSA A25, 2693 (2008)
- Spitzer M101
URL: http://gallery.spitzer.caltech.edu/Imagegallery/image.php?image_name=ssc2005-11a