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TITLE: DDA Computations of Porous Aggregates with Forsterite Crystals: Effects of Crystal Shape and Crystal Mass Fraction

ABSTRACT BODY:

Abstract Body: Porous aggregate grains are commonly found in cometary dust samples and are needed to model cometary IR spectral energy distributions (SEDs). Models for thermal emissions from comets require two forms of silicates: amorphous and crystalline. The dominant crystal resonances observed in comet SEDs are from Forsterite (Mg2SiO4). The mass fractions that are crystalline span a large range from $0.0 \le f$ crystal ≤ 0.74 . Radial transport models that predict the enrichment of the outer disk (>25 AU at 1E6 yr) by inner disk materials (crystals) are challenged to yield the highend-range of cometary crystal mass fractions. However, in current thermal models, Forsterite crystals are not incorporated into larger aggregate grains but instead only are considered as discrete crystals. A complicating factor is that Forsterite crystals with rectangular shapes better fit the observed spectral resonances in wavelength (11.0-11.15 µm, 16, 19, 23.5, 27, and 33 µm), feature asymmetry and relative height (Lindley et al. 2013) than spherically or elliptically shaped crystals. We present DDA-DDSCAT computations of IR absorptivities (Qabs) of 3 μ m-radii porous aggregates with 0.13 \leq *f*crystal \leq 0.35 and with polyhedral-shaped Forsterite crystals. We can produce crystal resonances with similar appearance to the observed resonances of comet Hale-Bopp. Also, a lower mass fraction of crystals in aggregates can produce the same spectral contrast as a higher mass fraction of discrete crystals; the 11µm and 23 µm crystalline resonances appear amplified when crystals are incorporated into aggregates composed otherwise of spherically shaped amorphous Fe-Mg olivines and pyroxenes. We show that the optical properties of a porous aggregate is not linear combination of its monomers, so aggregates need to be computed. We discuss the consequence of lowering comet crystal mass fractions by modeling IR SEDs with aggregates with crystals, and the implications for radial transport models of our protoplanetary disk.

AUTHORS (FIRST NAME, LAST NAME): Diane H. Wooden¹, Sean S. Lindsay², David Harker³, Charles Woodward⁴, Michael S. Kelley⁵, Ludmilla Kolokolova⁵

INSTITUTIONS (ALL):

- 1. Planetary Systems Branch, NASA Ames Research Center, Moffett Field, CA, United States.
- 2. Atmospheric, Oceanic and Planetary Physics, University of Oxford, Oxford, United Kingdom.
- 3. UCSD/CASS, La Jolla, CA, United States.
- 4. MN Institute of Astrophysics, Minnepolis, MN, United States.
- 5. University of Maryland, College Park, MD, United States.