

Analyses of Cometary Silicate Crystals: DDA Spectral Modeling of Forsterite

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Comets are the Solar System's deep freezers of gases, ices, and particulates that were present in the outer protoplanetary disk. Where comet nuclei accreted was so cold that CO ice ($\sim 50\text{K}$) and other supervolatile ices like ethane (C_2H_2) were preserved.

However, comets also accreted high temperature minerals: silicate crystals that either condensed ($\geq 1400\text{K}$) or that were annealed from amorphous (glassy) silicates ($>850\text{--}1000\text{K}$). By their rarity in the interstellar medium, cometary crystalline silicates are thought to be grains that formed in the inner disk and were then radially transported out to the cold and ice-rich regimes near Neptune. The questions that comets can potentially address are: How fast, how far, and over what duration were crystals that formed in the inner disk transported out to the comet-forming region(s)? In comets, the mass fractions of silicates that are crystalline, f_{cryst} , translate to benchmarks for protoplanetary disk radial transport models. The infamous comet Hale-Bopp has crystalline fractions of over 55%. The values for cometary crystalline mass fractions, however, are derived assuming that the mineralogy assessed for the submicron to micron-sized portion of the size distribution represents the compositional makeup of all larger grains in the coma. Models for fitting cometary SEDs make this assumption because models can only fit the observed features with submicron to micron-sized discrete crystals. On the other hand, larger ($0.1\text{--}100\ \mu\text{m}$ radii) porous grains composed of amorphous silicates and amorphous carbon can be easily computed with mixed medium theory wherein vacuum mixed into a spherical particle mimics a porous aggregate. If crystalline silicates are mixed in, the models completely fail to match the observations. Moreover, models for a size distribution of discrete crystalline forsterite grains commonly employ the CDE computational method for ellipsoidal platelets ($c:a:b=8.14\times 8.14\times 1$ in shape with geometrical factors of $x:y:z=1:1:10$, Fabian et al. 2001; Harker et al. 2007). Alternatively, models for forsterite employ statistical methods like the Distribution of Hollow Spheres (Min et al. 2008; Oliveira et al. 2011) or Gaussian Random Spheres (GRS) or RGF (Gielen et al. 2008). Pancakes, hollow spheres, or GRS shapes similar to wheat sheaf crystal habit (e.g., Volten et al. 2001; Veihelmann et al. 2006), however, do not have the sharp edges, flat faces, and vertices seen in images of cometary crystals in interplanetary dust particles (IDPs) or in Stardust samples. Cometary forsterite crystals often have equant or tabular crystal habit (J. Bradley). To simulate cometary crystals, we have computed absorption efficiencies of forsterite using the Discrete Dipole Approximation (DDA) DDSCAT code on NAS supercomputers. We compute thermal models that employ a size distribution of discrete irregularly shaped forsterite crystals (non-spherical shapes with faces and vertices) to explore how crystal shape affects the shape and wavelength positions of the forsterite spectral features and to explore whether cometary crystal shapes support either condensation or annealing scenarios (Lindsay et al. 2012a, b).

We find forsterite crystal shapes that best-fit comet Hale-Bopp are tetrahedron, bricks or brick platelets, essentially equant or tabular (Lindsay et al. 2012b), commensurate with high temperature condensation experiments (Kobatake et al. 2008). We also have computed porous aggregates with crystal monomers and find that the crystal resonances are amplified. I.e., the crystalline fraction is lower in the aggregate than is derived by fitting a linear mix of spectral features from discrete subcomponents, and the crystal resonances 'appear' to be from larger crystals (Wooden et al. 2012). These results may indicate that the crystalline mass fraction in comets with comae dominated by aggregates may be lower than deduced by popular methods that only employ ensembles of discrete crystals.