Systematic Constraints on Chemical Compositions of Amorphous Silicate Dust Using New Optical Constants

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Amorphous silicate, a major component of circumstellar and interstellar refractory dust, is predominantly formed in asymptotic giant branch (AGB) stars (Henning 2020). Infrared spectroscopic observations of M-type AGB stars show diverse amorphous silicate dust spectra. However, the dust composition of individual stars remains poorly constrained. Previous experiments of amorphous silicate dust analogues have focused on Mg–Si–Fe–O mineral compositions (e.g., Dorschner et al. 1995, Mutschke et al. 1998, Jäger et al. 2003), and one-to-one comparisons between observed spectra and experimental products with specific mineral compositions have been insufficient to explain the observed spectral diversity. Experiments on non-stoichiometric systems including Al and Ca, two major silicate-forming elements after Mg and Fe, are limited. Therefore, the relationships between Al and Ca content, degree of SiO_4 polymerization, and spectral features of amorphous silicate remain poorly understood. As a result, quantitative estimation of dust compositions outside experimentally explored compositional ranges remains difficult. In this study, we experimentally investigated how the chemical composition and internal structure of amorphous silicate dust affect their mid-infrared spectral features by systematically varying Ca/Mg ratios, Al/Si ratios, and degree of SiO_4 polymerization.

Condensation experiments in a Ca–Al–Mg–Si–O system were carried out using the induction thermal plasma (ITP) system (JEOL TP-40020NPS, Kim et al. 2021) to produce dust analogs with systematically varied Al/Si and Ca/Mg ratios based on CI chondritic composition. The products were analyzed by XRD (Rigaku RINT-2100) and EPMA (JEOL JXA-8530F). Absorption and reflectance spectra were measured using FTIR spectrometers (JASCO FT/IR-4200, IRT5200; Thermo Nicolet 6700). We derived optical constants from absorption and reflectance spectra using a Lorentz oscillator model (Enomoto et al. 2026). We also derived optical constants using iterative Kramers–Kronig analysis (Takigawa 2026).

The results provide the first systematic constraints on how Al and Ca abundances and polymerization degree affect the infrared spectra of amorphous silicates in non-stoichiometric regions. The 10 μm peak shifts toward longer wavelengths with depolymerization of the SiO_4 network. In addition, this trend varies with Al/Si ratios (0, 0.08, and 0.5), which can be attributed to the weaker Al–O bond relative to the Si–O bond. In contrast, the 18 μm peak shifts toward shorter wavelengths with decreasing polymerization degree, which may reflect decreases of Si–O–Si bond angles. Furthermore, the 18 μm peak position depends on the Ca/(Ca+Mg) ratio, shifting toward longer wavelengths with increasing Ca content. Our new optical constants of amorphous silicate over a broad compositional range enabled us to identify systematic relationships between Al and Ca content, polymerization degree, and spectral features. These trends provide a framework for constraining dust compositions beyond conventional mineral-based one-to-one comparisons. Using this framework together with physical parameters such as grain size and shape, we constrained the chemical compositions of dust around M-type AGB stars. This approach can also be applied to dust in the interstellar medium and protoplanetary disks.