OXYGEN ISOTOPE EXCHANGE AND CRYSTALLIZATION OF AMORPHOUS SILICATE DUST IN PROTOPLANETARY DISKS: 3D MONTE CARLO SIMULATION

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Introduction: The Sun's oxygen isotope composition is enriched in ^{16}O compared with meteorites, cometary dust, Earth, Moon, and Mars [1]. To account for the enrichment, dust that formed Solar System bodies should have had ^{16}O-depleted oxygen isotope compositions, likely due to the oxygen isotope exchange between silicate dust and ^{16}O-depleted H_2O vapor [2]. Recent experimental studies [3, 4] have determined oxygen isotope exchange kinetics between amorphous Mg silicates and H_2O vapor under the protoplanetary disk-like low pressure conditions. The obtained kinetics suggests that oxygen isotope exchange may occur at lower temperatures than that for crystallization of amorphous silicate, except for short-duration high temperature heating [3, 4]. Because crystallization of amorphous silicates suppresses the effective oxygen exchange due to extremely sluggish exchange reaction between crystalline silicates and H_2O vapor [3, 4], it is important to understand both crystallization and oxygen isotope exchange behaviors of amorphous silicate dust in protoplanetary disks.

Methods: In this study we aim to examine the progress of oxygen isotope exchange and crystallization reactions of amorphous silicate dust particles in steady-state accretion disks.

Monte Carlo simulation. We made three-dimensional Monte Carlo simulations to evaluate trajectories of dust particles in the steady-state accretion disk [5–7], where the inner part of disk is heated by viscous heating (α viscosity model) [7]. Dust size was assumed to be 0.08 μm, well coupled with gas, within the size range of silicate grains in the matrix of chondritic meteorites [8]. We adopted α of 10^{-2} and 10^{-3} and the steady accretion rate of $\dot{M}$ of 10^{-6}, 10^{-7} and 10^{-8} M_{Sun} yr^{-1}.

Oxygen isotope exchange and crystallization reactions. We used diffusive oxygen isotope exchange kinetics of amorphous silicate dust having the forsterite (Mg_2SiO_4) stoichiometry with H_2O vapor [3] and its crystallization kinetics in vacuum [9]. The reported reaction kinetics was simplified into the Avrami equation to include in the present disk model.

One thousand amorphous silicate dust particles were released at 5.2 au from the central star, near the H_2O snowline, and the progresses of reactions were calculated for dust moving inward radially by accretion and outward/vertically by diffusion at each time step [5–7]. Calculation continued for 10^6 yr, and the highest temperatures (T_{ox} and T_{cr}), where dust had experienced by the time when oxygen isotope exchange and crystallization reactions completed, respectively, were recorded.

Results and Discussion: Different particles show different T_{ox} and T_{cr}, and we here use the mode temperatures of T_{ox}- and T_{cr}-distributions (T^m_{ox} and T^m_{cr}) for discussion. We found that T^m_{ox} and T^m_{cr} depend on the disk parameters (α and $\dot{M}$). In the case of α=10^{-3}, T^m_{ox} and T^m_{cr} (in kelvin) are (~690, ~850), (~700, ~860), and (~730,~870) for $\dot{M}$ of 10^{-6}, 10^{-7} and 10^{-8} M_{Sun} yr^{-1}, respectively. In the case of α=10^{-2}, they are (~760, ~890), (770, ~900), and (~790, ~910) for $\dot{M}$ of 10^{-6}, 10^{-7} and 10^{-8} M_{Sun} yr^{-1}, respectively. T^m_{ox} is lower than T^m_{cr} for amorphous forsterite dust moving in protoplanetary disks irrespective of disk parameters. In all calculations, there is no particle that completed crystallization before the completion of oxygen isotope exchange. These results suggest that oxygen isotope exchange of amorphous silicate dust with forsterite stoichiometry occurs in the accretion disk prior to crystallization. We also conclude that the oxygen isotope exchange temperature and the crystallization temperature of amorphous forsterite dust exist at temperatures of 700–800 K and 850–900 K, respectively, in protoplanetary disks.

References: [1] McKeegan, K. D. et al. (2011) *Science* 332:1528-1532. [2] Yurimoto, H. & Kuramoto, K. (2004) *Science* 305:1763-1766. [3] Yamamoto, D. et al. (2018) *The Astrophysical Journal*, 865:98. [4] Yamamoto, D. et al. (2020) *Meteoritics & Planetary Science*, 5:1281-1292. [5] Ciesla, F. J. (2010) *The Astrophysical Journal*, 723:514-529. [6] Ciesla, F. J. (2011) *The Astrophysical Journal*, 740:9-20. [7] Okamoto, T. & Ida, S. (2022) *The Astrophysical Journal*, 928:171-183. [8] Koike, C. et al. (2010) *The Astrophysical Journal*, 7098:983-992 [9] Yamamoto, D. & Tachibana, S. (2018) *American Chemical Society Earth and Space Chemistry* 2:778-786.