

Chemical Reactions of Dynamically Moving Dust in a Protoplanetary Disk

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Elemental variations among different chemical groups of chondrites suggest that the chemical fractionation occurred in the early Solar System before parent body accretion. We made 3D Monte Carlo simulations of irreversible chemical reactions for dynamically moving dust in an accreting protoplanetary disk, and proposed prediction formulas for effective reaction temperatures of various chemical reactions of dust in the disk [1]. The predicted formulas for the effective reaction temperature well explain those for irreversible reactions occurring at 200–1400 K.

In this work, we apply these prediction formula to various cosmochemical issues. (i) Crystallization of amorphous silicate dust with forsterite and enstatite compositions occurs at 850–900 and 1050–1100 K, respectively, based on experimentally determined crystallization kinetics of these amorphous silicates [e.g., 2]. Crystallization temperatures of amorphous alumina dust (~800 K) and phase-transition from g-alumina to a-alumina (~1050 K) are also predicted using the reaction rates [3]. (ii) Oxygen isotope exchange of amorphous silicate dust with disk H₂O vapor occurs at 680–800 and 750–880 K for 0.1 mm-sized amorphous silicates with forsterite and enstatite compositions, respectively [e.g., 4]. The effective O isotope evolution would have occurred for amorphous silicate dust moving inward in the disk under the condition where ¹⁶O-poor H₂O is enriched compared to ¹⁶O-rich CO. (iii) Degradation and combustion of macromolecular organics are irreversible reactions. With proper kinetic data, effective temperatures for modification of organics (loss of N, H, and O) are expected to be predicted [e.g., 5].

[1] Ishizaki L. et al. (2023) *LPSC* 54, #1394. [2] Yamamoto D. and Tachibana S. (2018) *ACS Earth Space Sci.* **2**, 778–786. [3] Kobayashi K. et al. (2023) *LPSC* 54, #1128. [4] Yamamoto D. et al. (2020) *MaPS* **55**, 1281–1292. [5] Nakano H. et al. (2003) *ApJ* **592**, 1252–1262.