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# Molecular diffusion mechanism of atmospheric gases trapped in ice-Ih

## Content

Paleoatmospheric records can be better resolved from polar ice if trapped gases have been less diffused. The gas diffusion has been shown to be negligible on a laboratory time scale, but additional consideration should be given to whether its cumulative effects on old glacial ice can be also ignored. To address this issue, we will need to comprehensively understand the molecular diffusion mechanism of the atmospheric gases trapped in ice. Here, we employ density functional theory calculations to investigate the gas diffusion in ice-Ih from the atomistic level. The calculation results confirm that the diffusion energy barrier between interstitial sites within the ice-Ih lattice structure is primarily dependent on the atomic size and charge distribution of hopping gases. Consistent with the previous results of classical molecular dynamics simulation, the interstitial mechanism appears to govern the diffusion of noble gases (He, Ne, Ar, Kr, and Xe). However, the bond-breaking mechanism formerly proposed to explain the diffusion of CO2, O2, and N2 may be unnecessary because these molecular gases prefer to hop along the hexagonal channel also via the interstitial mechanism. We believe that the refined understanding of the gas diffusion mechanism can help future studies to investigate the gas dissolution at the gas-ice interface and the diffusion-induced elemental and isotopic fractionation in old glacial ice.

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