Light element diffusion in liquid Fe for P-T conditions of the Earth's interior

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Abstract

Chemical diffusion of light elements in liquid Fe plays an important role both during core formation and the growth of the inner core. However, relevant conditions are difficult to achieve in the laboratory, and first-principle determination of the diffusion constants have lacked benchmarking with experiments. Here we present results that combine experimental and computational estimates on diffusivities of Si and O in liquid Fe, covering the whole P-T range from ambient pressure to conditions of the Earth's inner core. We show that both approaches are compatible and use structural information from the molecular dynamics simulations to analyze the experimental results. Si diffuses at a comparable rate to Fe over the whole P-T range considered, which is consistent with the short-range structure in the liquid. For O in Fe, an analysis of the radial distribution function and coordination number reveals that Fe and O compress in a very different manner up to a density of approximately 8 g/cc, with initial compression primarily accommodated by an increase in coordination. This behavior can account for the very anomalous diffusion behavior observed in experiments with no appreciable P-dependence up to 25 GPa.

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