

Outer core composition estimated from thermoelastic properties of liquid Fe alloys

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The Earth's core is thought to include substantially large amounts of light elements (LEs), which account for observed density deficits of ~10% for the liquid outer core and ~5% for the solid inner core (e.g. Birch, 1964; Brown and McQueen, 1986; Jephcoat and Olson, 1987; Uchida et al., 2001; Anderson et al., 2003; Dewaele et al., 2006; Ichikawa et al., 2014). The density jump across the inner-outer core boundary (ICB) evaluated by seismic wave observations is ~4.5-6.7 % (Shearer and Masters, 1990, Masters and Gubbins, 2003), which cannot be accounted for by the melting phase transition of pure iron alone and requires a LEs partitioning more into the outer core (Alfè et al., 2002a). Although oxygen, silicon, carbon, nitrogen, sulfur, and hydrogen have been proposed as candidates for the LEs (Stevenson, 1981), little is known about the amount and the species so far. However, experimental determination of these properties for the liquid states are still not practical at the outer core pressure and temperature (from ~136 GPa to ~329 GPa and from ~4,000 K to ~6,000 K) due to technical limitations. The ab initio density functional computation method is instead quite powerful to investigate liquid properties under such extreme condition. Here, we show integrative analyses of the compositional model of the Earth's outer core based on the ab initio thermoelasticity of iron-nickel-LE alloy liquids. Results indicate that combination of LEs in the outer core cannot be fully constrained only by the comparison between elastic properties and seismic observation. Comprehensive considerations covering density jump at the ICB, phase relations, geochemical constraints, and the ΔV_p of low-velocity anomalies in the outermost core are used to refine the compositions of the outer core.

Keywords: Composition of the Earth's outer core, Light elements, ab initio molecular dynamics simulation