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Science Research Bldg. 1, 4th floor.

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Keywords:

1. Sulfur
2. iron-silicate partitioning
3. ab initio calculation

Effects of Si and O in the metal on the S partitioning between liquid metal and molten silicate at high pressure and temperature based on ab initio calculations

S is one of the most likely elements to explain the density deficit in the Earth's core (e.g., Birch, 1952). To constrain the S concentration in the core, various S partitioning experiments between liquid iron and molten silicate have been conducted in the past (e.g., Rose-Weston et al., 2009; Suer et al., 2017). These experiments show containing O and Si in liquid iron significantly affects S partitioning. However, experimental conditions have been limited in pressure and temperature. This study employs theoretical methods to examine the effects of O and Si in liquid iron on S partitioning between liquid iron and molten silicate under higher pressure and temperature conditions (20-135 GPa, 4000-5000 K). In this study, the reaction free energy is calculated using the ab initio thermodynamic integration molecular dynamics method.

Results reveal that O notably reduces the siderophilicity of S, especially at 135 GPa with 20 mol% O in liquid iron, where the partition coefficient ($\log D_s$) decreases from ~ 3.5 to ~ 1.5 . For 20 mol% Si, $\log D_s$ decreases from ~ 3.5 to ~ 2.5 at 135 GPa but shows minimal reduction at 60 GPa. Analysis of the local structure and electronic structure of liquid iron suggests that Si weakens S-Fe interactions through Si-Fe correlation, while the effect of O is attributed to volume reduction caused by its containing.

In most cases, the siderophilicity of S is reduced when O or Si is contained in liquid iron. However, this effect is not large enough to say that the light elements in the core are not S. Therefore, from the perspective of S partitioning, it can be said that it is feasible for the light elements in the Earth's core to have a composition of coexisting S, O, and Si.