The 484th Geodynamics Seminar

Ab initio predictions of K, He and Ar partitioning between silicate melt and liquid iron under high pressure

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Element partitioning is an important property in recording geochemical processes during the core-mantle differentiation. However, experimental measurements of element partitioning coefficients under extreme temperature and pressure condition are still challenging. Theoretical modeling is also not easy, because it requires estimation of high temperature Gibbs free energy, which is not directly accessible by the standard molecular dynamics method. We recently developed an original technique to simulate Gibbs free energy based on the thermodynamics integration method. We apply it to element partitioning of geochemical intriguing trace elements between molten silicate and liquid iron such as potassium, helium and argon as starting examples.

Radiogenic potassium in the core can provide energy for Earth's magnetic field, convection in the mantle and outer core. However, its partitioning behavior between silicate and iron remains unclear under high pressure. Our calculations suggest that a clear positive temperature dependence of the partitioning coefficient but an insignificant pressure effect. Unlike sulfur and silicon, oxygen dissolved in the metals considerably enhances potassium solubility. Calculated electronic structures reveal alkali-metallic feature of potassium in liquid iron, favoring oxygen with strong electron affinity. Our results suggest that ^{40}K could serve as a potential radiogenic heat source in the outer core if oxygen is the major light element therein. We now further extend our technique to partitioning behaviors of other elements, helium and argon, to get insides into the 'helium paradox' and 'missing argon' problems.

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