Ab initio prediction of potassium partitioning into the Earth's core

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Silicate earth is depleted in potassium compared with chondrites [Wasserburg et al., 1964, Science]. Barely varying ratios of potassium isotope in chondrite, lunar and earth samples suggesting evaporation cannot be responsible for the missing of potassium [Humayun and Clayton, 1995, GCA]. The finding of a change in electronic structure of potassium from alkaline- to transition metal-like at high pressure highlighted the possibility of its incorporation into the core [Parker, 1996, Science]. If potassium is present, even ~ppm, the radiogenic heat produced by ^{40}K could be an important energy source for geodynamics [Labrosse, 2001, EPSL]. The potassium content in the core is determined by its partitioning behavior between silicate and metal system, which could be affected by many factors such as temperature, pressure, compositions of the metal (the type and content of light elements) and silicate systems (nbo/t: the ratio of non-bridging oxygen to tetrahedral cations) [Bouhifd etal., 2007, EPSL; Muthy etal., 2002, Nature]. However, previous experimental studies provided contradictory results of potassium incorporation into Fe-alloys, leaving its concentration in the core uncertain.

Ab-initio free energy simulations based on molecular dynamics conbined with thermodynamics integration[Taniuchi, 2014] are performed to investigate whether and how much potassium can enter the metal system. Potassium partition coefficient(D_k=Kwt%$_{metal}$/Kwt%$_{silicate}$) is determined as a function of pressure, temperature and composition by calculating the Gibbs free energy changes of its exchange reactions in different conditions. Helmholtz free energy is estimated with “thermodynamic integration” by computing the difference between two systems with different potential energy functions[Kirkwood, JCP, 1990].

Calculations performed from 3000 K to 5000 K suggest that temperature has no distinct effect in potassium incorporation into Fe-alloys. Results of D_k obtained from 20 GPa to 135 GPa at constant temperature and composition reveal that potassium partitioning behavior has a negligible pressure dependence. Besides, the potassium partial density of states (pDOS) shows its electronic structure remains to be alkaline metallic even at 135 GPa. Simulations show a limited effect of Al concentration in silicate composition to potassium solubility into metal system.

Influences of the light elements (O and S) proposed to be responsible for the density deficits of the core to potassium partitioning are also investigated in this study. Potassium solubility seems unchanged when the S content of the metal system increases. Simulations with oxygen free metal composition suggest that potassium will completely sequester into silicate system. However, with the presence of oxygen in metal, potassium will start its incorporation into metal system. Our results suggest that effects of temperature, pressure, silicate composition and S content are insignificant, while oxygen controls potassium partitioning between silicate and metal system.

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