The 453rd Geodynamics Seminar

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

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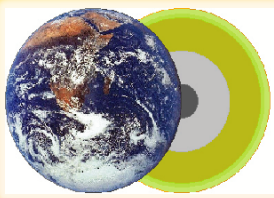

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

Silicate earth is in strong depletion of K compared with chondrites. Barely varying ratios of K isotope in chondrite, lunar and earth samples suggesting evaporation cannot be responsible for the missing of K. The finding of a change in electronic structure of K from alkaline- to transition metal-like at high pressure highlighted the possibility of its incorporation into the core. If K is present, even in ~ppm, the radiogenic heat produced by ^{40}K could be an important energy source for mantle dynamics. The K content in the core is determined by its partitioning behavior between silicate and metallic system, which could be affected by many factors such as temperature, pressure, compositions of the metallic (the type and content of light elements) and silicate systems (NBO/T: the ratio of non-bridging oxygen to tetrahedral cations). However, previous experimental studies provided contradictory results of K incorporation into Fe-alloys, leaving its content in the core uncertain.

Ab-initio free energy calculations based on molecular dynamics simulations are performed to investigate whether and how much K can enter the metallic system. K 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 corresponding to different conditions. Helmholtz free energy was obtained based on "thermodynamic integration" by computing the difference between two systems with different potential energy functions ($F_1 - F_0 = \int_0^1 < U_1 - U_0 >_\lambda d\lambda$). In this presentation, first I'll report about the influences of temperature, pressure, composition of silicate and metallic systems to the partitioning behavior of K, and then discuss the possibility of K existence in the Earth's core.

詳細は当センターホームページ: http://www.grc.ehime-u.ac.jp/をご覧ください
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