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Hf and W partitioning between liquid metal and silicate melt based on first principle calculation and the early earth's evolution of ^{182}W isotope

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^{182}Hf has a geologically short half-life of 8.9 million years,. Hf is thought to remain in the silicate melt phase while W is distributed in the metal melt phase during the Earth core formation. As a result, the metalic core should have low ^{182}W compared with that of mantle. Ocean island basalts (OIBs) from the islands such as Hawaii and Samoa whose sources would be the lowermost mantle show low $\mu^{182}W$ (deviation from present-day upper mantle values in ppm) (i.e. Mundl et al. 2017; Rizo et al. 2019), and these are considered the evidence for the inclusion of core material. To understand what these ^{182}W isotopes indicate in the evolution of the Earth, it is necessary to look at the behavior of Hf and W under high pressure and the effects of meteorite impact.

We investigated the partitioning of Hf-W between silicate melts and molten iron using first-principles free energy calculations under high-temperature and high-pressure condition, which is difficult to achieve by laboratory experiments. We also calculated whether the partition coefficient changes when iron is mixed with silicate or vice versa. As a result, it was confirmed that W is distributed in iron and Hf is distributed in silicate melt in all cases. The partition coefficients of W and Hf were not largely affected by the addition of Fe to the silicate melt, while those of W and Hf were decreased and increased, respectively, when Fe contained O. This proves that Hf-W partitioning can occur due to partitioning between core and mantle, resulting in negative $\mu^{182}W$ values of core. Thus, one of the most probable reasons why some OIBs from the deep mantle have low (negative) $\mu^{182}W$ values is that the core material with low $\mu^{182}W$ values is involved in the source of such OIBs.

Mundl, A., et al. (2017) Science 356, 66. Rizo, H. et al. (2019) Geochem. Perspectives Lett. 11, 6-11.