Grain boundary diffusion of W and Pt at the core-mantle boundary

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The negative $\mu^{182}W$ anomalies associated with high ${}^{3}\text{He}/{}^{4}\text{He}$ ratios in some ocean island basalts may derive from the Earth's core through long-term core-mantle interactions. Atomic diffusion along grain boundaries is typically orders of magnitude faster than its lattice counterpart. It has been proposed that the grain boundary diffusion of siderophile elements is an efficient mechanism for core-mantle interaction and may effectively modify the W isotopic compositions of the plume-source mantle. In this study, we perform large-scale molecular dynamics simulations driven by machine learning potentials of ab initio quality to investigate the grain boundary diffusion of W and Pt in ferropericlase. The recently found complexions with chargeneutral vacancy pairs are used to construct the polycrystalline systems. We will report the first-hand data of W and Pt diffusion at the core-mantle boundary conditions. Implications for the core-mantle interactions and the origin of ocean island basalts will be discussed.