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Diamonds in the Deep: Unveiling the Role of Water-Induced Reactions in Earth's Lower Mantle

FEIWU ZHANG, XU ZHENG, JOSHUA MUIR AND YI WANG

Institute of Geochemistry, Chinese Academy of Sciences

The carbon and hydrogen cycles in the Earth's interior are linked to key planetary processes, impacting mantle melting, degassing, and chemical differentiation, but the fate of hydrogen in chemical interactions by subducted slabs to the deep Earth remains poorly understood. Using first-principles density functional theory (DFT) calculations, this study investigates the chemical reaction processes between hydrous minerals and iron-carbon alloys under extreme lower mantle conditions, focusing on analyzing changes in chemical reaction energy and elastic properties. Our study reveals that phase H reacts with Fe_3C at the Core-Mantle Boundary (CMB), resulting in the formation of diamond, $FeH_{(fcc),}$ and $FeOOH_{(pyrite\text{-}type)}$, as the equation below illustrates:

$Fe_3C+MgSiO_4H_2 \rightarrow FeO + 2FeH + MgSiO_3+ C$ (1)

$Fe_3C+MgSiO_4H_2 \rightarrow 3FeOOH + 9FeH + 6MgSiO_3+ 4C$ (2)

These reactions indicate that subducted water reaching the CMB can release core carbon as diamonds while enriching the deep mantle with hydrogen and oxygen. The released core carbon accounts for a significant portion of the mantle's carbon, thereby linking Earth’s carbon and hydrogen cycles.

We calculated the wave velocity (V_P, V_S) and density of diamond, $FeH_{(fcc)}$, and $FeOOH_{(pyrite\text{-}type)}$ in the deep lower mantle along the geotherm of the cold slab. Diamonds may become locally enriched in the lowest mantle, creating anomalous structures of low density and high seismic velocities . When these produced diamonds are transported upwards by mantle flow, they may create regions with unusually high seismic velocities. Additionally, the formation of diamond also yields $FeH_{(fcc)}$ and $FeOOH_{(pyrite\text{-}type)}$. These products exhibit high density and ultra-low seismic velocities, suggesting a potential origin for ultra-low velocity zones (ULVZs) in the D" layer. Therefore, the interaction between hydrogen from subducted slabs and the core's iron-carbon reservoir could generate deep mantle diamonds and promote the accumulation and thickening of an oxygen-rich layer, with profound global geological implications.

Our model suggests that the interaction between hydrous minerals in subducted plates and the iron-carbon alloy in the core may transfer carbon and hydrogen in the deep lower mantle, significantly influencing our understanding of deep mantle dynamics, seismic anomalies, and geochemistry.