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Carbon in the deep upper mantle and transition zone under reduced conditions: Insights from high-pressure experiments and machine learning models

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Carbon in the deep upper mantle and transition zone under reduced conditions: Insights from high-pressure experiments and machine learning models

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The petrological storage of carbon in Earth's mantle is an important consideration within the framework of the deep carbon cycle. In the deep (>250 km depth) reduced mantle, carbon storage mechanisms differ greatly from those in the oxidized shallow mantle. To investigate the stability of carbon-bearing phases in Earth's deep mantle, we experimentally constrained compositional effects on phase stability in the Fe-Ni-S-C system at conditions relevant to the deep upper mantle and mantle transition zone. Our experiments suggest that carbide is absent at 10 GPa and 1450 °C in the Ni-poor (molar Ni/(Ni+Fe) = 0.2) portion of the metal-sulfide-carbon ternary, with carbon occurring as diamond or dissolved in the Fe-Ni-S-C melt. At 19 GPa and 1600 °C, $(Fe, Ni)_7C_3$ saturates in the melt with C-rich (4.8–9.5 wt.%), S-poor (2.3–6.4 wt.%) bulk compositions. In comparison, Fe-Ni alloy only saturates with the C- and S-poor bulk composition of 77.9 wt.% Fe, 19.5 wt.% Ni, 1.9 wt.% S, and 0.7 wt.% C. Based on these results, we trained machine learning models to predict carbon solubility in Fe-Ni-S-C melts. Compared to classical regression models, machine learning models significantly improve the accuracy of carbon solubility predictions. Combined, our experimental and machine learning results suggest that diamond and Fe-Ni-S-C melt are the primary hosts of carbon in the convecting deep upper mantle and throughout most of the mantle transition zone. In the deepest parts of the transition zone, however, carbide is likely to precipitate in C-rich mantle sources at adiabatic temperatures.