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The high-pressure Fe-FeH phase diagram: Experiments and thermodynamic modelling

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Hydrogen may be one of major light elements in the metallic cores of terrestrial planets, and the Fe-FeH phase diagram is of great importance to understand core composition and temperature. However, since metallic iron incorporates negligible amounts of hydrogen at ambient pressure, the study of the Fe-FeH system has been limited. Here we obtained the Fe-FeH phase diagram at high pressures to 330 GPa, corresponding to Earth's inner core boundary conditions, based on a combination of high-pressure experiments and thermodynamic modelling. Both melting and subsolidus experiments were carried out up to 130 GPa and 4200 K in a laser-heated diamond-anvil cell combined with in-situ synchrotron X-ray diffraction measurements. We then developed a thermodynamic model based on the present and earlier experiments on the Fe-FeH system including Fe- and FeH-endmembers. It predicts the Fe-FeH phase diagram at 330 GPa, showing a higher Fe-FeH eutectic temperature than the extrapolation of a melting curve reported by earlier experiments, a concentration-dependent hcp-Fe/liquid partition coefficient of hydrogen, and the non-linear effect of hydrogen on the depression of melting temperature. With these findings, we estimated the possible ranges of Earth's core composition and temperature, suggesting that both the outer and inner cores contain hydrogen and silicon as important light elements with oxygen a minor component in the outer core liquid.