

Supporting Information

Group 8 metallocenes as single-source precursors for the synthesis of light-element-stabilized FCC phases under extreme conditions

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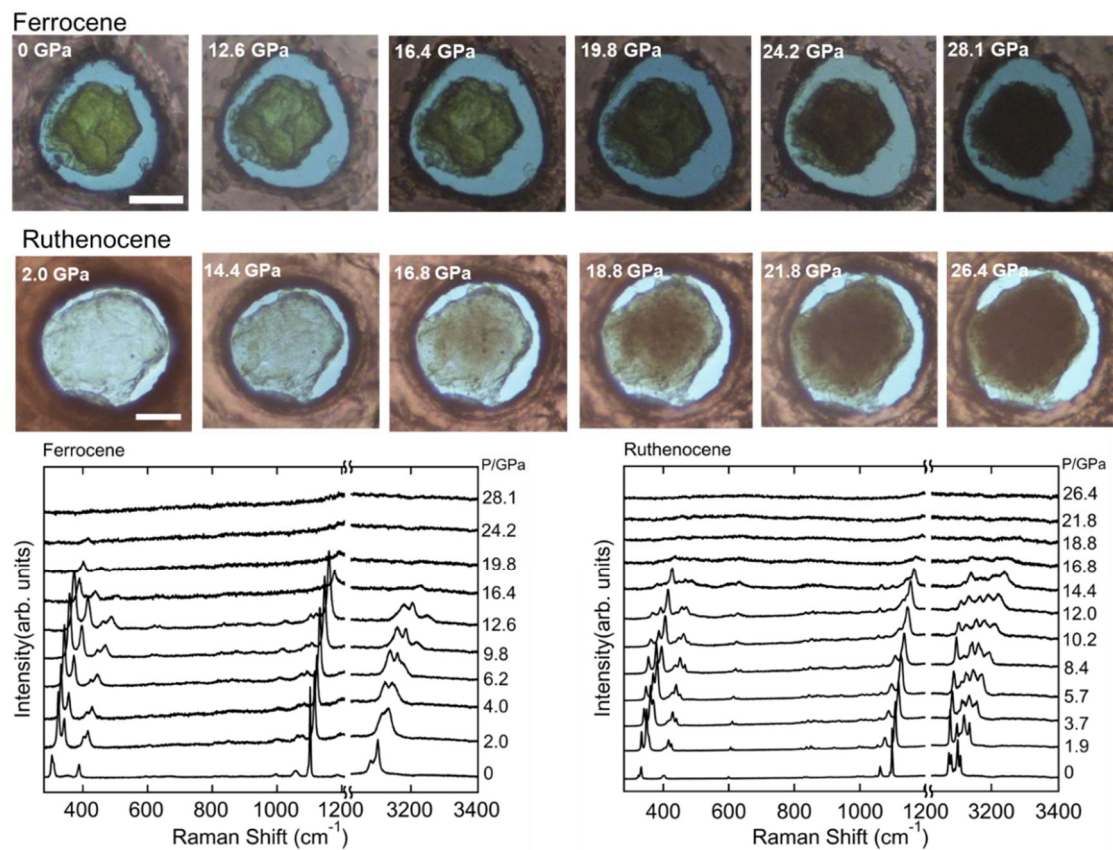


Figure S1

Optical micrographs of ferrocene and ruthenocene were obtained at room temperature under high-pressure conditions (#15, #28). Both compounds exhibited a transition to an opaque state upon compression. While sharp Raman peaks were clearly observed at low pressures, their intensities monotonically decreased with increasing pressure, eventually becoming negligible above 20 GPa.

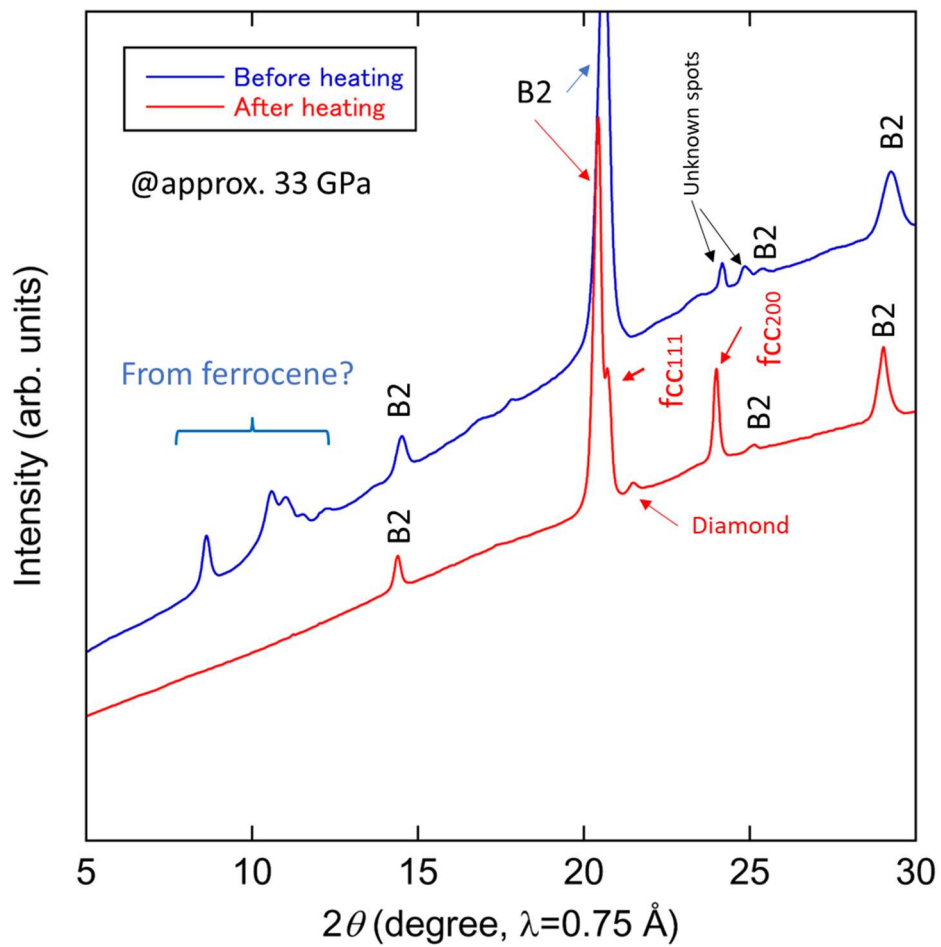


Figure S2

XRD patterns of ferrocene were collected before and after laser heating at approximately 33 GPa (#12). Prior to heating, a few broad peaks were observed at low 2θ angles; these peaks were no longer detectable after laser heating.

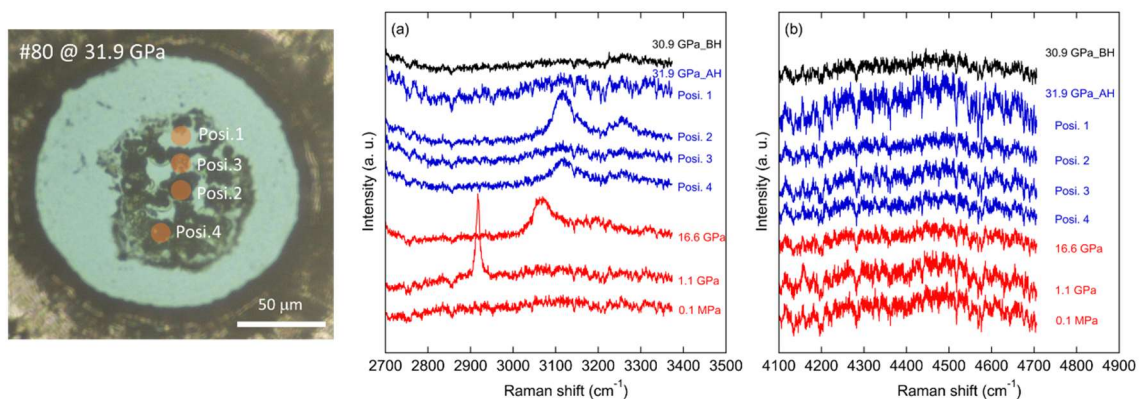


Figure S3

Raman spectra of ferrocene were collected before and after laser heating at approximately 30 GPa, and during the decompression process (Run #80). Left side figure represents the measurement position. Spectra in (a) and (b) are collected with the center of wavenumber at 3000 and 4400 cm^{-1} , respectively. BH and AH denote “before heating” and “after heating,” respectively. “Posi. n ” indicates the specific location on the heated sample where the spectra were acquired (left side figure). The bottom three profiles were recorded at Posi. 2 during the decompression process.

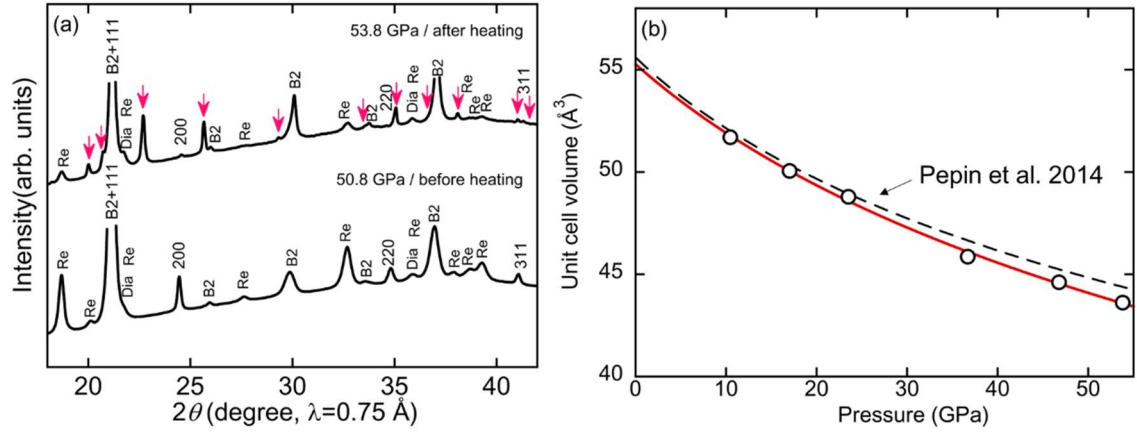


Figure S4

(a) XRD patterns collected at approximately 50 GPa before and after laser heating (#26). Labels hkl and Dia denote reflections from the fcc phase and diamond, respectively, while B2 and Re correspond to the NaCl pressure medium and rhenium gasket. The initial fcc phase underwent a significant intensity reduction upon laser heating, accompanied by the emergence of a new peak (indicated by the arrow) consistent with the double hexagonal close-packed (dhcp) structure of FeH. The peaks of the residual fcc phase observed after heating at 53.8 GPa were also measured during the decompression process, and the corresponding volumes are plotted in Fig. 2(b). (b) Pressure–volume relationship for the synthesized dhcp phase. The solid and dashed lines represent the present and previously reported equation of state (EOS) for dhcp-FeH, respectively.

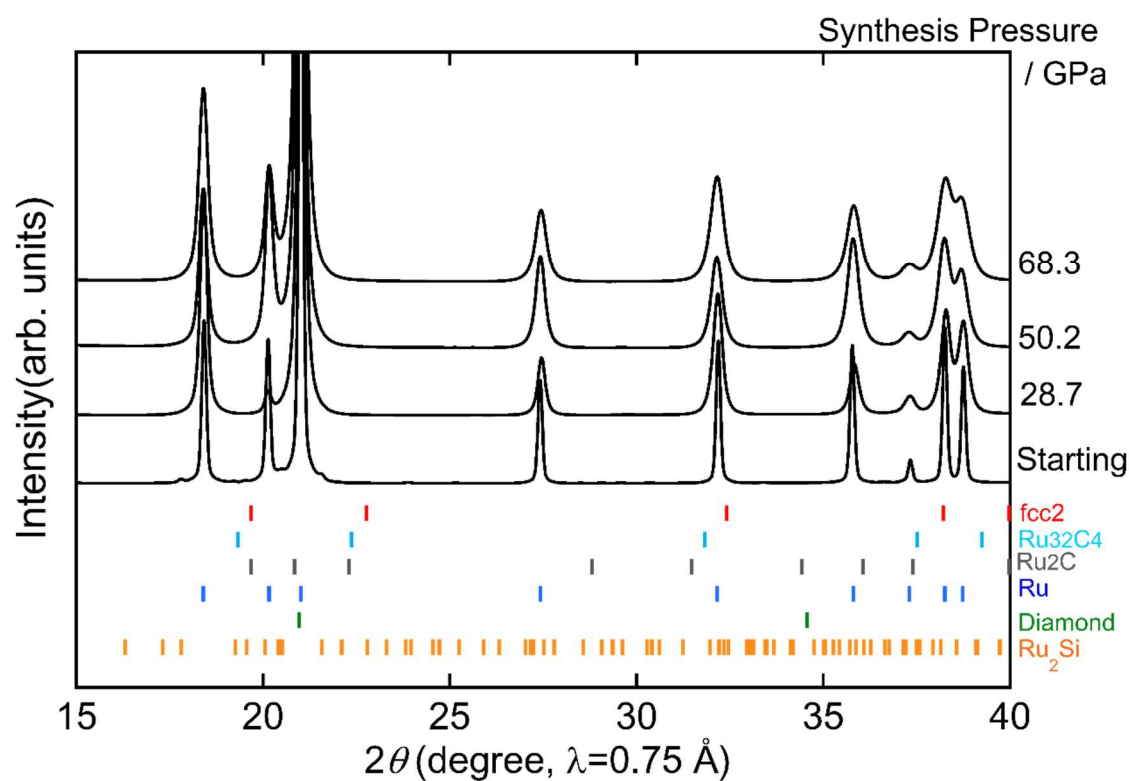


Figure S5

XRD pattern of the sample synthesized under high pressure. The starting material was prepared via arc melting and liquid rapid quenching; trace amounts of Ru_2Si , resulting from Si contamination from the nozzle, were detected. In the high-pressure synthesized product, neither the fcc phase nor the previously reported Ru_2C phase was observed.