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Pure Iron Compressed and Heated to Extreme Conditions¹ ARKADY MIKHAYLUSHKIN, SERGEI SIMAK, Theory and Modeling Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, S-581 83, Linköping, Sweden, LEONID DUBROVINSKY, Bayerisches Geoinstitut, Universitat Bayreuth, D-95440 Bayreuth, Germany, NATALIA DUBROVINSKAIA, Mineralphysik und Strukturforschung, Mineralogisches Institut, Universität Heidelberg, 69120 Heidelberg, Germany, BORJE JOHANSSON, Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), SE-10044 Stockholm, Sweden, IGOR ABRIKOSOV, Theory and Modeling Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, S-581 83, Linkóping, Sweden — The results of a first-principles study supported by the temperature-quenched laser-heated diamond anvil-cell experiments on the high-pressure high-temperature structural behavior of pure iron are reported. We show that in contrast to the widely accepted picture, the face-centered cubic (fcc) phase becomes as stable as the hexagonal-close-packed (hcp) phase at pressures around 300360 GPa and temperatures around 50006000 K. Our temperaturequenched experiments indicate that the fcc phase of iron can exist in the pressuretemperature region above 160 GPa and 3700 K, respectively. This, in particular, means that the actual structure of the Earth's core may be a complex phase with a large number of stacking faults.

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Arkady Mikhaylushkin Theory and Modeling Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, S-581 83, Linköping, Sweden

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