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Single crystal crystallography of geomaterials at 100 GPa and above LEONID DUBROVINSKY, BGI Bayeuth University, NATALIA DUBROVINSKAIA, ELENA BYKOVA, Bayeuth University, KONSTANTIN GLAZYRIN, TIZIANA BOFFA BALLARAN, CATHERENE MCCAMMON, ANASTASIA KANTOR, BGI Bayeuth University, MARCO MERLINI, MICHAEL HANFLAND, ALEXANDER CHUMAKOV, ESRF — Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single crystal diffraction experiments. Advances in diamond anvil cell techniques (DACs) and modern X-ray sources have increased the accessible pressure range for structural research up to several dozens of gigapascals. We have developed a methodology to perform single crystal X-ray diffraction experiments in double-side laser-heated DACs and demonstrated that the solution of crystal structures, their refinement, and accurate measurements of the thermal equation of state of metals, oxides, and silicates from single crystal diffraction data are possible in a megabar pressure range at temperatures of thousands degrees. Particular attention is paid to the in situ study of silicate perovskite (Pv) at extreme conditions. By tracking the changes of crystallographic parameters at pressures above 120 GPa and temperatures up to 2200 K, we found that (a) there is no a spin state crossover in ferric iron occupying the bi-capped trigonal prism ("A") crystallographic site, and (b) ferric iron does not enter the octahedral ("B") site at any conditions of our experiments. We demonstrate that incorporation of ferric iron and aluminum significantly increases the compressibility of Pv and show that the oxidation state of iron is a critical parameter for interpretation of seismic tomography data.

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