New insights into the composition of Earth's deep lower mantle: Multigrain analysis at megabar pressures

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Models of the Earth's deep interior have been built upon the basic assumption that the lower mantle down to the top of the D" layer mainly consists of perovskite (pv) with nominally 10 mol% Fe. However, seismic observations suggest compositional heterogeneity in the bottom 1000 km of the lower mantle, implying variations in the mineralogical constitution of this region. Our recent study using laser-heated diamond anvil cell (DAC) technology coupled with synchrotron x-ray diffraction (XRD) has demonstrated the disproportionation reaction of (Mg,Fe)SiO3 perovskite (pv) to a nearly Fe-free pv and an Fe-rich H-phase with a previously unknown hexagonal structure at 95-101 GPa and 2200-2400 K. This finding further complicates the geochemistry and geophysics of the bottom half of the lower mantle. It has been long challenging for structure identification and accurate unit-cell calculations in mineral assemblages when multiple low symmetry phases coexist. Applying the multigrain method to megabar pressures, the crystal chemistry and unit-cell parameters are investigated in situ at high pressure for each individual phase in lower mantle mineral assemblages. The high-pressure structures are solved using heavy atom method by merging crystallographic data sets from multigrains. The unit-cell parameters are calculated for each phase with exceptional accuracy based on hundreds of reflections from multigrains. The crystal chemistry and phase relations of minerals at high *P*-*T* are used to understand the composition and dynamics of the lower mantle.