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Local and Long Range Symmetry in Ferroelastic Lead Phosphate at High Pressure. Ross Angel, Ulrich Bismayer, William Marshall, Dept Geosciences, Virginia Tech, Blacksburg, VA 24060 USA.

Pure lead phosphate, $\text{Pb}_3(\text{PO}_4)_2$, undergoes a phase transition from $C2/c$ to $R-3m$ symmetry at approximately 1.8 GPa at room temperature. High-pressure neutron powder diffraction measurements were used in combination with high-pressure single-crystal X-ray diffraction to show that there is no significant change in the local structure at the high pressure phase transition; the structure of the $R-3m$ phase at pressures just above the phase transition includes disordered positions for several atoms. The further observation of diffuse scattering from the $R-3m$ phase at high pressure suggests that the disorder is static and arises from the presence of several orientations of ordered microdomains of monoclinic local structure. The observation of the same behavior in Ba-doped lead phosphate supports these conclusions. The macroscopic transition from monoclinic to trigonal symmetry therefore appears to correspond to a pressure at which the coherency strains between the locally monoclinic microdomains are sufficient to create a dimensionally trigonal lattice within which local displacements of atoms are still significant. At higher pressures these displacements are suppressed and the structure appears to have true local and global trigonal symmetry. This is in complete contrast to the high-temperature phase transition from $C2/c$ to $R-3m$ that involves dynamic disorder of the Pb atoms.