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Local atomic structure of BaFe₂As₂ by neutron powder diffraction JENNIFER NIEDZIELA, Dept. of Physics and Astronomy, U. Tennessee, Knoxville; ORNL - Neutron Sciences Directorate, TAKESHI EGAMI, Dept. of Mat. Science and Engineering, Dept. of Physics and Astronomy, U. Tennessee, Knoxville; ORNL - Joint Institute for Neutron Sciences — All structures of iron-based superconductors (FeSC) have planar layers of iron, tetrahedrally coordinated by pnictogens or chalcogens, and the structural details of this layer impact the superconducting and magnetic properties. Local structural studies of the iron-coordinated layer show evidence for local distortions resulting from models that allow for overall reductions in local symmetry. BaFe₂As₂, a parent compound of several families of FeSC, undergoes a transition at T $\approx = 140$ K, resulting in the onset of AFM ordering following a small lattice distortion. Here we report the results of a by time of flight neutron diffraction study on BaFe₂As₂, analyzed using Rietveld and pair distribution function techniques. This work produces a comprehensive view of the local structure of BaFe₂As₂ as a function of temperature. The results are consistent with previous work showing stratification of the As-As bond length, and show that models accounting for an overall reduction in local symmetry provide the best fit to the experimental data. Further, the results show that local distortions are present up to room temperature. Details of the experiment and implications for the paramagnetic and magnetic states will be discussed.

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