Crystal and magnetic structures of $BaSrFe_2O_{5+\delta}$

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The oxygen-deficient perovskite, $BaSrFe_2O_{5+\delta}$, was synthesized in air at 1100 C. The crystal structure is cubic, *Pm*-3*m*, with long-range disorder of oxygen vacancies. Rietveld refinements using neutron diffraction data (Figure 1) led to the determination of the oxygen stoichiometry, $\delta = 0.52(2)$. The neutron data, down to 3.6 K, show no indication of long-range magnetic order, consistent with the magnetic susceptibility results. However, a comparison between the data at 3.6 K and 285 K (Figure 2) shows broad, temperature dependent peaks at ~ 17 deg and 29 deg, indicating the presence of short-range magnetic domains. A fit to the 17 deg peak in the 3.6 K data to the Ornstein-Zernike model, $I(Q) = A/[(Q-Q_0)^2 + \kappa^2]$, where A is an amplitude, $Q = 4\pi\sin\theta/\lambda$, Q_0 is the peak centre and $\kappa = 1/\xi$ with ξ being the correlation length is shown in Figure 3. The fitting shows a correlation length of 11(1) Å for the magnetic domains in $BaSrFe_2O_{5.5}$. This is in sharp contrast to the Sr-only analogue, $Sr_2Fe_2O_{5.5}$ [1], which shows long-range ordering of oxygen vacancies, *Cmmm* space group, and also long-range magnetic order. The magnetic structure of $Sr_2Fe_2O_{5.5}$ is a C-type antiferromagnetic [2], where the magnetic moment on each site is aligned antiparallel to the nearest neighbors within the same layer but parallel to the nearest neighbors in the adjacent layers.

References

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[2] Schmidt, M.; Hofmann, M.; Campbell, S.J. J. Phys.: Condensed Matter, 2003, 15, 8691-8701

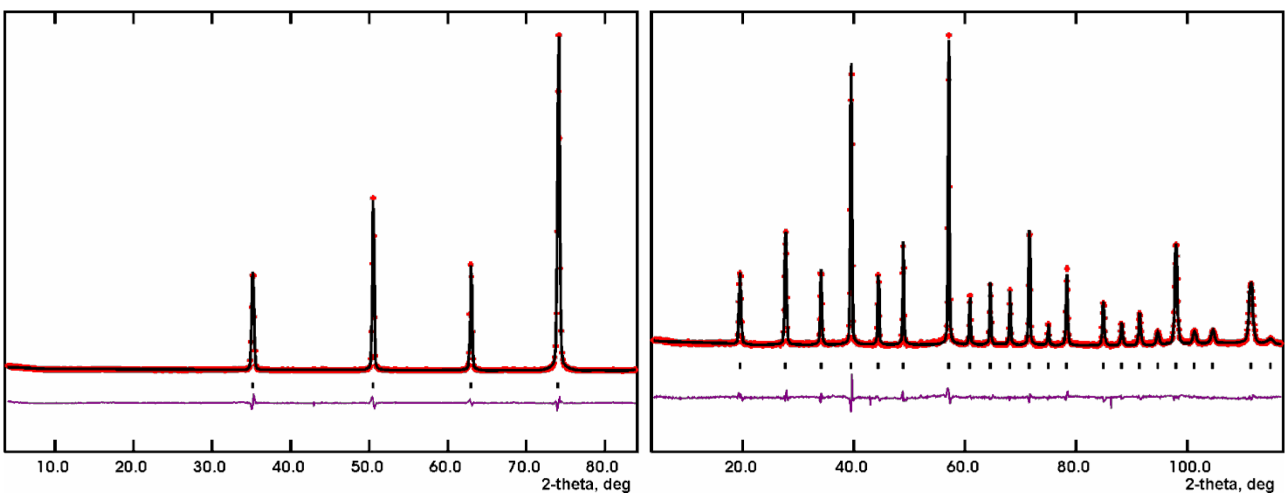

Figure 1 The Rietveld refinement profiles for the neutron diffraction data with $\lambda = 2.27$ Å (left) and $\lambda = 1.33$ Å (right). Note the absence of the magnetic Bragg peaks.

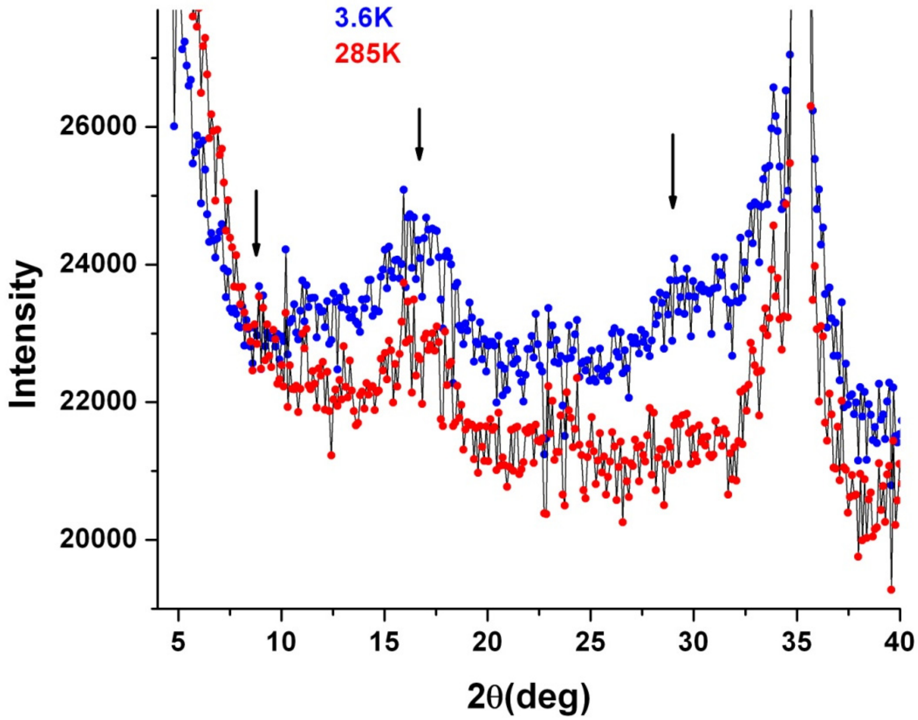

Figure 2 A comparison between the neutron diffraction data at 3.6 K (blue) and 285 K (red). Note the presence of the magnetic features (↓) that diminish as the as temperature increases, and also the cross over at 2θ ~ 8 deg.

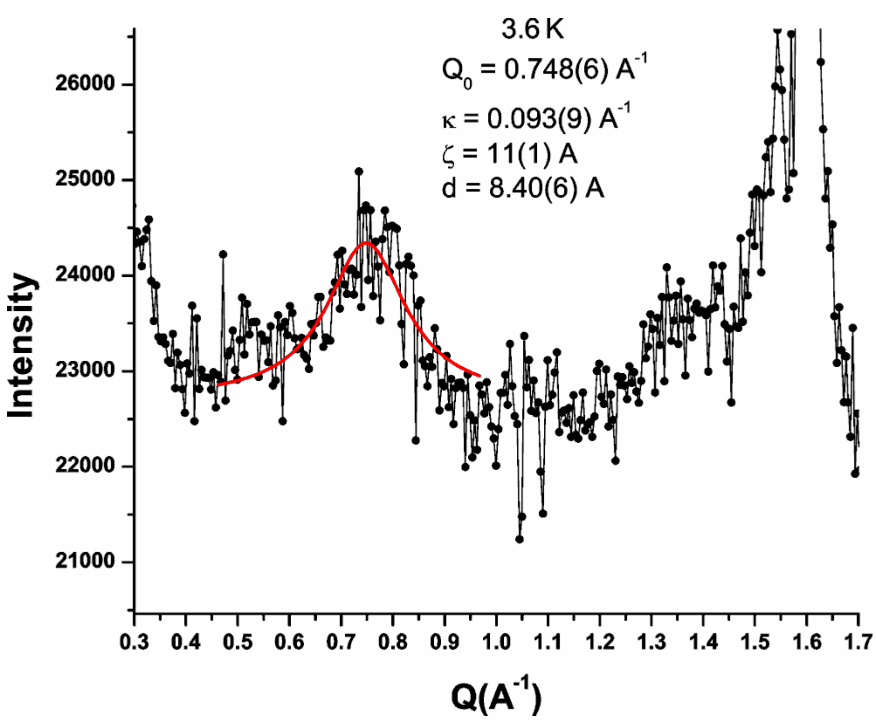

Figure 3 The fit to the Ornstein-Zernike model for one of the magnetic features in the neutron data at 3.6 K. The correlation length for the magnetic domains was found to be 11(1) Å and the d-spacing is incommensurate with the chemical cell.