ESRF	**Experiment title:** Nematic structural transition in the Fe-based superconductor FeSe	**Experiment number**: HC-2944
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Report: We performed powder XRD measurements on an iron-based superconductor FeSe with the aim of investigating the local atomic distortions above and below the nematic phase transition temperature $T_s \approx 87$ K. We used pair distribution function (PDF) analysis to unravel the local atomic distortions. In the temperature dependence of $G(r)$, we observed an unusual broadening in the peak corresponding to the Fe-Fe distance below 30 K suggesting a precursor-state phenomenon occurring prior to the superconducting transition at 8.5 K in FeSe. Our results indicate that the partial suppression of the density of states (or pseudogap) observed in the temperature range of 20 - 30 K [1,2] also contains a structural distortion with short range correlations.

As a first step, we performed several diffraction measurements in the temperature range 5 – 190 K. The lattice parameters were obtained from the Rietveld analysis. The temperature dependence of the lattice parameters display the expected behaviour corresponding to the tetragonal (*P4/nmm*) to orthorhombic (*Cmma*) distortion at T_s as can be seen in Fig. 1.

An analysis of the interatomic distances make use of the reduced PDF, $G(r)$, which is a sine Fourier transform of the experimental total scattering function, $S(Q)$, defined as [3]

$$G(r) = 4\pi r[\rho(r) - \rho_0] = \frac{2}{\pi}\int_{Q_{min}}^{Q_{max}} Q\,[S(Q) - 1]\sin(Qr)\,\mathrm{d}Q$$

where $\rho(r)$ is the atomic number density function and indicates the probability of finding an atom at a distance r from another atom while ρ_0 is the average atom number density. The $G(r)$ function measures deviations from the average atomic density.

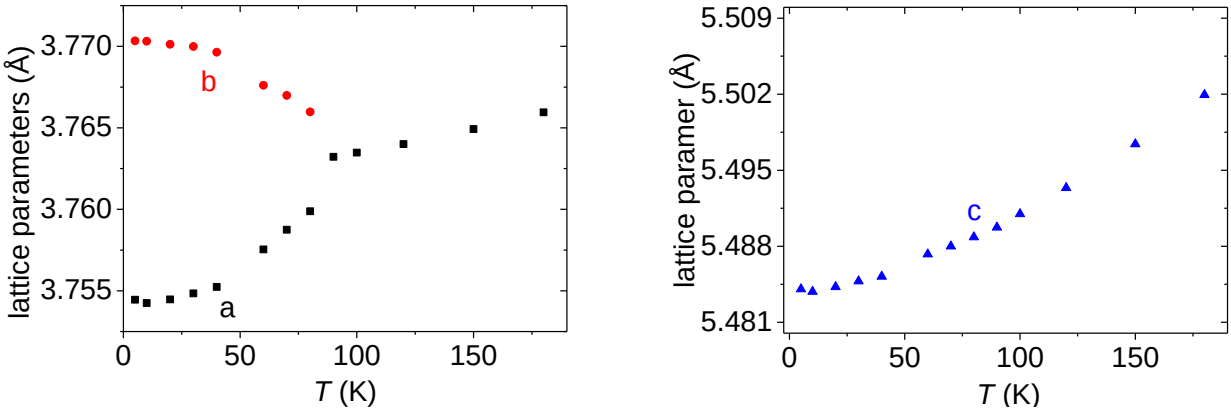

Fig. 1 The temperature dependence of the lattice parameters of FeSe displaying a tetragonal to orthorhombic distortion at $T_s \approx 87$ K

At temperatures encompassing the nematic transition, we did not observe a significant change in $G(r)$. This implies that the changes in the atomic distances at the structural transition are rather small. The analysis of G(r) functions in this temperature range is still in progress. However, when the temperature was lowered to below 30 K, some of the peaks at low r values began to broaden, with a strong effect visible in the case of the Fe-Fe distance at $r \approx 2.69$ Å, marked by the red arrow in Fig.2. The results suggest that the local symmetry is lower than that of the *Cmma* space group below 30 K [4]. This is the temperature at which also a pseudogap-like behaviour has been reported [1,2]. Whether the pseudogap is originating from the pre-formed Cooper pairs, or is due to a competing order such as a charge or spin density wave (CDW or SDW) is an open question. Since pressure strongly affects the transition to the superconducting state, a similar PDF experiment under pressure would help to distinguish among different scenarios and a goal of our future proposal at ESRF.

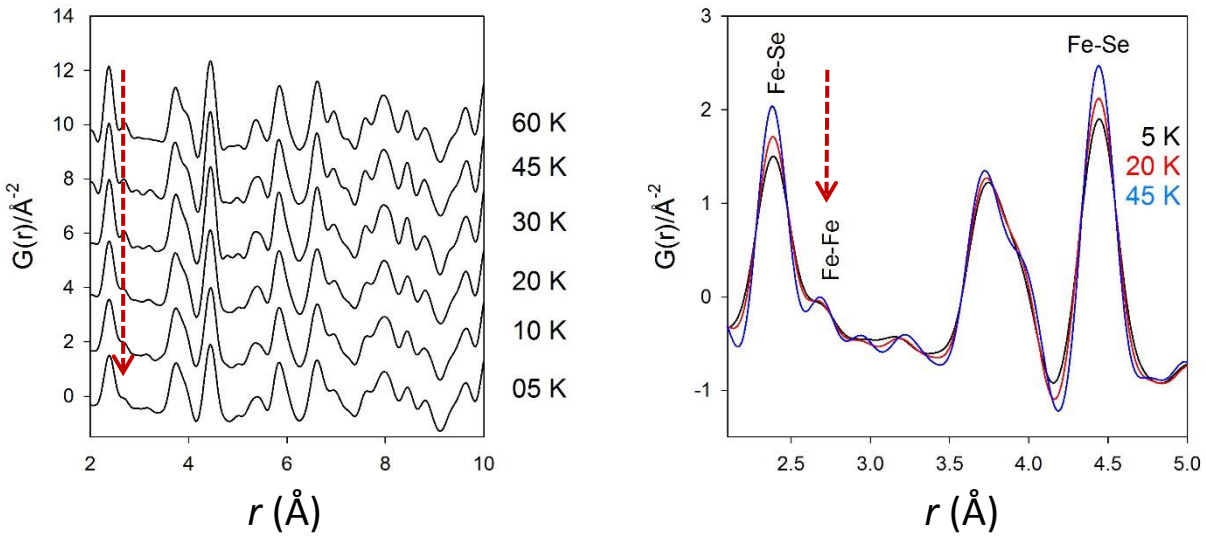

Fig. 2. Left panel: low r range of all the $G(r)$ collected in the cryostat. Right panel: details of selected $G(r)$ functions indicating a broadening of the peak correponding to the Fe-Fe distance.

References

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