ESRF	**Experiment title:** The nature of nematicity in superconducting FeSe from diffraction studies	**Experiment number**: HC-1879
Beamline: BM01A	**Date of experiment**: from: 23 Apr 2015 to: 27 Apr 2015	**Date of report**: 26 Feb 2018
Shifts: 12	**Local contact(s)**: P. Pattison	*Received at ESRF:*

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Experiment:

High quality single crystals of FeSe were selected for diffraction studies as a function of temperature in a 10 – 300 K range. Full 3D reciprocal spheres were reconstructed in fine details. Experimental intensities were integrated and all the corresponding structural models were successfully refined (atomic coordinates, isotropic and anisotropic displacement parameters etc.)

Results

Objectives of the experiment were successfully fulfilled. The nematic transition was observed at 100 K (Fig. 1), in according to the literature data. In addition, anomaly prior to the nematic state was observed around 120 K (Fig. 1, black arrow). This anomaly was found to be correlated with the behaviour of the Fe-Se distances which exhibit change in the slope at this temperature (not shown in the report).

Nematic transition below 100 K was found to be correlated with a change in the domain structure. Upon cooling, single crystals of FeSe exhibit uniform domain spread which is the most pronounced at the base superconducting temperatures (not shown in the report). This feature certainly influences the superconducting properties of this material. Upon temperature increase the FeSe recovers its original domain microstructure.

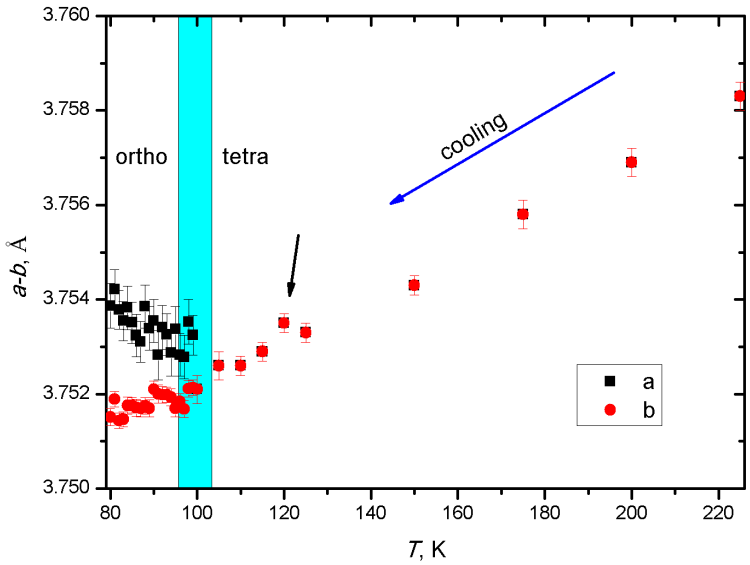

Figure 1. Behaviour of the FeSe cell parameters as a function of temperature featuring an anomaly at 120 K and a following nematic transition at 100 K

Summary

The obtained results shed light on the origin of the nematicity in FeSe, i.e. it is also related to the domain spread observed upon cooling. Moreover, the persisting domain spread at base superconducting temperatures indicates the existence of possible correlation between microstructure and superconducting properties of FeSe. These correlations are to be discovered with a help of ab initio calculations. The anomaly at 120 K is related to the FeSe bonding interactions.