



	<b>Experiment title:</b> Crystal structure study of superconducting $X_yFe_{2-x}Se_2$	<b>Experiment number:</b> 01-02-965
<b>Beamline:</b> BM01A	<b>Date of experiment:</b> from: 2/10/2011 to: 4/10/2011	<b>Date of report:</b> 27/02/2012
<b>Shifts:</b> 9	<b>Local contact(s):</b> D. Chernyshov	<i>Received at ESRF:</i>
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## Report:

### *Experiment*

Single crystals of  $X_yFe_{2-x}Se_2$  ( $X = K, Rb, Cs$ ) were investigated at BM01A station of Swiss-Norwegian Beam Lines at ESRF using MAR345 detector with a 0.7 Å wavelength. Fe-vacancy order-disorder transitions with temperature were studied. Full detailed reciprocal space 3D map with diffuse scattering was obtained for  $Cs_{0.8}Fe_{1.6}Fe_2$  at room temperature.

## Results and discussion

For  $\text{Cs}_{0.8}\text{Fe}_{1.6}\text{Se}_2$  in addition to the expected pattern for the tetragonal phase with ordered Fe vacancies [1], a diffuse scattering from Cs occupational disorder has been observed, together with an extra Bragg contribution from a minor phase (Figure 1) [2]. The minor phase, in agreement with previous findings, is compressed in the tetragonal  $a$ - $b$  plane and expanded along the  $c$ -direction; a set of modulated Bragg rods evidences a planar disorder (Figure 1, c). Fourfold splitting of the rods as well as the main Bragg peaks for  $L \neq 0$  imply that symmetry of the minor phase is not higher than *monoclinic*. The monoclinic distortion was estimated to be 90.7 degrees. Structured diffuse scattering, observed on top of the Bragg component, relates to the major phase and is attributed to a correlated distribution of Cs ions, as follows from observed weakening of the X-ray diffuse signal in the series  $A=\text{Cs}, \text{Rb}, \text{K}$ .

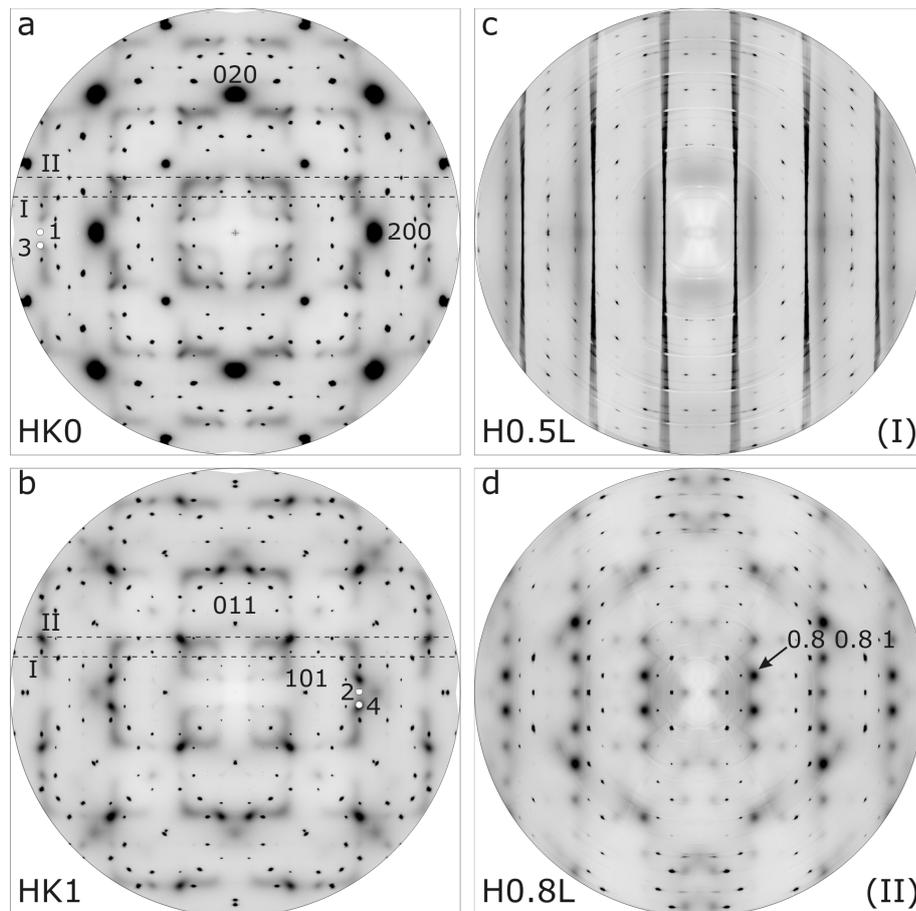


Fig. 1. Reciprocal space cuts for  $\text{Cs}_{0.8}\text{Fe}_{1.6}\text{Se}_2$ : (a) HK0; (b) HK1; (c) H0.5L; (d) H0.8L.

We suggest that the observed 3D diffuse signal contrasts a perturbation of inter-atomic interactions at a certain set of q-vectors corresponding to effective nesting of the Fermi surface. Detailed analysis of the observed diffuse features together with other probes of Fermi surface and *ab initio* calculations should help to reveal more details about the electronic structure of novel  $A_x\text{Fe}_{2-y}\text{Se}_2$  superconductors.

### ***References***

1. V. Yu. Pomjakushin, D. V. Sheptyakov, E. V. Pomjakushina, A. Krzton-Maziopa, K. Conder, D. Chernyshov, V. Svitlyk, and Z. Shermadini. *Phys. Rev. B* **83**, 144410 (2011)
2. A. Bosak, V. Svitlyk, A. Krzton-Maziopa, E. Pomjakushina, K. Conder, V. Pomjakushin, A. Popov, D. de Sanctis, D. Chernyshov. *arXiv:1112.2569* 2012.