ESRF	**Experiment title:** Temperature-dependent behavior of Bragg and diffuse scattering of phase-separated $Cs_{0.8}Fe_{1.6}Se_2$ superconductor	**Experiment number**: **01-02-1003**
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Report:

Experiment

Single crystals of $Cs_{0.8}Fe_{1.6}Se_2$ were studied in details at the SNBL BM01A at ESRF using PILATUS 2M detector with a 0.6997 Å wavelength. At least three phases were experimentally observed as a function of temperature. Third phase with the satellites appeares at least at the T = 500 K. The satellites were found to be quenched at the room temperature.

Results and discussion

A family of the $A_xFe_{2-y}Se_2$ (A – alkali metals) phases, even in a state commonly reffered to as a monocrystalline, consist of at least two phases [1- 3]. In the $Cs_{0.8}Fe_{1.6}Se_2$ sample the main phase crystallizes in a *I*4*/m* symmetry with a partially ordered Fe vacancies [4]. The second phase is compressed in the tetragonal *a-b* plane and expanded along the *c* direction [1]. A set of modulated Bragg rods indicates a planar disorder [1]. From the previouse powder synchrotron radiation diffraction experiments we have observed a merging of the main and secondary phases in the $Rb_yFe_{2-x}Se_2$ sample [2].

From the recently obtained high resolution single crystal synchrotron radiation diffraction data we have observed that the second phase (Fig.1) is trasformed into the third phase with longer *a-b* unit cell parameters upon heating. A set of satellites can be observed as well. The transition takes place at the temperature of at least 500 K (Fig. 2) and is kinetically inhibited. Upon annealing at the 500 K the amount of the third phase increases and the second phase dissapears completely. Upon cooling down to the room temperature the second phase reemerges but the sattelites are quenched. (Fig. 3).

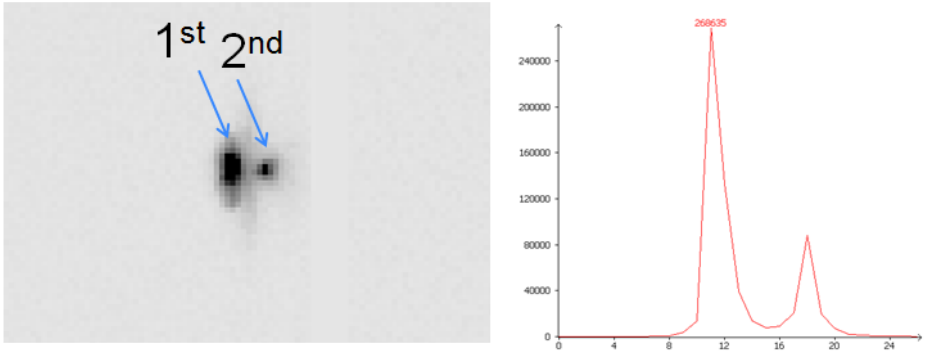

Fig. 1. First and the second phase in $Cs_{0.8}Fe_{1.6}Se_2$ at 300 K

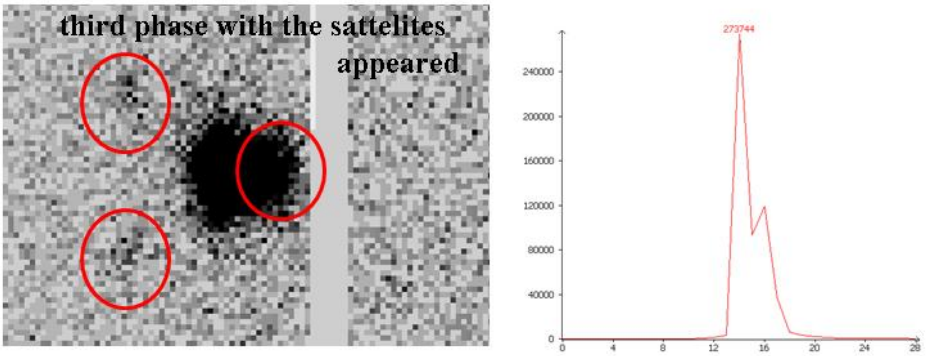

Fig. 2. Appearance of the third phase in $Cs_{0.8}Fe_{1.6}Se_2$ at 500 K

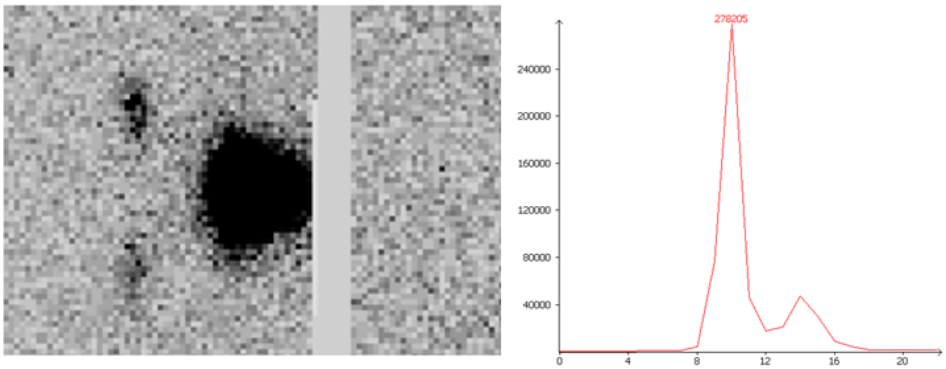

Fig. 3. Quenching of the satellites in $Cs_{0.8}Fe_{1.6}Se_2$ at 300 K

Summary

At least three phases were observed in the $Cs_{0.8}Fe_{1.6}Se_2$ sample as a function of temperature. The second phase is transformed into the third phase with longer *a-b* unit cell parameters at the temperature of the least 500 K. Since the $Cs_{0.8}Fe_{1.6}Se_2$ sample is superconductive before and after annealing at 500 K, the main phase is likely to be responsible for the observed superconductivity since it is remained unaltered.

References

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