Crystal structure of the new superconductor FeSe$_{1-x}$S$_x$

Kirill V. Frolov$^1$, Anna G. Ivanova$^1$, Dmitry Yu. Chemishov$^2$, Iurii Dovgaliuk$^2$, Dmitry A. Chareev$^3$, Ivan A. Troyan$^1$

$^1$FSRC Crystallography And Photonics RAS, Moscow, Russian Federation, $^2$Swiss-Norwegian Beamlines at the ESRF, Grenoble, France, $^3$Institute of Experimental Mineralogy RAS, Chernogolovka, Moscow Region, Russian Federation

E-mail: green@crys.ras.ru

The discovery of superconductivity in iron-based pnictides and chalcogenides has been at the forefront of interest over the last few years [1,2]. Fe(Se,Te,S) compounds considered as the simplest Fe-based superconductors useful for study correlations between structural, electron, magnetic and superconducting properties. Among these materials FeSe$_{1-x}$S$_x$ is the least studied compound and single crystal X-ray diffraction (XRD) experiments for it was not conducted. FeSe$_{1-x}$S$_x$ ($x = 0 - 0.2$) single crystals were grown in evacuated quartz ampoules using the AlCl$_3$/KCl flux technique [3] in a temperature gradient (from 400°C to $\sim$50°C) for 45 days. Crystals have a platelike shape with the c axis oriented perpendicular to the crystal plane. Two samples with $x = 0.03$ and 0.09 were selected for single crystal synchrotron XRD measurements. Both of them were superconducting with $T_c = 9.5$ and 10.1 K respectively. The XRD data were collected in 90 – 300 K temperature range at the ESRF beamline BM01 using PILATUS@SNBL diffractometer ($\lambda = 0.7458\AA$, PILATUS2M detector) equipped with Oxford Cryojet cryogenic nitrogen jet system.

Complete single crystal XRD measurements were performed for good quality FeSe$_{0.91}$S$_{0.09}$ sample at the room temperature. Crystal structure of FeSe$_{0.91}$S$_{0.09}$ was refined in sp.gr. P4/n ($a=3.809(1)$, $c=5.529(1)$, $R=3.5\%$). It was found that atoms of S and Se statistically occupy 2c position of the structure. Percentage ratio S/Se was defined in the result of the site occupancies refinement. Test XRD room temperature experement for FeSe$_{0.97}$S$_{0.03}$ crystal showed that sample was polycrystalline. Polycrystalline low temperature XRD measurements were performed in temperature interval 90-300 K. Some additional peaks not corresponding to sp.gr. P4/n were revealed at temperatures below 170 K.

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