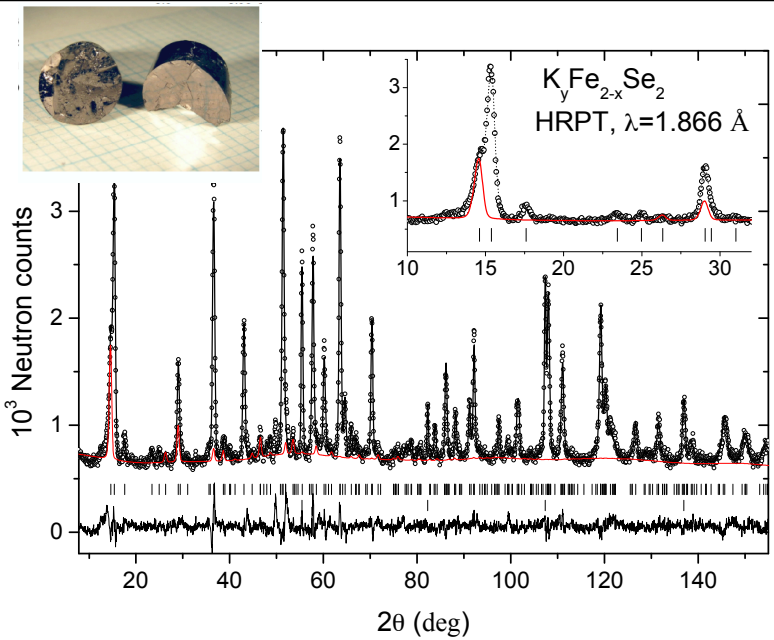
Iron vacancy superstructure and antiferromagnetic order in superconducting $X_yFe_{2-x}Se_2$ (X=K, Cs, Rb)

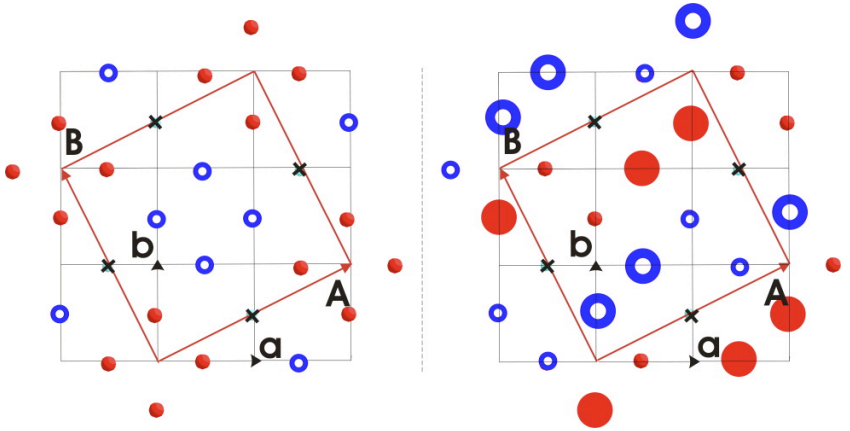
Vladimir Pomjakushin, Denis Sheptyakov, Ekaterina Pomjakushina, Anna Krzton-Maziopa, Kazimierz Conder, Dmitry Chernyshov, Volodymir Svitlyk and Zurab Shermadini

LNS, LDM, SmuS, PSI and Swiss-Norwegian Beam Lines at ESRF

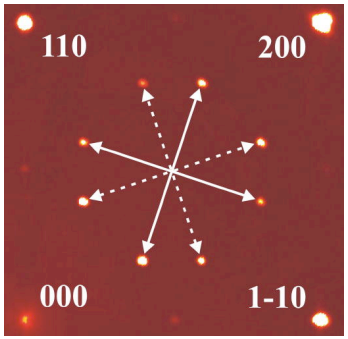
A unique feature of the new alkali-metal intercalated iron selenides $X_yFe_{2-x}Se_2$ (X = K, Cs, Rb) discovered towards the end of 2010 is the presence of robust antiferromagnetism with an extraordinary high Néel temperature above 500 K, and high-temperature superconductivity with a critical temperature at around 30 K. Another interesting specific feature of this new class of magnetic superconductors is the presence of an iron vacancy superstructure. Concomitantly with the vacancy ordering, the ordering of the rest of the iron atom spins have the same propagation wave vector at almost the same temperature with the iron magnetic moment ranging from 2.1 to 2.6 μ_B at 300K. The presence of such strong magnetism may come as a surprise to superconductivity experts and increases the demand for new ideas to rationalize this phenomenon.



The Rietveld refinement pattern and difference plot of the neutron diffraction data. The magnetic contribution together with the background is shown by a red line.



Two best-fit symmetry adapted magnetic configurations in a projection of one layer of Fe on the *ab*-plane. Iron vacancy positions are shown by crosses. Open blue and filled red circles show Fe down and up spins. Large red unit cell (**A,B**) corresponds to the supercell with vacancy ordered structure.



The satellite reflections are indicated by arrows for **k**1 = [2/5 ,1/5 ,1] and **k**2 = [1/5 ,2/5 ,1] by solid and dashed lines These two *k* vectors correspond to two twin domains.

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