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Superstructures in Iron-Based Superconductors

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This presentation will look at the various superstructures in iron-selenide superconductors and we will discuss the importance of understanding long range superstructures in functional materials.

The alkaline iron selenides $A_xFe_{2-y}Se_2$ (A = K, Rb, Cs) have attracted much interest recently due to the observation of superconductivity with T_c~30K in conjunction with antiferromagnetism with an unusually high ordering temperature T_N of up to 559K and large ordered moment of about $3.3\mu_B$ per Fe. This observation suggests the possibility of coexistence between these two orthogonal phenomena, superconductivity and magnetic ordering. Other iron pnictide superconductors have phase diagrams that indicate coexistence of magnetism and superconductivity in certain regions, however the highest T_c's and bulk superconductivity are only found when the magnetic state has been suppressed. The basic principles of superconductivity indicate that magnetic fields cannot permeate a superconducting region.

Single crystal neutron diffraction is combined with synchrotron x-ray scattering to identify the different superlattice phases present in $Cs_{0.8}Fe_{1.6}Se_2$. A combination of single crystal refinements and first principles modelling are used to provide structural solutions for the $\sqrt{5} \times \sqrt{5}$ and $\sqrt{2} \times \sqrt{2}$ superlattice phases. The $\sqrt{5} \times \sqrt{5}$ superlattice structure is predominantly composed of ordered Fe vacancies and Fe distortions, whereas the $\sqrt{2} \times \sqrt{2}$ superlattice is composed of ordered Cs vacancies. The Cs vacancies only order within the plane, causing Bragg rods in reciprocal space. By mapping x-ray diffraction measurements with narrow spatial resolution over the surface of the sample, the structural domain pattern was determined, consistent with the notion of a majority antiferromagnetic $\sqrt{5} \times \sqrt{5}$ phase and a superconducting $\sqrt{2} \times \sqrt{2}$ phase.

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