Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Thermal evolution of antiferromagnetic correlations and tetrahedral bond angles in superconducting $FeTe_{1-x}Se_x$

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— We will present neutron scattering measurements of low energy magnetic excitations from superconducting $FeTe_{1-x}Se_x$ samples. A model with short-range correlated spin plaquettes characterized by particular antiferromagnetic wave vectors is used to describe the measured magnetic scattering data in the (HK0) plane. We show that the characteristic antiferromagnetic wave vector evolves from that characteristic of the bicollinear structure characteristic of $FeTe_{1-x}Se_x$ (at high temperature) to that associated with the stripe structure of antiferromagnetic iron arsenides (at low temperature). We also present powder neutron diffraction results for lattice parameters in $FeTe_{1-x}Se_x$ indicating that the tetrahedral bond angle tends to increase towards the ideal value on cooling, with a corresponding reduction in crystal-field splitting of the Fe 3d orbitals. We suggest that the thermal change in spin correlations implies a relative change among the exchange couplings, and that this is associated with changes in orbital occupancies. Finally, while the magnitude of the low energy magnetic spectral weight is substantial at all temperatures, it actually weakens somewhat at low temperature, where the charge carriers become more itinerant.

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Date submitted: 06 Nov 2015 Electronic form version 1.4