Neutron scattering study of correlated phase behavior in Sr_2IrO_4

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Recently there has been a surge of interest in the study of iridium oxide based materials which are members of Ruddelsden-Popper series $Sr_{2n+1}Ir_nO_{3n+1}$. The competition between spin orbit interaction and electron-electron correlation changing the conventional energy hierarchy in these materials holds the promise of potentially stabilizing exotic electronic ground states [1-3]. In particular, Sr_2IrO_4 (n = 1) and $Sr_3Ir_2O_7$ (n = 2) have rather unusual antiferromagnetically (AF) ordered insulating electronic ground states despite the presence of their extended 5d Ir^{4+} ions. Currently, there are two competing proposals to explain the resulting insulating ground state: (a) A cooperative interplay of spin-orbit induced bandwidth narrowing and on-site Coulomb interactions which generates the necessary J_{eff} = 1/2 Mott insulating ground state, and (b) the stabilization of a weakly-correlated band insulator in which the formation of magnetic order continuously builds the bandgap and where the effects of electron-electron correlations are secondary [3]. It is also proposed that with increase in dimensionality n, the system changes continuously into the metallic regime where the energy gap of $Sr_3Ir_2O_7$ (n = 2) is substantially smaller than that of Sr_2IrO_4 (n = 1); consistent with the idea of dimensionality driven insulator metal transition. However, the low temperature phase behavior of these systems remains quite complex and poorly understood [1]. A direct comparison of correlated magnetism and structural phase behavior in these two materials is one way of looking at their respective correlation strengths.

In our recent experiments on the C5 triple axis spectrometer, we performed a diffraction study of the correlated phase behavior within a single crystal of Sr_2IrO_4. Within this experiment, we are able to generate a direct comparison of ordered AF moment in Sr_2IrO_4 with that of $Sr_3Ir_2O_7$ which was measured at C5 previously [1]. Our study demonstrates that both materials exhibit magnetic domains originating from crystallographic twinning as well as comparable moment sizes contrary to theoretical predictions. Weakly temperature-dependent superlattice peaks violating the tetragonal space group of Sr_2IrO_4 were also observed supporting the notion of a lower structural symmetry and a high temperature lattice distortion in this material. Our results demonstrate that the correlated spin order and structural phase behaviors in both single and bilayer $Sr_{n+1}Ir_nO_{3n+1}$ system are remarkably similar and suggest comparable correlation strengths in each system. Fig. 1(a) shows the radially integrated intensities of the (1, 0, L) magnetic peaks originating from crystallographic twinning. Fig.1 (b) shows the comparison of magnetic order parameters for Sr_2IrO_4 and $Sr_3Ir_2O_7$. Both order parameters track each other and follow simple power law $M^2 = (1 - T/T_N)^{2\beta}$ with the same exponent. Fig. 2(c) shows the in-plane projection of model of canted antiferromagnetic order used to calculate correlated moment in Sr_2IrO_4 [4].

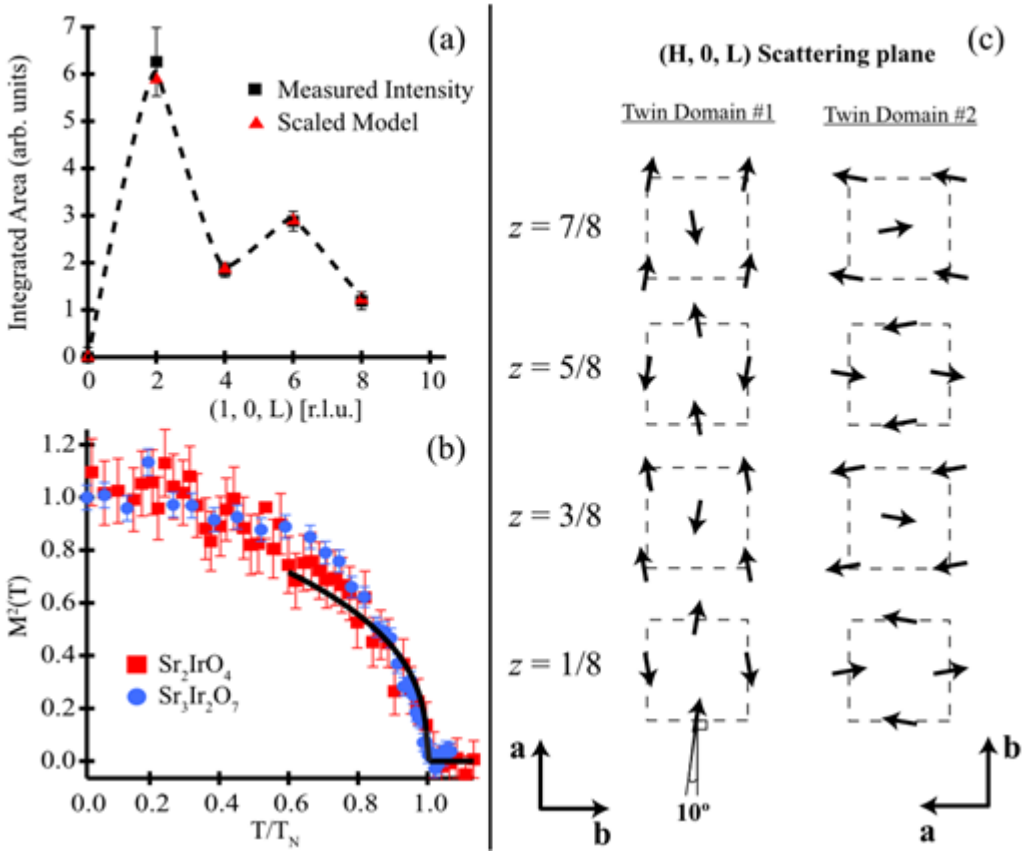

Fig.1: (a) Radially integrated intensities (black squares) of magnetic Bragg peaks are plotted as function of (1,0,L). Expected intensities from the two domain magnetic model discussed in the text are overplotted as red triangles. (b) Magnetic order parameters squared plotted as a function of reduced temperature for Sr-214 (square symbols) and Sr-327 (circle symbols). (c) In-plane projections of the model of canted AF order utilized in the calculation for Sr-214 moment. Relative c-axis locations of each plane within the unit cell are denoted to the left of each corresponding plane. The correlated moment was found to be **m** = 0.36 ± 0.06 μ_B/Ir which is close to that for $Sr_3Ir_2O_7$ (0.35 ± 0.06 μ_B/Ir).

References:

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