Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Local structural aspects of metal-metal transition in $IrTe_2$ from x-ray PDF[1] RUNZE YU, MILINDA ABEYKOON, Brookhaven National Laboratory, Upton, NY 11973, USA, HAIDONG ZHOU, University of Tennessee,Knoxville, TN 37996, USA, WEIGUO YIN, EMIL S. BOZIN[2], Brookhaven National Laboratory, Upton, NY 11973, USA — Evolution of local atomic structure across the metal-metal transition in $IrTe_2$ is explored by pair distribution function (PDF) analysis of x-ray total scattering data over 80 K <T <300 K range. Local and average structures are found to be in accord at all temperatures conforming to P-1 and P-3m1 symmetry at low and high temperature, respectively. We find no evidence of short-range Ir-dimers surviving into the high-T regime, in stark contrast to the earlier EXAFS study proposing Ir-dimer order-disorder mechanism. Phase fraction obtained from explicit 2-phase structural modeling displays hysteretic behavior across the transition, in agreement with electronic transport measurements, indicative of a strong tie between the lattice and electronic configurations. Bond valence methodology applied to structural parameters further indicates significant bond charge disproportionation in association with the transition.

[1]Work at Brookhaven National Laboratory was supported by US DOE, Office of Science, Office of Basic Energy Sciences (DOE-BES) under Contract No. DE-SC0012704.
[2]Experimental; Oral;11.1.2: Emergent Properties of Bulk Complex Oxides

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Date submitted: 07 Nov 2016 Electronic form version 1.4