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, HAI DDONG 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.

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