Combined Atomic Pair Distribution Function and EXAFS Analysis Of Local Structural Study Of $MoTe_2$

Sumit Khadka[1], Byron Freelon[2], Leighhane Gallington[3], Yu-Cheng Shao[4], Milinda Abeykoon[5]

[1]Texas Center for Superconductivity, [2]University of Houston, Houston, [3]Advanced Photon Source (X-ray Science Division),

[4]National Synchrotron Radiation Research Center, Hsinchu Science Park,

[5]Brookhaven National Laboratory

skhadka3@uh.edu

At temperatures below 250K, standard scattering methods have revealed that 1T' $MoTe_2$ experiences a first-order structural phase transition (SPT) to a non-centrosymmetric orthorhombic T_d phase, resulting in the emergence of Weyl points protected by the broken inversion symmetry. However, because these two distinct phases have very similar structures and a low energy barrier between them, various distortions occur on both macroscopic and atomic scales. In this study, we use scattering techniques that are better suited for examining atomic or local structures to investigate the local structure of 1T' $MoTe_2$ over a range of temperatures from 95K to room temperature. We found that as the temperature decreases, the interlayer atomic distances change significantly, while the intralayer distances remain the same. We further analyzed this phenomenon using both small and large box models and showed that stacking faults and layer rotations have an impact on the interlayer atomic distances, which is consistent with the experimental results. Understanding the interlayer behavior of $MoTe_2$ through local structure analysis can help to answer some of the outstanding questions about the SPT on $MoTe_2$ and its effect on the emergence of Weyl points at low temperatures.