

Two dimensional ordering phase brought on by the destabilization of the VO₂ rutile structure in V_{0.81}Mo_{0.19}O₂

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VO₂ has a known temperature driven, structural phase transition from a tetragonal (R) phase to a monoclinic (M1) phase at which the material also undergoes a metal-to-insulator transition (MIT). Additionally, chemical doping into the VO₂ structure is known to change the temperature of this transition as well as introducing new structural phases. Molybdenum doping has been shown to depress the temperature of this structural transition until the low temperature M1 phase disappears at some critical molybdenum concentration with no previously known additional phases present in this region of dopant composition.

We will present total x-ray scattering data obtained from beamline 6-ID-D at the APS on single crystal samples of V_{0.81}Mo_{0.19}O₂. Results from these experiments show the existence of a first order phase transition from the tetragonal (R) phase to a previously unknown two-dimensional, long range ordering phase at this critical molybdenum concentration. Additionally, we will present 3D- Δ PDF data on this 2D ordered phase and a yell model of the atomic correlations that contribute to this structural change. Modeling of this data shows a preference towards the geometric frustration contribution, giving new insights into its importance for modeling the MIT in VO₂.