Abstract Submitted
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**X-ray and neutron scattering studies of microstructure and dynamics in $VO_2$**[1] JOHN BUDAI, JIAWANG HONG, MICHAEL MANLEY, OLIVIER DELAIRE, ELIOT SPECHT, CHEN LI, Oak Ridge National Lab, JON TISCHLER, AYMAN SAID, Argonne National Lab, DOUGLAS ABERNATHY, Oak Ridge National Lab, BOGDAN LEU, Argonne National Lab, ALEXANDER TSELEV, LYNN BOATNER, ROBERT MCQUEENEY, Oak Ridge National Lab — Vanadium dioxide is a strongly correlated material that exhibits a well-studied, but poorly understood, metal-insulator transition coupled with a tetragonal-monoclinic structural phase transition near 340 K. We have combined synchrotron x-ray and spallation neutron scattering measurements to investigate microstructure and lattice dynamics in $VO_2$. Submicron-resolution x-ray microdiffraction studies reveal local phase coexistence driven by strain effects within individual single-microcrystals. Macroscopic diffuse scattering and inelastic x-ray and neutron scattering measurements reveal unusual features in the rutile phonon dispersions at particular locations in reciprocal space, including temperature-dependent dispersions near the R-point. Comparisons of measurements with ab initio molecular dynamics calculations indicate that anharmonicity plays a central role in determining the lattice vibrations and hence physical properties in this system.

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