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Neutron and x-ray scattering studies of the lattice dynamics in VO2 OLIVIER DELAIRE, JOHN D. BUDAI, JIAWANG HONG, MICHAEL MANLEY, CHEN LI, ELIOT SPECHT, Oak Ridge National Laboratory, AYMAN SAID, BOGDAN LEU, JON TISCHLER, Argonne National Laboratory, DOUGLAS ABERNATHY, LYNN BOATNER, ROBERT MCQUEENEY, Oak Ridge National Laboratory, ORNL-ANL COLLABORATION — Vanadium dioxide exhibits a metal-insulator transition at 340K, concomitant with a structural distortion from rutile to monoclinic on cooling. While much attention has been given to purely electronic aspects of the transition and the band-gap opening, less information has been available about the lattice dynamics (phonons), and their role in the thermodynamics of this important phase transition. We report detailed x-ray and neutron scattering measurements of the phonon dispersions and density of states in VO2, and their influence on the thermodynamics [1]. We show that the entropy of the transition is dominated by the large phonon entropy of the rutile phase, which stabilizes it at high temperature. This phonon entropy arises from soft, strongly-anharmonic phonons across much of the Brillouin zone. The origin of this softness and strong anharmonicity are discussed. [1] J. D. Budai*, J. Hong*, M. E. Manley, E. D. Specht, C. W. Li, J. Z. Tischler, D. L. Abernathy, A. H. Said, B. M. Leu, L. A. Boatner, R. J. McQueeney, and O. Delaire, Nature 2014, DOI:10.1038/nature13865 Support by DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division; APS and SNS facilities supported by DOE-BES.

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