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First-principles calculations of phonons in VO_2[1] ERIC J. WALTER, HENRY KRAKAUER, TYLER HUFFMAN, M.M. QAZILBASH, College of William and Mary — Vanadium dioxide (VO_2) undergoes a metal-insulator transition at 340K. This is accompanied by a structural transition from a metallic, high-temperature rutile phase to a low-temperature monoclinic insulating phase. Recently, it has become possible to produce single crystal platelets of VO_2 deposited on a oxidized silicon substrate. These micro-crystals are under strain which can potentially alter their properties compared to bulk samples. Infrared micro-spectroscopy on these samples permits accurate measurements of their electronic and phonon properties as the mircro-crystals are driven reversibly across the temperature-driven insulator-to-metal transition (IMT). We present *ab-initio* calculations of phonons in the rutile and monoclinic phases of VO_2. These calculations were performed using first-principles density functional theory using both LDA and LDA+U. The effect of the Hubbard parameters and strain on both phases is discussed. We compare our results to the single crystal measurements and previous experimental results.

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