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Infrared absorption studies of OH centers in the metal-insulator-transition oxide VO2 YING QIN, WEIKAI YIN, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University, LYNN BOATNER, Oak Ridge National Laboratory — VO_2 is an unusual solid-state material that undergoes a metal insulator transition at approximately 68 °C that accompanies a structural transition from monoclinic to rutile. The introduction of hydrogen into VO2 has been found to suppress the monoclinic insulating phase, providing a means to tune the metal-insulator-transition temperature. Single crystals of VO2 have been grown recently at the Oak Ridge National Laboratory. We have introduced hydrogen and deuterium into VO_2 single crystals for study by low temperature IR spectroscopy. OH and OD vibrational lines (4.2K) have been found at 3289 and 2446 cm^{-1} that provide information about the structure of the OH (and OD) center in VO_2. The vibrational frequencies are similar to those found for OH and OD modes in other oxides with the rutile structure, for example SnO_2 and TiO_2. The frequency ratio, r $= \omega H/\omega D$, is r = 1.345, consistent with H (and D) being bonded to a light element like oxygen. Furthermore, our experiments determine the polarization of the OH vibrational mode and the thermal stability of H centers in VO_2. Supported by NSF Grant DMR-1160756.

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