Raman scattering in VO_2

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VO_2 shows a metal insulator transition at 340 K, which is connected with a structural phase transition from the tetragonal rutile structure to a distorted monoclinic rutile structure. Despite intense experimental and theoretical investigations on the mechanism of the metal insulator transition of VO_2 the nature of this transition is not clear until now. Proposed mechanisms for the phase transition are e.g. a Mott-Hubbard transition or a Peierls transition. Although there has been a number of experimental investigations of the lattice vibrations of VO_2 the position and the nature of the modes at the Γ-point are not clear until now. Therefore, we studied the lattice vibrations of VO_2 with Raman spectroscopy again to get more information about the lattice part of the phase transition.
From the 18 Raman allowed modes in the low temperature phase we were able to observe 17. In accordance with former investigations we observed a softening of the lowest Raman active mode. A shell model calculation has been performed, which reproduces quite well the observed Raman modes at the Γ-point. We discuss the nature of the soft mode within the shell model and it's role in the phase transition and compare the results of the shell model in the metallic phase with the observed structures in the Raman spectra of the high temperature phase.