

Abstract Submitted
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Localized Vibrational Modes of O_{Te} and $(O_{Te} - V_{Cd})$ Centers in CdTe: Fundamentals and Second Harmonics* GANG CHEN, Purdue Uni., I. MIOTKOWSKI, S. RODRIGUEZ, A. K. RAMDAS — In CdTe, grown with excess Cd vacancies (V_{Cd}), oxygen replacing Te (O_{Te}) displays a pair of fundamental localized vibrational modes (LVMs), $\nu_1 = 1096.78 \text{ cm}^{-1}$ and $\nu_2 = 1108.35 \text{ cm}^{-1}$. They are ascribed to the non-degenerate Γ_1 (ν_1) and the doubly degenerate Γ_3 (ν_2) LVMs of $(O_{Te} - V_{Cd})$ centers with nearest neighbor Cd missing, having C_{3v} symmetry and \hat{c} axis along $\langle 111 \rangle$. In CdTe grown with conditions suppressing V_{Cd} , O_{Te} occurs with all the four Cd nearest neighbors, and exhibits a triply degenerate Γ_5 LVM at $\nu_0 = 349.79 \text{ cm}^{-1}$ of T_d symmetry.[1] The harmonics of $(O_{Te} - V_{Cd})$, i.e., of ν_1 and ν_2 occur at $\nu_4 = 2198.66 \text{ cm}^{-1}$ and $\nu_5 = 2210.5 \text{ cm}^{-1}$. The temperature dependence of both (ν_1, ν_2) and (ν_4, ν_5) pairs display a remarkable behavior: ν_1 and ν_2 approach each other and coalesce at $T^* \sim 300 \text{ K}$, as do ν_4 and ν_5 ; beyond T^* they behave as a triply degenerate ν_0^* and ν_s^* , respectively. The relative intensity of $\nu_2 : \nu_1$ approaches 2 as $T \rightarrow T^*$ while that of $\nu_5 : \nu_4$ approaches 1/2. These features find a convincing explanation on the basis of the dynamic switching of the $(O_{Te} - V_{Cd})$ dangling bond among the four $\langle 111 \rangle$ axes and, for $T \geq T^*$, these centers “acquire” T_d symmetry. With its T_d symmetry, O_{Te} displays a single second harmonic ν_s at 695.72 cm^{-1} . [1] Chen *et al.*, Phys. Rev. Lett., **96**, 035508 (2006).
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