## Abstract Submitted for the MAR07 Meeting of The American Physical Society

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  $\Gamma_1$  ( $\nu_1$ ) and the doubly degenerate  $\Gamma_3$  $(\nu_2)$  LVMs of  $(O_{Te} - V_{Cd})$  centers with nearest neighbor Cd missing, having  $C_{3\nu}$ symmetry and  $\hat{\mathbf{c}}$  axis along (111). In CdTe grown with conditions suppressing V<sub>Cd</sub>, O<sub>Te</sub> occurs with all the four Cd nearest neighbors, and exhibits a triply degenerate  $\Gamma_5$  LVM at  $\nu_0 = 349.79$  cm<sup>-1</sup> of  $T_d$  symmetry.[1] The harmonics of (O<sub>Te</sub> - V<sub>Cd</sub>), i.e., of  $\nu_1$  and  $\nu_2$  occur at  $\nu_4 = 2198.66 \text{ cm}^{-1}$  and  $\nu_5 = 2210.5 \text{ cm}^{-1}$ . The temperature dependence of both  $(\nu_1, \nu_2)$  and  $(\nu_4, \nu_5)$  pairs display a remarkable behavior:  $\nu_1$ and  $\nu_2$  approach each other and coalesce at  $T^* \sim 300$  K, as do  $\nu_4$  and  $\nu_5$ ; beyond  $T^*$  they behave as a triply degenerate  $\nu_0^*$  and  $\nu_s^*$ , respectively. The relative intensity of  $\nu_2$ :  $\nu_1$  approaches 2 as  $T \to T^*$  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<sub>Te</sub> - V<sub>Cd</sub>) dangling bond among the four (111) axes and, for  $T \ge T^*$ , these centers "acquire"  $T_d$  symmetry. With its  $T_d$  symmetry,  $O_{Te}$  displays a single second harmonic  $\nu_s$  at 695.72 cm<sup>-1</sup>. [1] Chen *et al.*, Phys. Rev. Lett., **96**, 035508 (2006). \*Work supported by NSF (DMR 0405082)

> Anant K Ramdas Purdue University

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