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d-CORE TRANSITIONS IN ZnTe AND CdTe

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The strong interest in the II-VI zincblende semiconductors and their mixed compounds for technical applications is well known. We have started a research program on the conduction states of these materials and on the influence of the d states on their valence bands by measuring their reflectivity mainly in the region of excitation of the uppermost d core states of the cation. In this report we present high resolution reflectivity measurements of ZnTe and CdTe single crystals performed between 10 and 20 eV at room temperature on the vacuum ultraviolet beam line of the Italian synchrotron radiation facility PULS at the Frascati National Laboratories run by the Istituto Nazionale di Fisica Nucleare. Fig. 1 shows the reflectivities of ZnTe and CdTe in the region of the d excitations and the suggested assignment of the observed structures.

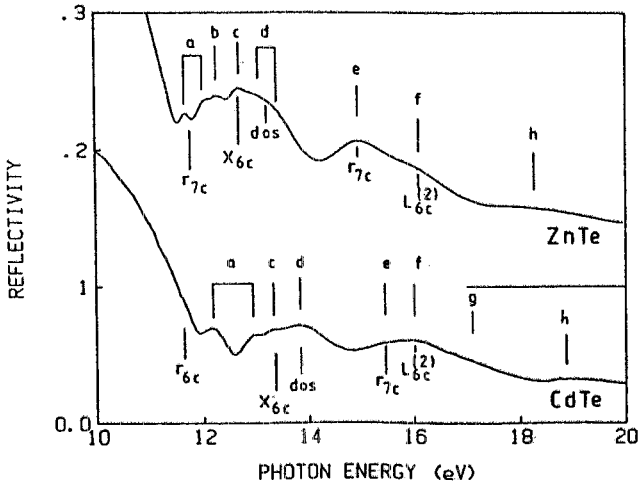

Fig. 1

The threshold for the d transitions (Γ_{7c} in Fig. 1) has been determined by adding the fundamental band gap to the binding energy of the d states with respect to the top of the valence bands. The assignment of the structures present in the d spectra should be based on the cation p-like projected density of states of the conduction bands, i.e. on that portion of the total density of states that is modulated by the transition matrix element between the metal d states and the fraction of the conduction states with p symmetry around the metal atoms. Since a calculation of the projected density of states is not available for these compounds, we assigned the observed structures trying to identify the transitions with a strong matrix element using group-theoretical arguments and from the comparison with other zincblend semiconductors (GaP and GaAs). Finally, in the case of ZnTe and CdTe we suggest that the first strong, sharp d structure near the threshold corresponds to a core exciton bound to a high lying conduction band minimum, possibly at the L or X points of the Brillouin zone.