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THEORETICAL STUDY OF OPTICAL AND XANES SPECTRA FOR CdTe WITHIN THE k -DEPENDENT MATRIX ELEMENT APPROACH

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The reflectivity and X-ray absorption near-edge structure spectra for CdTe were calculated with the inclusion of the transition matrix elements from band structure obtained within self-consistent, relativistic linear muffin tin orbital method. The results were compared with experimental data for the case of CdTe and with our previous calculations.

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The LMTO method which we used in this study of the optical properties and XANES spectra of CdTe is described elsewhere [1] and the details of its application to the calculation of the electronic structure of the zinc-blende-type compounds are presented in other papers [2, 3]. The band structure was calculated with the inclusion of the "combined correction term" in the "frozen core approximation" [4]. LSDA potential was used in the form proposed by Vosko, Wilk and Nusair [5]. The openness of the zinc-blende structure was dealt in standard way by placing additional "empty spheres" into the unit cell. Scalar relativistic corrections were consistently applied in the self-consistent procedure. In the final band-structure calculation the spin-orbit coupling was included as a formal perturbation term in the Hamiltonian [1]. The self-consistent energy eigenvalues and wave functions were used to determine the complex dielectric functions.

The optical absorption is proportional to the imaginary part of the dielectric function $\epsilon_2^b(\hbar\omega)$ given by the following expression [6]:

$$\epsilon_2^b(\hbar\omega) = \frac{\text{const}}{\omega^2} \sum_i \sum_f \int_{\text{BZ}} d^3k |M_{fi}^k|^2 \delta(E_f^k - E_i^k - \hbar\omega),$$

where $M_{fi}^k = \langle f\mathbf{k} | \mathbf{P} | i\mathbf{k} \rangle$ is the dipole matrix element of the momentum operator. The calculations were carried out in a single energy panel using $5s$, $5p$ and $5d$ basis functions for Te and $5s$, $5p$ and $4d$ basis functions for Cd. The finite lifetime was incorporated in the results by convoluting them with a Lorentzian function of a width that depends on the final state energy. We also took into account the experimental resolution in the Gaussian form. In general, our calculations allow for a consistent assignment of structures in the experimental reflectivity spectrum and

for understanding the physical mechanism of the transitions observed in the $R(\omega)$ spectrum. We show (Fig. 1) that interpretation of the UV part of the spectra proposed by Cardona et al. [7] and Kisiel et al. [8] is entirely correct, when all relativistic terms are included in the calculation procedure. In papers [2, 3] we suggested that the structure assigned to core excitons can be described within the framework of a band-to-band transition formalism. However, the structure is removed when the convolution with a Lorentzian function is included.

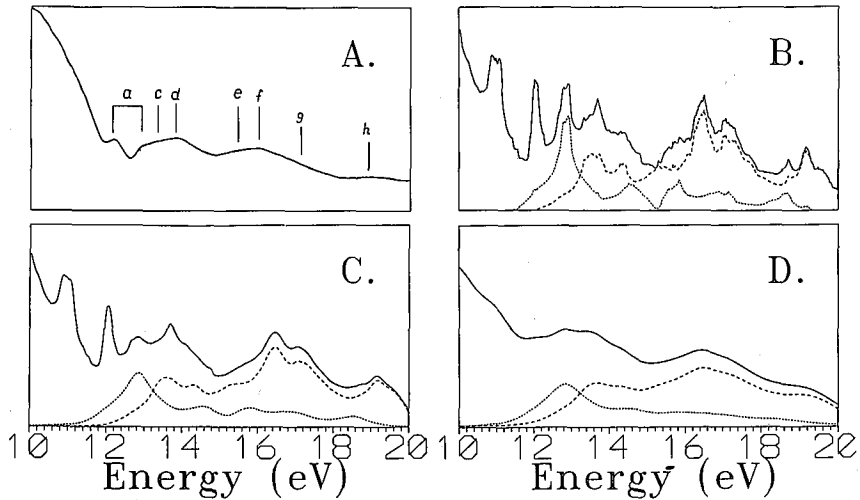


Fig. 1. Reflectivity spectrum of CdTe in the UV energy range: (A) experimental spectrum measured at room temperature in the region of the cation d excitations [8]; (B) theoretical "raw" result: the broken curve (short dashes) represents the contribution of band 1, the broken curve (long length dashes) the contribution of bands 2 to 6, the full curve represents the total absorption spectrum; (C) theoretical "convoluted" result: Γ_L does not depend on the final state energy; (D) theoretical "convoluted" result: Γ_L depends on the final state energy [11].

In the one-electron approximation the X-ray absorption coefficient from a core state $|c\rangle$ with energy E_c to final unoccupied conduction states $|fk\rangle$ with energy E_f^k is given by the expression [6]:

$$\mu_0(\hbar\omega) = \text{const} \sum_f \int_{\text{BZ}} d^3k |M_{fc}^k|^2 \delta(E_f^k - E_c - \hbar\omega),$$

where $M_{fi}^k = \langle fk|P|c\rangle$ is the dipole transition matrix element. The core states were calculated by self-consistent Dirac-Slater method on the basis of modified Liberman program [9]. The final conduction states have finite lifetime, therefore the Müller correction was taken into account [10]. The absorption coefficient was finally convoluted with Gaussian and Lorentzian functions. The value of Lorentzian width Γ_L was optimized to obtain the best agreement of the theoretical spectrum

with the experimental one in the surrounding of the absorption edge (about 8 eV around the edge first inflection point). The calculation was carried out in two energy panels using $6s$, $5p$, $5d$ basis functions for Te and $5s$, $5p$, $5d$ basis functions for Cd.

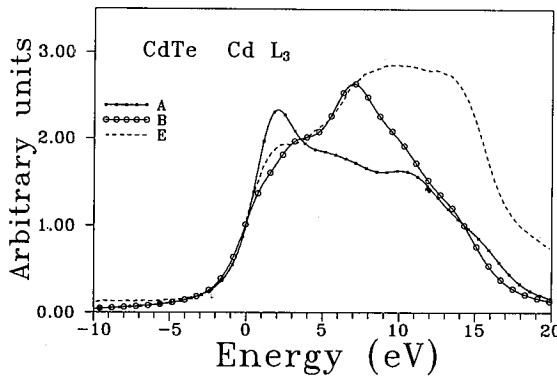


Fig. 2. The calculated Cd L_3 X-ray edge spectra for CdTe. The curve A — the calculations with inclusion of dipol transition matrix elements and Cd $4d$ basis functions. The curve B — the calculations with inclusion of dipol transition matrix elements and Cd $5d$ basis functions. The curve E — experimental spectrum.

From comparison of the theoretical results with experimental data it follows that the Cd L_1 and Te L_1 theoretical X-ray absorption edges results give almost equivalent good description of the experimental spectra [11]. Figure 2 presents the results for the Cd L_3 X-ray absorption edge which arises from superposition of the transitions to s -like and d -like conduction states. The worst agreement between theory and experiment exists for Cd L_3 edge when the basis function set includes the $4d$ Cd functions but does not include the $5d$ Cd functions [6, 11]. When the basis function set contains $5d$ Cd functions, the agreement between theory and experiment is much better.

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