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BULK BAND STRUCTURE OF CdTe ALONG THE $\Gamma - L$ DIRECTION*

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The valence band structure $E(\boldsymbol{k})$ for CdTe (111) Cd side surface 2×2 reconstructed was investigated along the $\Gamma - L$ direction of the bulk Brillouin zone by high-resolution angle-resolved photoemission spectroscopy method in the energy range between 9.5 eV and 30.0 eV. The $E(\boldsymbol{k})$ dependence was determined as well for bulk as for some of the surface states in the whole width of the valence band. Obtained results are compared with available calculated bulk band structure along $\Gamma - L$ direction.

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The Angle Resolved Photoemission Spectroscopy was used intensively during last years to determine experimentally the electronic structure of CdTe (in the whole energy range of the valence band of CdTe [1–5]). The most of these photoemission measurements were done for clean surface obtained by cleavage of the crystal in UHV conditions. The presented results are the continuation of this effort [5] and they are concerned to the electrons emitted perpendicularly to the CdTe (111), Cd side surface 2×2 reconstructed and cleaned by argon ion bombardment and annealing in ultra high vacuum ($p = 10^{-10}$ Torr) conditions. Used in the presented experiment cleaning procedure gave a background for investigation of electronic properties of another, not only cleavage, plane of CdTe crystal. The synchrotron radiation of the DORIS storage ring at HASYLAB in Hamburg in the energy range of 9–30 eV was used. The following energy and angle resolution was used 130 meV and 0.5° respectively.

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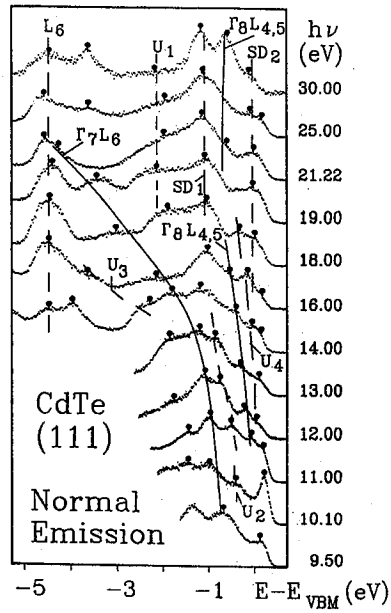

Fig. 1. The selected set of Angle Resolved Energy Distribution Curves (AREDC) obtained in normal emission at different photon energies $h\nu$ in the range from 9.5 to 30 eV, indicated on the right hand side of the figure. The SD_1 and SD_2 peaks are interpreted as the surface states: $\Gamma_8 L_{4,5}$, $\Gamma_7 L_6$, and L_6 peaks are interpreted as the volume states and U_1, U_2, U_3, U_4 are correlated to the umklapp process.

A selected set of angle resolved photoemission spectra taken in normal emission along the $\Gamma - L$ direction of the bulk Brillouin zone is shown in Fig. 1. The bulk valence band maximum Γ_8 energy position was experimentally determined by the comparison of its binding energy relatively to the Cd $4d$ core level measured on the (111) surface with that measured on the (110) surface [5]. This procedure was necessary because within the used photon energy range the uppermost valence band overlaps with the surface states SD_2 at the valence band maximum. The obtained reach structure of the spectra is interpreted as consisting of surface states (SD_1 and SD_2), and volume states ($\Gamma_8 L_{4,5}$, $\Gamma_7 L_6$, and L_6) with correlating to them structures originating from an Umklapp process (U_1, U_2, U_3, U_4).

The wave vector normal to the surface was determined by:

$$k_\perp = \left[(2m/h^2) \left(E_{\text{kin}} \cos^2 \theta + V_0 \right) - g_\parallel^2 \right]^{\frac{1}{2}} - G_\perp$$

$G_\perp$ is the normal component of a reciprocal lattice vector $\boldsymbol{G} = [G_\parallel,\ G_\perp]$ and $g_\parallel$ is in general, a linear combination of a $G_\parallel$ with a reciprocal surface lattice vector component $G_{s\parallel}$, here from the reconstructed (2×2) surface. The inner potential V_0 was found experimentally for (111) surface as equal 7 eV. The $\theta = 0°$ corresponds

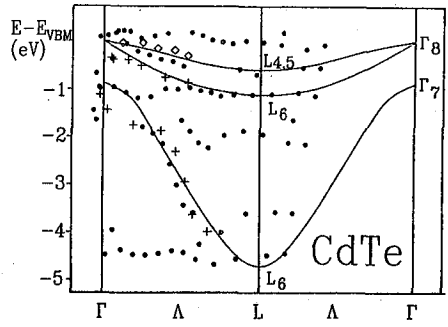

Fig. 2. The experimental band structure shown together with the calculated bulk band structure [5] along $\Gamma - L$ direction. The circles assign emissions with $k_\perp$ value for which $g_\parallel = 0$ and $\boldsymbol{G} = (111)$, the crosses for which $\boldsymbol{G} = (00\underline{2})$, and the rhombs for which $\boldsymbol{G} = (\underline{111})$.

to the $\boldsymbol{k}$ perpendicular to the (111) surface and to the direction $\Gamma - L$ in the bulk Brillouin zone. The value of E_{kin} was determined from energy distribution curves presented on Fig. 1, for each particular considered peak. All experimental structures, showing dispersion with $\mathbf{k}_\perp$, are due to bulk derived states. The umklapp process U_1 denotes emission which we interpret to originate from a part in the bulk band structure of high density of states, here from the bottom of the $\Gamma_7 X_6$ band (X_6 point [5]). The U_2 can be folded on $\Gamma_8 L_6$ while U_3 on $\Gamma_7 L_6$ and U_4 on $\Gamma_8 L_{4,5}$ with appropriate lattice vectors. In Fig. 2, the circles assign emissions with $k_\perp$ value for which $g_\parallel = 0$ and $\boldsymbol{G} = (111)$, the crosses for which $\boldsymbol{G} = (00\underline{2})$, and the rhombs for which $\boldsymbol{G} = (\underline{111})$.

In summary, the calculated high symmetric points L_6, $L_{4,5}$ and Γ_7 are in very good agreement with the experiment. The presented experimental results are taken for not cleaved surface (cleavage surface is (110)) but for cleaned CdTe (111) surface (2×2) reconstructed obtained with high energy and angle resolution, and contribute new precise data with taking into account transitions with two possible final states (umklapp process) of different precisely adjusted values of $\boldsymbol{G}$.

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