

ANGULAR RESOLVED UV PHOTOEMISSION OF THE  
PbTe (111) SURFACE

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A six fold symmetry of the peak positions is observed in the angular resolved photoemission spectrum from a PbTe (111) surface, when measuring in the threefold mirror plane where  $k_{\parallel}$  is along the LU or LK direction. This is direct evidence for indirect transitions, sampling the 1 dimensional-density of states along  $k_{\perp}$ . The remnant of the  $k_{\parallel}$  conservation manifests itself in the intensities of the peaks in the spectra. The occurrence of two non-dispersive bands at 5.75 and 6.25 eV are assigned to states due to Te vacancies at the surface.

## I. Introduction

Angle resolved photoemission spectroscopy (ARPES) has been widely used to determine the electronic structure of solids [1]. Here we wish to report on ARPES measurements on the (111) surface of PbTe. The objective of this work is threefold.

(i) It is an extension of the work of Grandke et al. [2] on the PbTe(100) surface in order to obtain the band energies of further directions in the Brillouin zone (BZ).

(ii) It is used to test the validity of the indirect transition model for  $k_{\perp}$ , the electron momentum perpendicular to the surface, invoked earlier for the interpretation of ARPES data on the lead salts [2].

(iii) It is the first ARPES measurement on a polar surface of PbTe. Since these surfaces are particularly prone to Te vacancies, we would expect Te-defect induced states in the ARPES spectrum of PbTe(111). The band structure of PbTe with Te-defects has been calculated by Parada and Pratt [3].

## II. Experimental

The PbTe sample was grown on a BaF<sub>2</sub>(111) surface by the hot wall technique [4]. The sample surface was cleaned by bombardment with 2kV Ar ions in the UHV system of the spectrometer. After sputter cleaning the sample showed the LEED pattern expected for an unreconstructed (111) surface. It improved in brightness after a heat treatment of 10 min. at 290°C. A few sputter and heat cycles were necessary to obtain a reproducible, oxygen free photoelectron spectrum. The photoemission spectrometer used was a VG ADES 400 system with an energy resolution of 0.3 eV and a total acceptance angle of 3°. Electron beam and light direction were coplanar.

III. Results and Discussion

One set of angle resolved spectra was taken with  $\vec{k}_{\parallel}$  in the direction LK (polar angle  $\theta > 0$ ) and in the direction LU ( $\theta < 0$ ), respectively (compare Fig.(1a)). Some representative spectra are shown in Fig.(2). If direct, i.e.  $k_{\perp}$  conserving transitions were to contribute mainly to these spectra, the peak positions would in general be different for each pair of spectra taken at an angle  $+\theta$  or  $-\theta$ . For a given magnitude of  $\theta$ , reference to Fig.(1b) shows that the values  $(\vec{k}_{\parallel}, k_{\perp})$  and  $(-\vec{k}_{\parallel}, k_{\perp})$  do not correspond to equivalent points in the BZ. In the indirect transition model all points along the line  $\vec{k}_{\parallel} = \text{const.}$  are sampled with equal probability and structure in the spectra arises from singularities in the 1-dimensional density of states. From Fig.(1b) it is apparent that positive and negative  $\vec{k}_{\parallel}$  values define equivalent lines in the BZ.

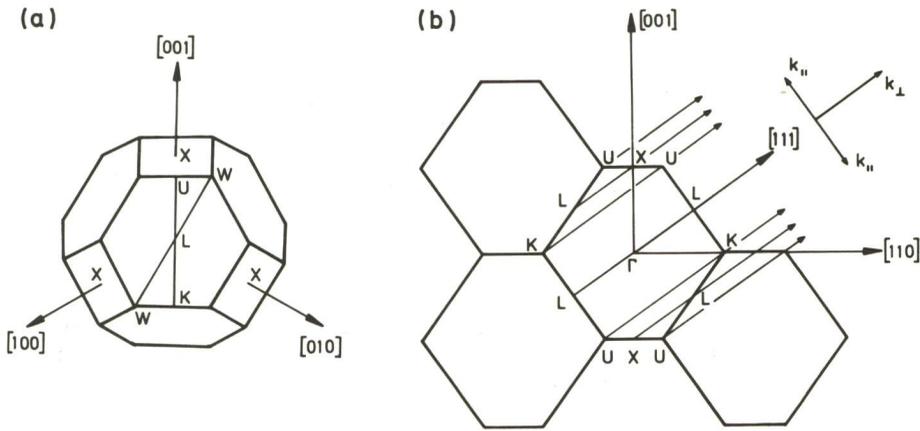


Fig. 1. Brillouin zone of PbTe in the repeated zone scheme  
 a) Top view onto the (111) surface: Measurements were confined to wave vectors  $\vec{k}_{\parallel}$  along LU, LK, and both LW directions as marked in the picture  
 b) Plane containing  $\Gamma$ , L, U, and  $k$

On the left hand side of Fig.(3) we have plotted the peak positions as a function of  $|\vec{k}_{\parallel}|$  for  $\theta > 0$  (open circles) and  $\theta < 0$  (full circles). We identify 4 bands between 0 and  $\sim 5$  eV binding energy originating from the Te 5p and Pb 6p like valence states. Despite a considerable energy dispersion there is perfect agreement in the peak positions for the two directions in accord with the indirect transition model.

The remnant of the conservation in  $k_{\perp}$  manifests itself in the intensities of peaks in the ARPES spectra. The normalised intensities of peaks contributing to bands I and IV are plotted for the LK and LU directions on the left hand side of Fig.(4). For band IV a strong enhancement of the transition intensity is observed for  $\vec{k}_{\parallel} = 0.8\text{\AA}^{-1}$  and a weaker relative maximum is seen in the opposite direction for  $-\vec{k}_{\parallel} = 0.3\text{\AA}^{-1}$ . We have calculated the corresponding  $k_{\perp}$  values in the kinematic approximation [5] with an inner potential  $V_0 = -10$  eV. The results show that the  $k$ -vectors of the two maxima correspond to equivalent points in the BZ about one third of the way from L to K. This region contributes as a primary cone emission to the maximum at  $+0.8\text{\AA}^{-1}$  and as a secondary cone emission to the shoulder at  $-0.3\text{\AA}^{-1}$ .

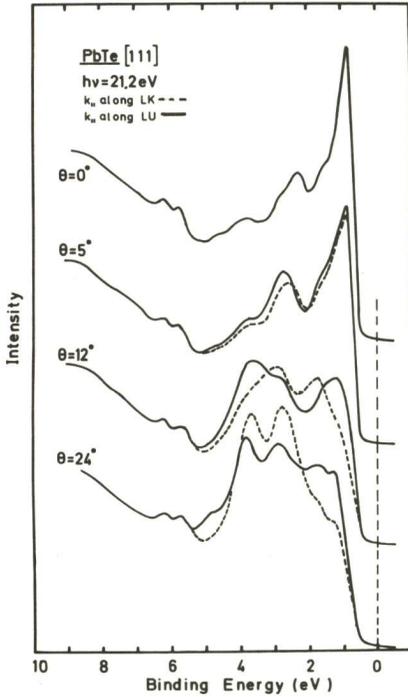


Fig. 2. Angle-resolved photo-electron spectra for PbTe (111) measured for various polar angles  $\theta$  with  $k_{\parallel}$  along LU (solid line) and  $k_{\parallel}$  along LK (dashed line): The photon incidence angle  $\phi = -45^\circ$  is in the opposite direction to  $\theta$

The right hand sides of Figs.(3) and (4) represent the energy dispersion of peak positions and the intensities of two bands from spectra taken in two directions in the WLF plane which (see Fig.(1a)) is perpendicular to one of the mirror planes ULF. Positive and negative values of  $\theta$  are therefore related by mirror symmetry and no differences are expected for the two sets of spectra independent of the transition model. This is indeed born out over most of the dispersion curves. Small deviations in bands I and III are likely to be due to a slight misalignment of the crystal as are differences in the intensities. The mirror symmetry holds only exactly for the plane WLF and the stabilizing effect  $(\partial E/\partial \phi) = 0$  of the mirror plane emission ( $k_{\parallel}$  in ULF) against azimuthal misalignment is absent in this case.

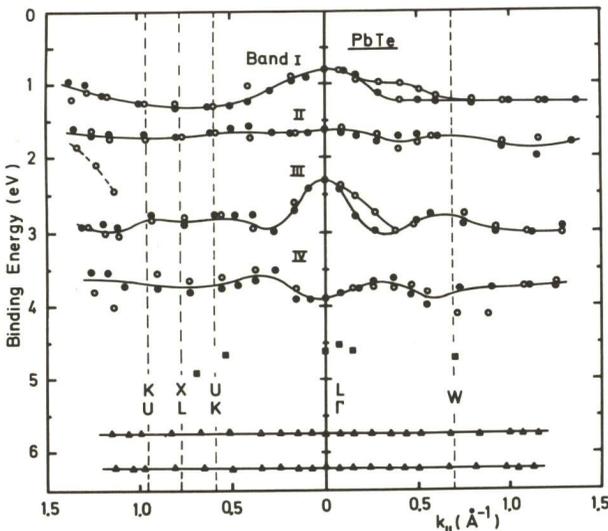


Fig. 3. The experimental determined valence band dispersion relation of PbTe. Left part: Peak positions versus momentum component  $k_{\parallel}$  along the direction LK (full circles) and LU (open circles). Right part:  $k_{\parallel}$  along the two LW directions. For the lowest two bands values for opposite  $k_{\parallel}$  are the same within the experimental errors and drawn by a filled triangle.

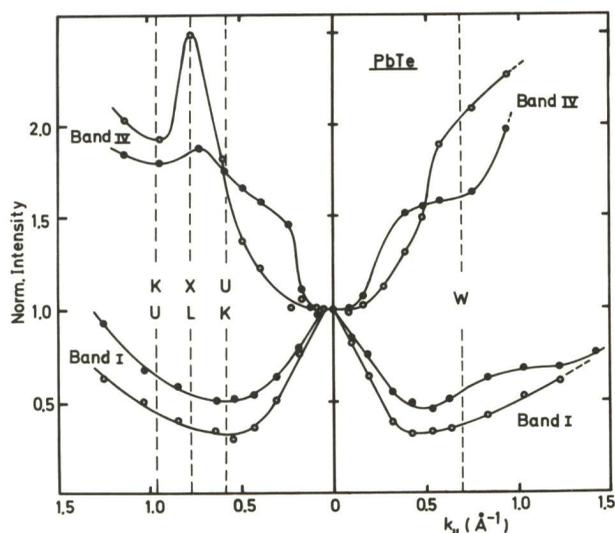


Fig. 4. Normalized peak intensity of band I and band IV as a function of  $k_{||}$  for the two emission planes

From the dispersion curves of Fig.(3) we can deduce energies (in eV) for a number of high symmetry points in the band structure of PbTe. These energies are compared with theoretical values [6] in the table below.

We finally note two non-dispersive lines at 5.75 eV and 6.25 eV below  $E_F$ . We tentatively assign these states to Te defect induced levels. The higher vapour pressure of Te makes Te defects likely at the surface of PbTe after heating. This leaves the surface n-type in agreement with the observed Fermi level position. The energies of these states are in reasonable agreement with a state at 5.7 eV calculated by Parada and Pratt [3] for a Te defect.

Symmetry designation	Experimental HeI	Theory EPM Ref. [6]
$\Gamma_8^-$	0.85	1.1
$L_6^+$	1.65	1.9
$\Gamma_6^-$	2.3	2.2
$X_6^-$	3.8	3.5
$X_6^-$	4.6	4.8

References

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