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SIMULTANEOUS INVERSE PHOTOEMISSION AND TARGET CURRENT SPECTROSCOPY: ADVANTAGES IN BAND MAPPING

D. FUNNEMANN and H. MERZ

Physikalisches Institut der Universität, Wilhelm-Klemm-Strasse 10, D-4400 Münster, F.R.G.

Abstract - The simultaneous measurement of inverse photoemission and target current spectra at single crystals allows to fix independently the position of the initial and final bands for the observed electron direct IPE transitions. The advantages of a combination of these two spectroscopic methods are demonstrated in the case of W(110).

With the method of Inverse Photoemission (IPE) the unoccupied part of the electronic band structure $E(k)$ of single crystals can be determined. For a location of the transition in $k$-space one needs information about energy $(E_i, E_f)$ and wave vector $(k_i, k_f)$ of the initial and final state. The condition for direct transitions gives $k_i = k_f$ within the first Brillouin zone. The peaks in the IPE-spectrum determine those energy values, where the energy difference of the involved energy-bands for direct transitions equals the photon energy used. But only the parallel component $k_\parallel$ is conserved (mod $G_\parallel$) in traversing the crystal surface whereas the normal component is changed. So $k$ can not be completely determined by one IPE measurement. To determine $k$ of the direct transition one often takes the position of the high lying bands from a calculation; a first approximation that often succeeded with simple metals so far. But for transition metals one often finds that the initial bands are displaced by a few eV when putting in an extra electron in the IPE-process. Those dynamical many-body correlations forbid the use of the calculated initial bands as a good approximation for the interpretation of the spectra.

The Target Current Spectroscopy (TCS) can fix the energy position of the IPE-initial bands. The combination of this spectroscopy with the IPE experiment has certain advantages: The target current is measured simultaneously with the IPE-spectrum. Many of the parameters of the measurement are identical for both...
spectroscopies i.e. surface condition of the target, energy and angle of incidence of the electron beam as well as its energy-distribution and its angle divergence. Up to now the advantages of this combination have seldom been used. Two deficiencies seem to be responsible for this situation. On the one hand the theory for the interpretation of target current spectra /7/ was restricted to polycrystalline samples. On the other hand a modulation of the primary electron energy - as in standard TC spectroscopy - would unacceptably degrade the energy resolution in the simultaneously taken IPE-spectrum. In the following we would like to explain how these problems may be overcome.

The interpretation of TC spectra of polycrystalline samples is accomplished by considering the inelastic scattering of the electrons in the target. A spectrum is build up by a convolution of three parts of the density of states (DOS) that take part in the energy-loss process. So the DOS structures in spectrum are broadened. In the case of single crystals sharp structures are due to the elastic electron scattering /10/. The initial state (its energy and wave vector) is prepared experimentally by the incoming nearly parallel beam. On varying energy or the incidence angle structures in the target current are to be expected. The probability for the elastic scattering is peaked in forward and backward direction /11/. The target current then reflects the one dimensional DOS in the direction of the incoming electrons. Relative maxima in the target current are to be expected. A small correction has to be applied: at the critical points the group velocity \(v_g = dE/dk\) of the electrons vanishes. So the target current reaches its maximum at a somewhat higher energy /10/.

For the combined TCS and IPE experiment no additional hardware is necessary. The target current is measured directly without a lock-in amplifier. Care has to be taken to compensate for the resultant loss in signal to noise (S/N) ratio. The time constant of the current measurement is extended to cover the accumulation time (here 10 s per energy value) chosen for the IPE-photon counting. The time averaged target current curve is differentiated by a numerical procedure. The best S/N ratio (without falsifying the structures) is found with the Savitzky-Golay-approximation /12/. The knowledge of the width of the energy distribution of the electrons and the fact that the data points are discrete is taken into account from the beginning. The noise is by fitting with a polynomial of third degree covering the range of the electron energy width. In comparison with a lock-in measurement the S/N ratio is only reduced by a factor of 0.735 /13/.

The advantages in combining the information from both spectroscopies are demonstrated for W(110) spectra taken at normal electron incidence. The mean energy of the photon-monochromator is 9.9 eV, its energy resolution (fwhm) 0.40 eV. The total energy resolution (fwhm) of the IPE-measurement (electrons and photons) is 0.55 eV /14/. The divergence of the electron beam \(\pm 4^\circ\).
Fig. 1 shows in its lower part the IPE-spectrum and the (first derivative of the) target current measured simultaneously on a common energy scale. The IPE-spectrum is shifted to lower energies by the monochromator energy (9.9 eV). The Fermi energy has been determined the usual way. The peak at 1.8 eV in the IPE spectrum is interpreted as a surface state /15/. It is very sensitive to contamination. The other three peaks are interpreted as direct transitions in the bulk band structure. But transitions with 9.9 eV energy difference do not fit in calculated band structures along \( r \mathbf{N} \).

The "fine" structure of the target current is superimposed to an increasing background. Relative Maxima of the target current are therefore found in the derivative at inflexion points with a negative slope (rather than at zeros). The arrows in Fig. 1 mark these inflexion points. The upper part of the figure displays a part of a calculated band-structure /16/ where the initial IPE-bands are adjusted according to our TCS-measurement. The TCS-spectrum shows that the high lying bands have to be shifted to higher energies by an amount of 1.3 eV for the lower and 2.1 eV for the upper band to fit the TCS-inflexion points (with an uncertainty of 0.5 eV for taking into account the vanishing group velocity at band edge. This experimentally determined shift changes the interpretation which bands are involved in the IPE-transitions. The major discrepancy between the calculated peak positions and the measured IPE-spectra is removed by shifting the initial bands.

Fig. 1 Inverse photoemission (IPE) and differentiated target current (TCS) in comparison with an adjusted band structure calculation /16/. The dashed lines show the direct bulk transitions. Arrows indicate inflexion points of the TCS-spectrum.
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