Using XPS or UPS, it is possible to measure energy vs. angle to obtain dispersion $E$ vs. $k$ as well as to measure intensity vs. energy.

![Graph showing emission intensity vs. binding energy for Cu(111)](image)

**Fig. 6.16.** Normal emission ARUPS data obtained from the Cu(111) surface with different photon energies. The sharp peak $S$ is due to a surface-state band [6.17]

Here for Cu(111), we see a peak which stays fixed vs. $E_F$ which makes it a surface state ($S$).

It lies just below $E_F$. The peaks starting at ~2 eV are $d$-bands (fully occupied $d$-shell so energy is lowered).

Lüth, p. 290
Again the dispersion is obtained by measuring at various angles $\Theta$. The surface state dispersion can be obtained for various parts of the Brillouin zone by looking at different crystal faces.

![Diagram showing dispersion curves for Cu(110) and Cu(111) surfaces.](image)

**Fig. 6.17.** Angle-resolved UV-photoemission spectra of surface-state bands on the Cu(110) and Cu(111) surface. The peak shifts as a function of detection angle $\Theta$ indicate a significant dispersion [6.17].
Fig. 6.18. Dispersion of the \( sp \)-derived surface state band on Cu(111) according to the ARUPS data of Fig. 6.17. Data points from measurements with two different photon energies \( \hbar \omega \) are plotted in the gap of the projected bulk bands (shaded). The inset gives the location in reciprocal space [6.17]

\[ \text{Lüth, p. 291} \]

Fig. 6.19. Dispersion of the \( sp \)-derived surface state band on Cu(110) according to the ARUPS data in Fig. 6.17. Data points from measurements with two different photon energies \( \hbar \omega \) are plotted in the gap of the projected bulk bands (shaded). The inset gives the location in reciprocal space [6.17]

\[ \text{Lüth, p. 292} \]
Cu is fcc

Cu (111) plane

normal is [111]
Transition metals having various numbers of electrons in the outer d-shell will display peaks which are related to the d-bands.

Fig. 6.20. Angle-resolved UV-photoemission curves measured with a photon energy of 21.22 eV on Cu(100) at different detection angles. The emission direction is in the (001) mirror plane containing the symmetry points $\Gamma$, $X$, $W$ and $K$ of the Brillouin zone [6.18]

Fig. 6.21. Dispersion of the d-derived surface-state band on Cu(100) according to the ARUPS data of Fig. 6.20. Data points from measurements with two different photon energies $\hbar \omega$ are plotted in the gap of the projected bulk sd bands (bounded by the shaded region). The inset gives the location in reciprocal space. The dashed-dotted curve results from a surface-state band calculation according to [6.18, 6.19]
Note that noble metals Cu, Ag, and Au have completely filled d-shells.

For unfilled (partially-filled) d-shells, the Fermi level will thus lie in the d-bands, or cut through the d-bands.

\[\text{W configuration:}\]
\[(\text{Xe}) 4f^{14} 5d^4 6s^2\]

Fig. 6.22. Layer-resolved Local Density Of States (LDOS) for W(100) as obtained by a slab calculation. For the topmost surface atomic layer surface states around the Fermi level \(E_F\) produce a strong band in an energy region where, in the bulk LDOS (center layer below), low density is found [6.20].

\[\text{Lüth, p. 294}\]

Fig. 6.23a,b. Surface state bands on the W(100) surface with (1 x 1) reconstruction [6.14]. (a) Experimental angle-resolved UPS data [6.21, 6.22]. (b) Theoretical results from a slab calculation [6.23].

\[\text{Lüth, p. 294}\]