

Surface Electronic States

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.

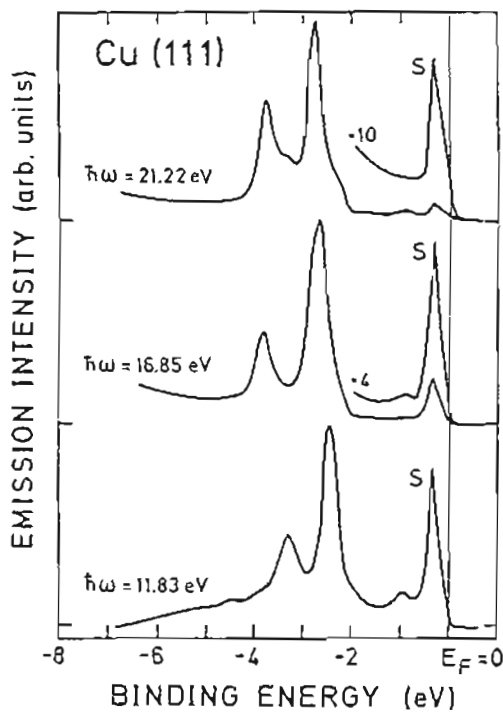


Fig. 6.16. Normal emission ARUPS data obtained from the Cu(111) surface with different photon energies. The sharp peak S is due to a surface-state band [6.17]

Lüth, p. 290

Here for Cu(111), we see a peak which stays fixed vs. E_γ (at $k_{||}=0$) which implies it's a surface state (S).

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

Again the dispersion is obtained by measuring at various angles θ . The surface state dispersion can be obtained for various parts of the Surf. Brillouin zone by looking at different crystal faces;

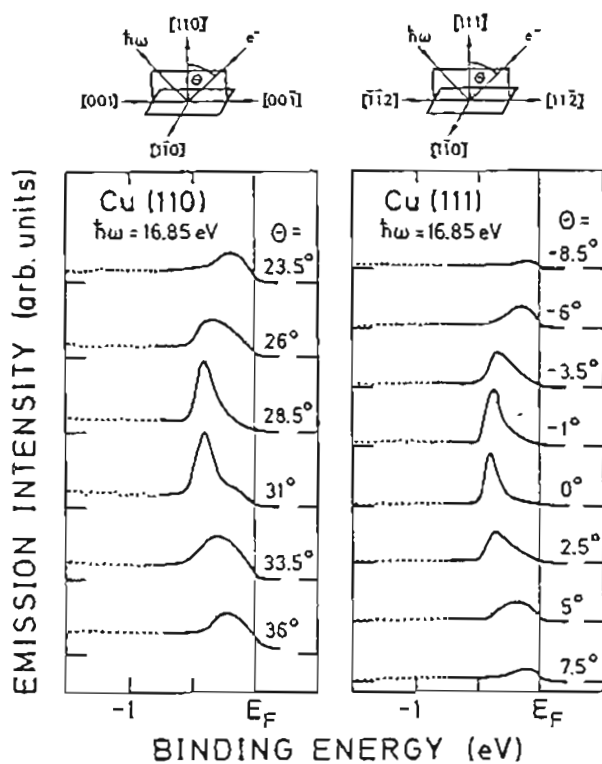


Fig. 6.17. Angle-resolved UV-photoemission spectra of surface-state bands on the Cu(110) and Cu(111) surface. The peak shifts as a function of detection angle θ indicate a significant dispersion [6.17]

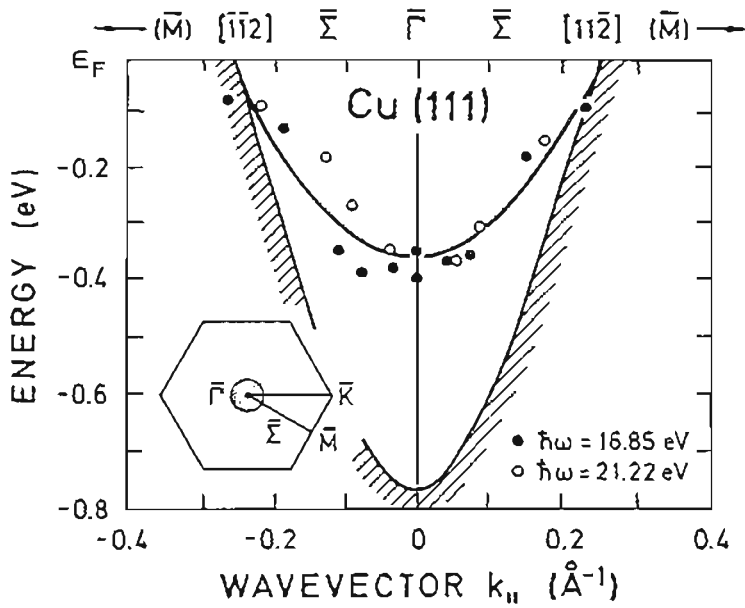


Fig. 6.18. Dispersion of the sp -derived surface state band on Cu(111) according to the ARUPS data of Fig. 6.17. Data points from measurements with two different photon energies $\hbar\omega$ are plotted in the gap of the projected bulk bands (shaded). The inset gives the location in reciprocal space [6.17]

Lüth, p. 291

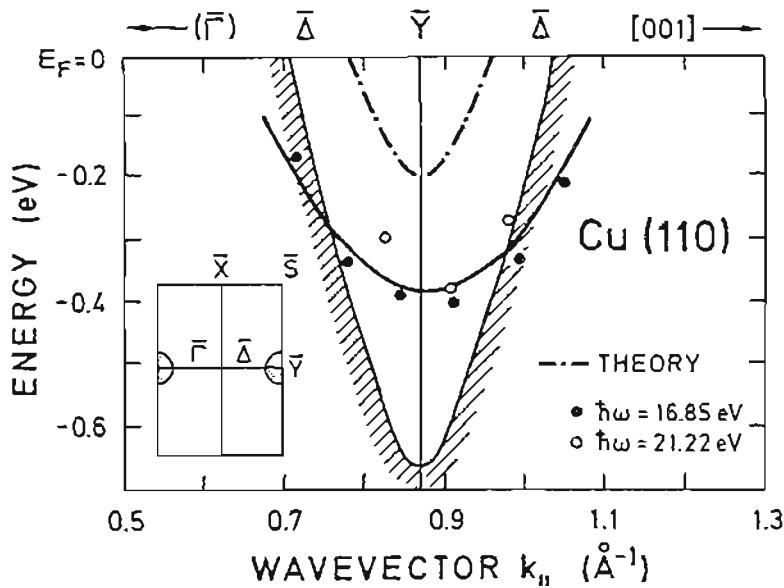
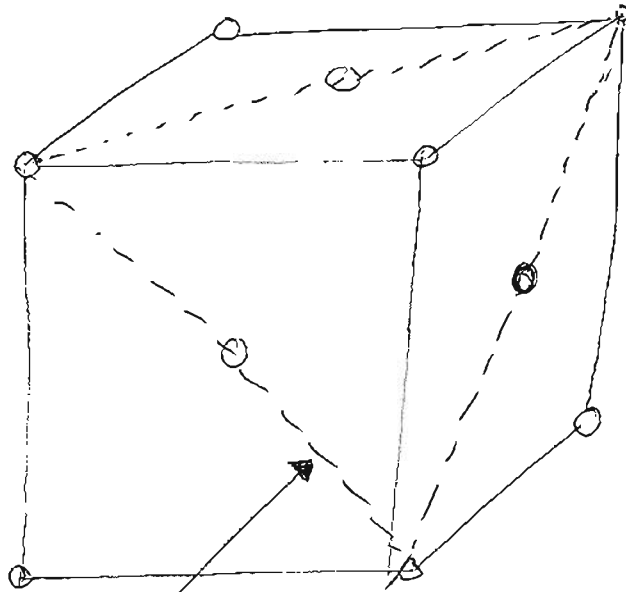


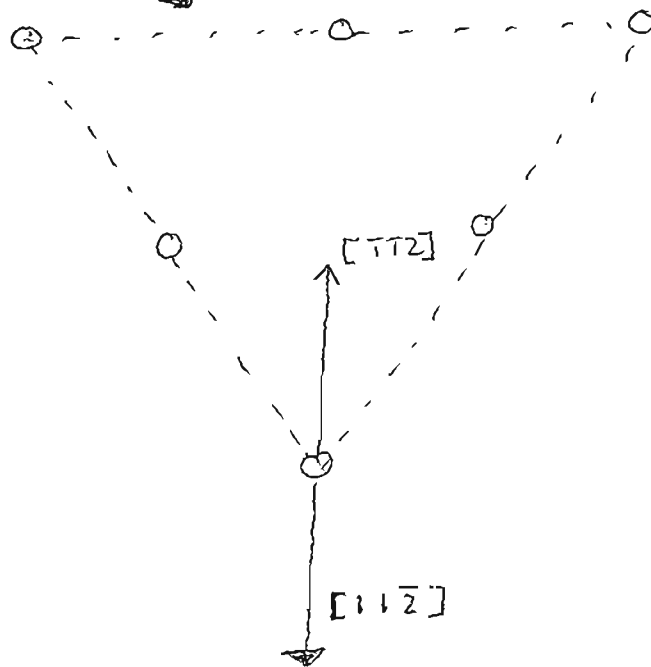
Fig. 6.19. Dispersion of the sp -derived surface state band on Cu(110) according to the ARUPS data in Fig. 6.17. Data points from measurements with two different photon energies $\hbar\omega$ are plotted in the gap of the projected bulk bands (shaded). The inset gives the location in reciprocal space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

Lüth, p. 292

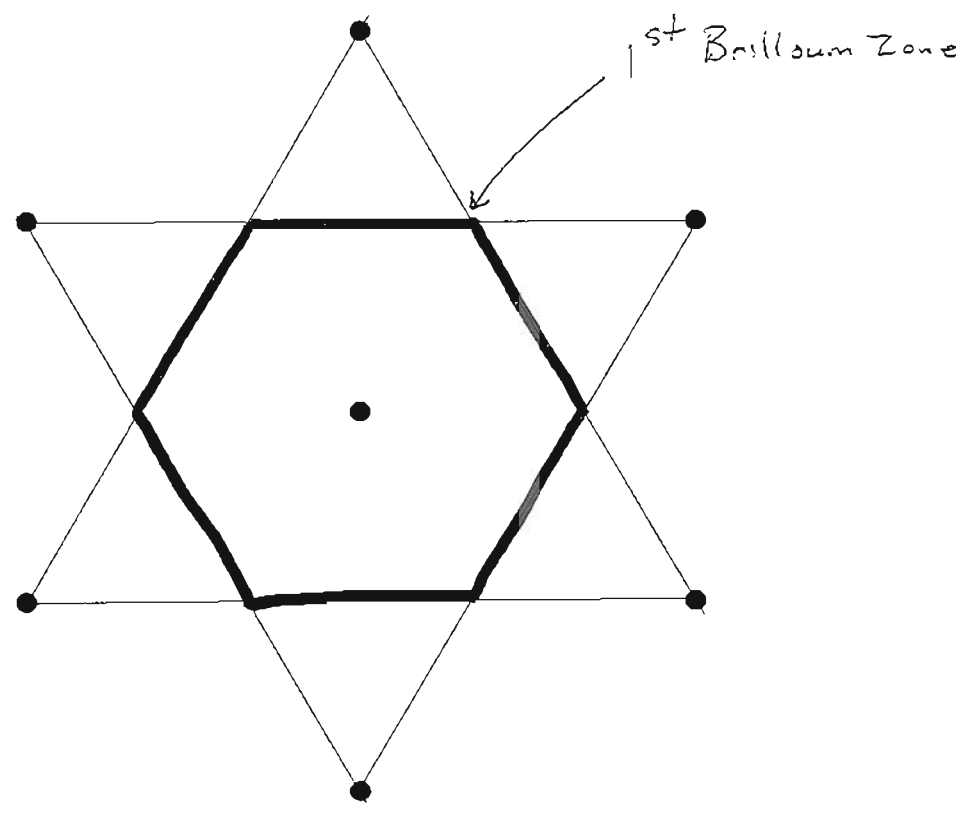
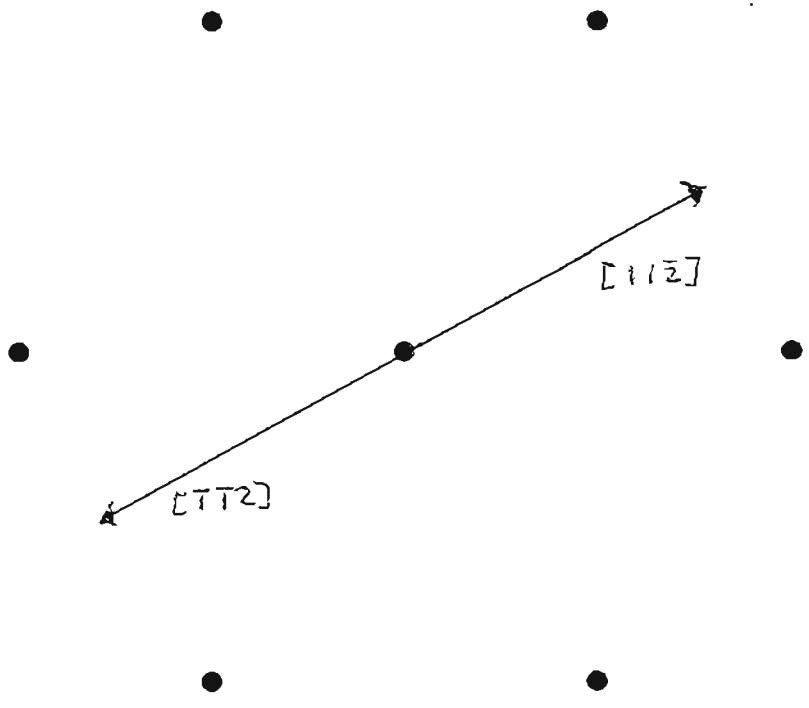
Cu is fcc



Cu (111) plane



normal is $[111]$



d-bands

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

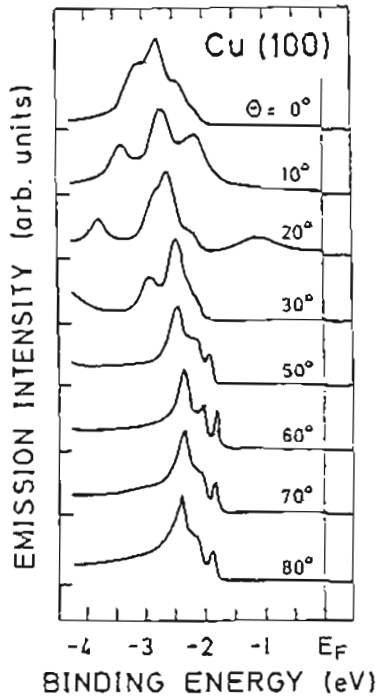


Fig. 6.20. Angle-resolved UV-photoemission curves measured with a photon energy of 21.22 eV on Cu(100) at different detection angles. The emission direction is in the (001) mirror plane containing the symmetry points Γ , X, W and K of the Brillouin zone [6.18]

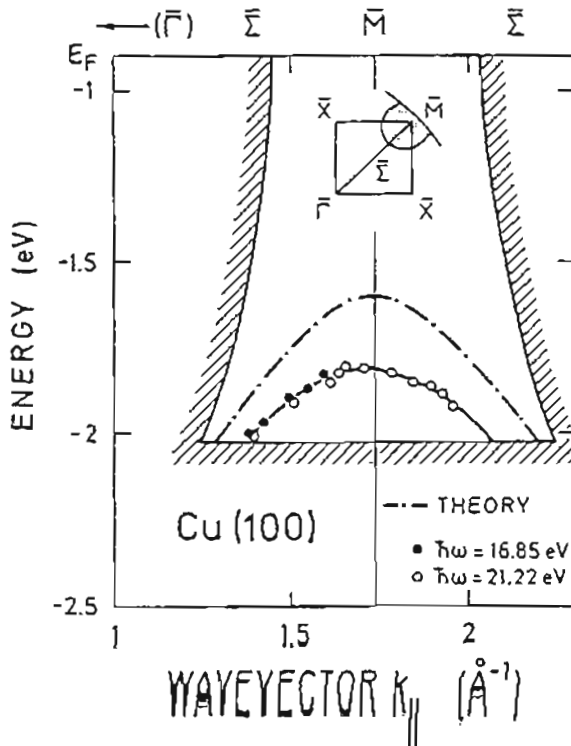


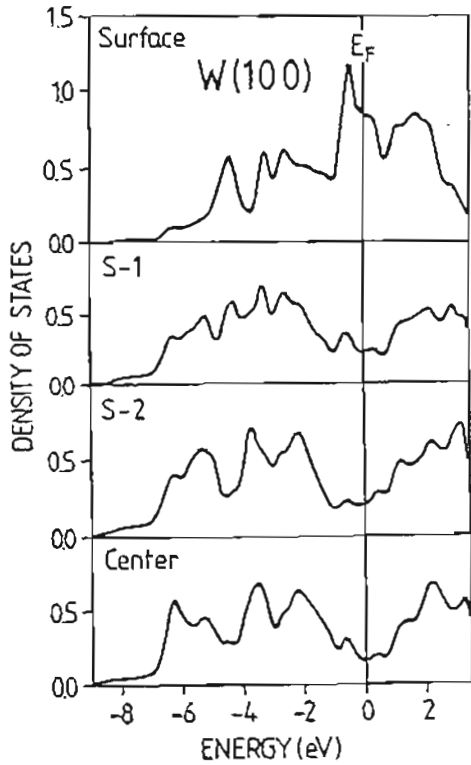
Fig. 6.21. Dispersion of the d-derived surface-state band on Cu(100) according to the ARUPS data of Fig. 6.20. Data points from measurements with two different photon energies $\hbar\omega$ are plotted in the gap of the projected bulk sd bands (bounded by the shaded region). The inset gives the location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

Lüth, p. 293

Lüth, p. 293

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).



W configuration:
 $[Xe] 4f^{14} \underline{5d^4} 6s^2$

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]

Lüth, p. 294

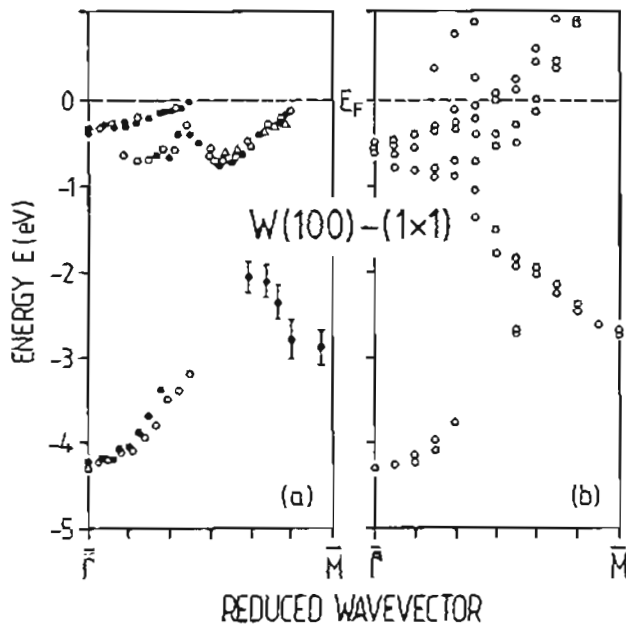


Fig. 6.23a,b. Surface state bands on the W(100) surface with (1×1) reconstruction [6.14]. (a) Experimental angle-resolved UPS data [6.21, 6.22]. (b) Theoretical results from a slab calculation [6.23]

Lüth, p. 294