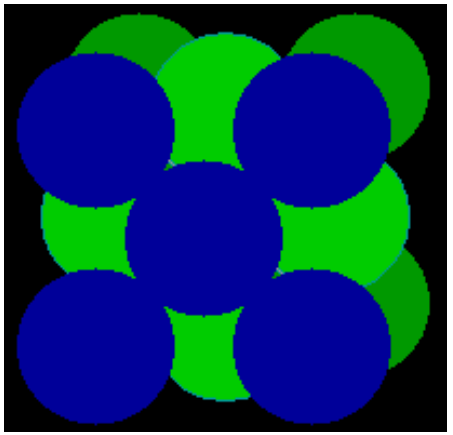
Surface physics

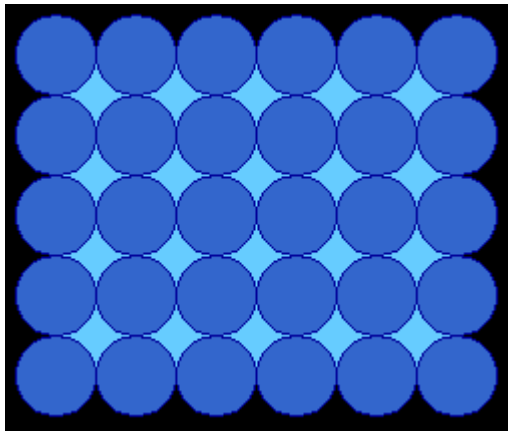
- Crystal surface structures; cleavage planes
- Surface reconstruction
- Surface energies; “work function”
- Electronic structure; bulk bands and surface bands
- Interfaces between crystals

Surface structure – example fcc lattice

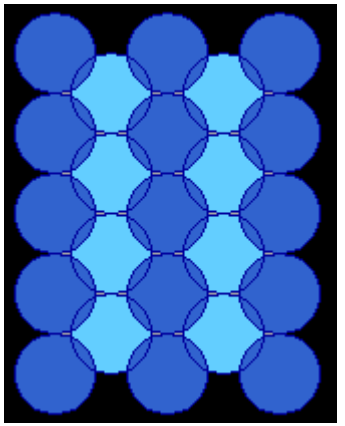
(pictures from http://www.chem.qmul.ac.uk/surfaces/scc/scat1_2.htm)



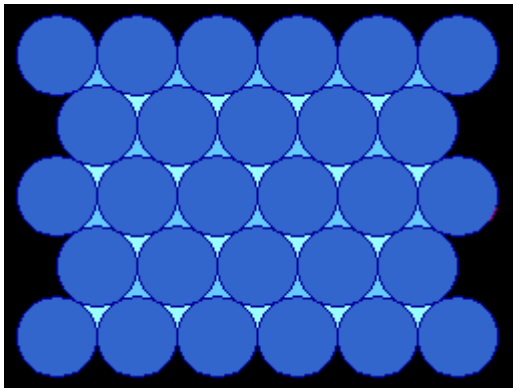
FCC bulk structure



(100) surface



(110) surface



(111) surface

From: PRB 20, 1444 (1982)

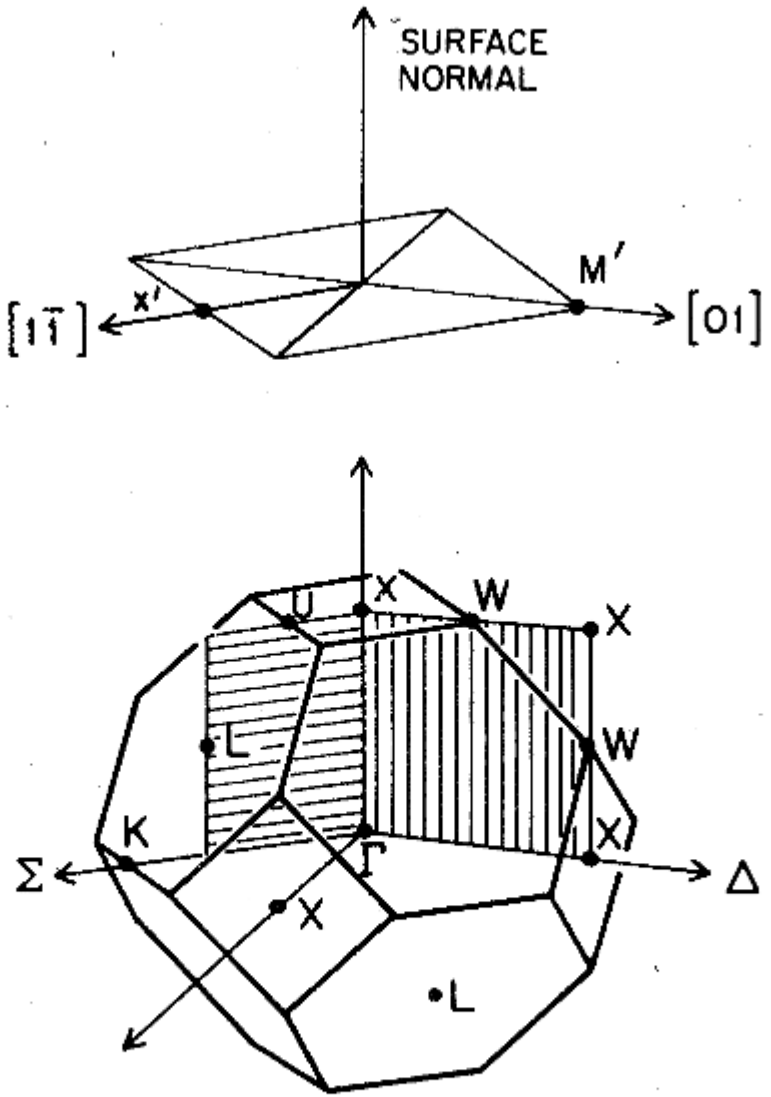


FIG. 5. Surface Brillouin zone at the top and bulk Brillouin zone at the bottom. The (100) and (110) planes are shown in the bulk zone.

Another view of the surface projections of an fcc lattice:
(PRB 18, 5365 (1978))

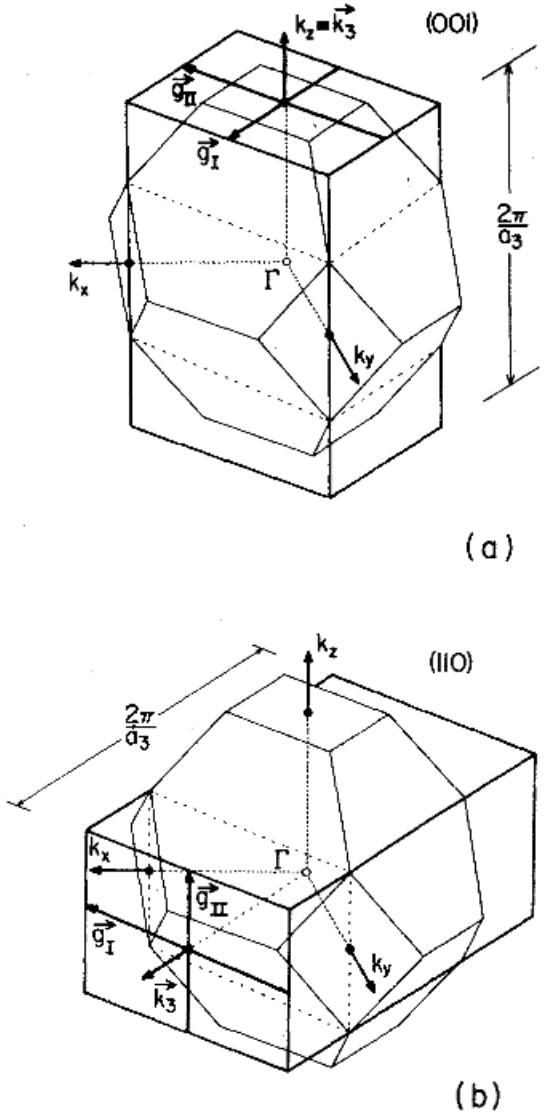
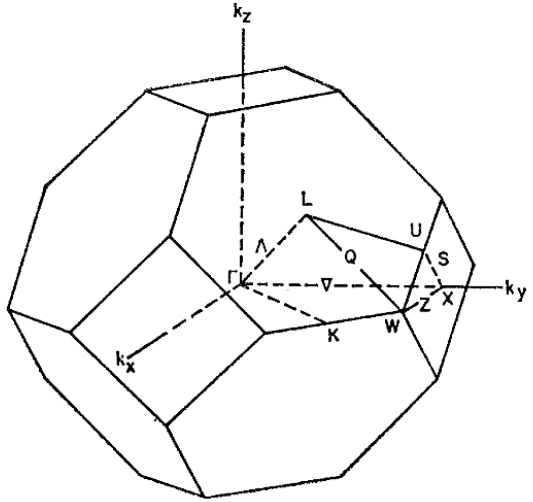
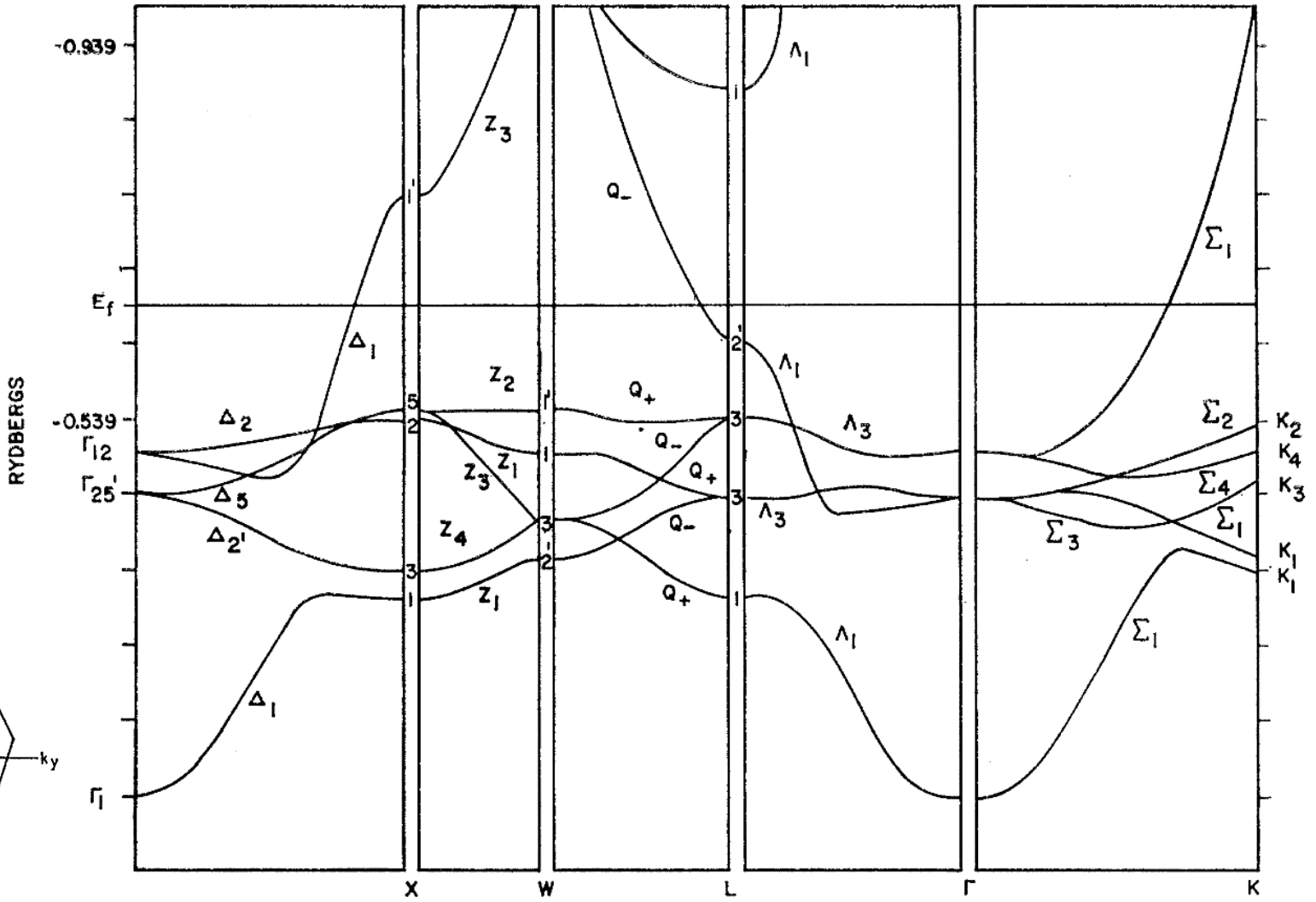


FIG. 3. (a) Brillouin zone for the (001) layers of a fcc lattice shown in relation to the fully symmetric Brillouin zone. (b) Similar construction for the (110) layers of a fcc lattice.

3-dimensional band structure of Cu (Burdick, PR 129, 138 (1963))





Calculated bands for 18 layer supercell of Cu (111) (PRB 28, 528 (1982))

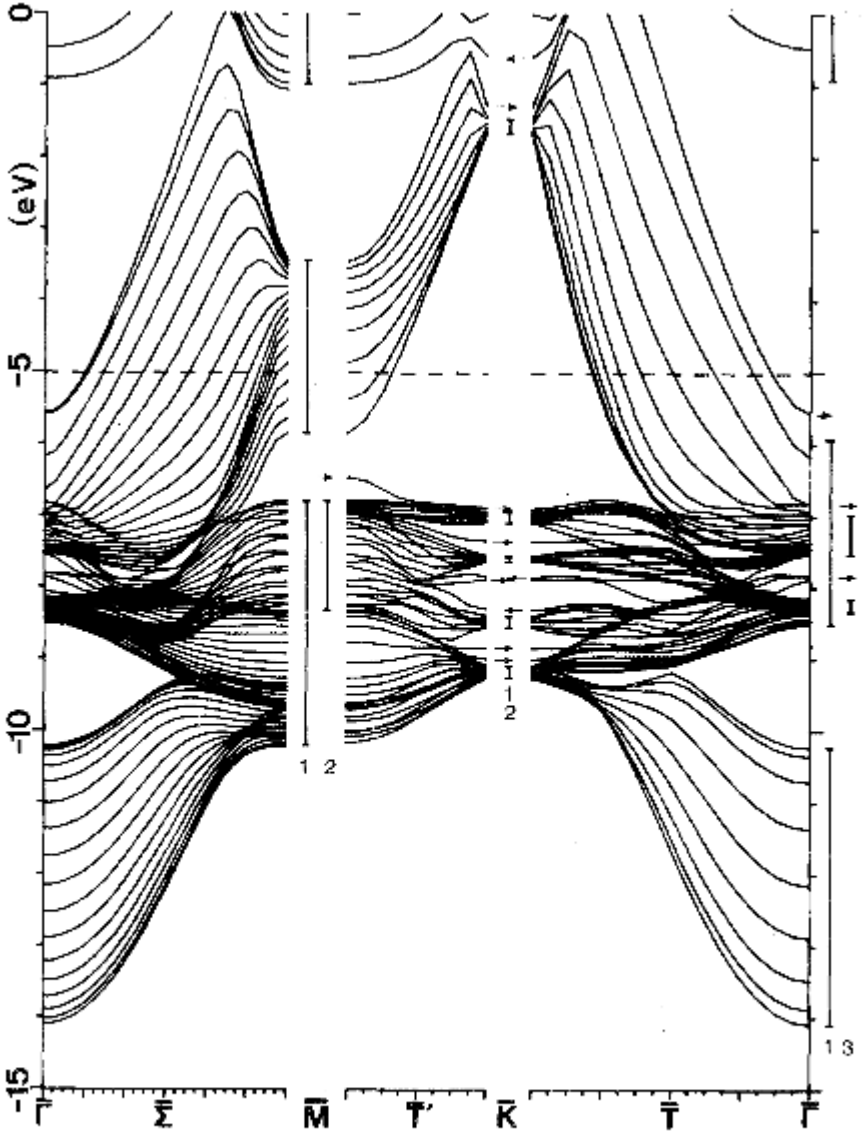
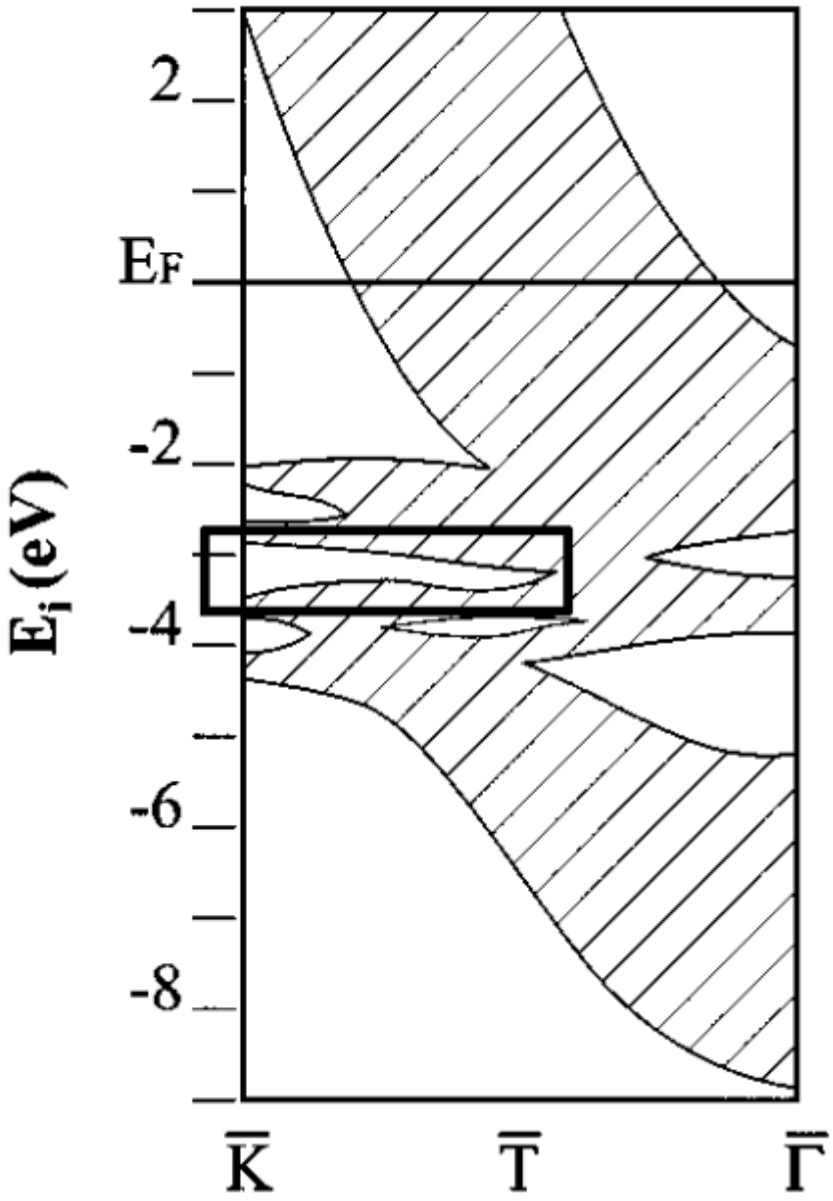
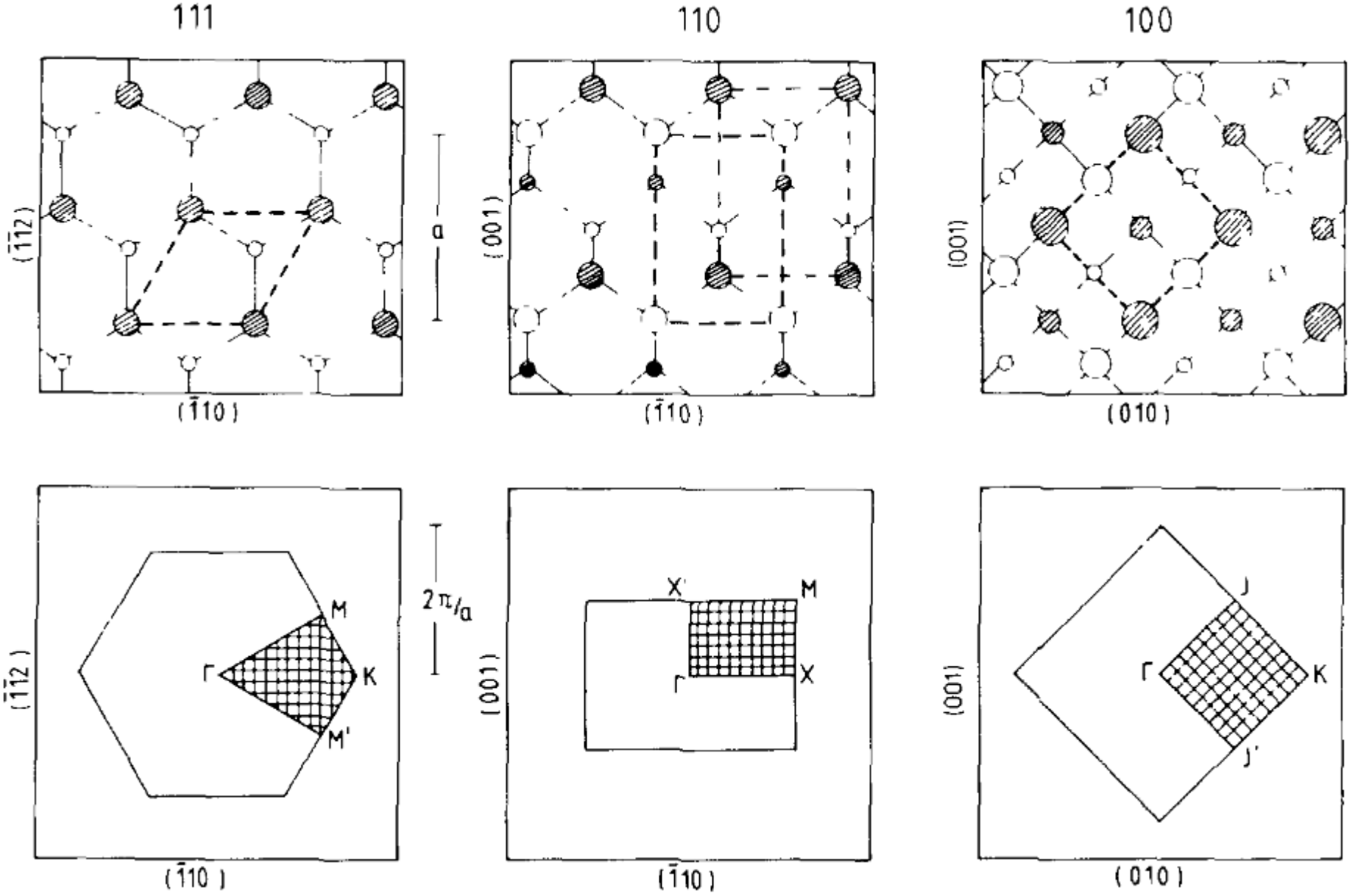


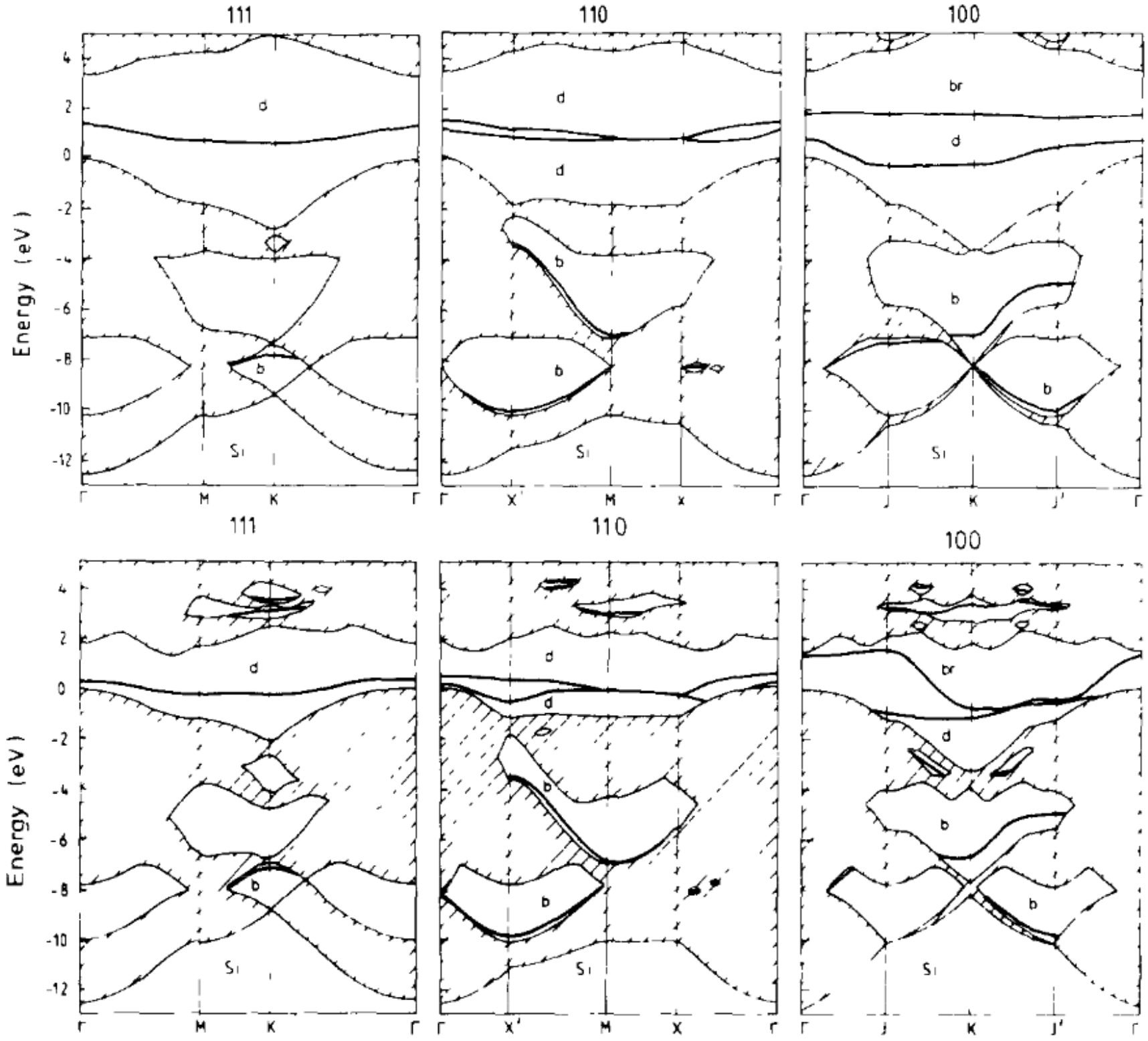
FIG. 5. Energy bands of $\bar{\Sigma}_1$, $\bar{T}'_1$, and $\bar{T}_1$ symmetry for the 18-layer Cu(111) film. The bulk continua and surface states at $\bar{\Gamma}$, $\bar{M}$, and $\bar{K}$ are as in Fig. 1.

Projected band structure of Cu (111) (PRB 54, 5092 (1996))



Surface reconstruction – Si (100)
(From Ivanov, Surface Science 92, 365 (1980))




111
110
100
Energy (eV)
4
2
0
-2
-4
-6
-8
-10
-12
d
b
br
Si
Γ
M
K
X'
X
J
J'

Analysis of Si dimer on (100) surface
(PRB 40, 11868 (1989)

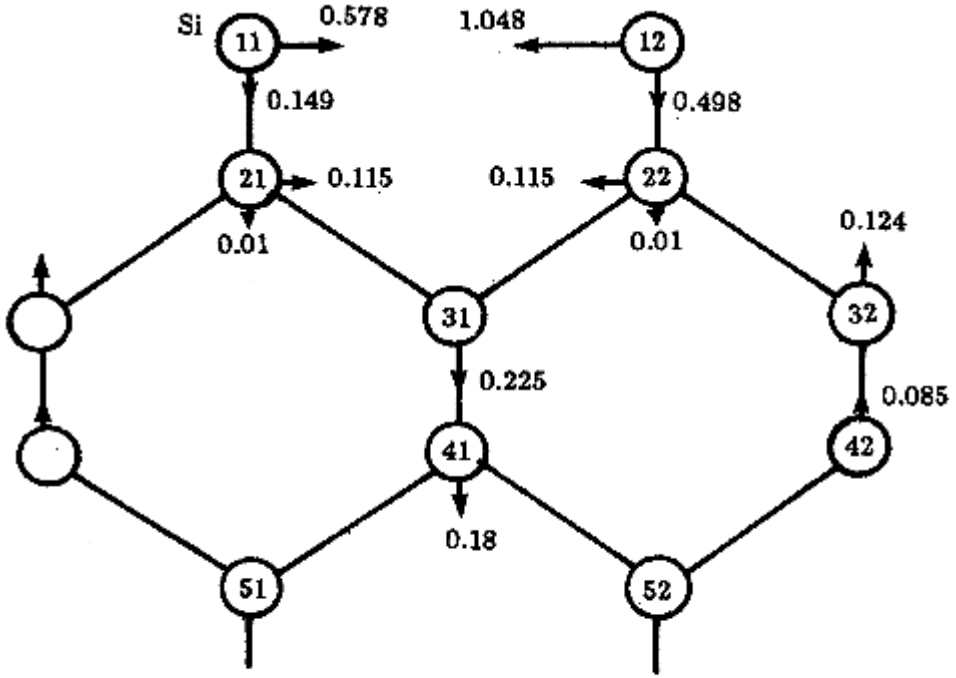


FIG. 2. Geometry of a single dimer used for comparing calculations of (2×1), $p(2\times2)$, and $c(4\times2)$ systems; units are Å.

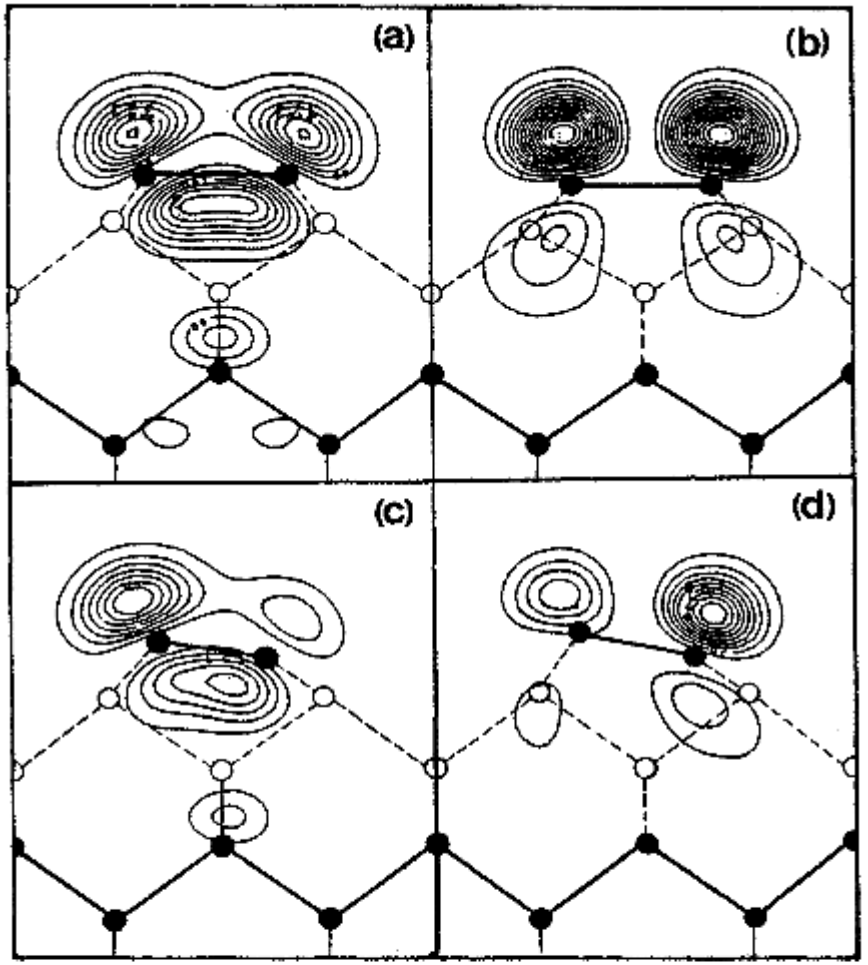


FIG. 4. Contour plots of square of wave functions at the J' point in (2×1) BZ. (a) Surface bonding and (b) antibonding states for symmetric dimer model. (c) Surface bonding and (d) antibonding states for the asymmetric dimer model. The plots are in a (110) plane cutting the surface at a right angle. The solid circles represent the Si atoms lying on the plane, and the solid lines between them represent the hypothetical covalent bonds. Si atoms not on the plane are denoted by open circles.

STM images of Si (100) dimers – PRB 70, 235411 (2004)