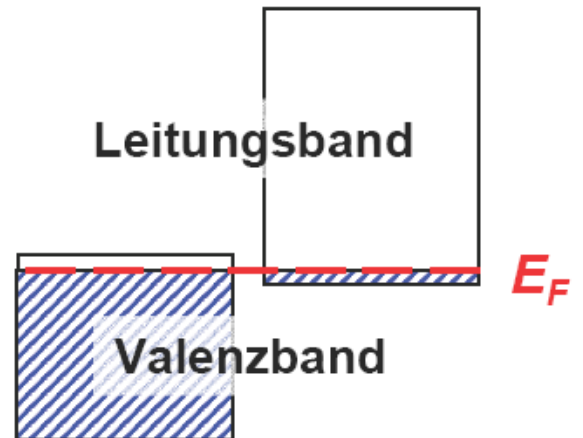
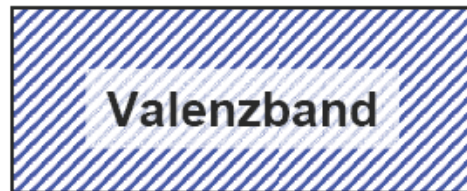
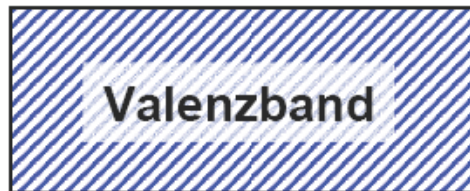
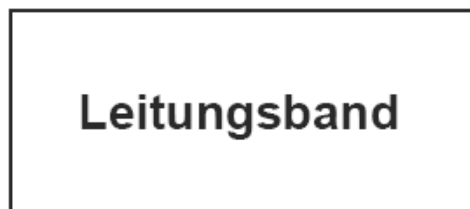
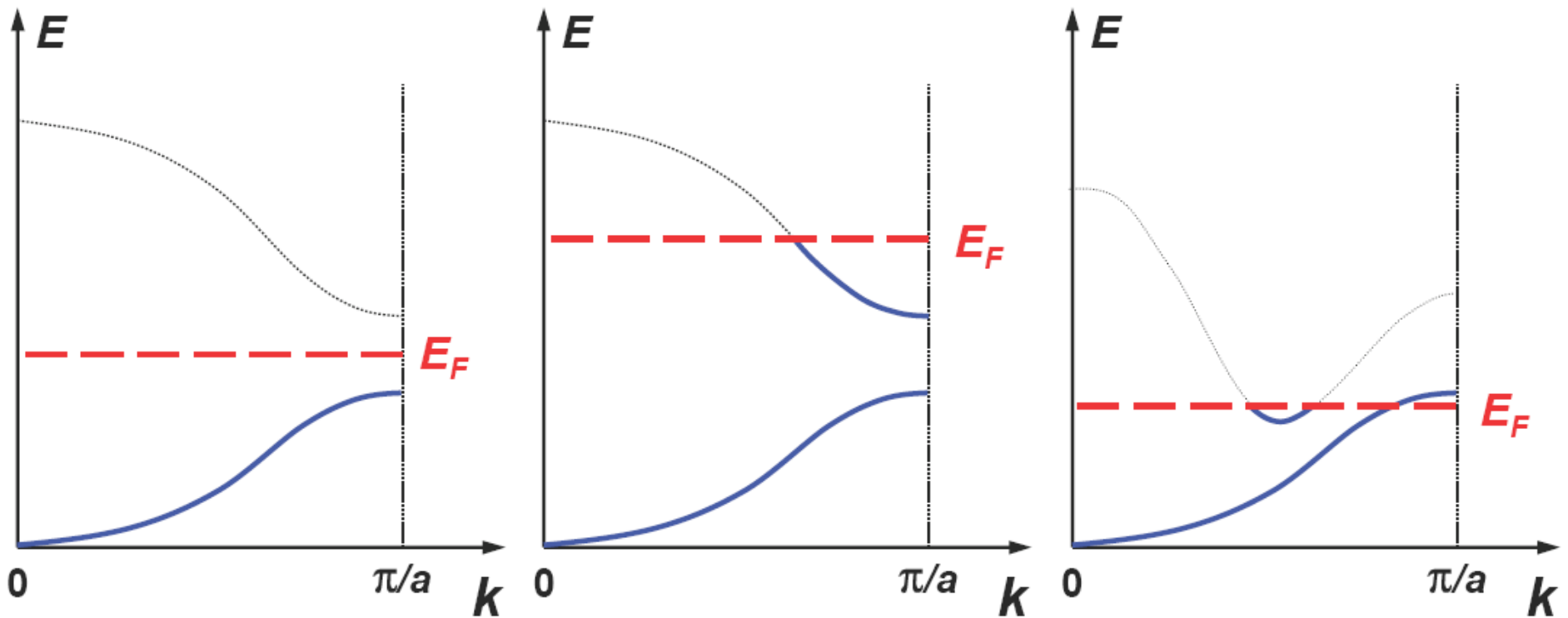


Je näher Zustand am Rand einer BZ,²
desto mehr beeinflusst Gitter die Energie



Isolator

Metall

Halbmetall

$n \ll 10^{22} \text{cm}^{-3}$
Sb As Bi

Zustände pro Band

1. Näherung fast freier Elektronen

Kristall mit Volumen V , monoatomare Basis, N Atome

also: $N = V/V_{\text{Zelle}}$ Einheitszellen

Elektronenzustand im k -Raum: $2\pi^3/V$

Volumen der BZ $2\pi^3/V_{\text{Zelle}}$

Zahl der Zustände in BZ: $N = V/V_{\text{Zelle}}$

Pro Band N verschiedene k -Werte, mit Spin $2N$ Elektronen je Band

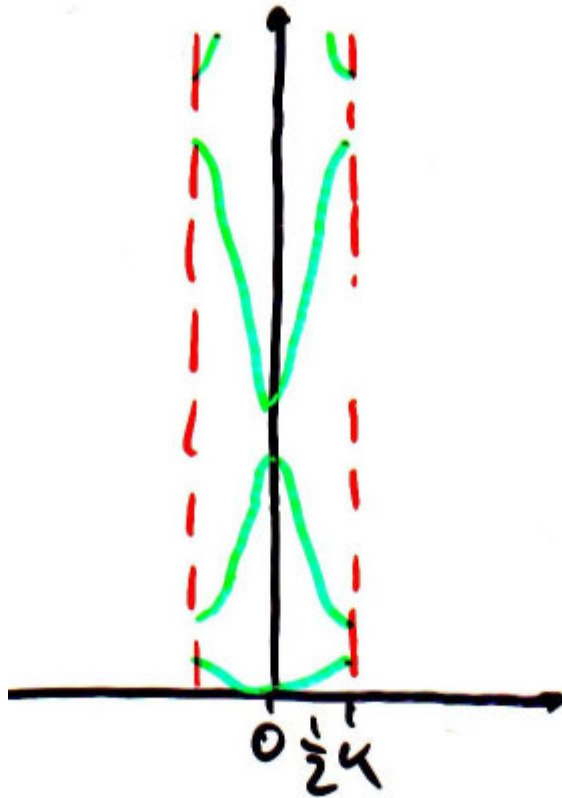
2. Näherung stark gebundener Elektronen

Gleicher Kristall

N -fach entartete atomaren Energieniveaus E_A^i

spalten in Bänder mit je N Zuständen (x 2 für Spinentartung)

Metal or Insulator: 1D case



Each band: 2 states per unit cell

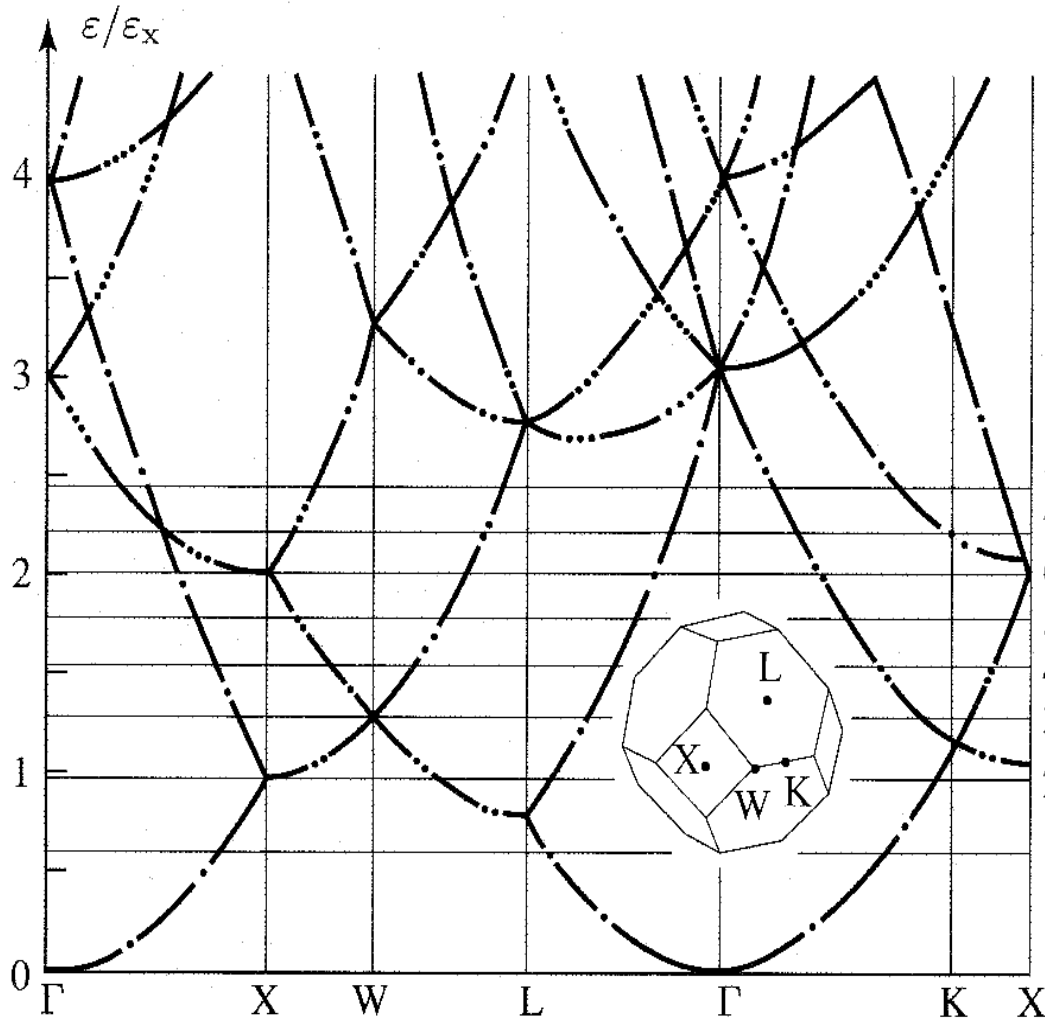
→ even number of electrons: **insulator**
(or **semiconductor**)

→ odd number of electrons: **metal**
Alkali **metals**: valency 1

But: Alkaline earths have valency 2
nevertheless: metals

3D effect: overlapping bands in different k-directions

Metal or Insulator: 3D case



Elektronen pro Einheitszelle

Energieniveaus freier Elektronen für ein fcc-Gitter längs der Richtungen von Γ ($k=0$) nach K, L, W und X.

ϵ_x ist die Energie im Punkt X ($[\hbar^2 k^2/2m] [2\pi/a]^2$).

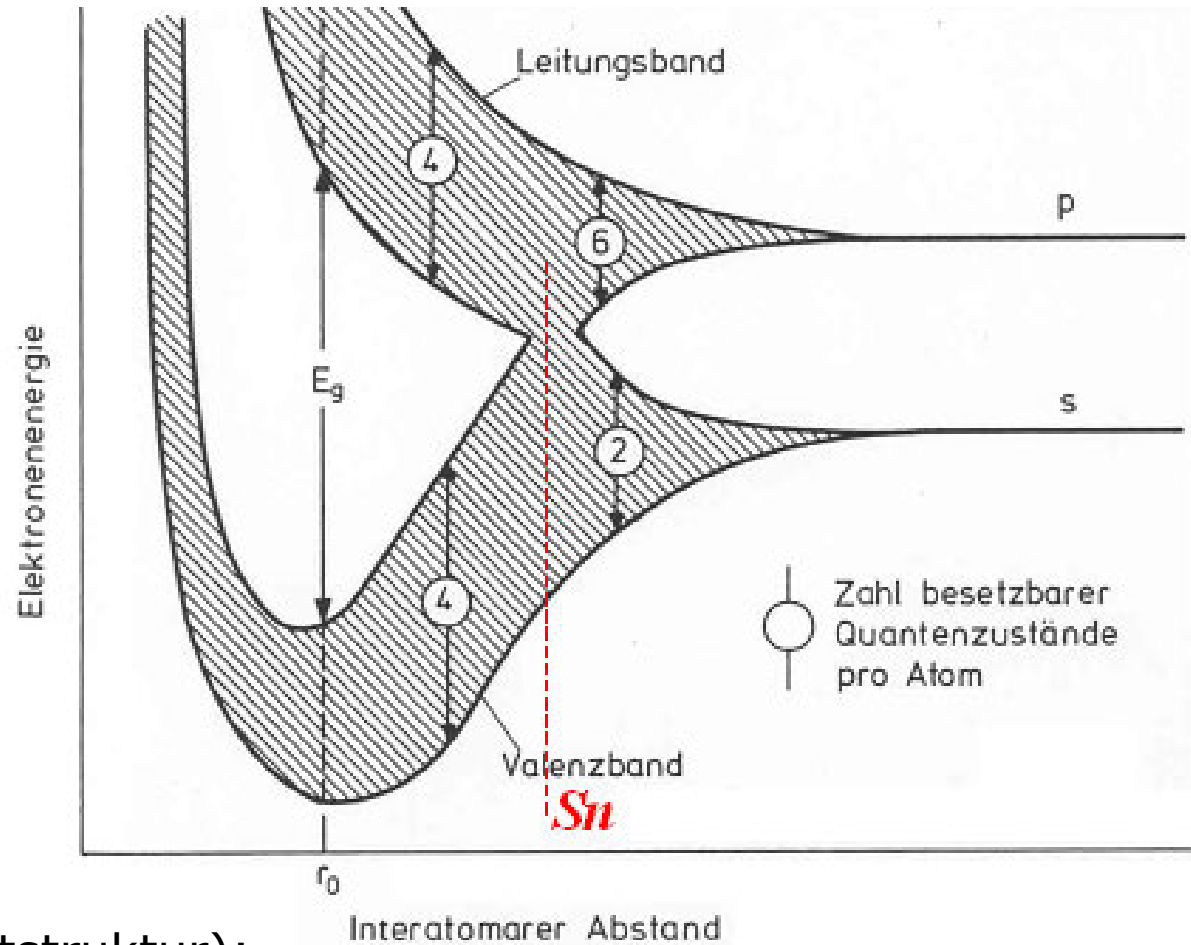
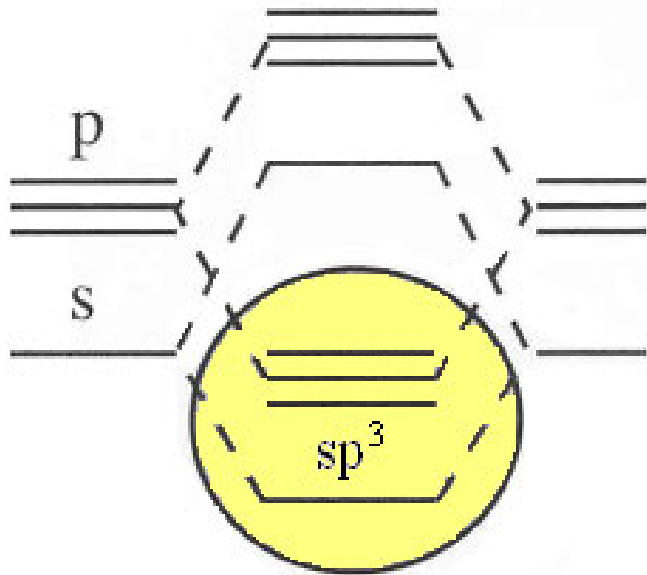
Horizontalen zeigen E_F für die angegebenen Elektronenzahlen.

Punkte auf den Kurven zeigen die Entartung der Niveaus freier Elektronen, die durch die Kurven repräsentiert werden.

aus F. Herman, „An Atomistic Approach to the Nature and Properties of Materials“, J. A. Pask, ed., Wiley, New York (1967)

Typical 3D dispersion with $U_G = 0$

(Some degeneracies lifted when $U_G \neq 0$)



Beispiel C ($1s^2, 2s^2, 2p^2$ mit Diamantstruktur):

atomaren s- und p-Orbitale bilden bindende & antibindende Zustände,
wobei die untersten 4 Zustände ein sp^3 -Hybrid bilden.

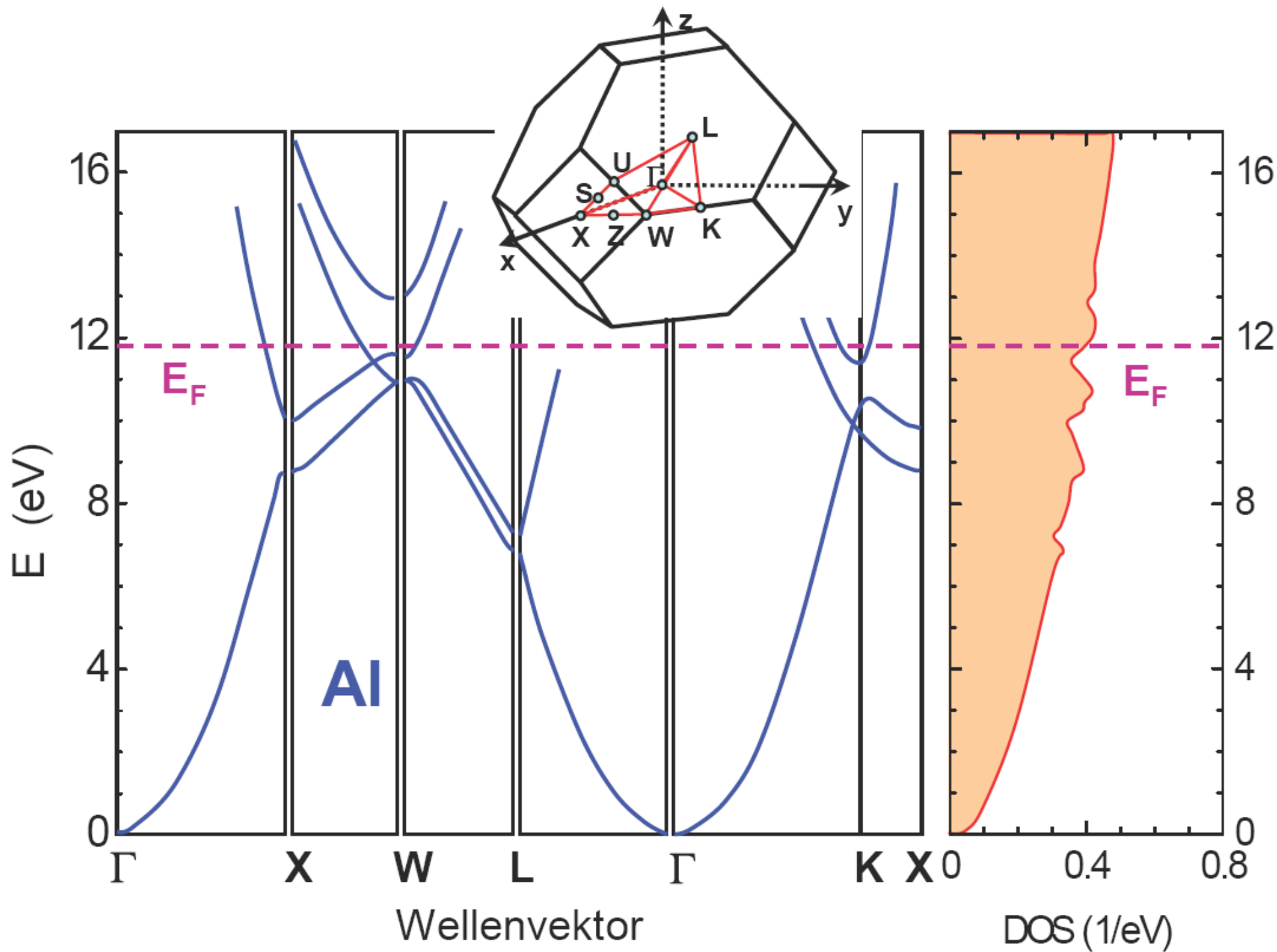
2 Atome in primitiver Einheitszelle, je mit 4 Elektronen

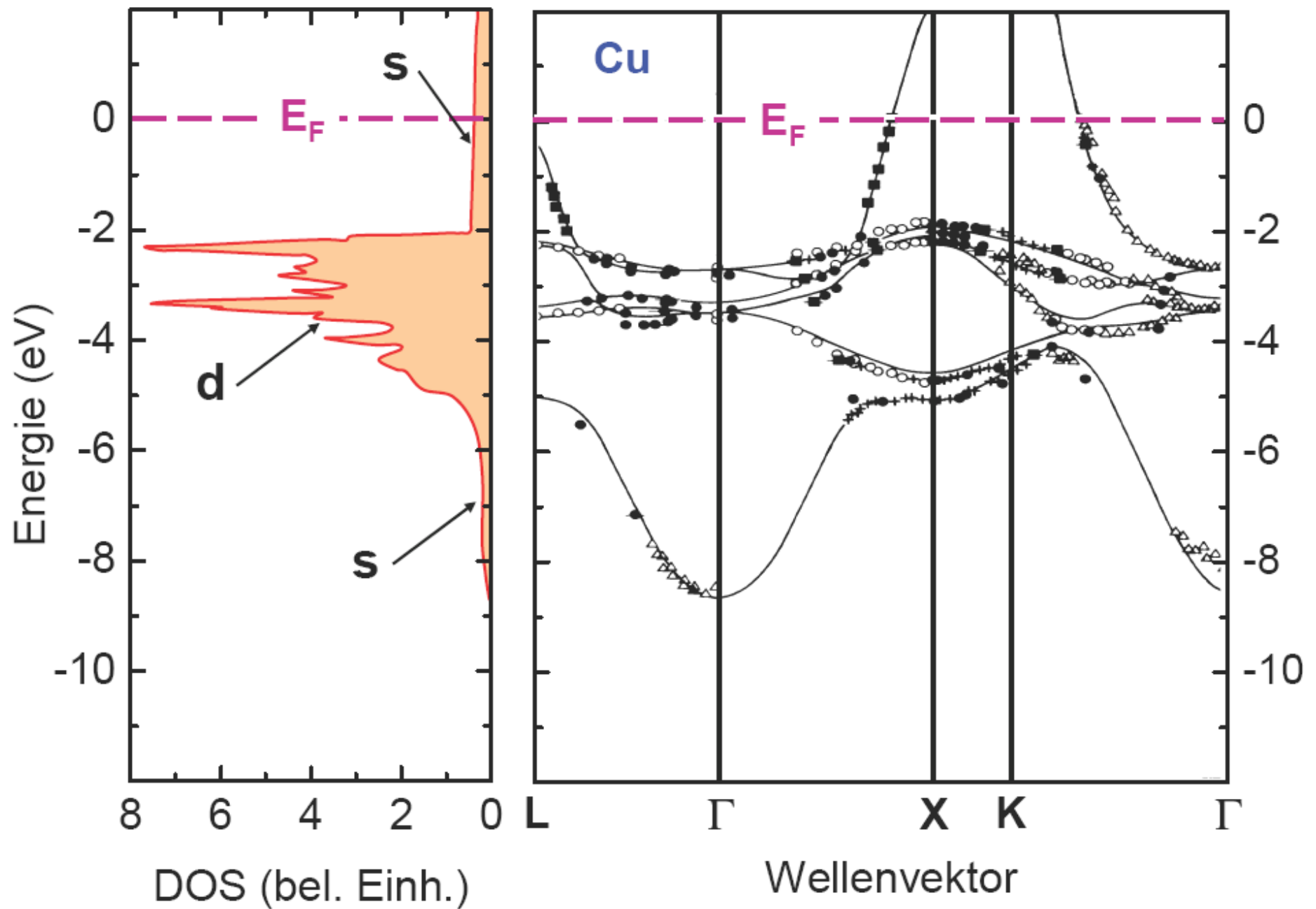
sp^3 -Band vollständig gefüllt

Lücke zum unbesetzten antibindenden sp^3 -Band

→ Diamant ist Nichtleiter, Zinn ein Metall (oder HL)

| | E_{gap}/eV | a/nm |
|----|----------------------------|---------------|
| C | 5 | 0.365 |
| Si | 1.1 | 0.534 |
| Ge | 1.0 | 0.566 |
| Sn | Metall | 0.646 |





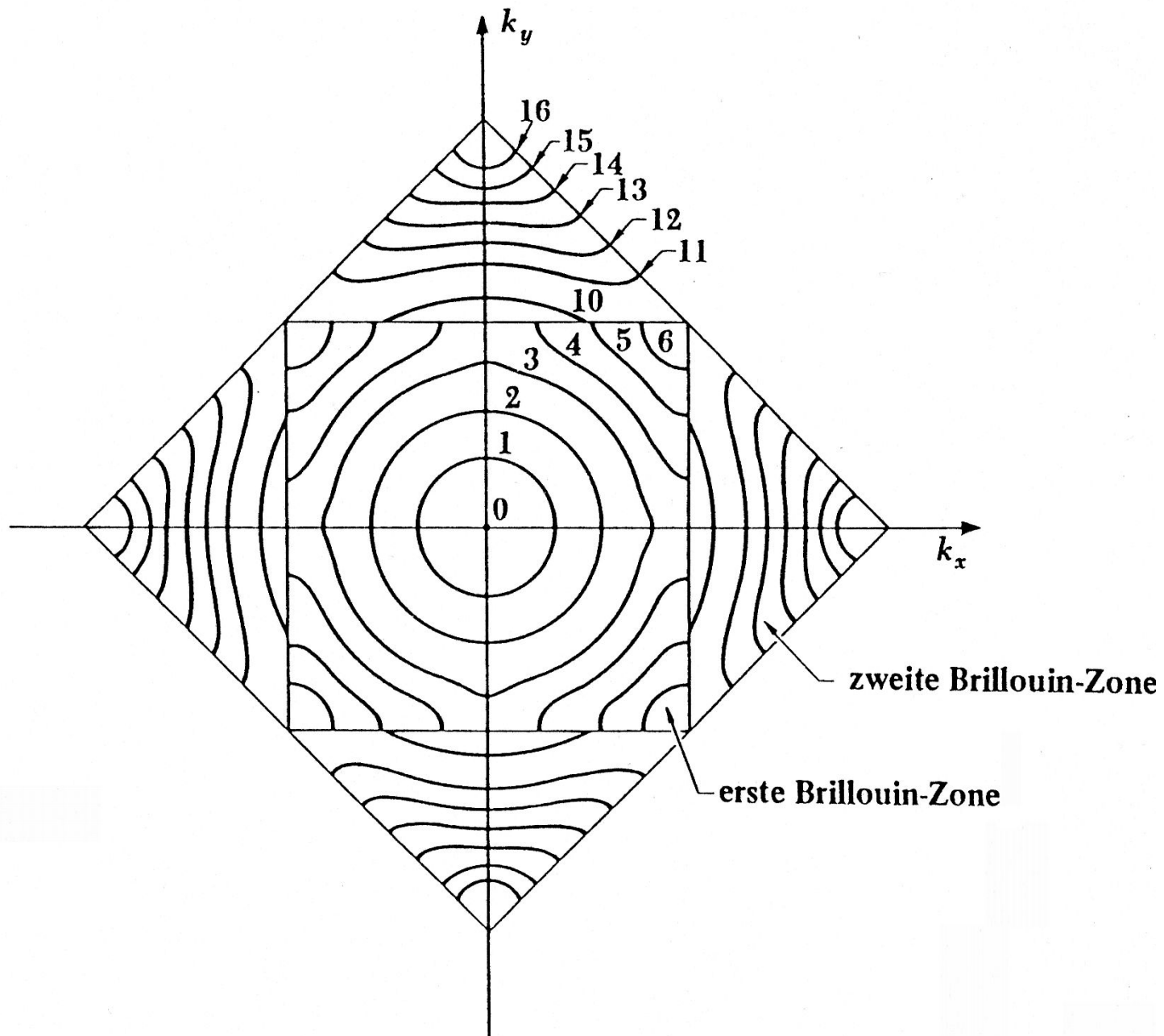
Bandstruktur von Cu Symbole: exp. Daten aus Courths & Hüfner, Phys. Rep. 112, 55 ('84)

lokalisiertere, anisotrope 3d-Orbitale ergeben fünf schmale Bänder mit komplexer Form⁹

4s-Band wesentlich breiter, Dispersion wie freie Elektronen

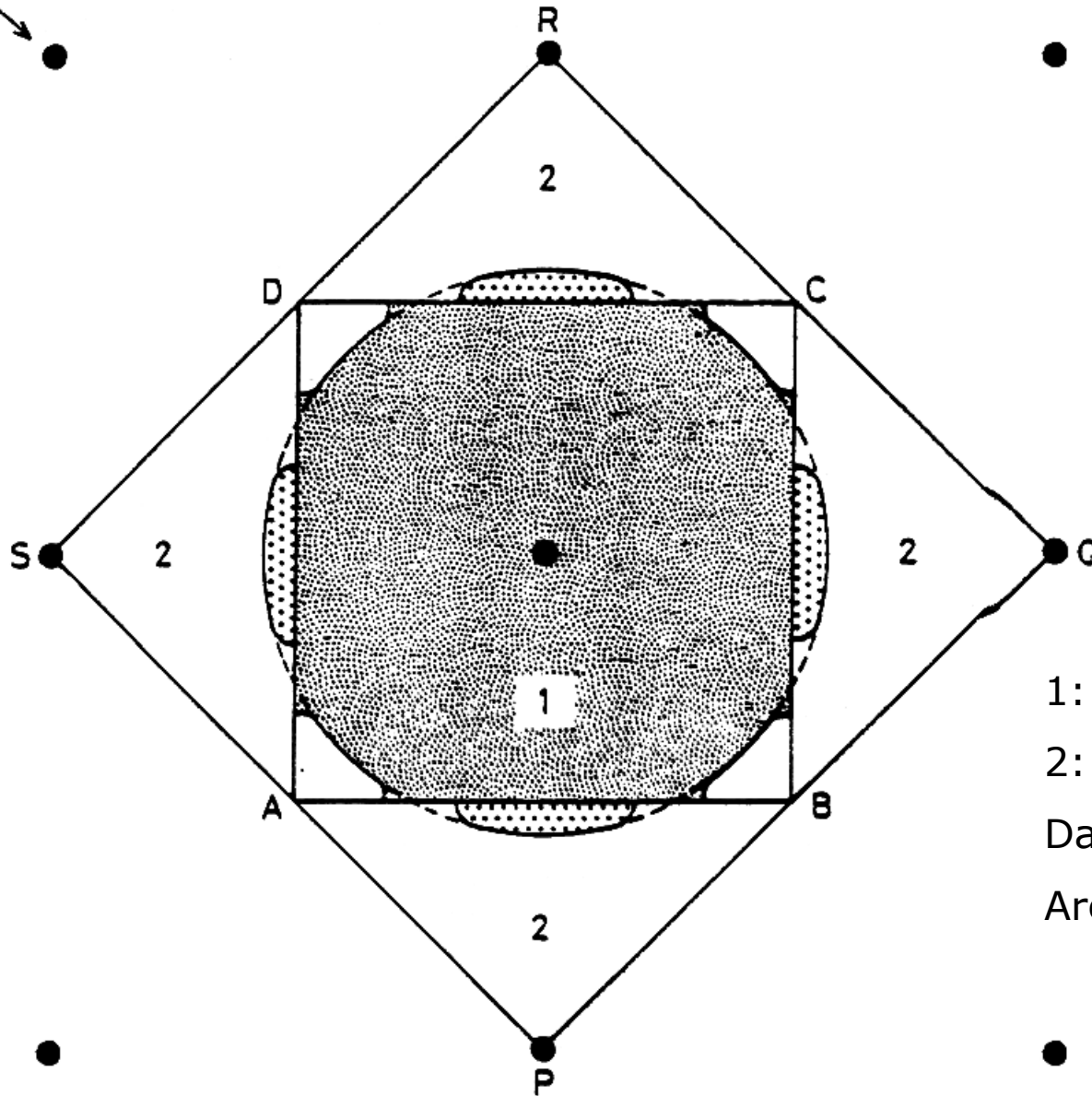
Fermiflächen

1. und 2. Brillouinzone eines Quadratgitters Linien konstanter Energie



Fermi surface of a divalent 2D-metal within the NFE-model

reciprocal lattice points



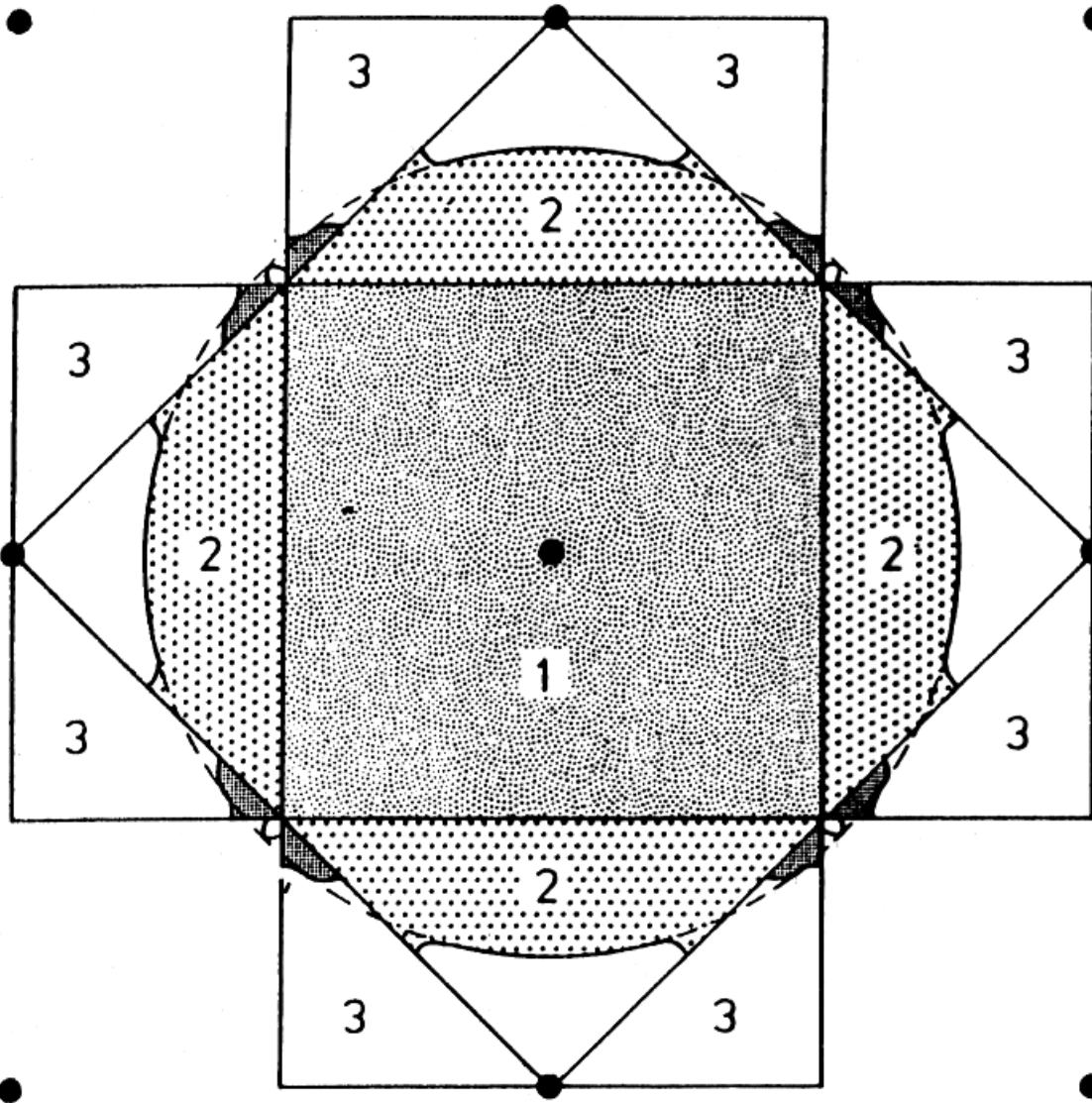
1: 1st BZ

2: 2nd BZ

Dashed circle: FEG Fermi surface

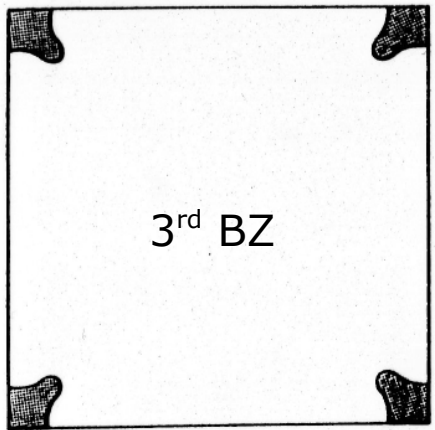
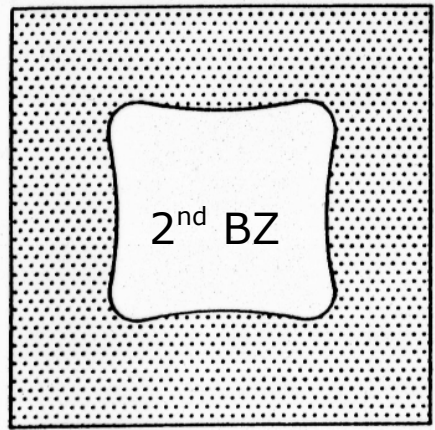
Area of circle = area of 1st BZ

Fermi surface of a trivalent 2D-metal within the NFE-model

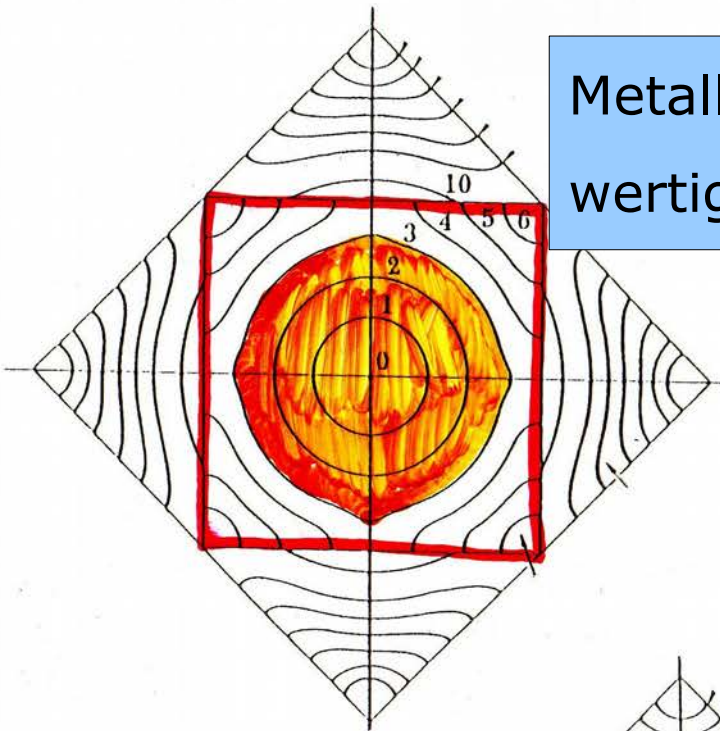


Reduced zone scheme

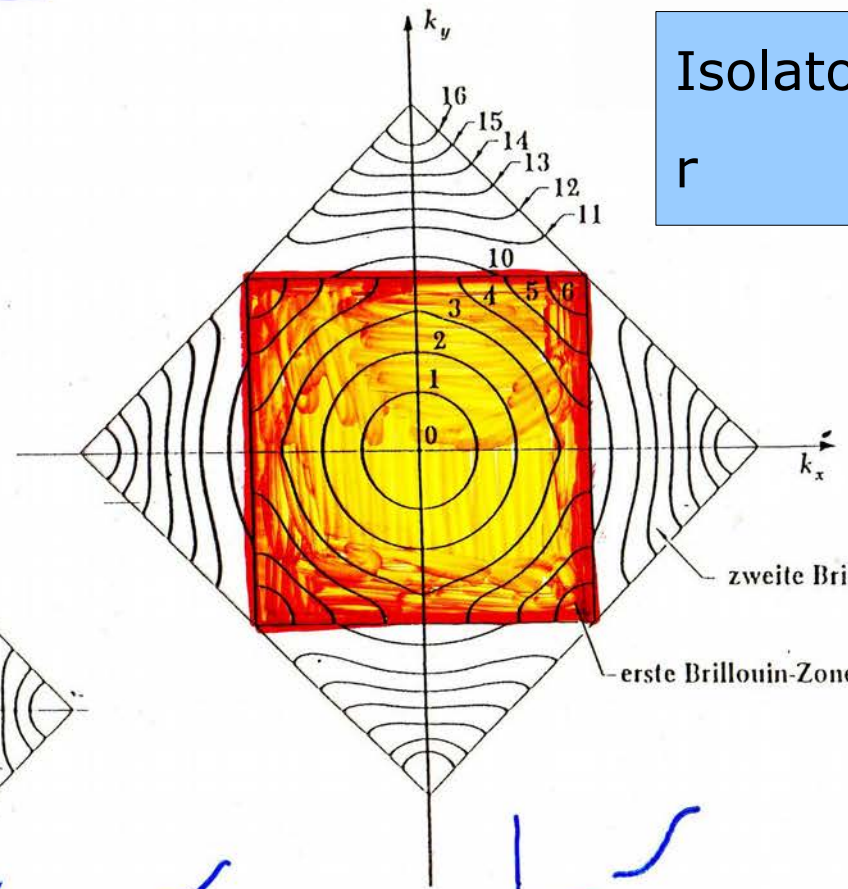
1st BZ: filled



Area of FE-circle (dashed) = 1.5 area of 1st BZ

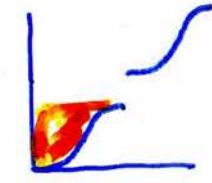
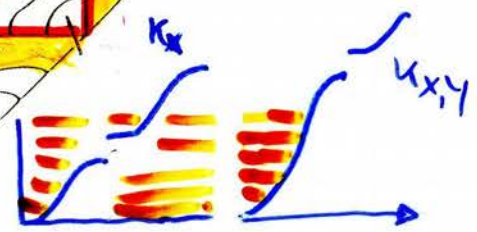
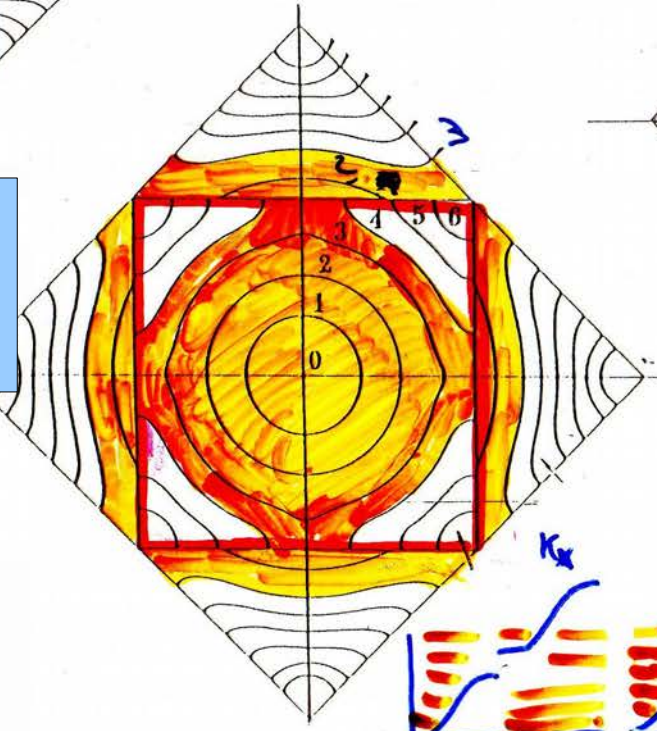


Metall-1-
wertig



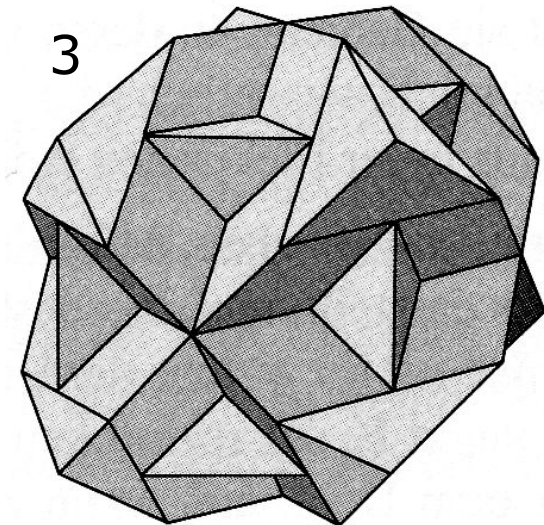
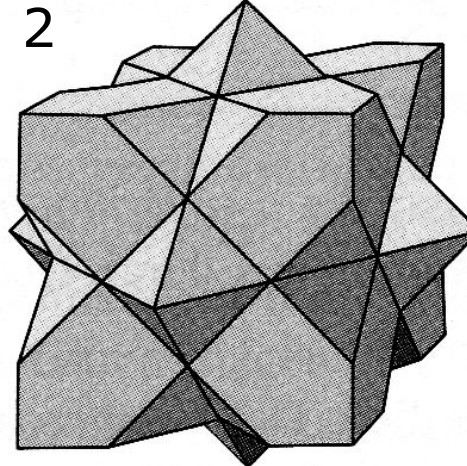
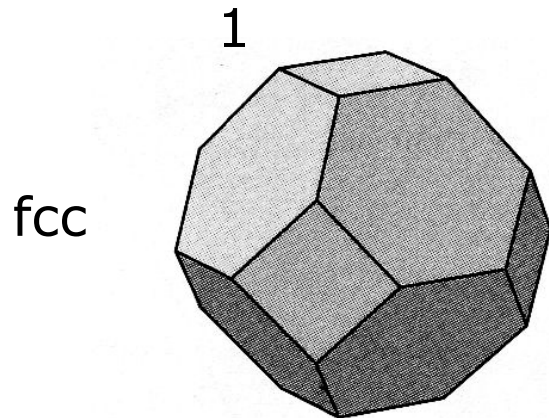
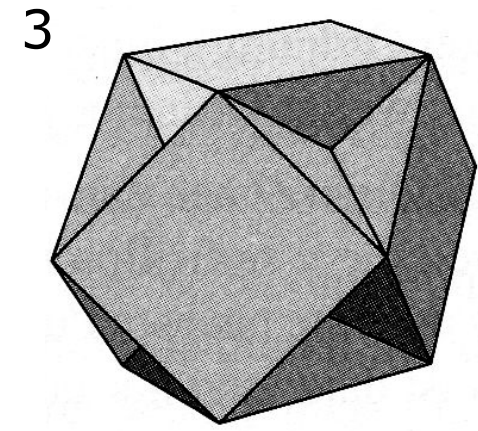
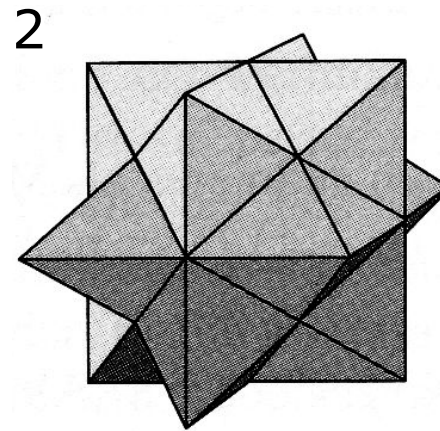
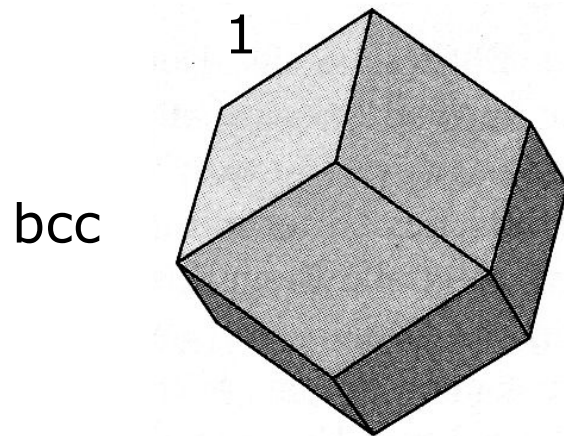
Isolato
r

Metall-2-
wertig

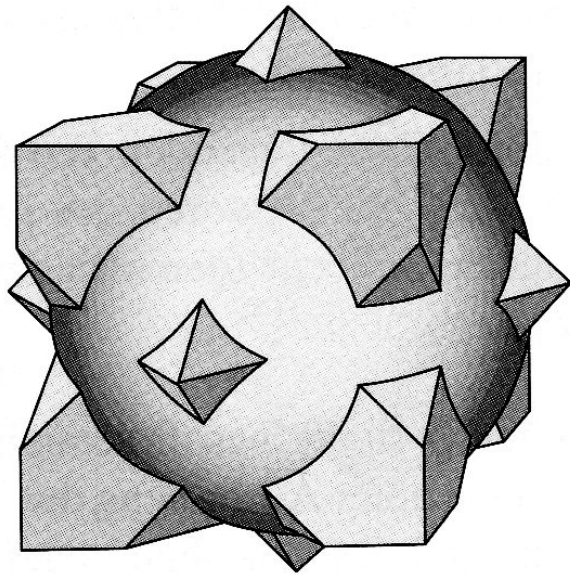


Äußere Oberflächen der 1., 2., 3. BZ

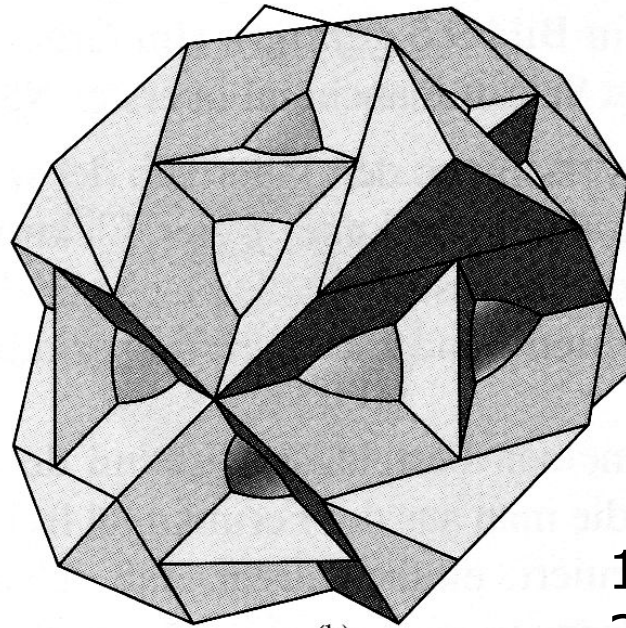
Innere Oberflächen der 2. = äußere der 1., usf.



Fermifläche vierwertiges fcc-Metall

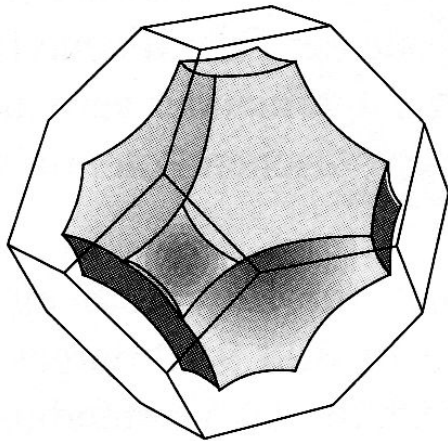


(a)

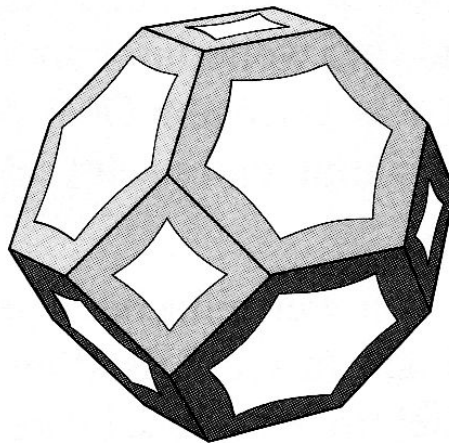


(b)

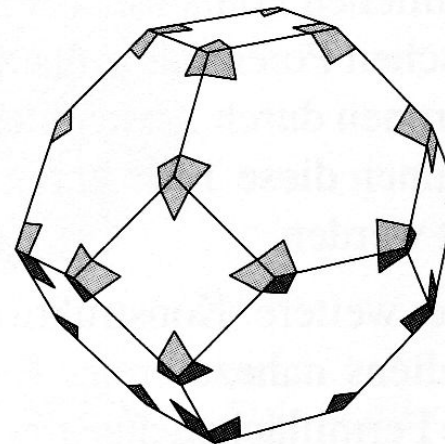
1. BZ voll in Fermikugel
2.-4. BZ teils.



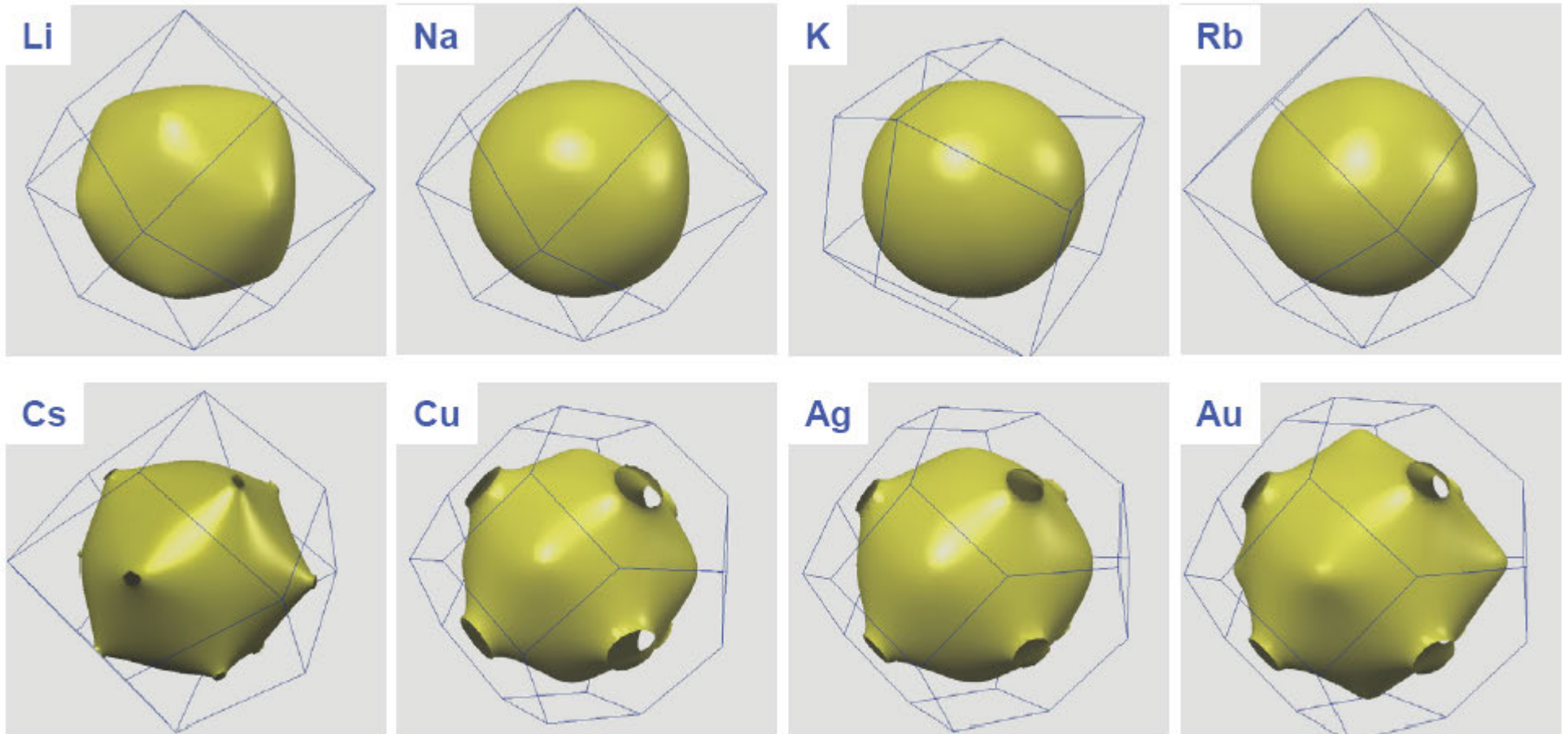
2. BZ



3. BZ



4. BZ

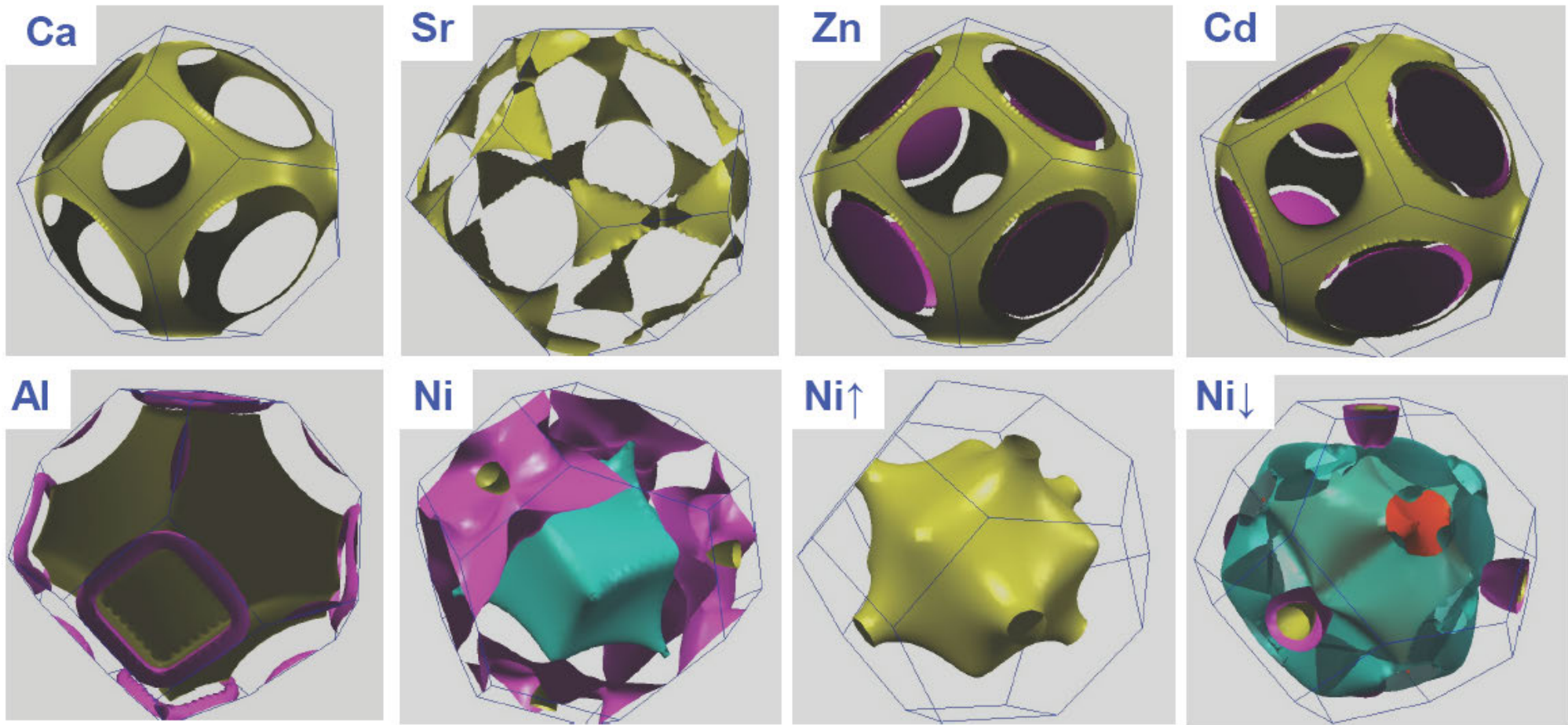


Fermiflächen einfacher Metalle

Alkalimetalle bcc

Münzmetalle fcc

(Quelle: Physics Department, University of Florida)



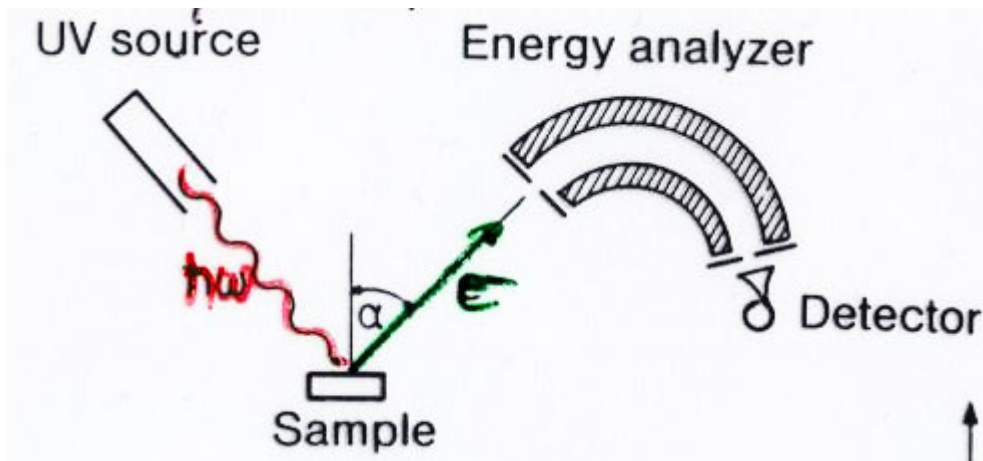
Fermiflächen

Ca, Sr, Al, Ni: fcc

Zn, Cd: eigentlich hcp, gezeigt ist fcc-Struktur zum Vergleich mit Ca, Sr

(Quelle: Physics Department, University of Florida)

Photoelectron Spectroscopy



occupied states

UPS: valence band (ARPES)

XPS: core levels (ESCA)

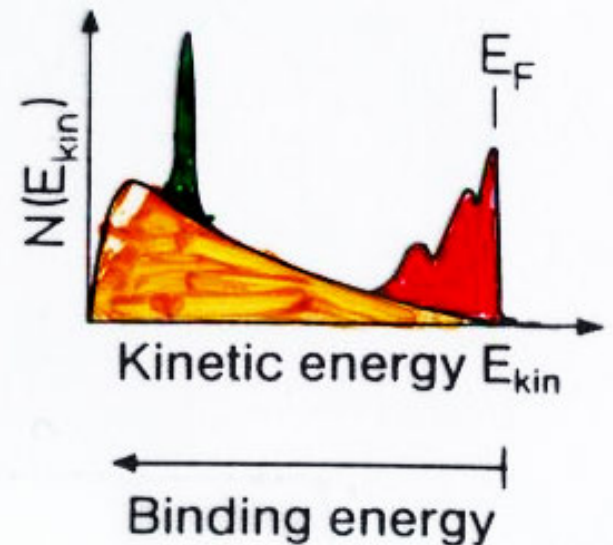
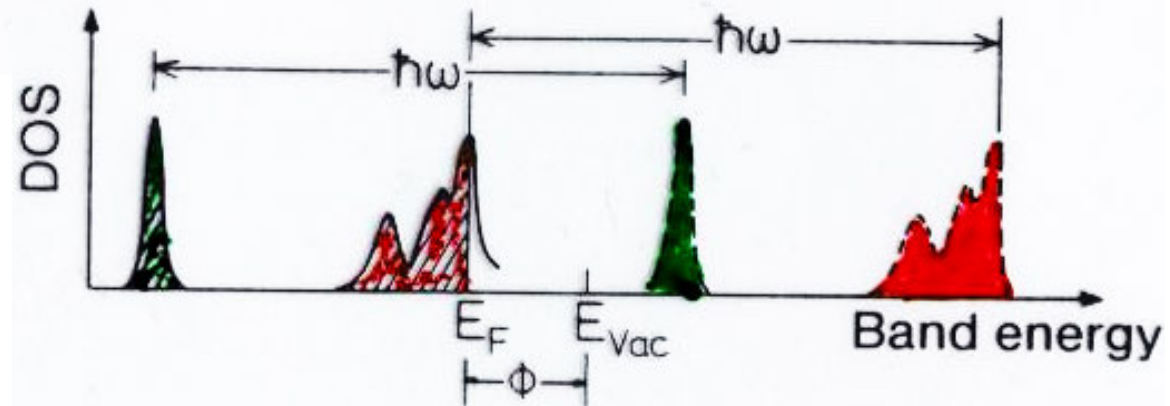
unoccupied states: IPES

conservation of energy

$$E_{kin} = h\omega - E_b$$

conservation of parallel momentum

$$\hbar K = \sqrt{2mE_{kin}} \sin(\alpha) = \hbar K_f = \hbar K_i$$



Angle Resolved Photoemission / Inverse Photoemission (ARUPS, KRIPES)

vertical transitions

IPES

vary E_{kin}

isochromat spectra



Today: Fermi surface mapping is a routine job

Constant- $|k|$ cut through Fermi surface of Cu(100)



ALS

model

data

