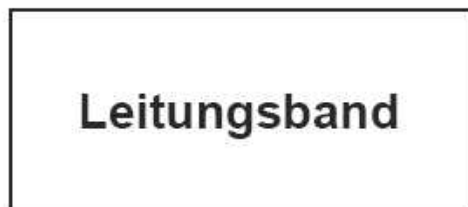
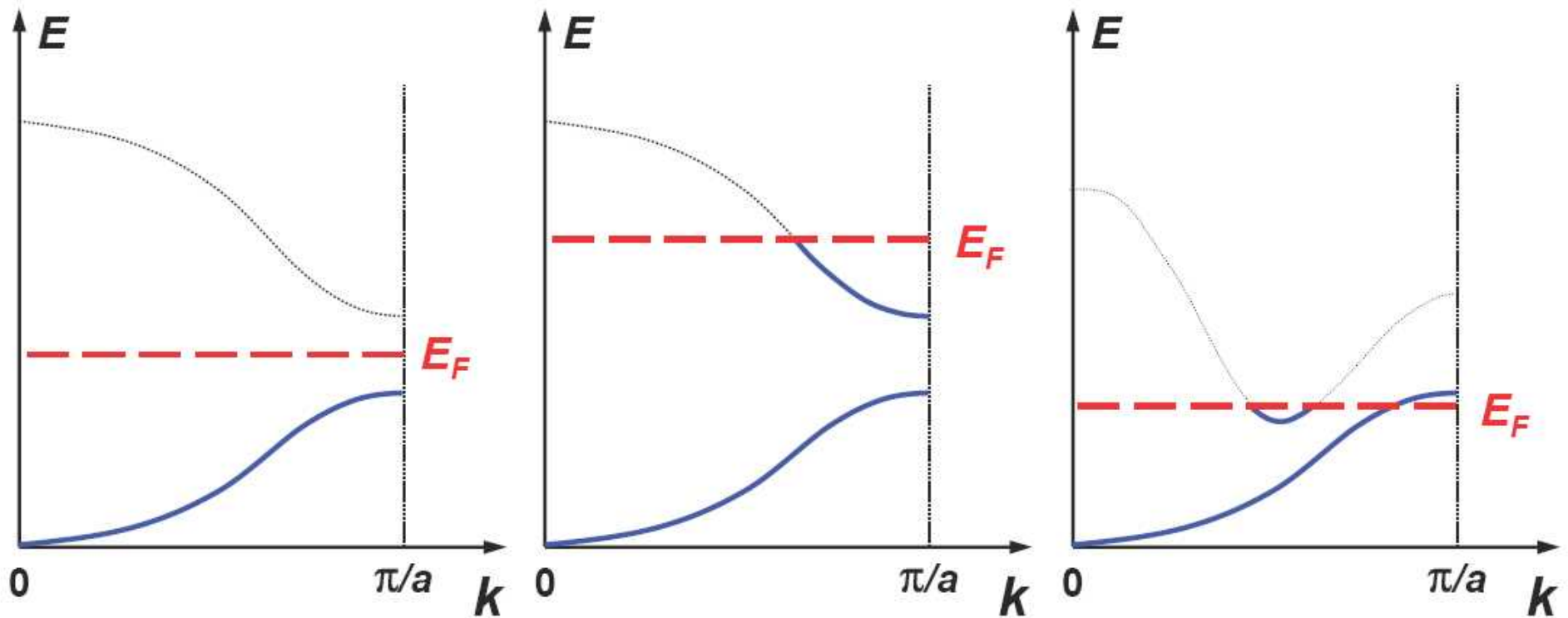


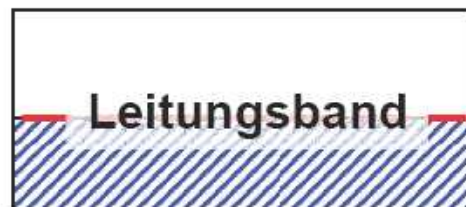
Je näher Zustand am Rand einer BZ, desto mehr beeinflusst Gitter seine Energie



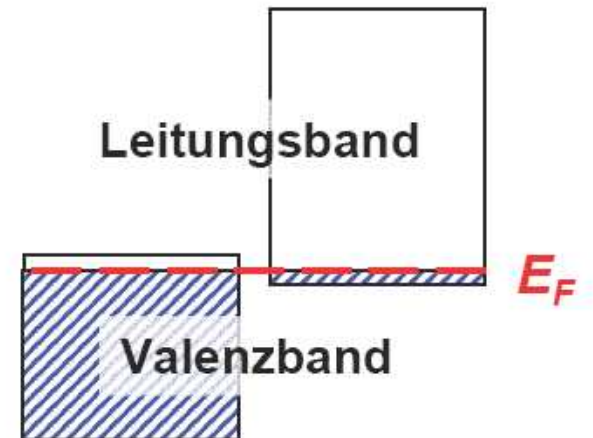
E_F



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 , N Atome, monatomare Basis

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 also N verschiedene k , mit Spin $2N$ Elektronen je Band

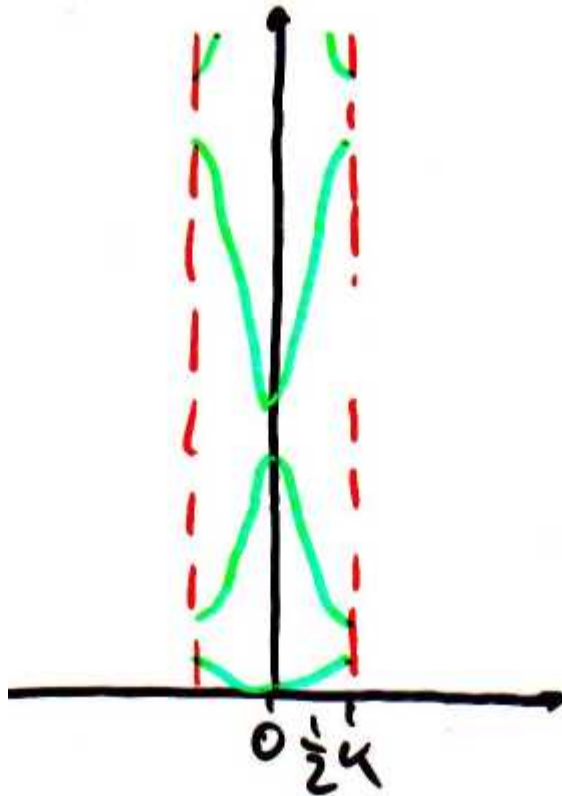
2. Näherung stark gebundener Elektronen

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**)

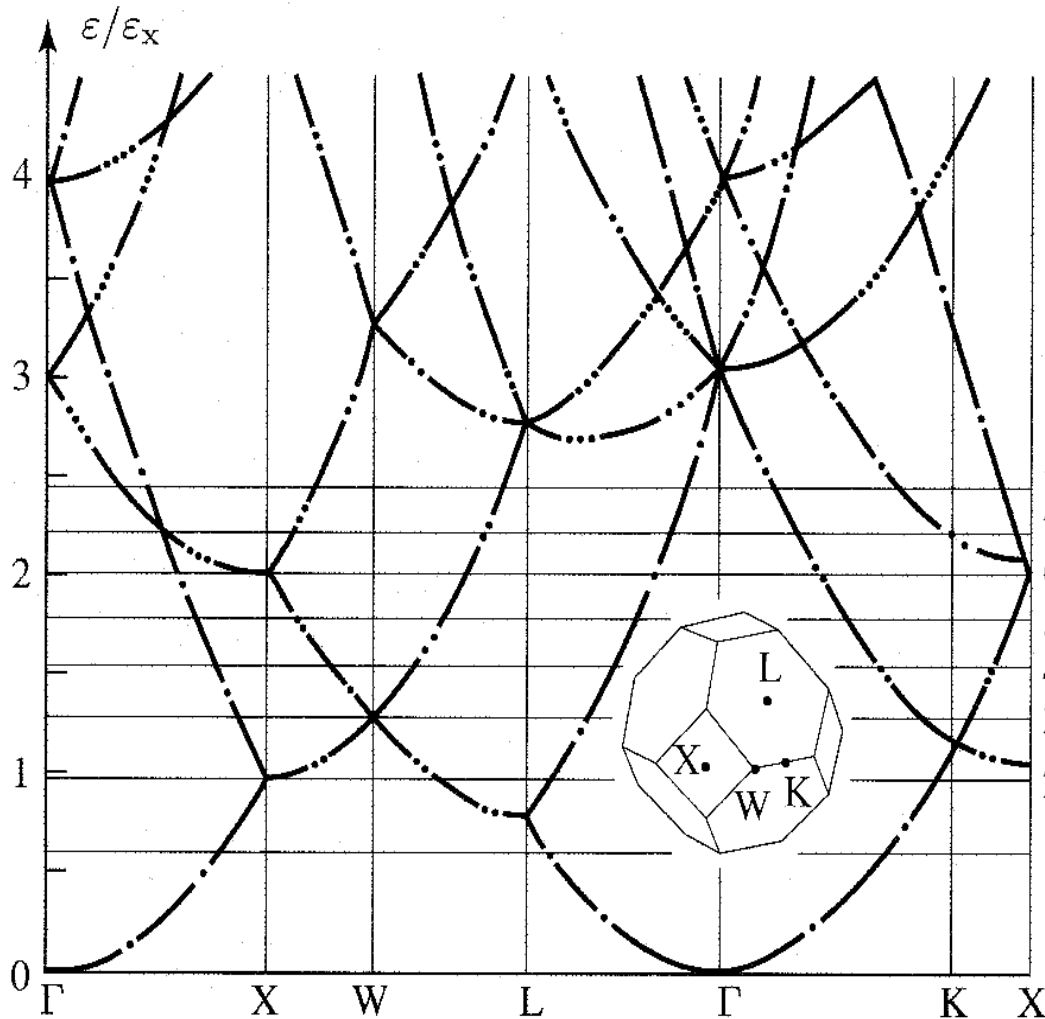
→ odd number of electrons: **metal**

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

ϵ_x : Energie im Punkt X, $\hbar^2/2m [2\pi/a]^2$

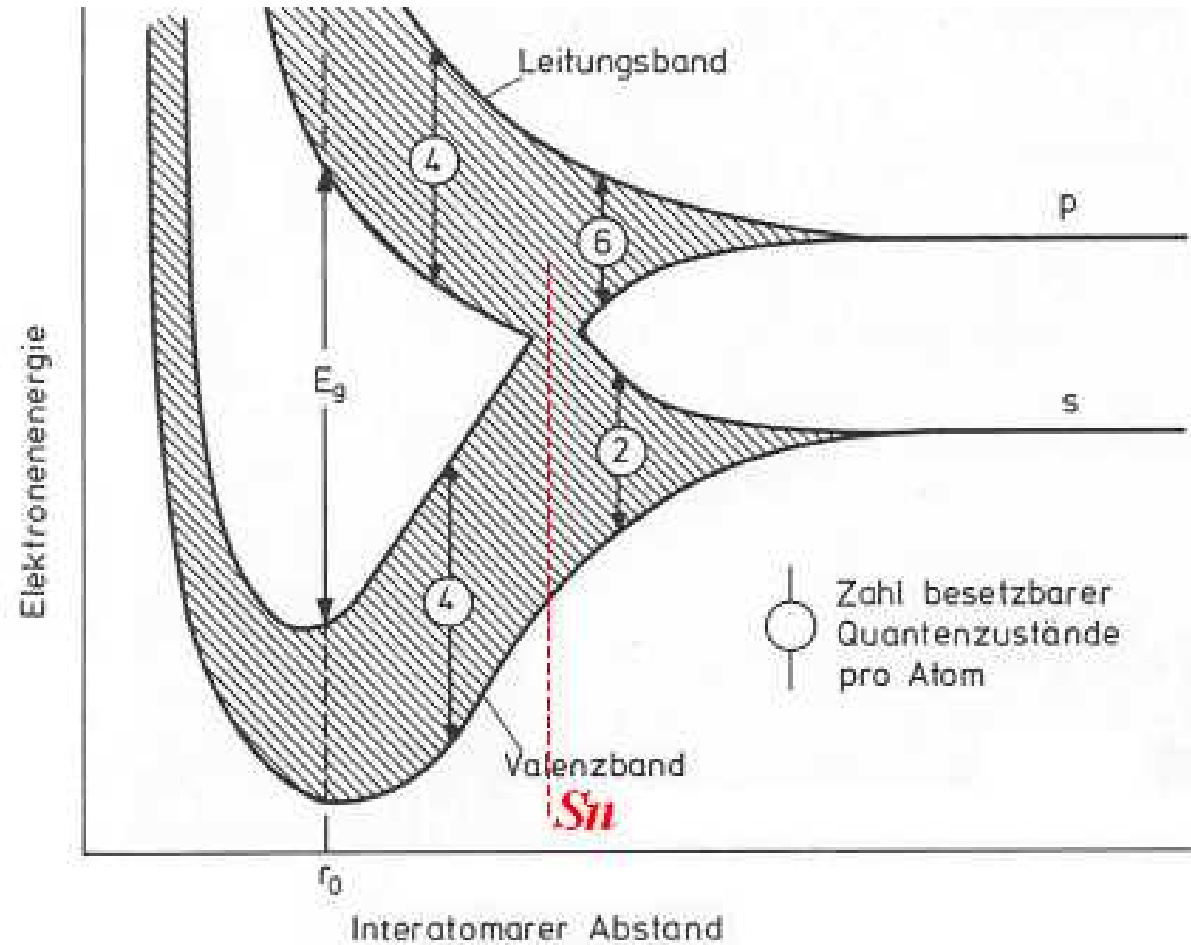
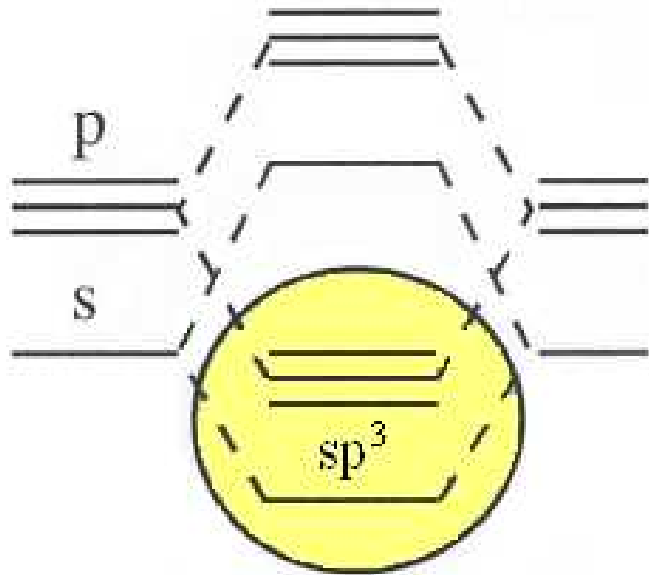
Horizontalen: E_F für angegebene Elektronenzahlen

Punkte auf den Kurven: Entartung der Niveaus

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

3D dispersion with $U_G = 0$

when $U_G \neq 0$: some degeneracies lifted
gaps open up



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

atomaren s - und p -Orbitale bilden ein sp^3 -Hybridorbital

bindende & antibindende Zustände

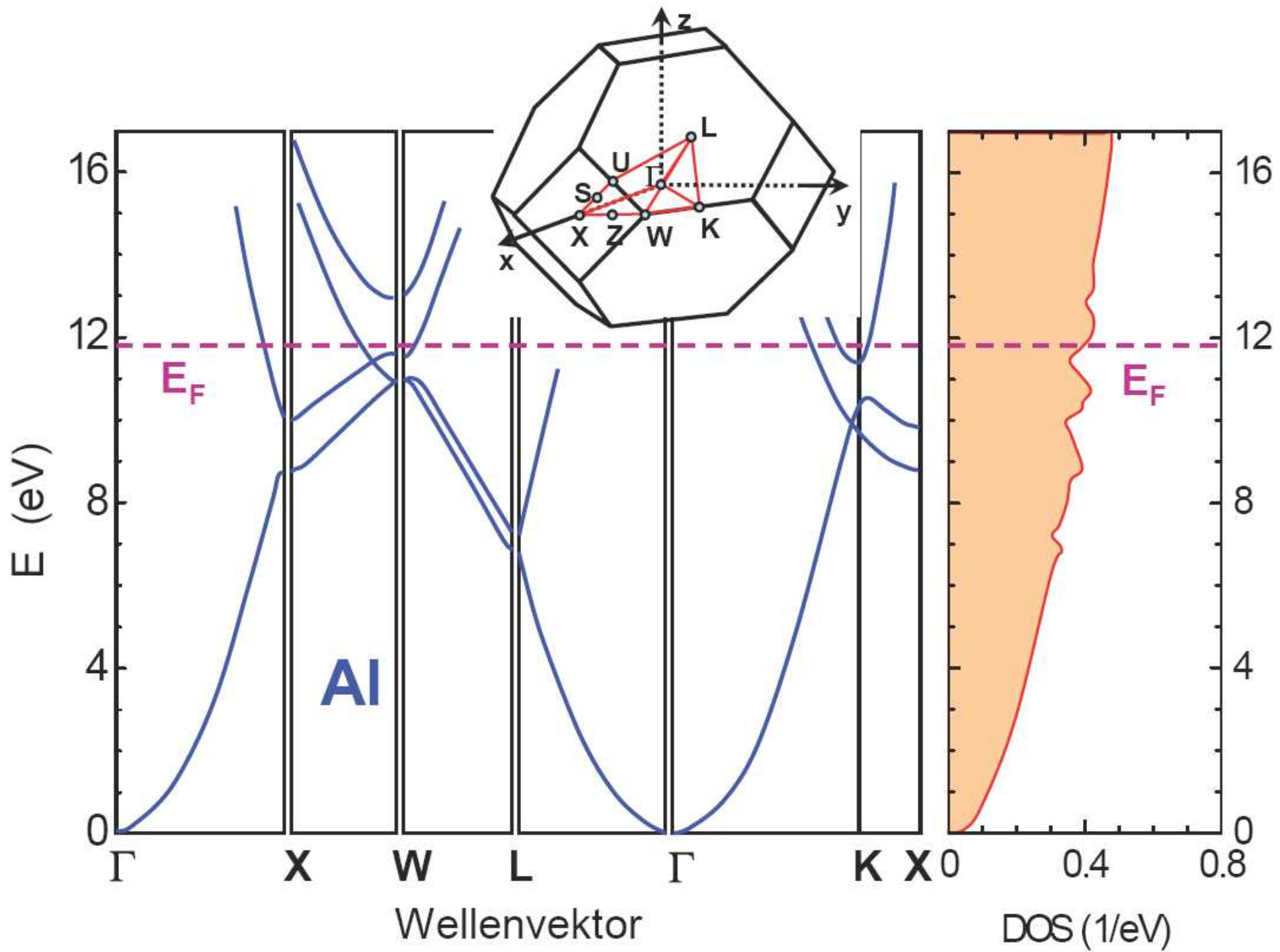
2 Atome in primitiver Einheitszelle, je mit 4 Elektronen

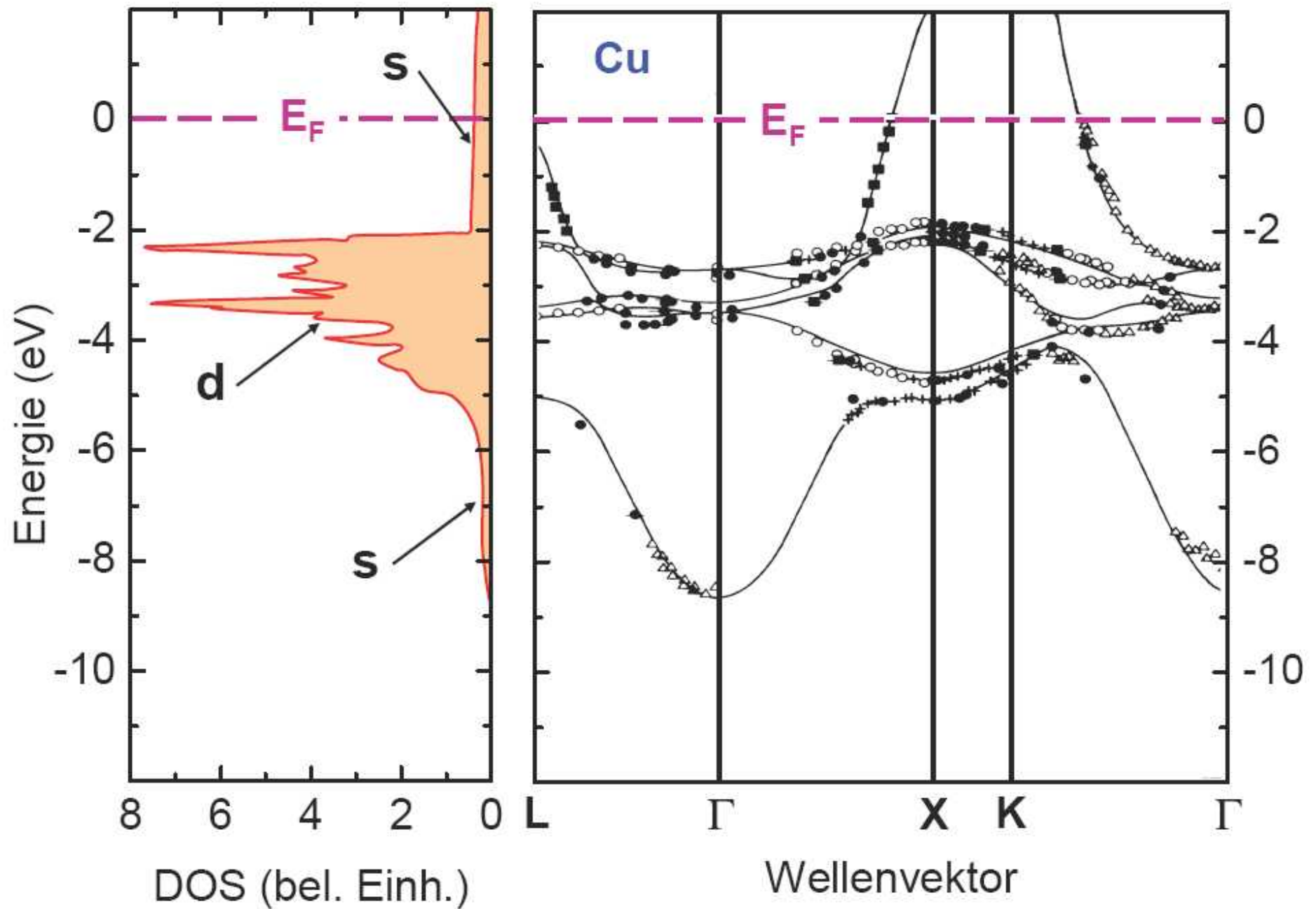
sp^3 -Band vollständig gefüllt

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 Courths & Hüfner, Phys. Rep. **112**, 55 (1984)

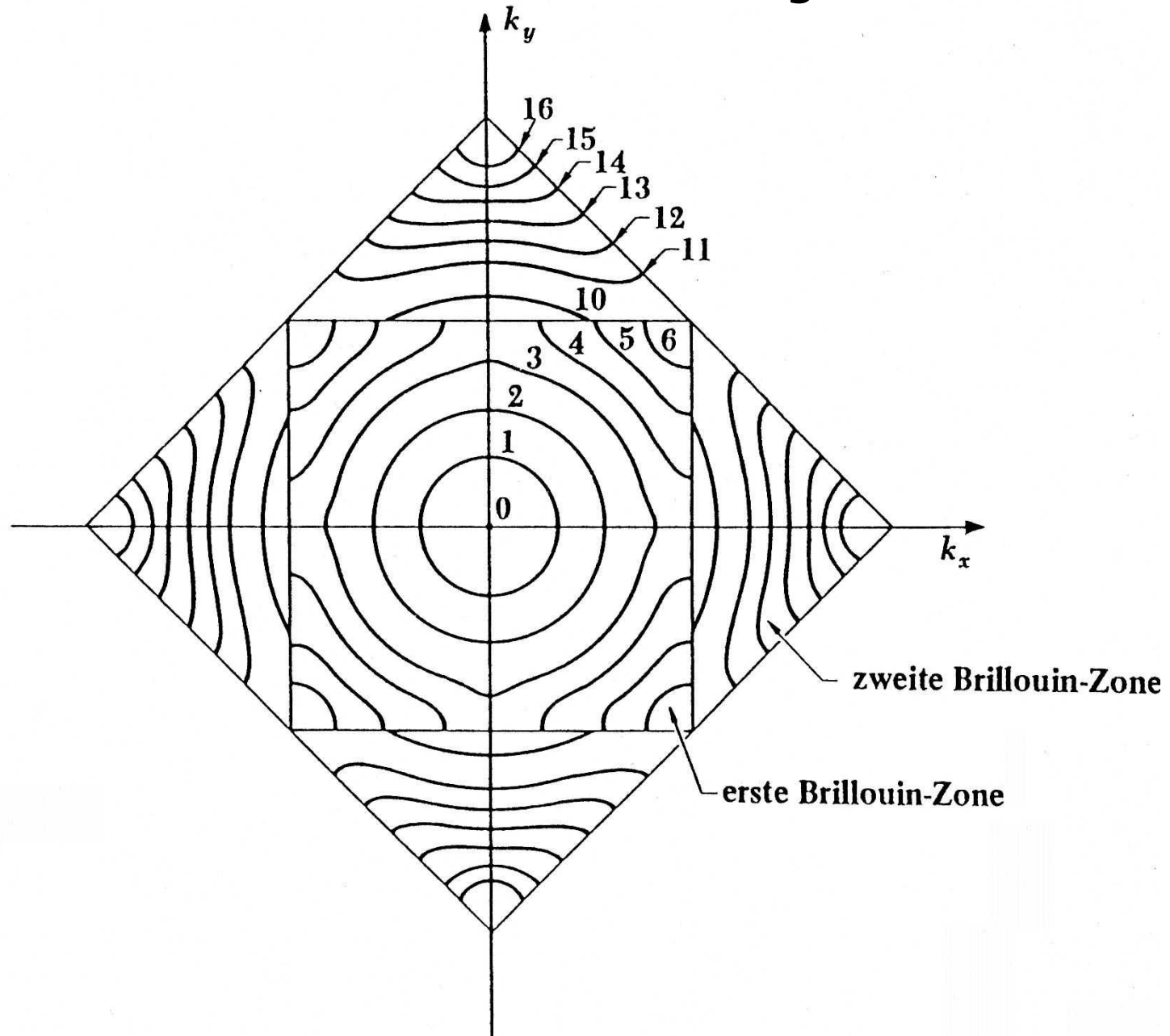
lokalisierte, anisotrope 3d-Orbitale ergeben fünf schmale Bänder

4s-Band wesentlich breiter, Dispersion wie freie Elektronen

Fermiflächen

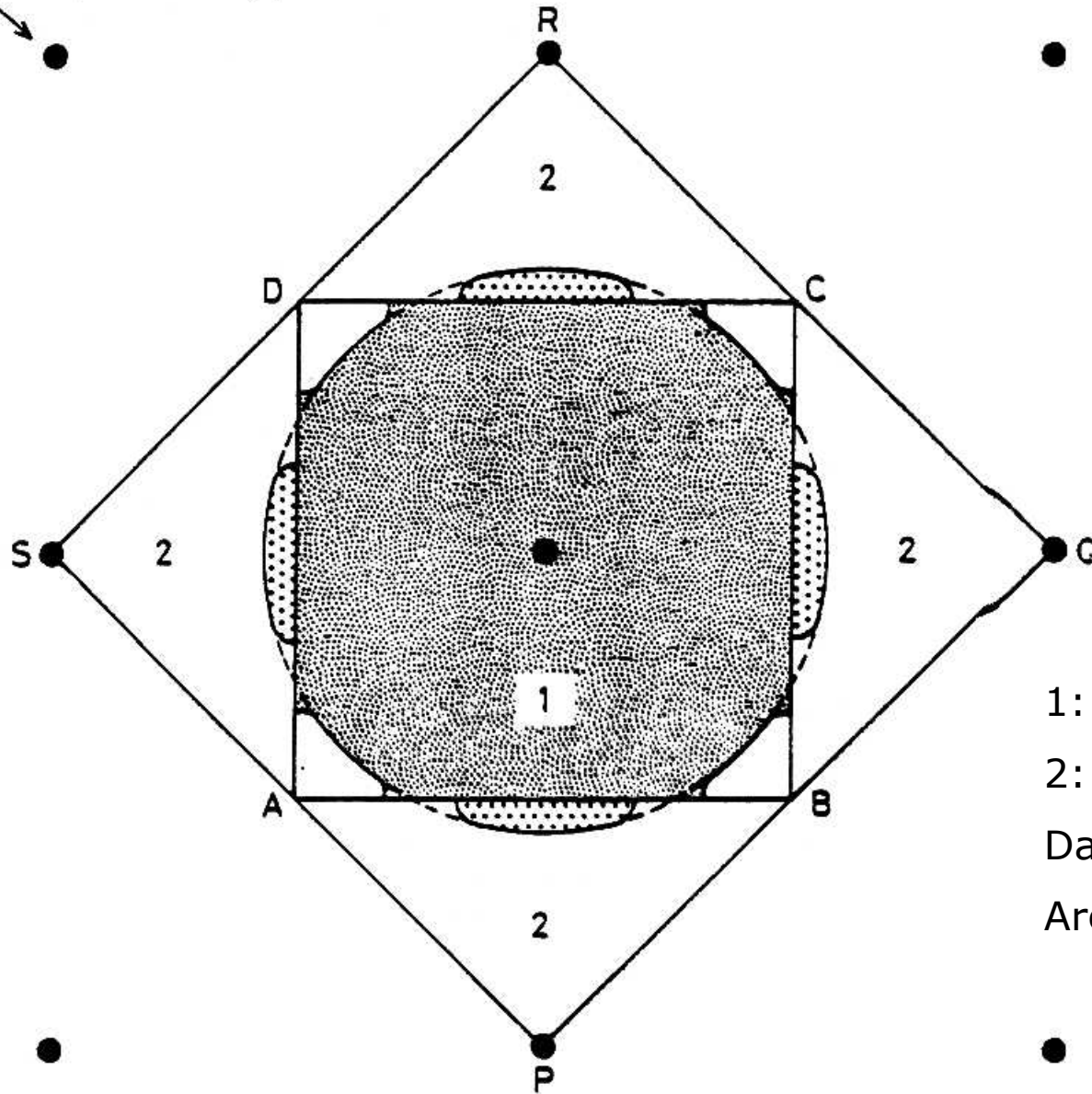
1. und 2. Brillouinzone eines Quadratgitters

Linien konstanter Energie



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

reciprocal lattice points



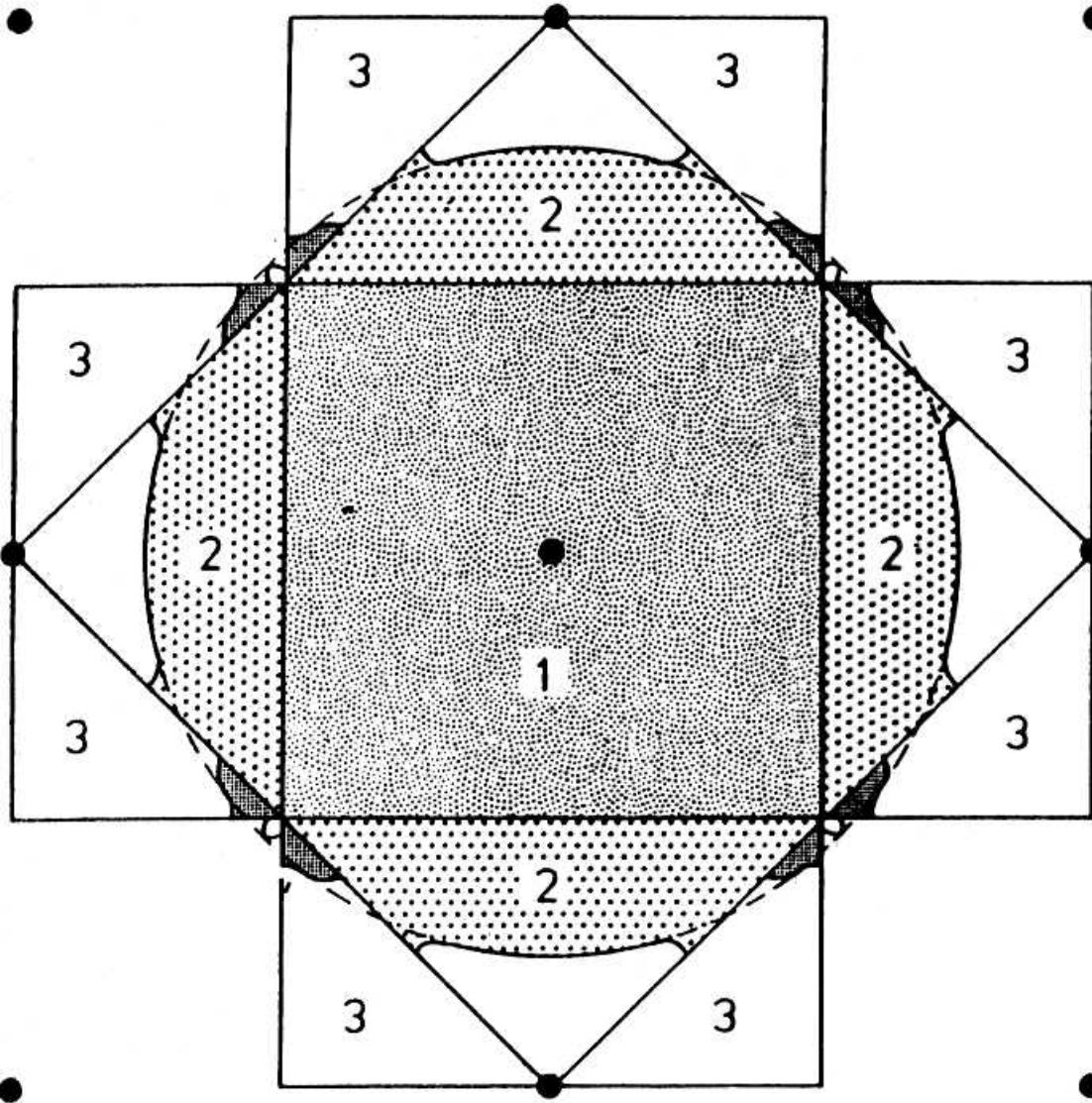
1: 1st BZ

2: 2nd BZ

Dashed circle: FEG Fermi surface

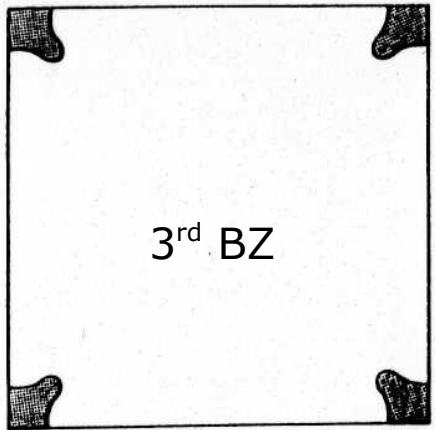
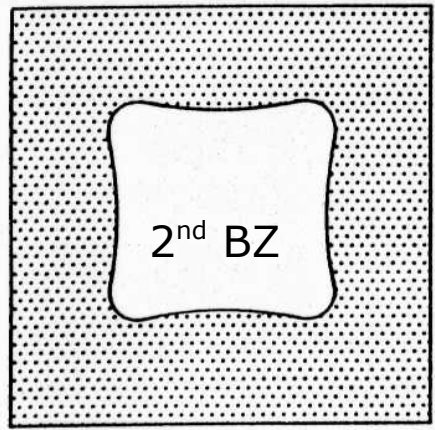
Area of circle = area of 1st BZ

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



Reduced zone scheme

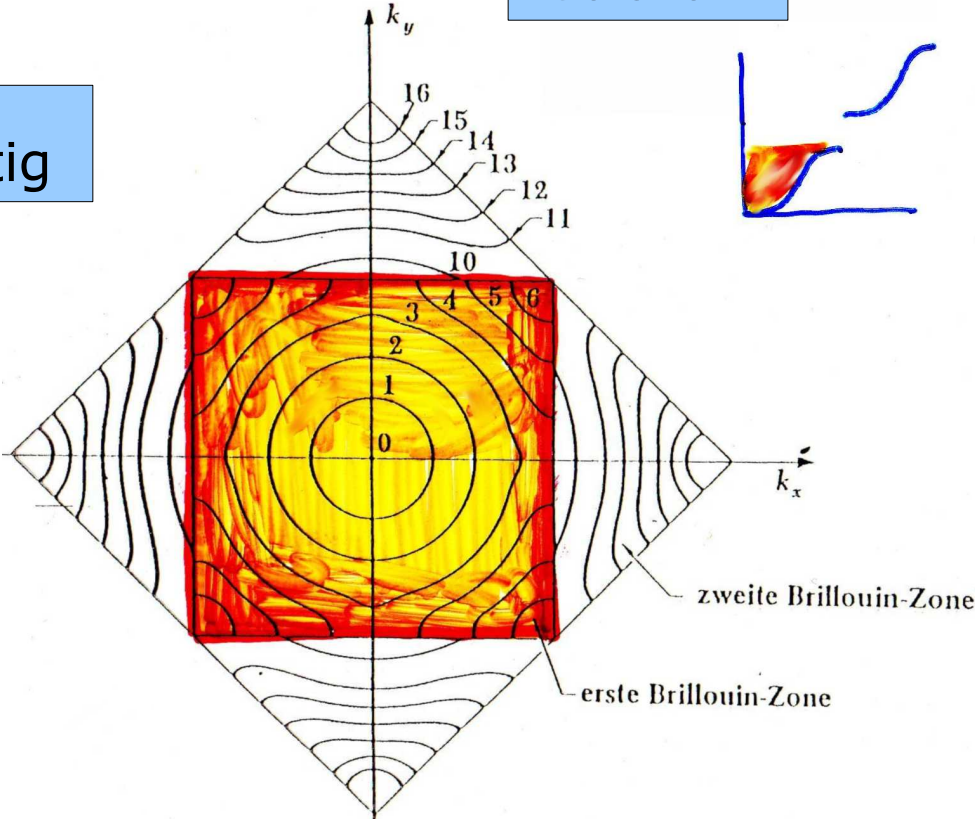
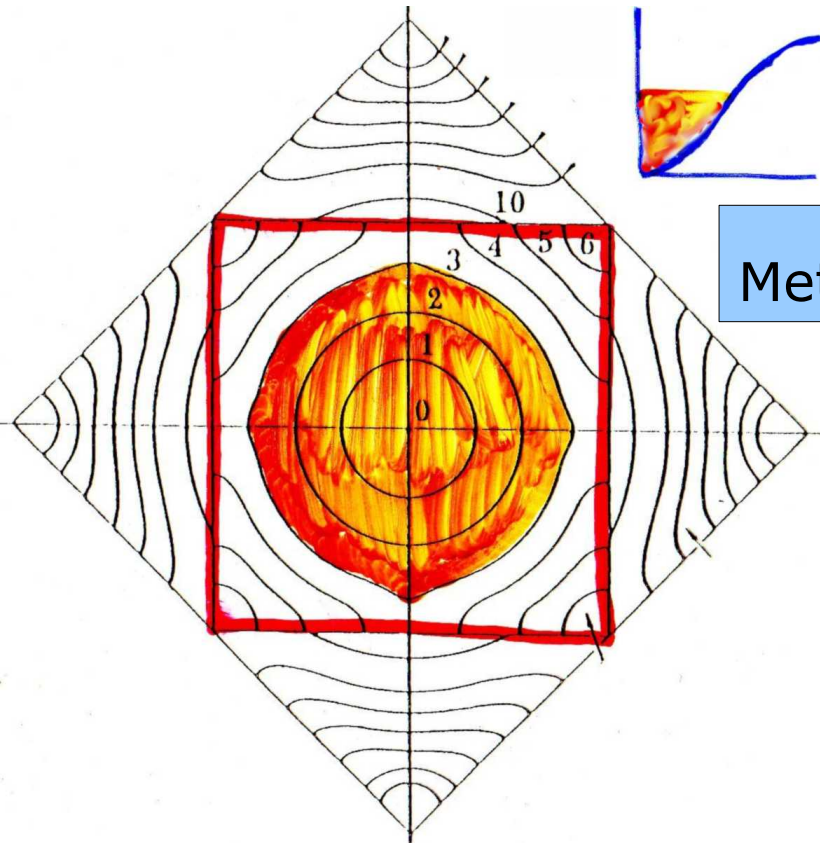
1st BZ: filled



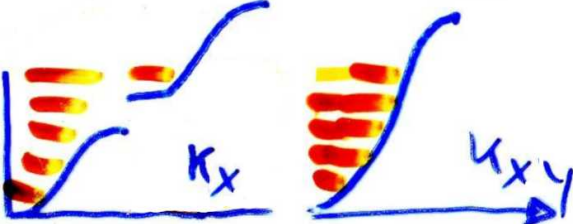
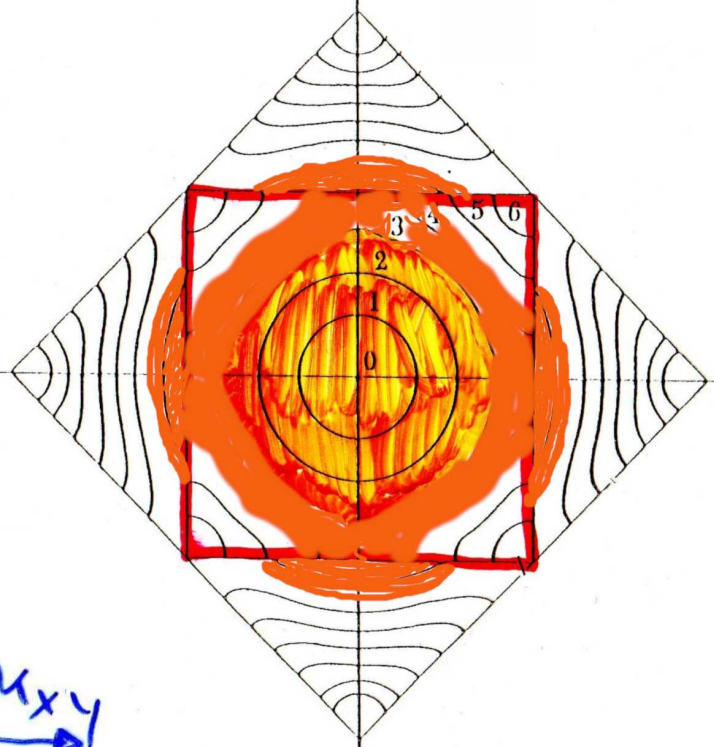
Area of Fermi-circle (dashed) = 1.5 area of 1st BZ

Isolator

Metall-1-wertig

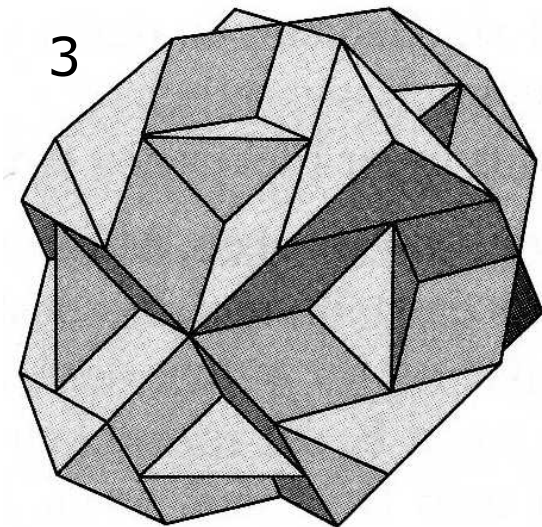
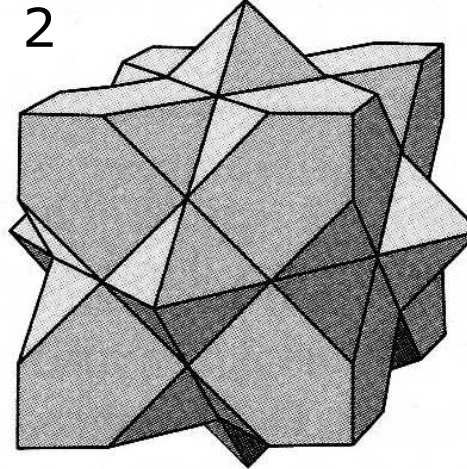
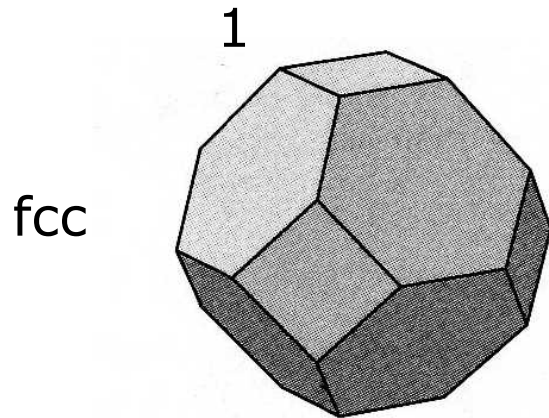
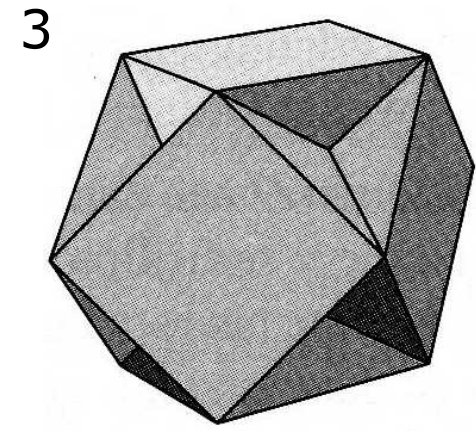
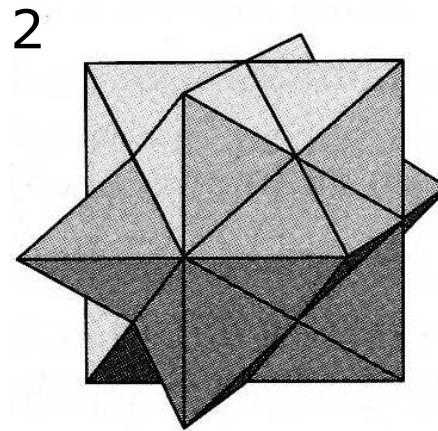
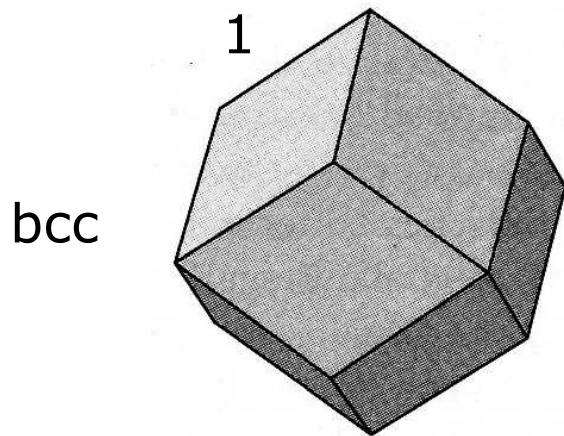


Metall-2-wertig

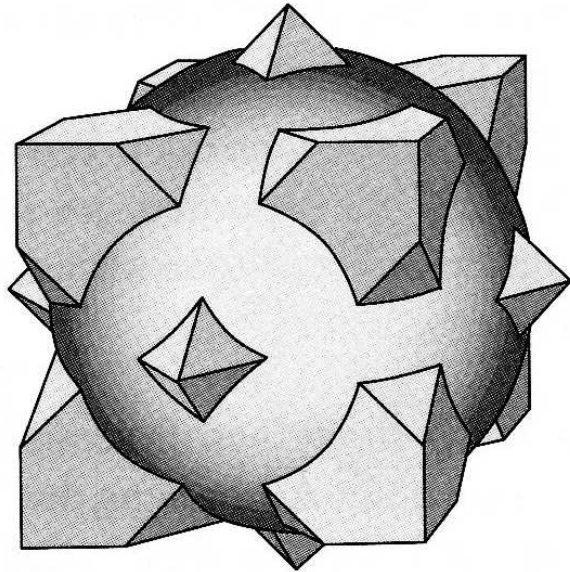


Äußere Oberflächen der 1., 2., 3. BZ

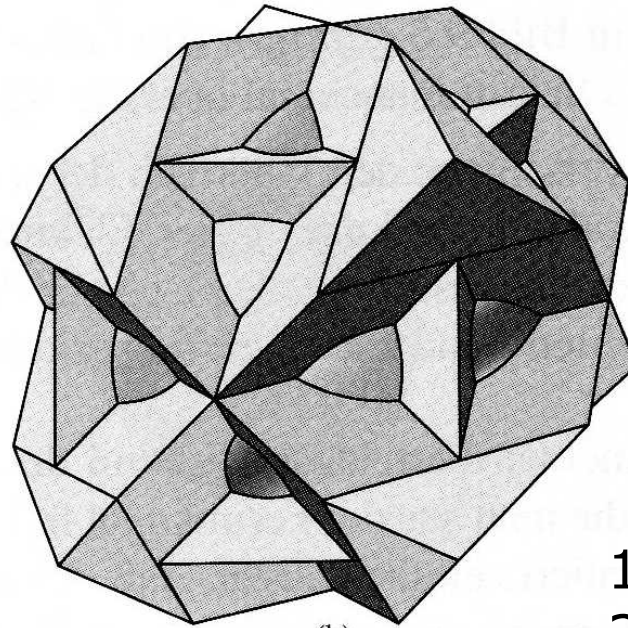
Innere Oberflächen der 2. = äußere der 1., usf.



Fermifläche **vierwertiges** fcc-Metall in 3D

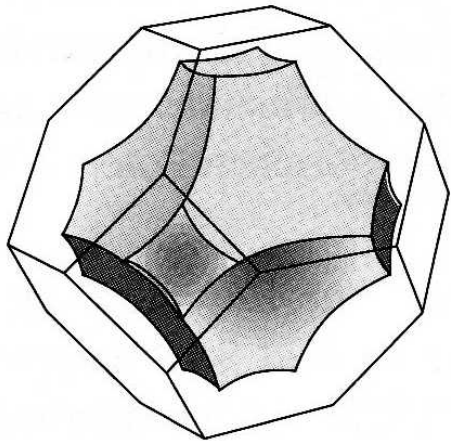


(a)

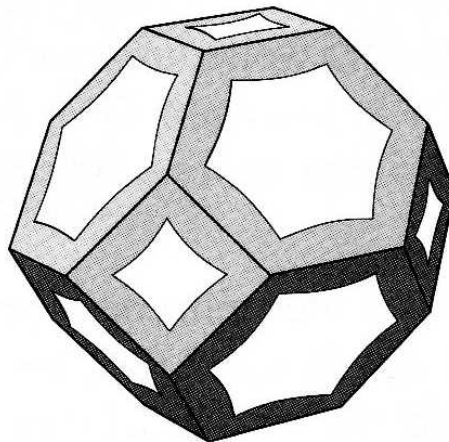


(b)

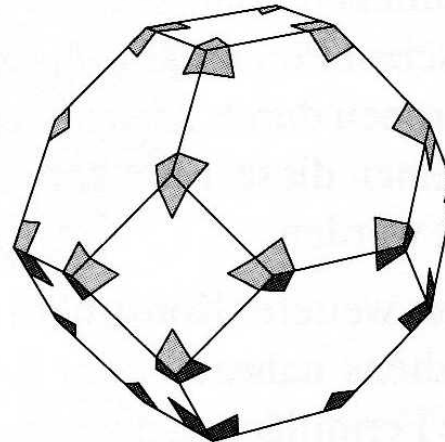
1. BZ voll in Fermikugel
2.-4. BZ teils.



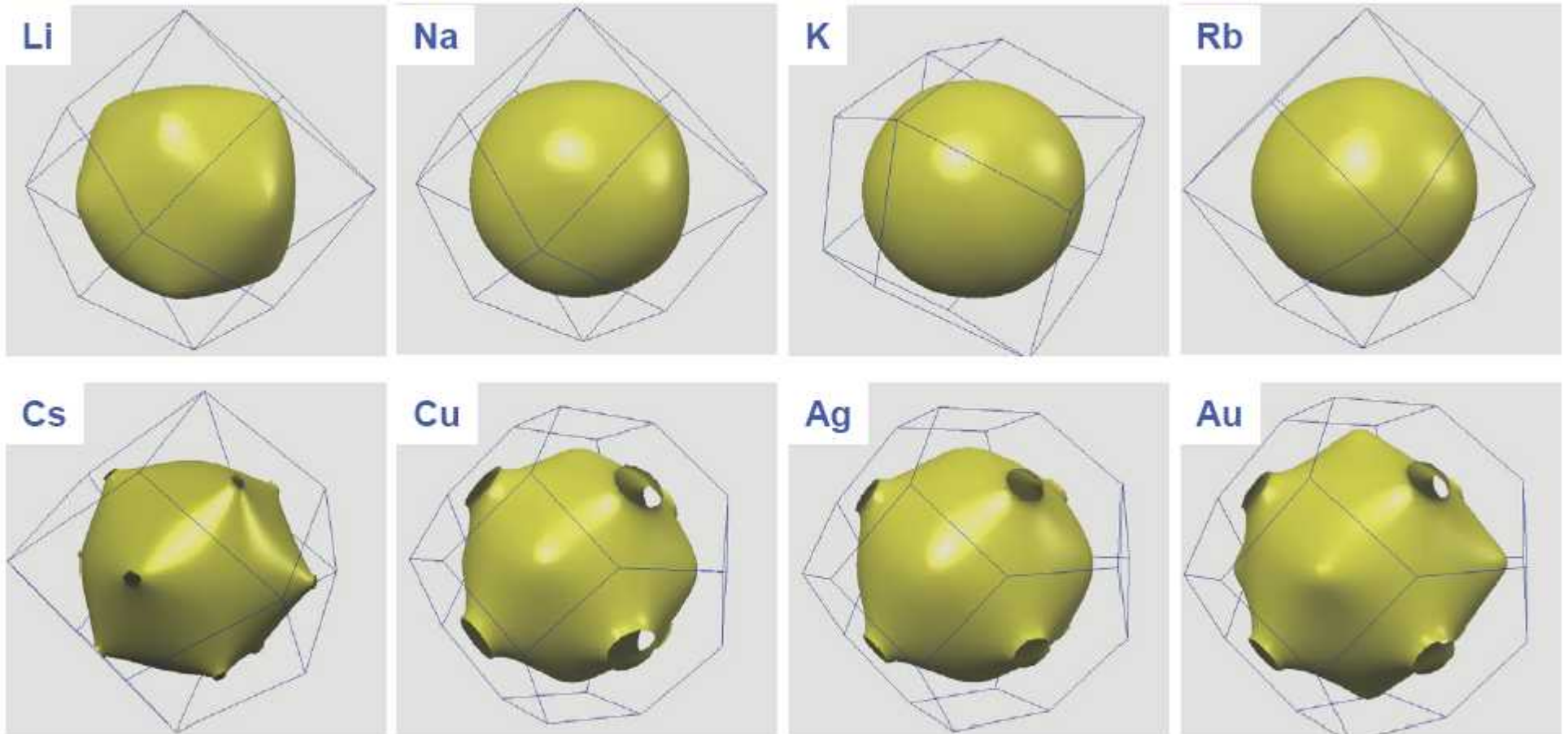
2. BZ



3. BZ



4. BZ

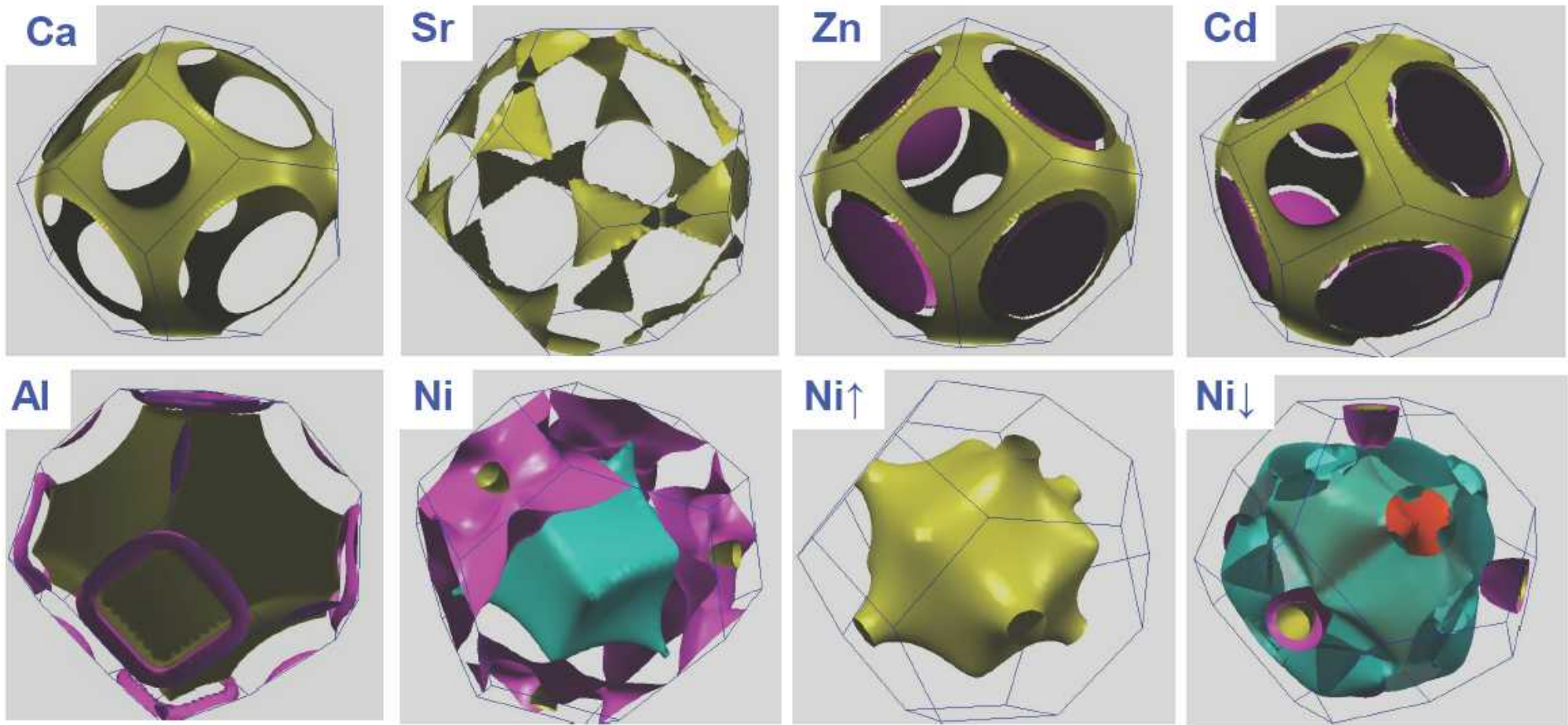


Fermiflächen einfacher Metalle

Alkalimetalle bcc

Münzmetalle fcc

(Quelle: Physics Department, University of Florida)



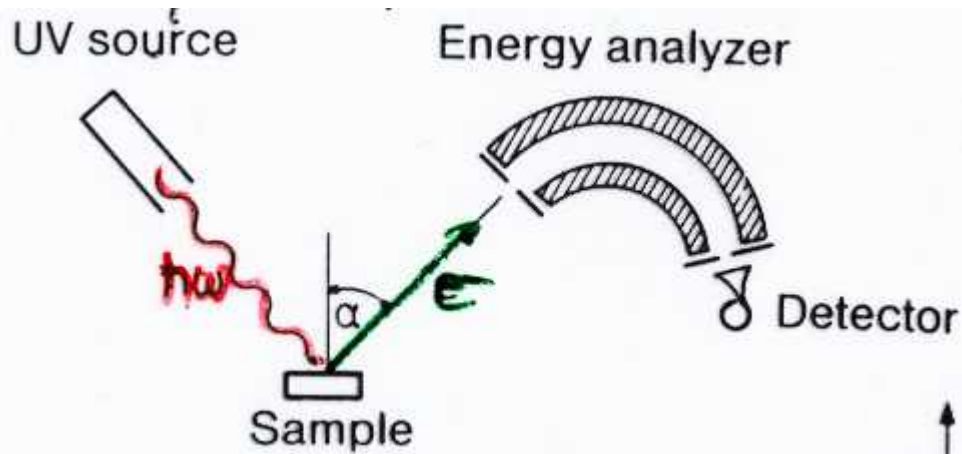
Fermiflächen

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)

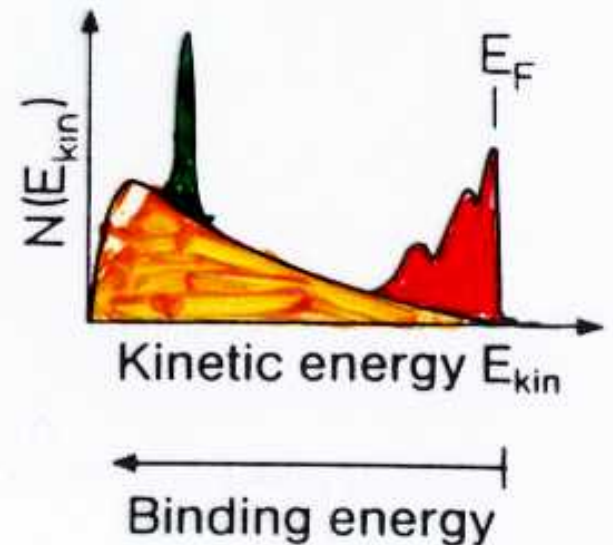
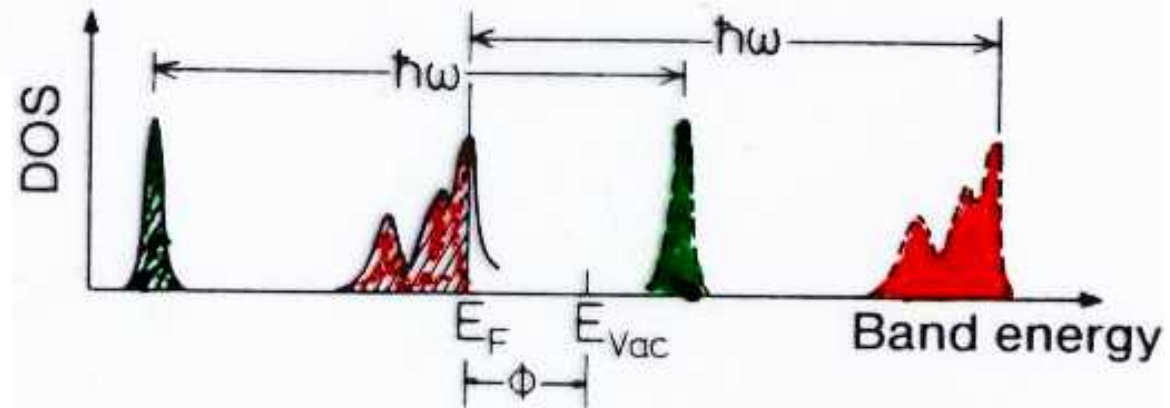
unoccupied states: IPES

conservation of energy

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

conservation of parallel momentum

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



Today: Fermi surface mapping is a routine job

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



ALS

model

data

