

Kristall = Gitter x Basis

Basis = periodisch
wiederkehrende Struktureinheit



Fig. 2.1a

Kristall = Gitter x Basis

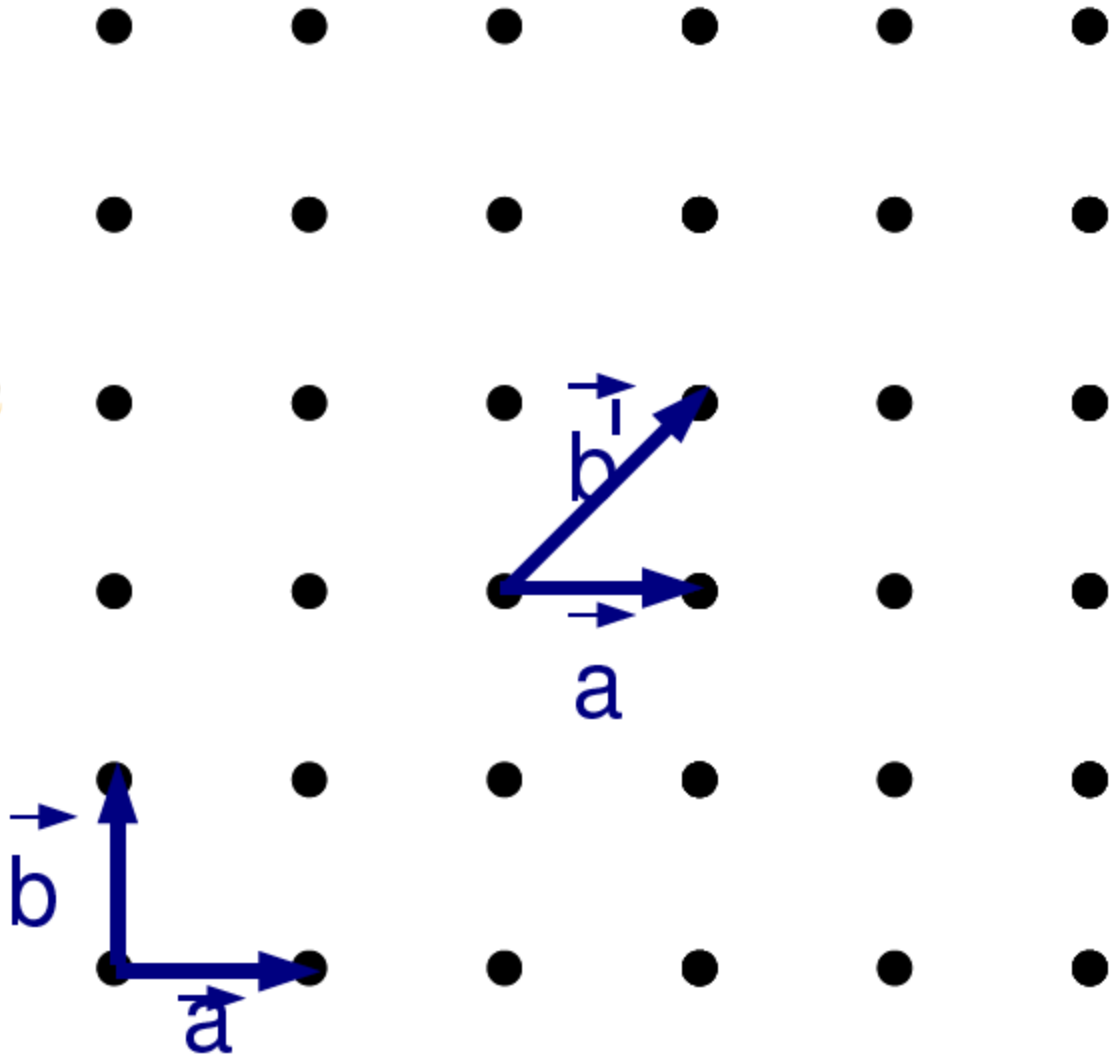
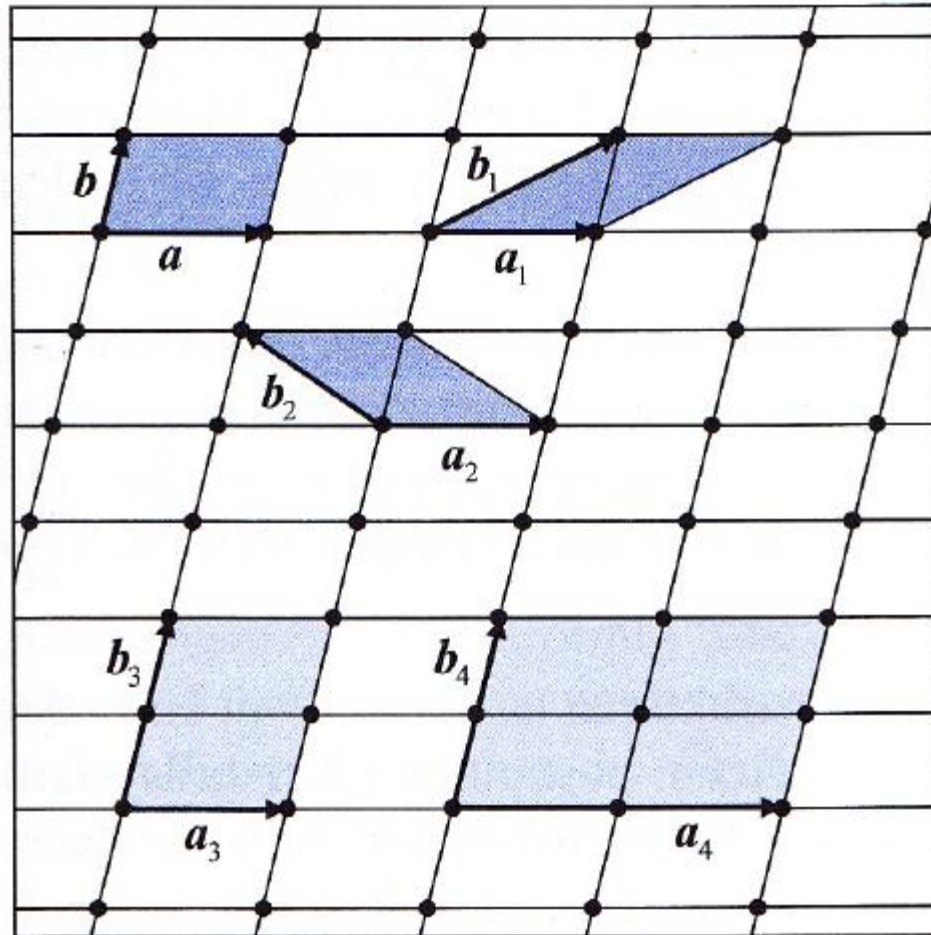


Fig. 2.1b

2 dimensionales Punktgitter: Verschiedene Elementarzellen



primitiv

Fig. 2.1c

3-dimensionale Bravais-Gitter

7 Kristallsysteme

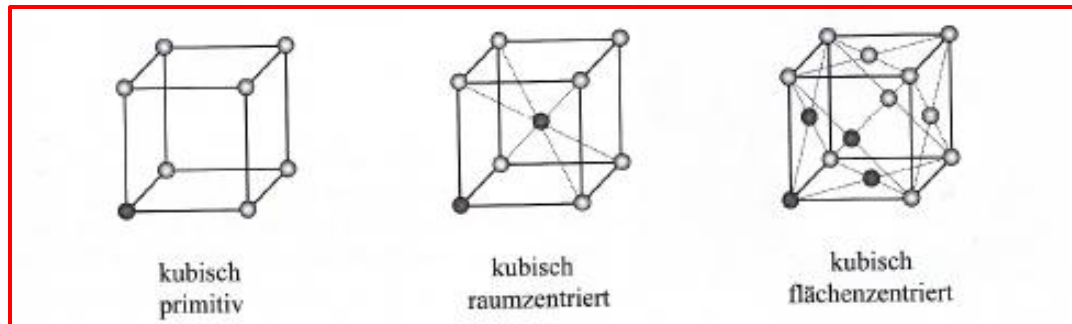
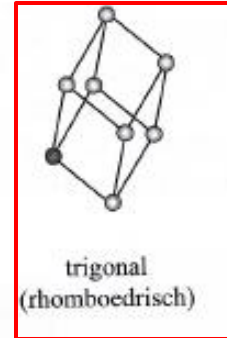
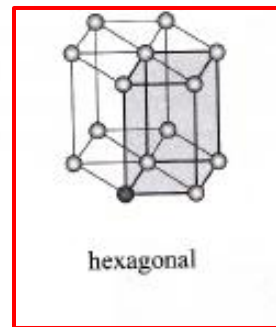
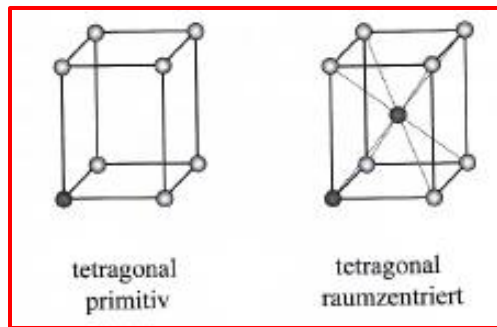
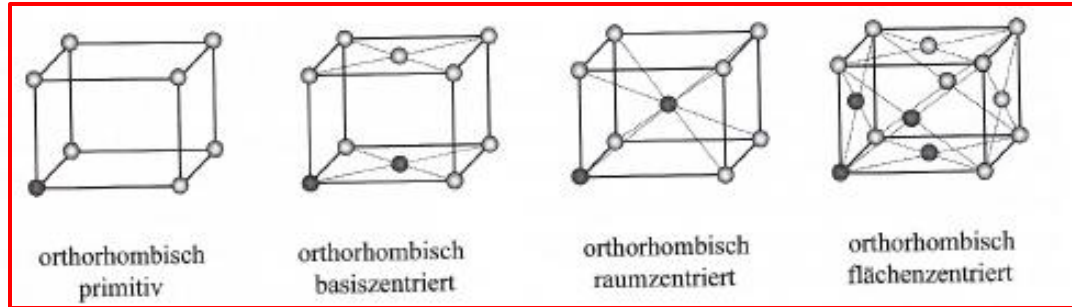
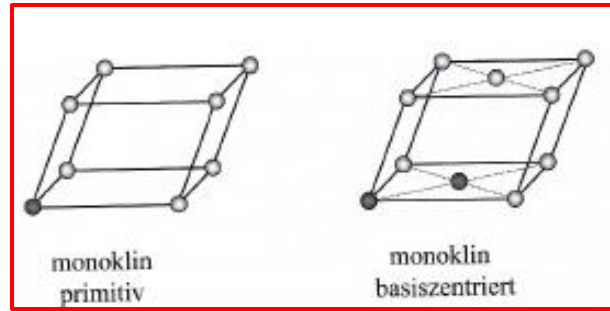
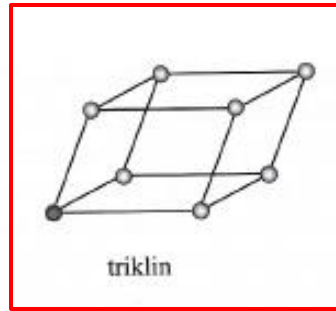
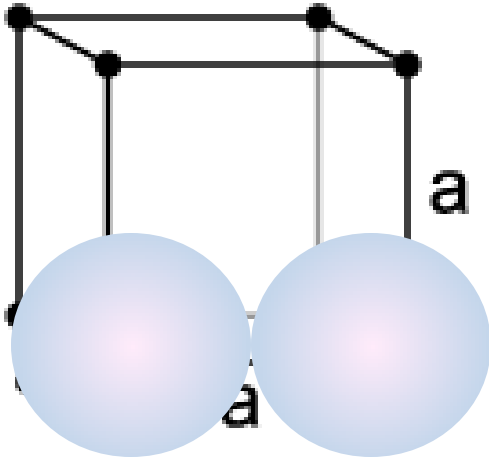


Fig. 2.1d

Kubische Kristallgitter - Packungsdichte

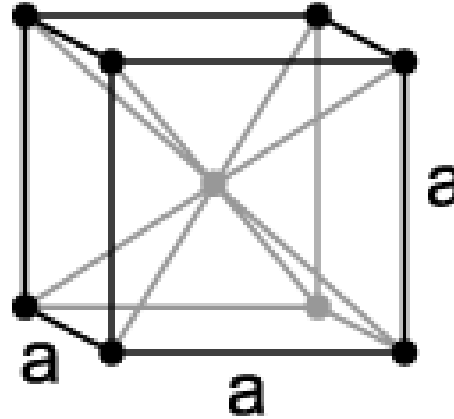
sc



$$a=2R$$

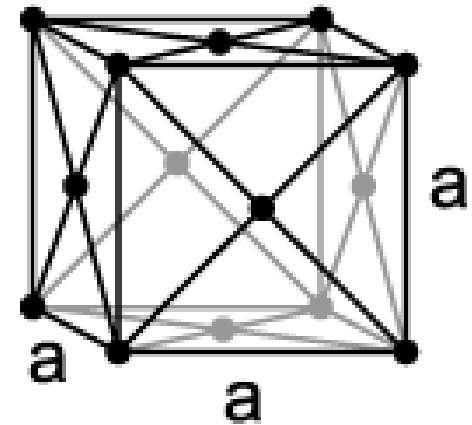
Raumerfüllung:
52%

bcc



Raumerfüllung:
68%

fcc

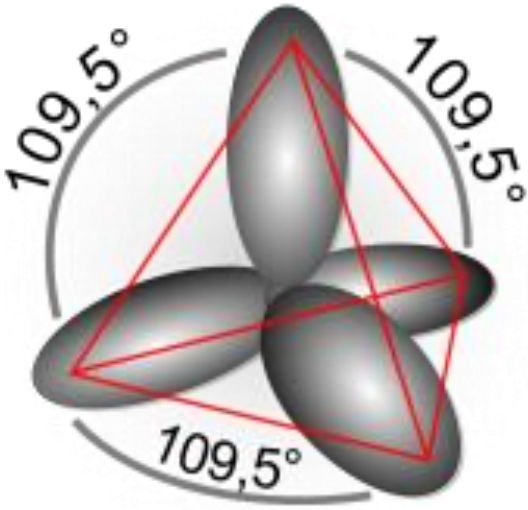


Raumerfüllung:
74%

$$1 \cdot \frac{4}{3} \pi R^3 / (2R)^3 = 0.52$$

Fig. 2.1e

Diamantstruktur



sp^3
orbitale

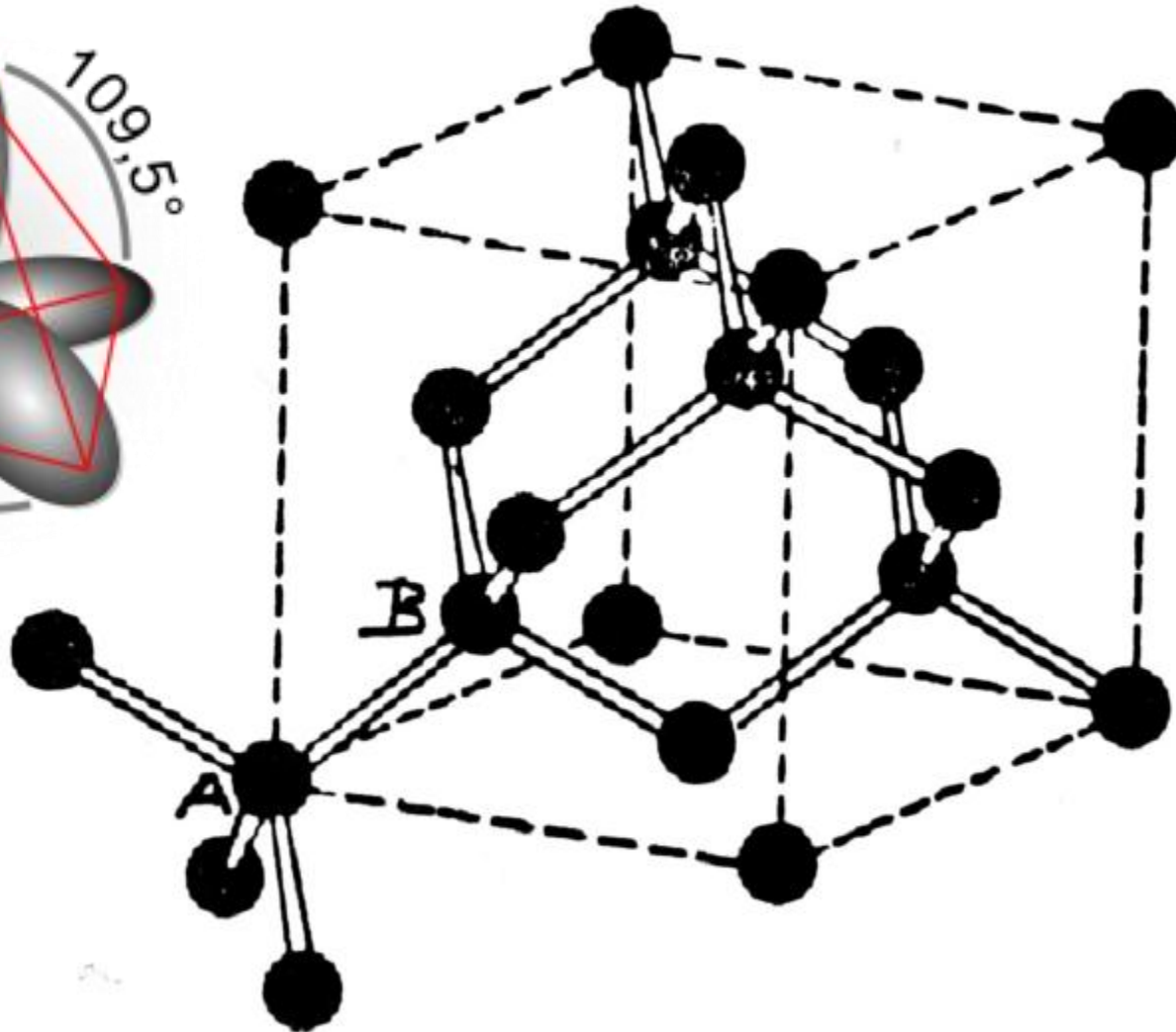


Fig. 2.1f

Diamantstruktur

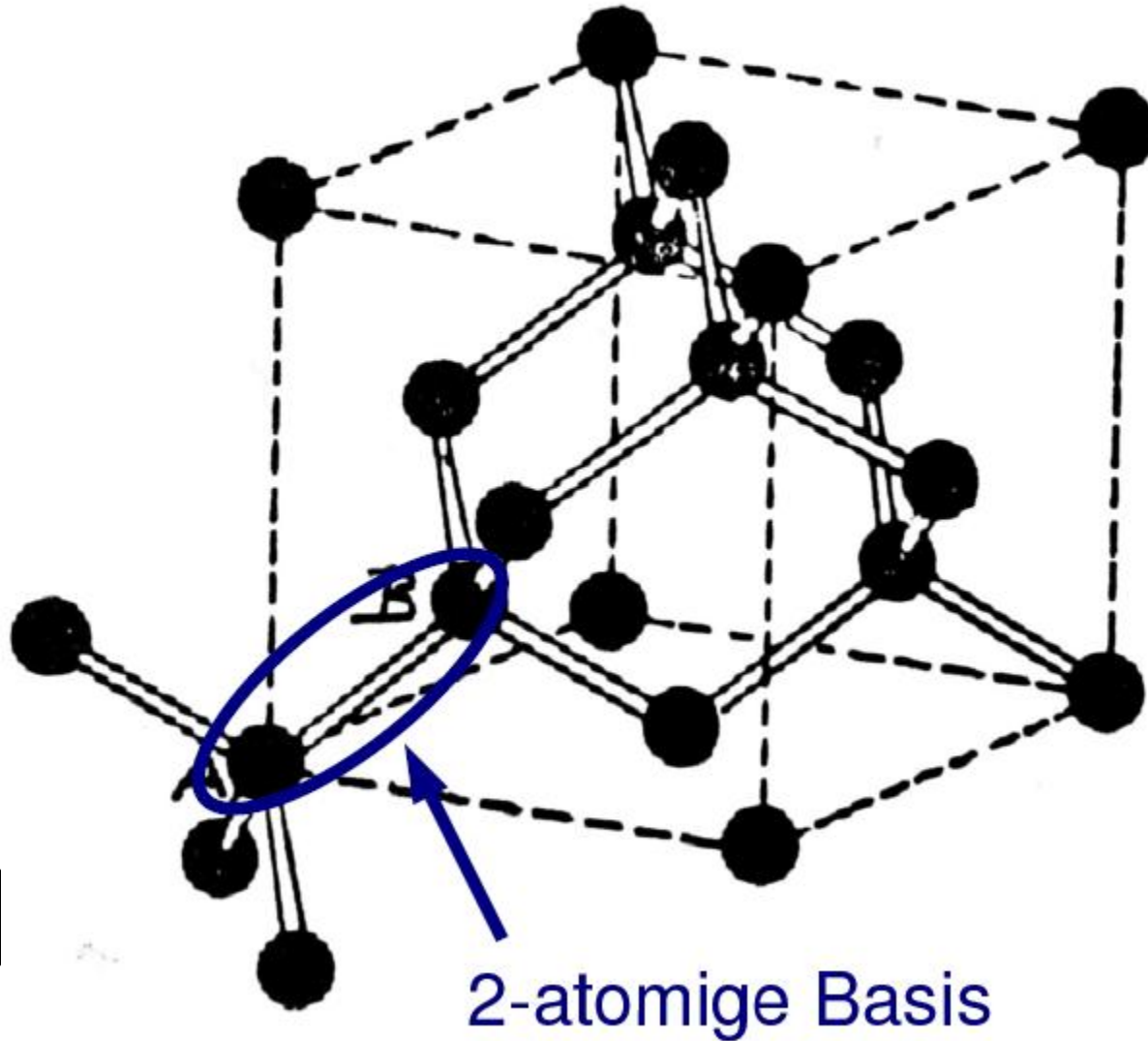


Fig. 2.1g

Diamantstruktur

fcc

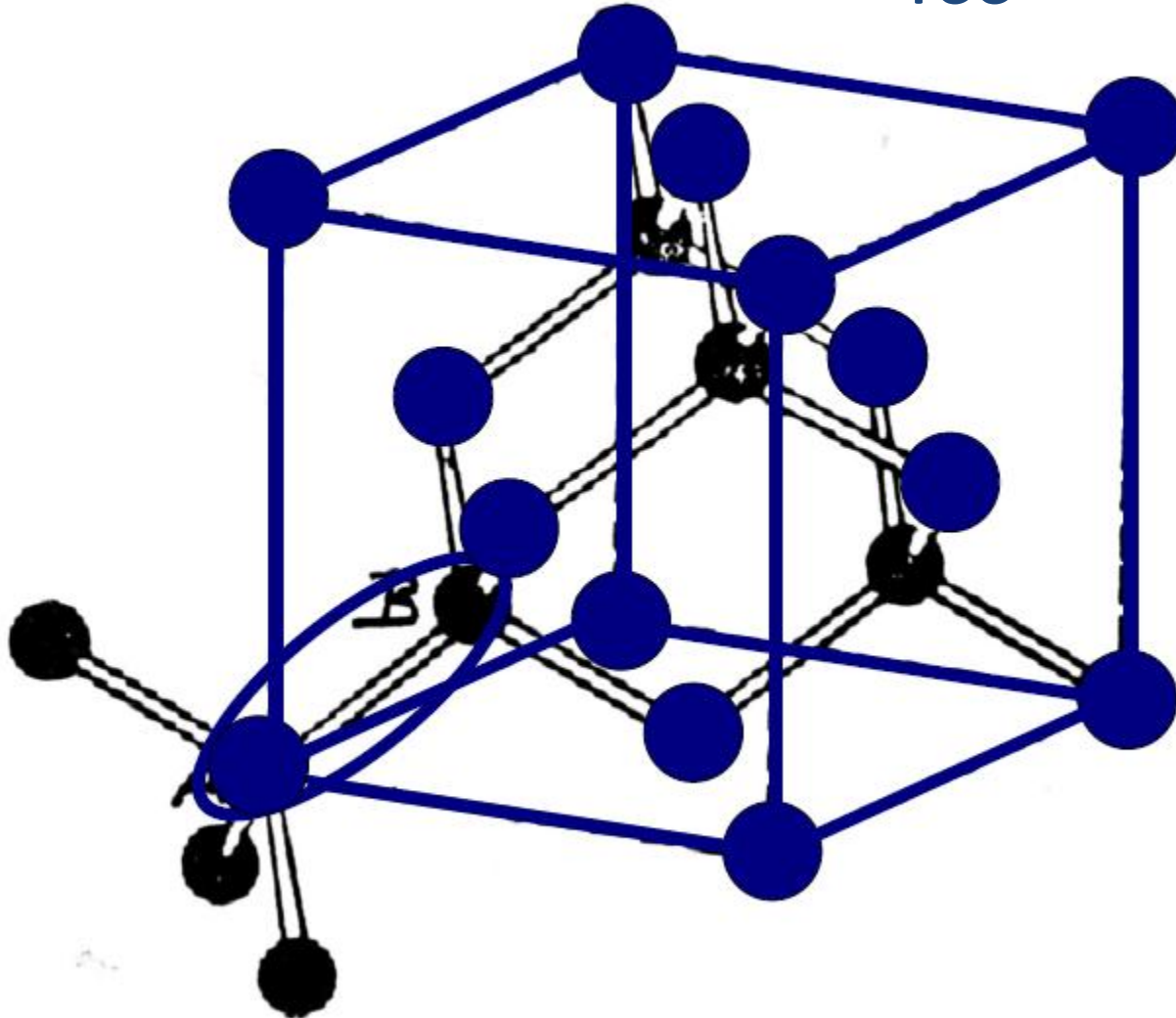


Fig. 2.1h

„Orangenstapel“: Dichteste Packungen:

fcc (ABCABC)

hcp (ABABABA)

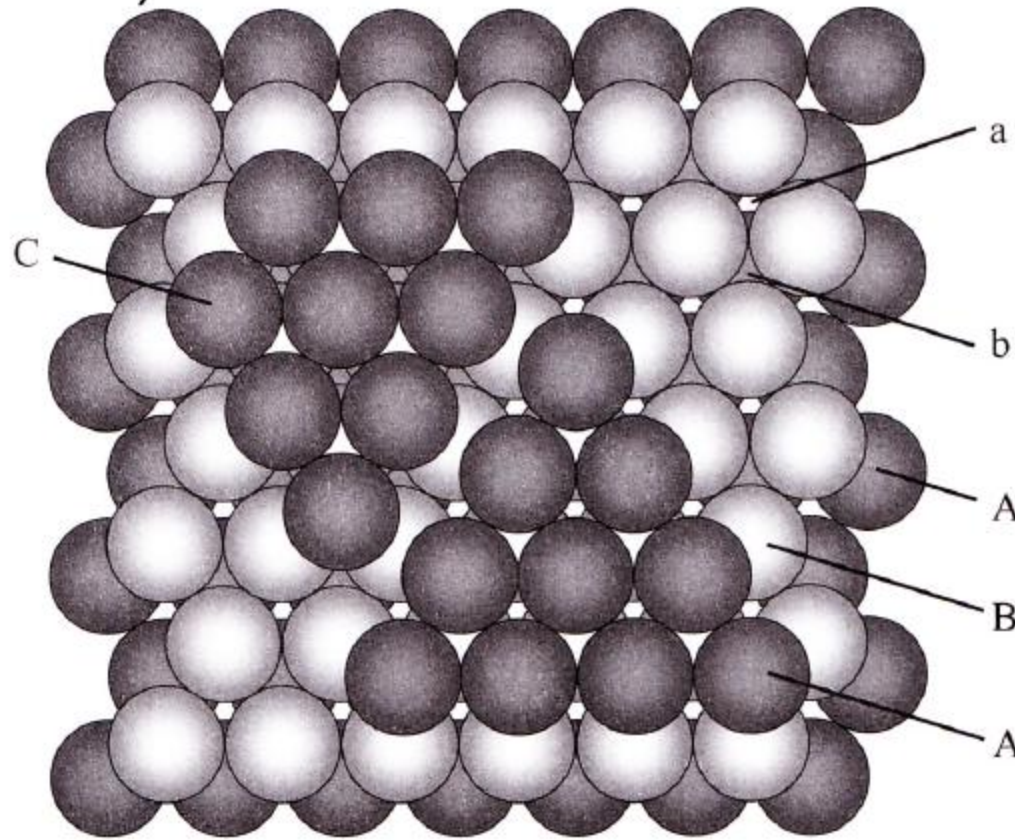
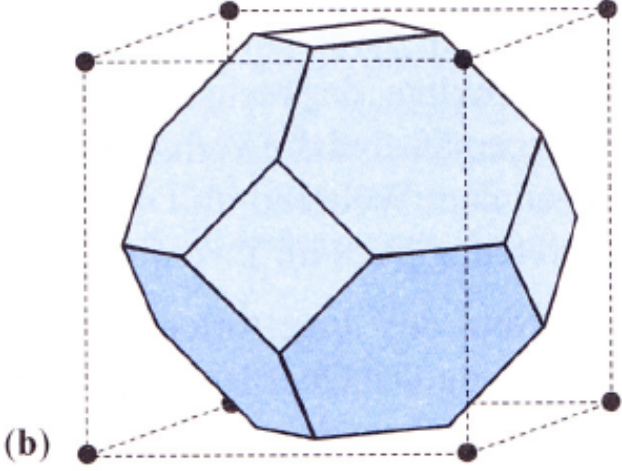
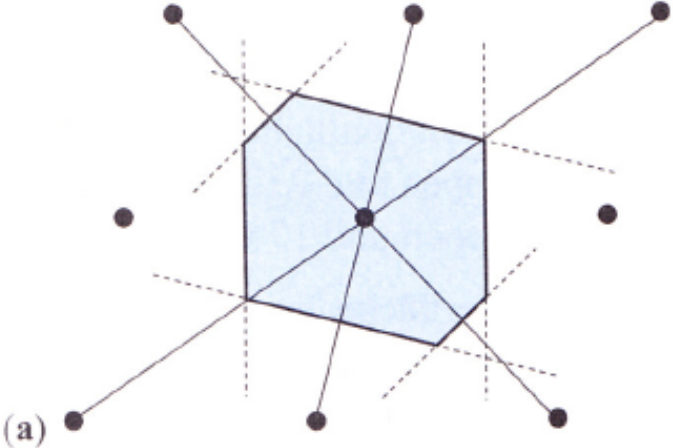


Fig. 2.1i

Packungsdichte 0,74

Wigner-Seitz-Zelle

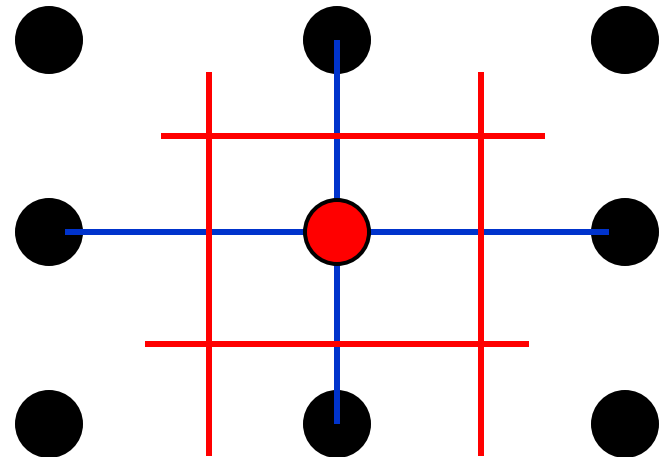
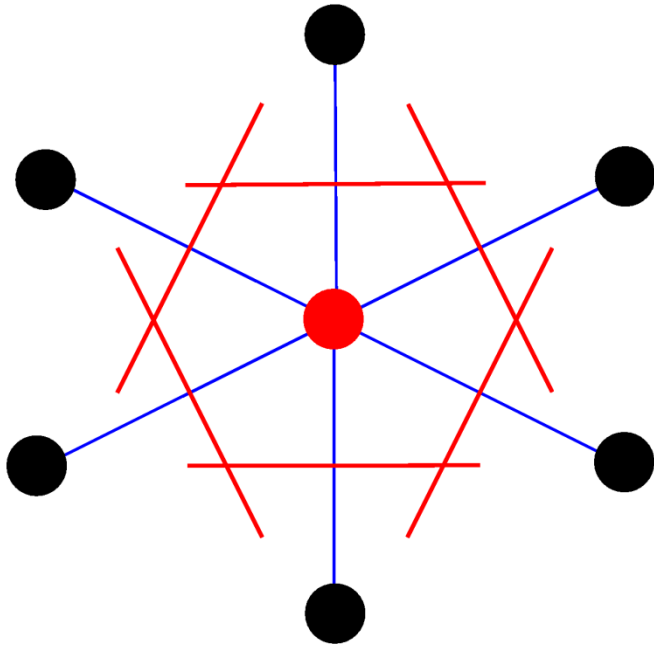


bcc

Fig. 2.2i

Wigner-Seitz Zelle

Fig. 2.2i++



Im reziproken Gitter bezeichnet man die WSZ als 1. Brillouin-Zone.
Die übernächsten Nachbarn definieren die nächsten Brillouin-Zonen.

Bragg-Reflexion

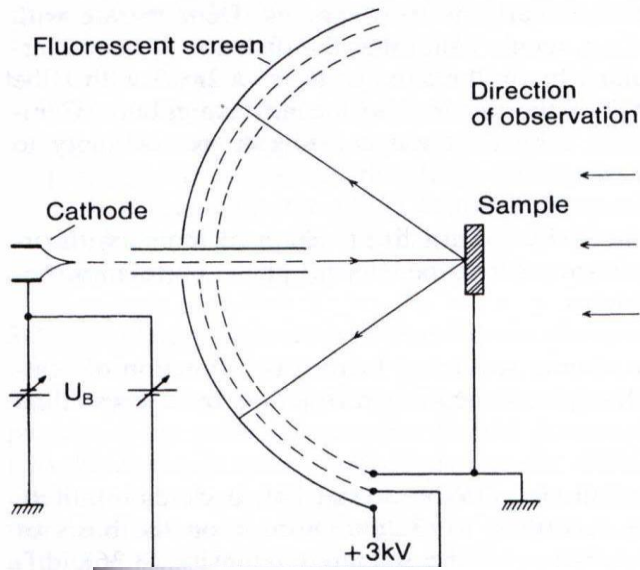
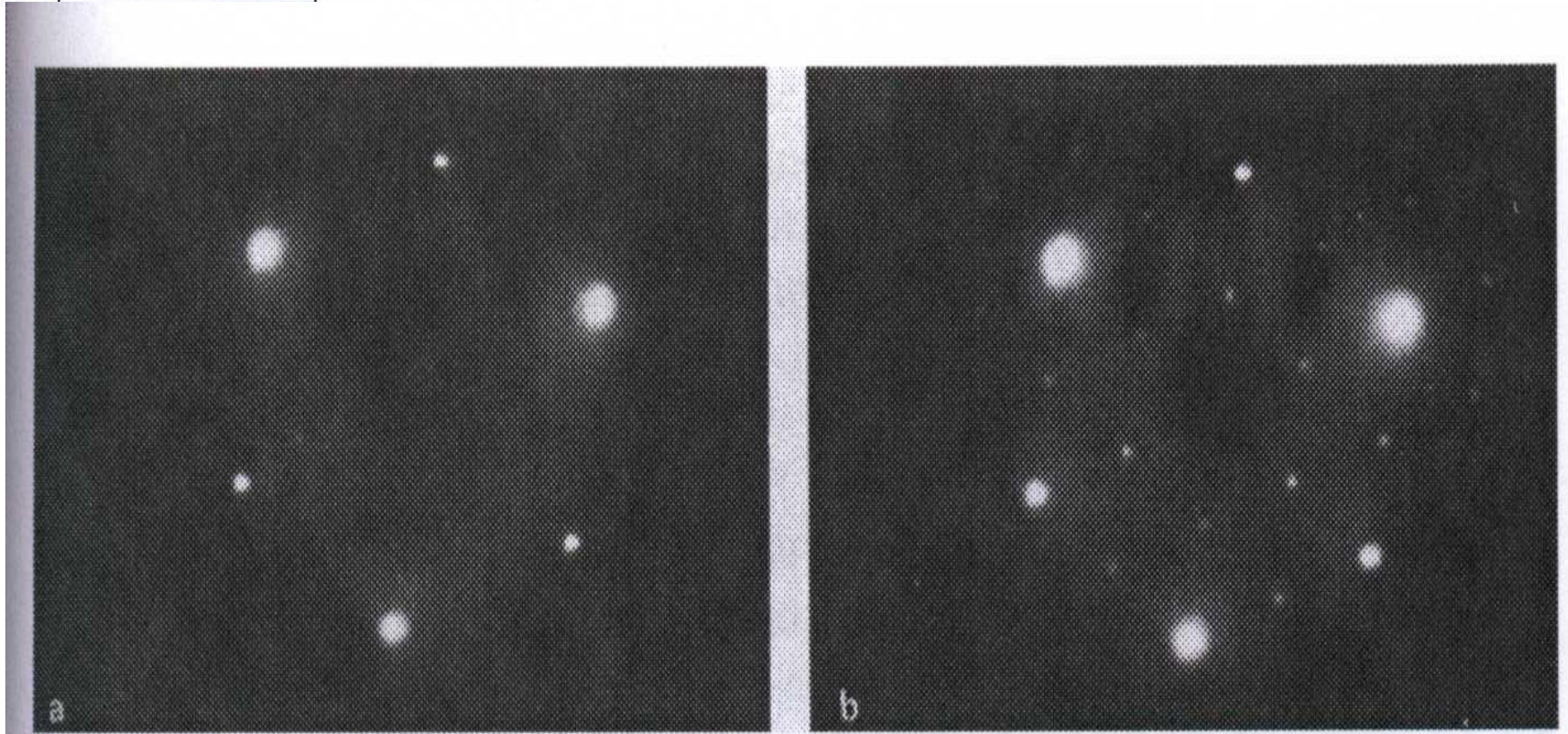
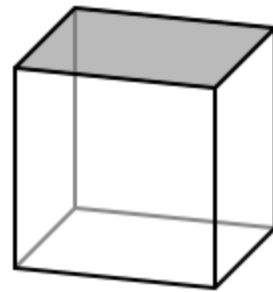
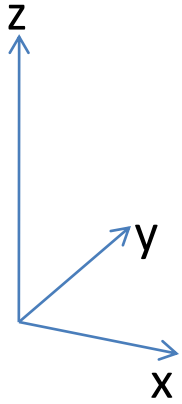


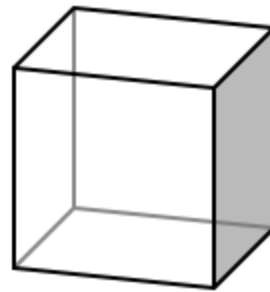
Fig. 2.2a



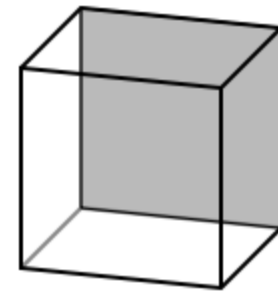
Millersche Indizes



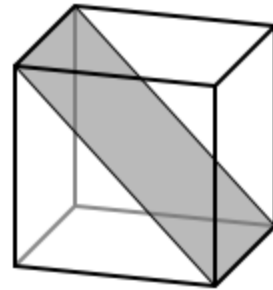
(001)



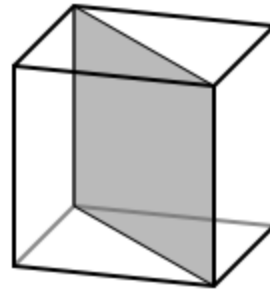
(100)



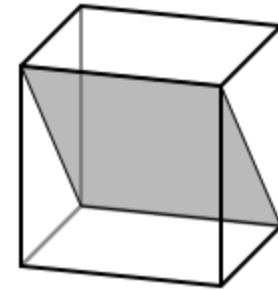
(010)



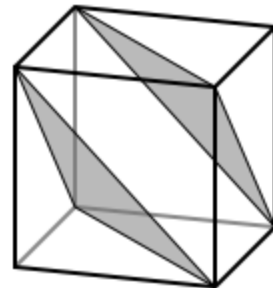
(101)



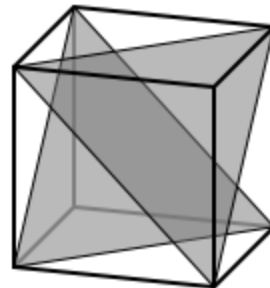
(110)



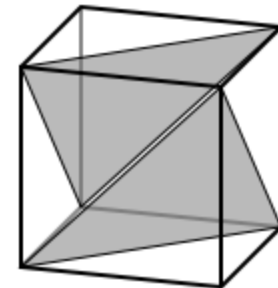
(011)



(111)



$(\bar{1}\bar{1}1)$



$(\bar{1}11)$

Fig. 2.2b

Für kubische Gitter mit Gitterkonstanten a findet man für den Abstand der Netzebenen ($h k l$):

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

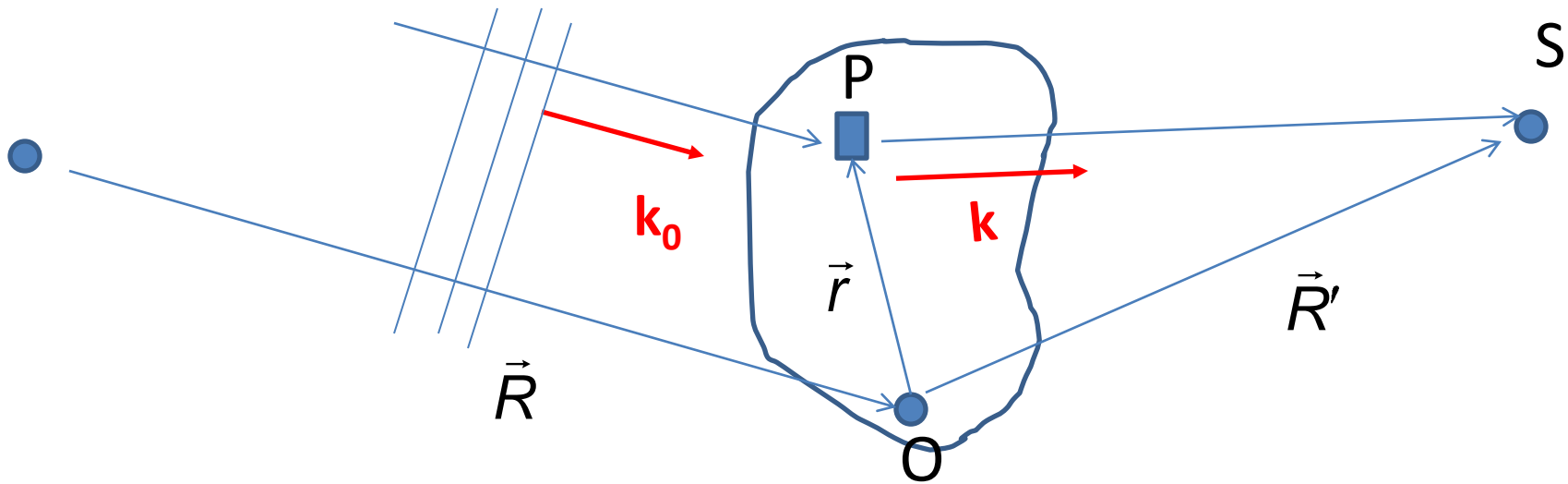
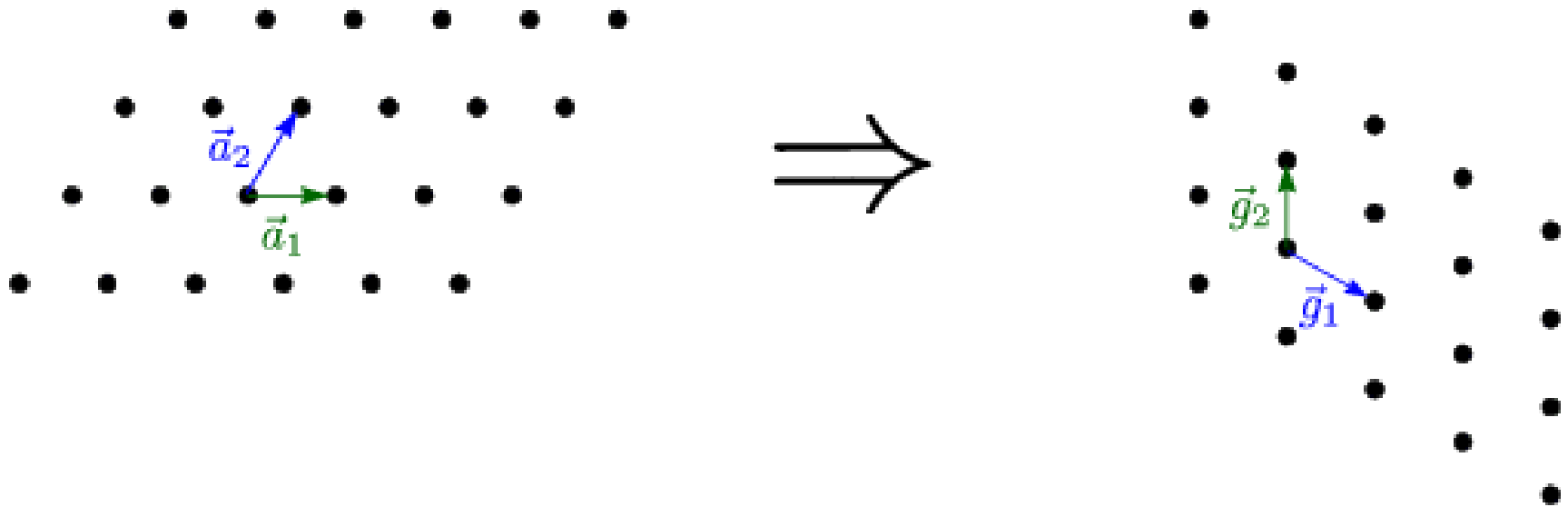


Fig. 2.2d

Reziproke Gittervektoren



Für kubisches Gitter

$$|\vec{a}_1| = |\vec{a}_2| = |\vec{a}_3| = |\vec{a}| \quad \left| \vec{b}_i \right| = \frac{2\pi}{a} \quad \left| \vec{G}_{hkl} \right| = \frac{2\pi}{a} \sqrt{h^2 + k^2 + l^2}$$

Fig. 2.2e

Ewald Konstruktion

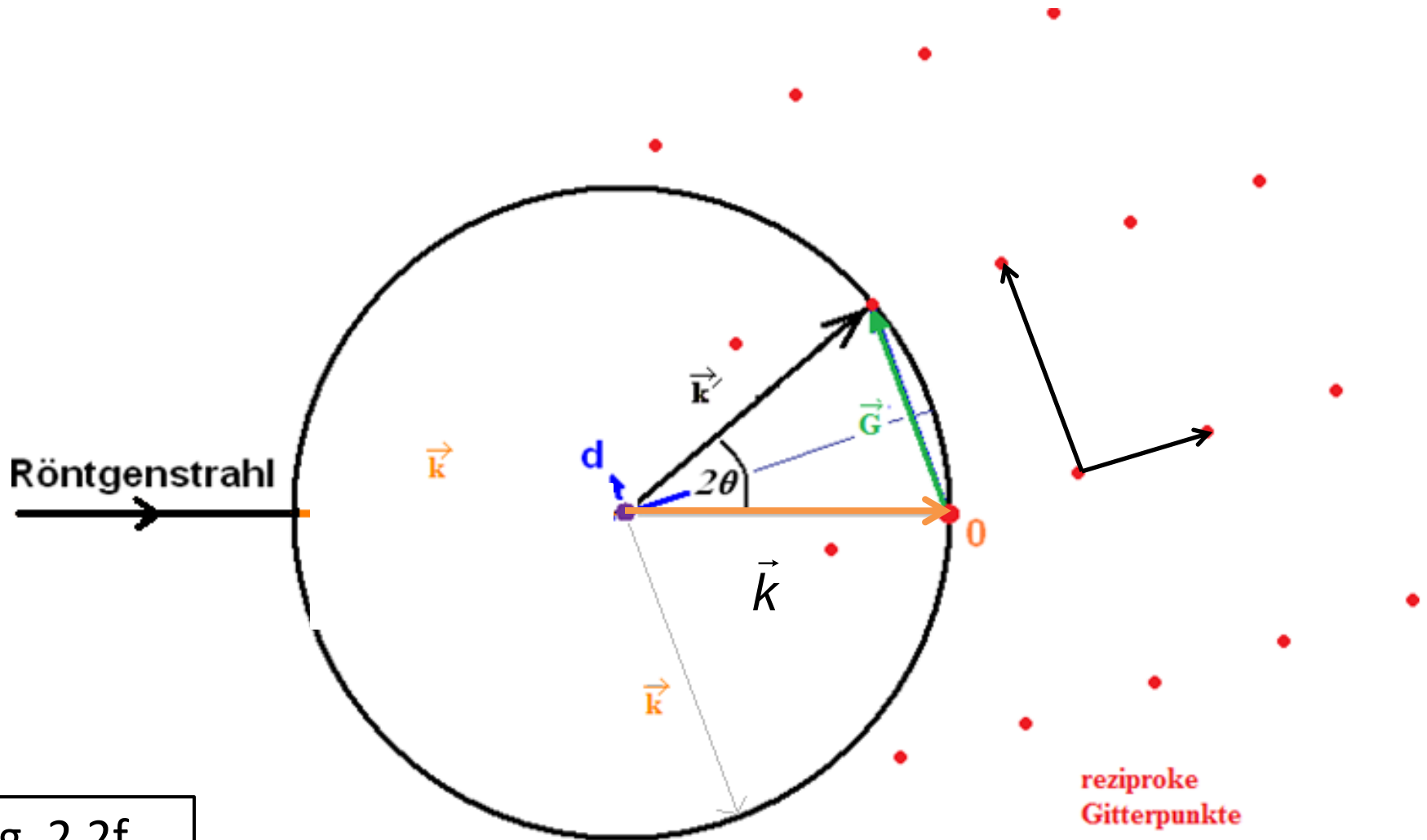


Fig. 2.2f

Strukturfaktor und mehratomige Basis

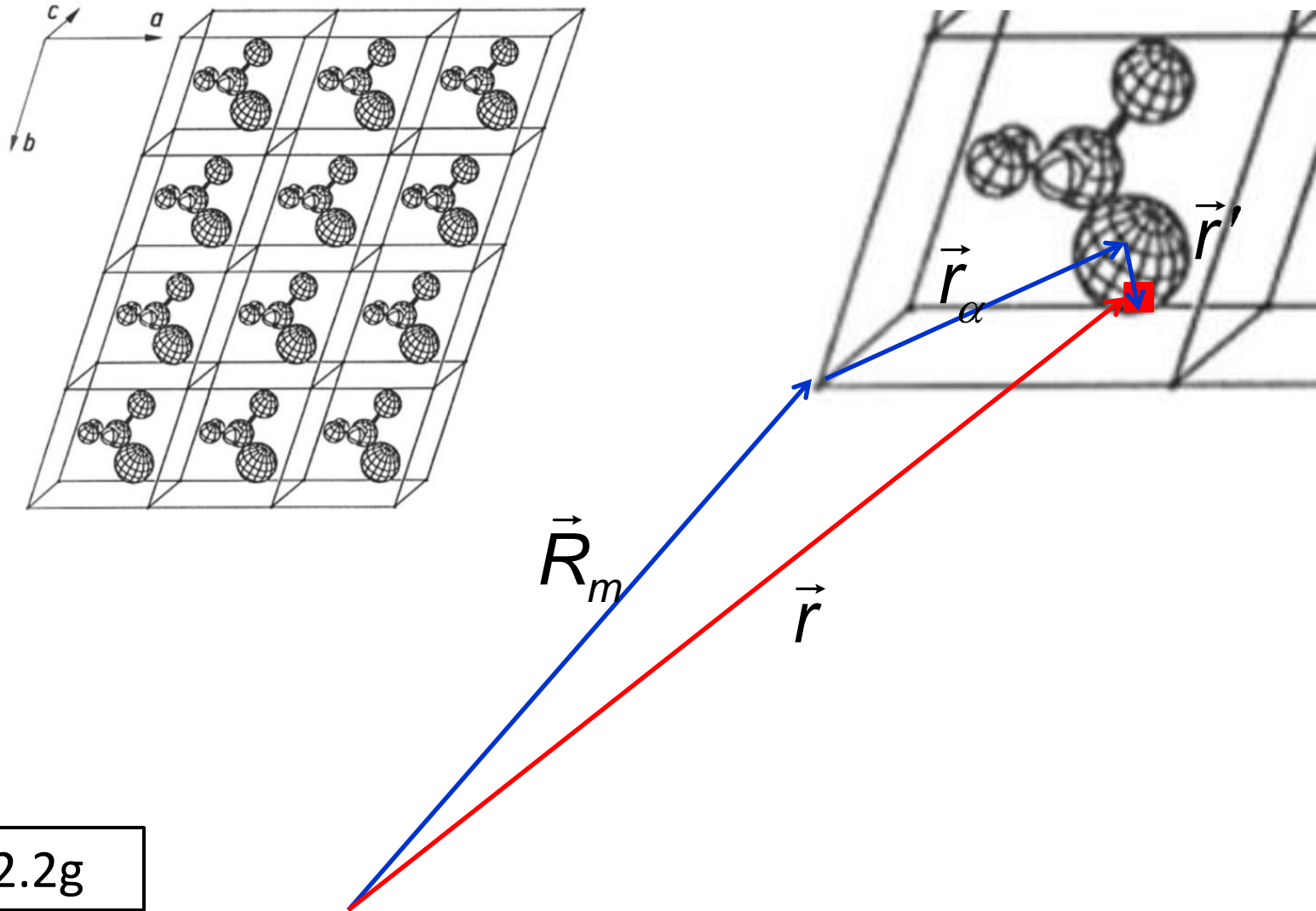


Fig. 2.2g