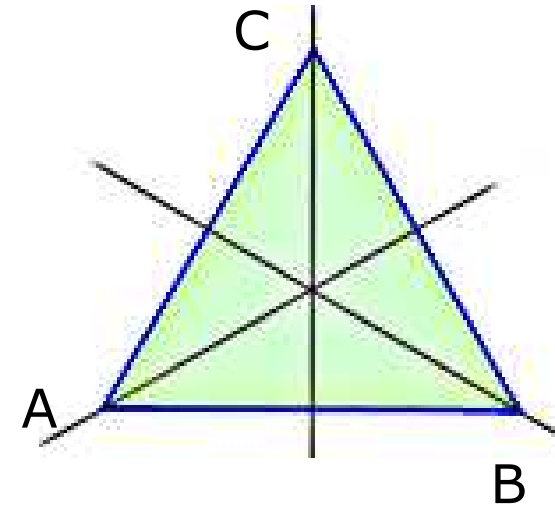


Bsp. einer Symmetriegruppe: Gleichseitiges Dreieck

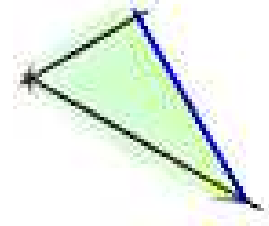
6 Elemente

3 **D**rehungen (um 0° , 120° , 240°)

3 **S**piegelungen



α	D0	D120	D240	Sp1	Sp2	Sp3
D0	D0	D120	D240	Sp1	Sp2	Sp3
D120	D120	D240	D0	Sp2	Sp3	Sp1
D240	D240	D0	D120	Sp3	Sp1	Sp2
Sp1	Sp1	Sp3	Sp2	D0	D240	D120
Sp2	Sp2	Sp1	Sp3	D120	D0	D240
Sp3	Sp3	Sp2	Sp1	D240	D120	D0



irred = $1/6$, z. B. n^3

Klassifikation der Kristallstrukturen

Die Symmetrieelemente eines Kristalls ...

Translationen

Punktoperationen

Kombinationen davon

... bilden Gruppe.

Punktoperationen (lassen einen Gitterpunkt fest)

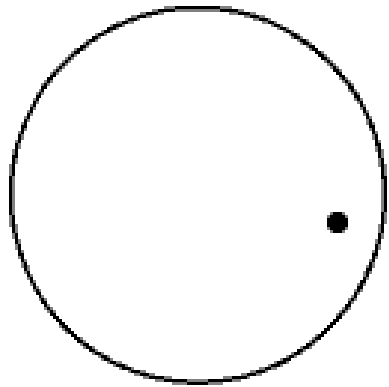
Drehachse mit Zähligkeit ***n*** (Drehung um $2\pi/n$)

Inversionszentrum ***i***

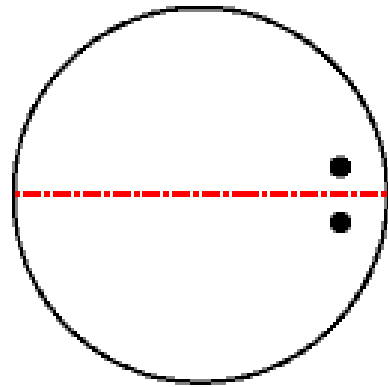
Spiegelebene ***m***

Drehspiegelachse (kann auch ohne ***n*** und ***m*** existieren!)

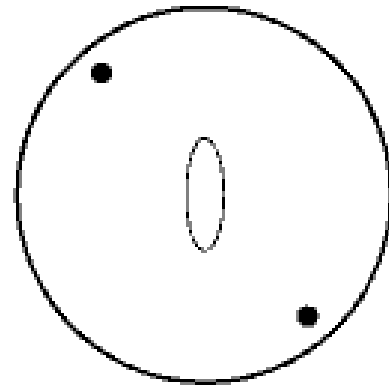
Drehinversionszentrum (kann auch ohne ***n*** und ***i*** existieren!)



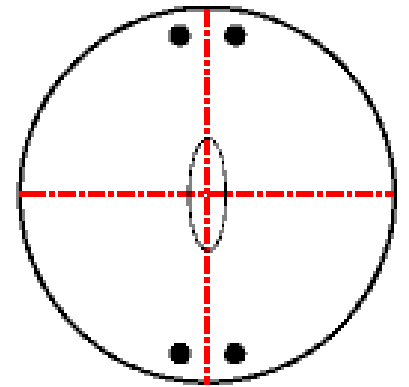
1



1m

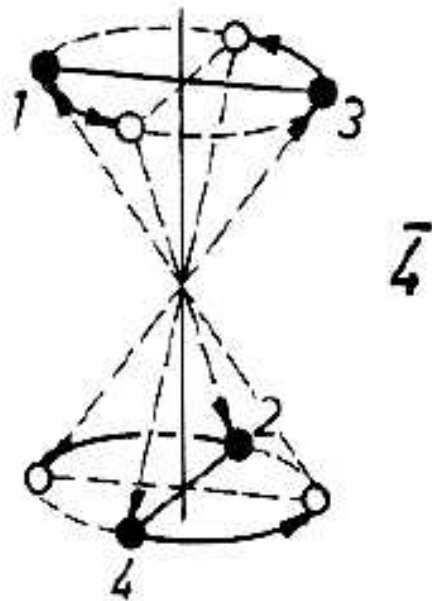


2

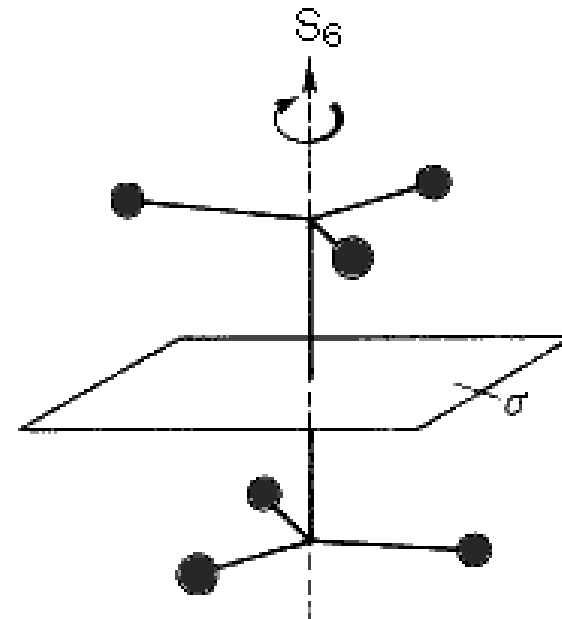


2mm

Vierzählige
Drehinversion
(ohne i)



Sechszählige
Drehspiegelachse



Klassifikation der Kristallstrukturen

Alle Symmetrieelemente eines Kristalls bilden Gruppe.

Punktoperationen auf Gitter mit kugelsymmetrischer Basis

7 Kristallsysteme

Alle Operationen auf Gitter mit kugelsymmetrischer Basis

14 Bravaisgitter

Punktoperationen auf Gitter mit beliebiger Basis

32 kristallographische Punktgruppen

Alle Operationen auf Gitter mit beliebiger Basis

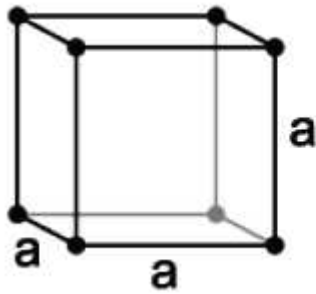
230 kristallographische Raumgruppen

	Bravaisgitter	Kristallstruktur
	(sphärische Basis)	(beliebige Basis)
Punktgruppen	7 Kristallsysteme	32 kristallograph. Punktgruppen
Raumgruppen	14 Bravaisgitter	230 Raumgruppen

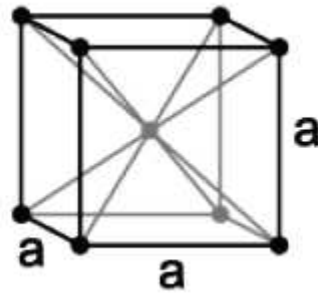
Kubisches Kristallsystem

Punktgruppe wie Würfel

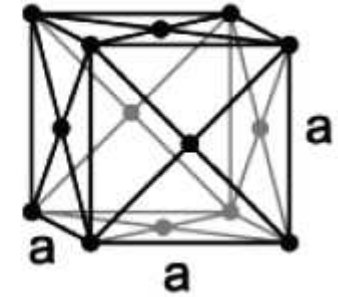
höchste Symmetrie, drei gleich lange, rechtwinklige Achsen



Kubisch-
primitiv (sc)



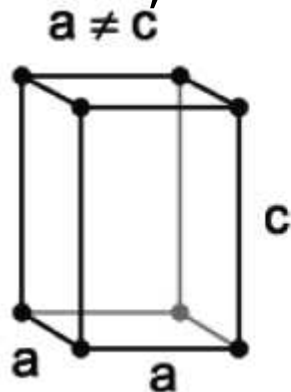
Kubisch-
raumzentriert (bcc)



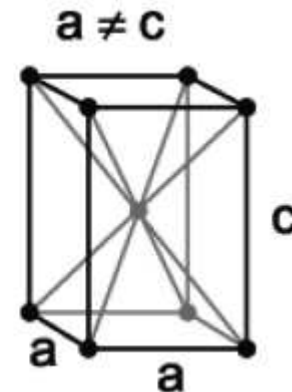
Kubisch-
flächenzentriert (fcc)

Tetragonales Kristallsystem

zwei gleich lange Achsen, drei 90°-Winkel



Tetragonal-primitiv

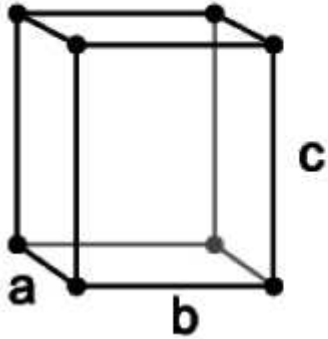


Tetragonal-raumzentriert

(ortho) Rhombisches Kristallsystem

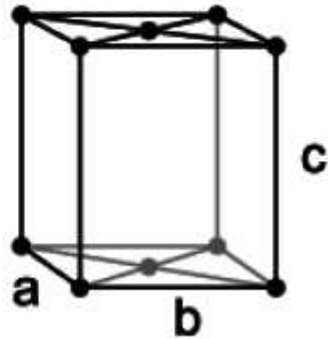
drei 90°-Winkel, keine gleichlangen Achsen

$$a \neq b \neq c$$



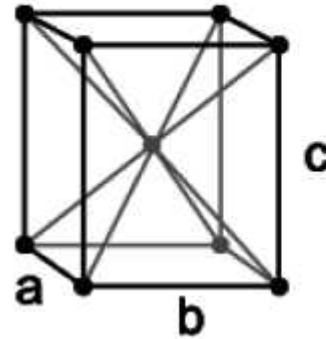
Rh.-primitiv

$$a \neq b \neq c$$



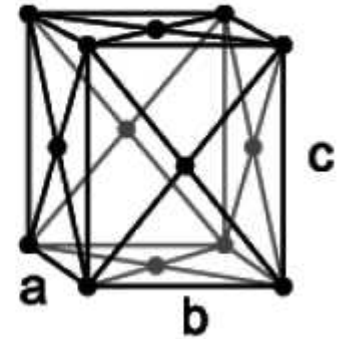
Rh.-
basiszentriert

$$a \neq b \neq c$$



Rh.-
raumzentriert

$$a \neq b \neq c$$

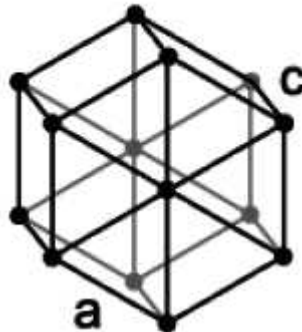


Rh.-
flächenzentriert

Hexagonales Kristallsystem

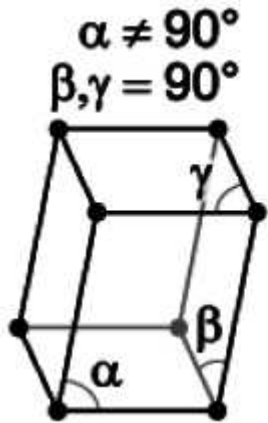
zwei gleichlange Achsen mit 120°-Winkel, dritte Achse senkrecht dazu

$$a \neq c$$

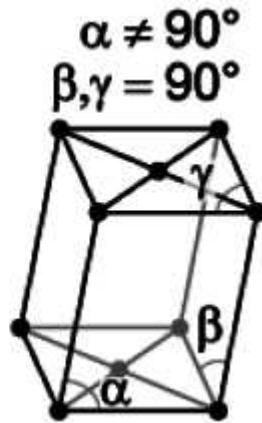


Monoklines Kristallsystem

zwei 90° -Winkel, keine gleichlangen Achsen



M.-primitiv

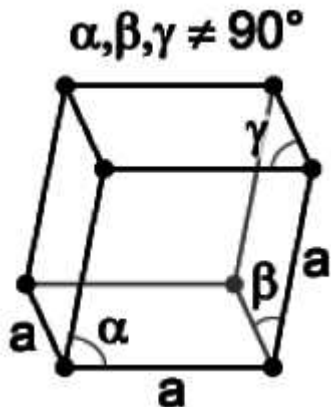


M.-basiszentriert

Trigonales o. rhomboedrisches System

drei gleichlange Achsen,

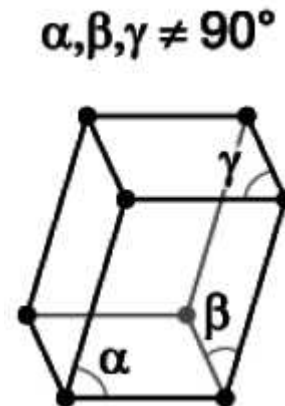
drei gleiche Winkel ungleich 90°



Triklines Kristallsystem

keine Winkel oder Achsen

geringste Symmetrie aller Gitter



Bravaisgitter

Kristallsystem (kristallographisch)	Basisvektoren bzw. Kristallachsen	Winkel	Anzahl Raumgitter
triklin	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	1
monoklin	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$	2
orthorhombisch	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	4
tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	2
hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	1
rhomboedrisch	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	1
kubisch	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	3

ELEMENTS WITH RHOMBOHEDRAL (TRIGONAL) BRAVAIS LATTICES*

ELEMENT	a (Å)	θ	ATOMS IN PRIMITIVE CELL	BASIS
Hg (5 K)	2.99	70°45'	1	$x = 0$
As	4.13	54°10'	2	$x = \pm 0.226$
Sb	4.51	57°6'	2	$x = \pm 0.233$
Bi	4.75	57°14'	2	$x = \pm 0.237$
Sm	9.00	23°13'	3	$x = 0, \pm 0.222$

* The common length of the primitive vectors is a , and the angle between any two of them is θ . In all cases the basis points expressed in terms of these primitive vectors have the form $x(\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3)$. Note (Problem 2(b)) that arsenic, antimony, and bismuth are quite close to a simple cubic lattice, distorted along a body diagonal.

ELEMENTS WITH TETRAGONAL BRAVAIS LATTICES*

ELEMENT	a (Å)	c (Å)	BASIS
In	4.59	4.94	At face-centered positions of the conventional cell
Sn (white)	5.82	3.17	At 000, $0\frac{1}{2}\frac{1}{2}$, $\frac{1}{2}0\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, with respect to the axes of the conventional cell

* The common length of two perpendicular primitive vectors is a , and the length of the third, perpendicular to these, is c . Both examples have centered tetragonal Bravais lattices, indium with a one-atom and white tin with a two-atom basis. However, both are more commonly described as simple tetragonal with bases. The conventional cell for indium is chosen to stress that it is a slightly distorted (along a cube edge) fcc structure. The white tin structure can be viewed as a diamond structure compressed along one of the cube axes.

ELEMENTS WITH ORTHORHOMBIC BRAVAIS LATTICES*

ELEMENT	a (Å)	b (Å)	c (Å)
Ga	4.511	4.517	7.645
P (black)	3.31	4.38	10.50
Cl (113 K)	6.24	8.26	4.48
Br (123 K)	6.67	8.72	4.48
I	7.27	9.79	4.79
S (rhombic)	10.47	12.87	24.49

* The lengths of the three mutually perpendicular primitive vectors are a , b , and c . The structure of rhombic sulfur is complex, with 128 atoms per unit cell. The others can be described in terms of an eight-atom unit cell. For details the reader is referred to Wyckoff.

Tetraeder: 24 Gruppenelemente T_d

Untergruppe der Oktaedergruppe (Würfelgruppe)

* 12 Drehungen

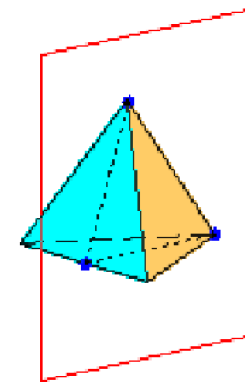
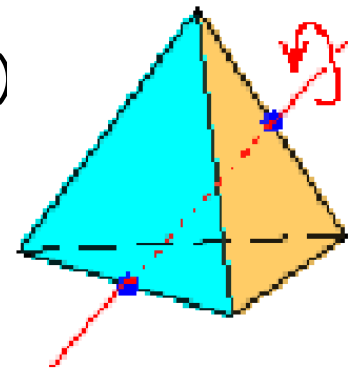
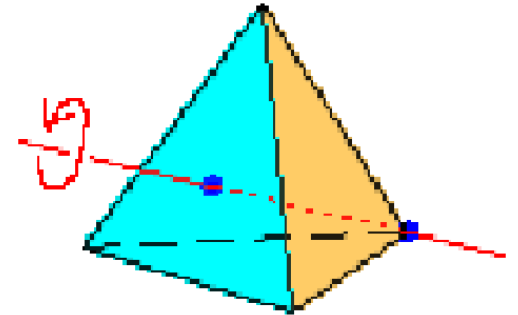
o identische Abbildung

o 4 3-zählige Achsen

(durch Ecke und Mittelpunkt der gegenüberliegenden Fläche, 2 Möglichkeiten für den Drehsinn)

o 3 2-zählige Achsen

(durch Mittelpunkte zweier gegenüberliegender Kanten)



* 6 Ebenenspiegelungen

* 6 Drehspiegelungen (90°-Drehung gefolgt von Ebenenspiegelung)

90° um Achse durch Mittelpunkte zweier gegenüberliegender Kanten; Spiegelung an zu dieser Achse senkrechter Ebene durch Mittelpunkt zwischen gegenüberliegenden Kanten

Oktaedergruppe: 48 Elemente

- * $90^\circ, 180^\circ, 270^\circ$ -Drehung um die 3 4-zähligen Drehachsen
(durch gegenüber liegende Ecken)
- * $120^\circ, 240^\circ$ -Drehung um die 4 3-zähligen Drehachsen
(durch gegenüber liegende Flächenmittelpunkte)
- * 180° -Drehung um die 6 2-zähligen Drehachsen
(durch gegenüber liegende Kantenmittelpunkte)
- * die Identität

$3 \times 3 + 4 \times 2 + 6 + 1 = 24$ Elemente der Drehgruppe,
kombiniert mit Spiegelungen:
 $2 \times 24 = 48$ Elemente der Symmetriegruppe.

$\#(O) = 24:$

Id + Drehungen:

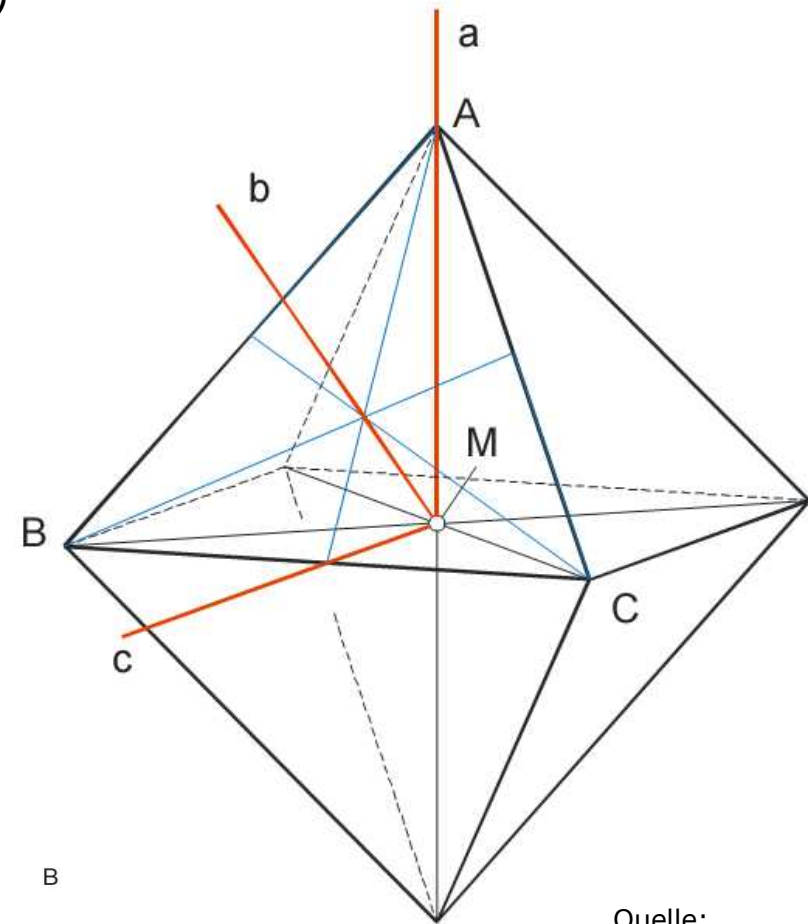
4-zählige Achsen ... *a*

3-zählige Achsen ... *b*

2-zählige Achsen ... *c*

Spiegelebene ...z.B.: [MBC]

→ O_h mit $\#(O_h) = 48$



Quelle:
Otto RÖSCHEL
Vortrag Strobl
TU Graz

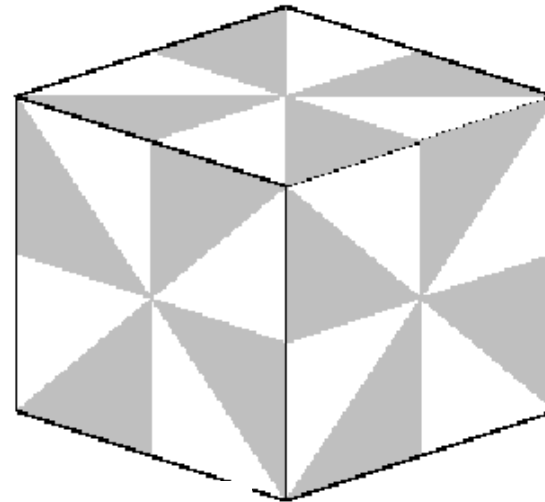
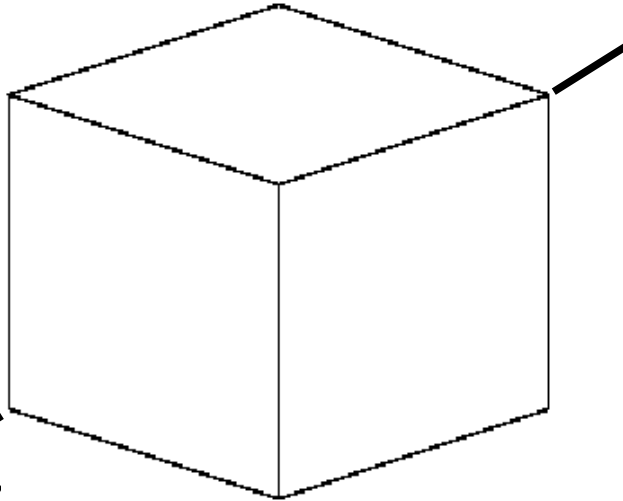
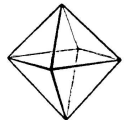
Punktsymmetrie der Basis: Schönflies-Nomenklatur

hier: Kubische kristallographische Punktgruppen

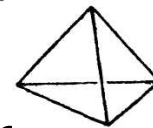
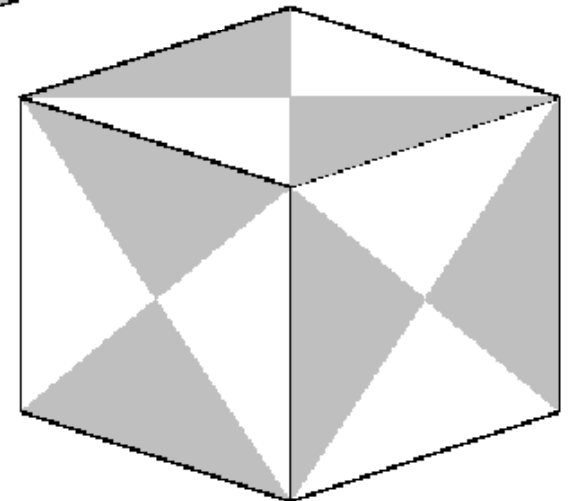
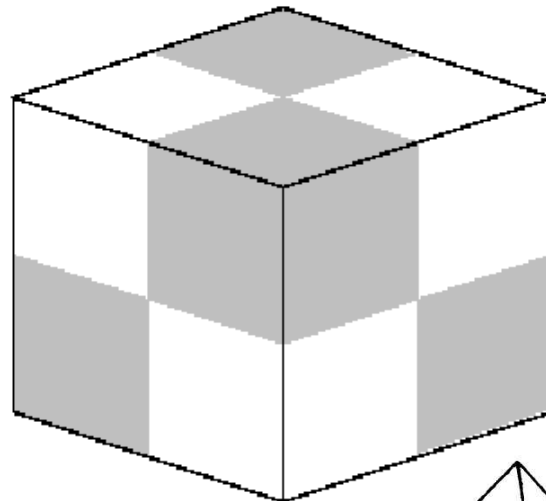
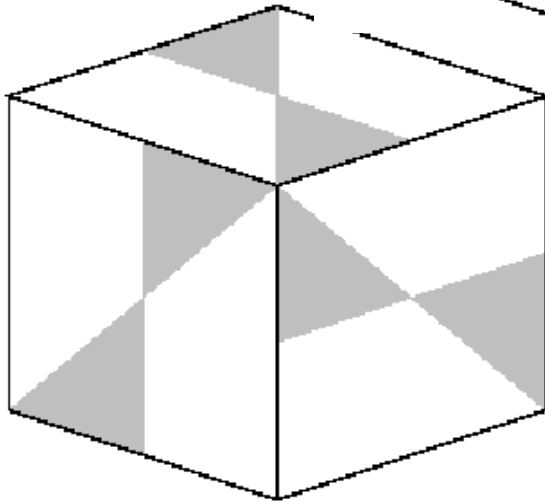
(Punktoperationen auf Gitter bei beliebiger Basis)

O_h : O + horizontale Spiegelebene

O)ktaedergruppe



Graphs:
U Newcastle upon Tyne

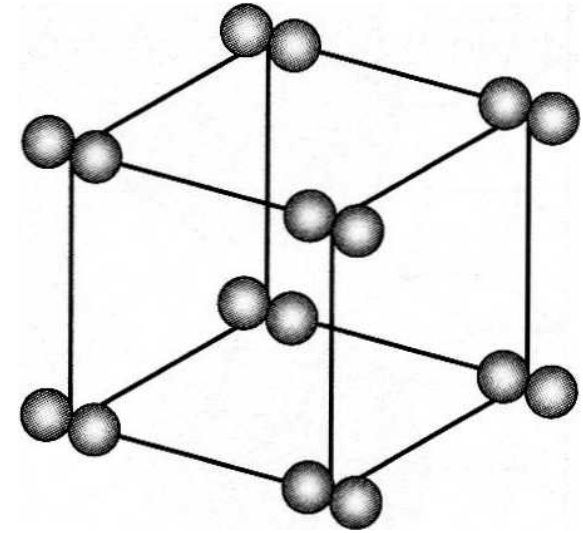
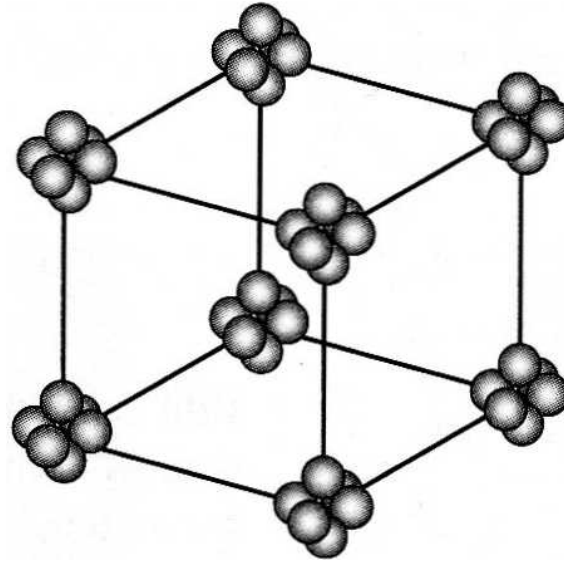
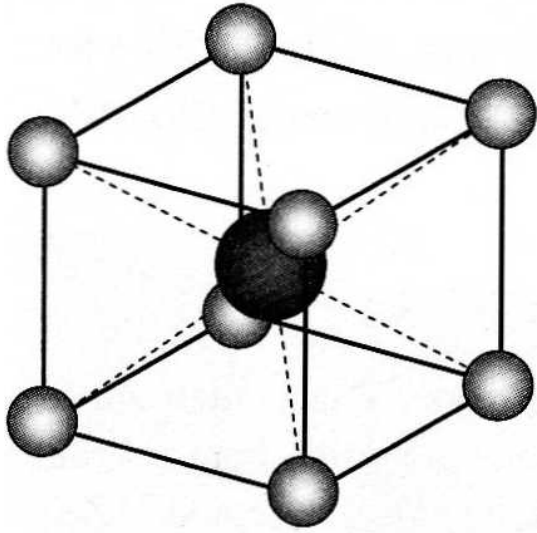


T)etraedergruppe

T_d : T + Inversion

T_h : T + Spiegelung

Kubische Elementarzellen mit unterschiedlichen Basen



mit kubischer Symmetrie verträglich

nicht zum kubischen Kristallsystem gehörig

Punktsymmetrie der Basis

Nicht-kubische Punktgruppen

C_n n-fache Drehachse

C_{nv} dazu noch m (enthält Achse)

+ die sich ergebenden m

C_{nh} n-fache Achse + dazu \perp m

S_n n-fache Drehspiegelachse

D_n n-fache Drehachse

+ 2fache \perp dazu

+ sich ergebende 2-fache




























D_{nh} D_n + m \perp zur n-Achse

D_{nd} D_n + m, die Winkel

zwischen n und 2 halbiert

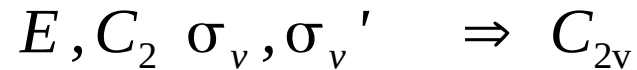
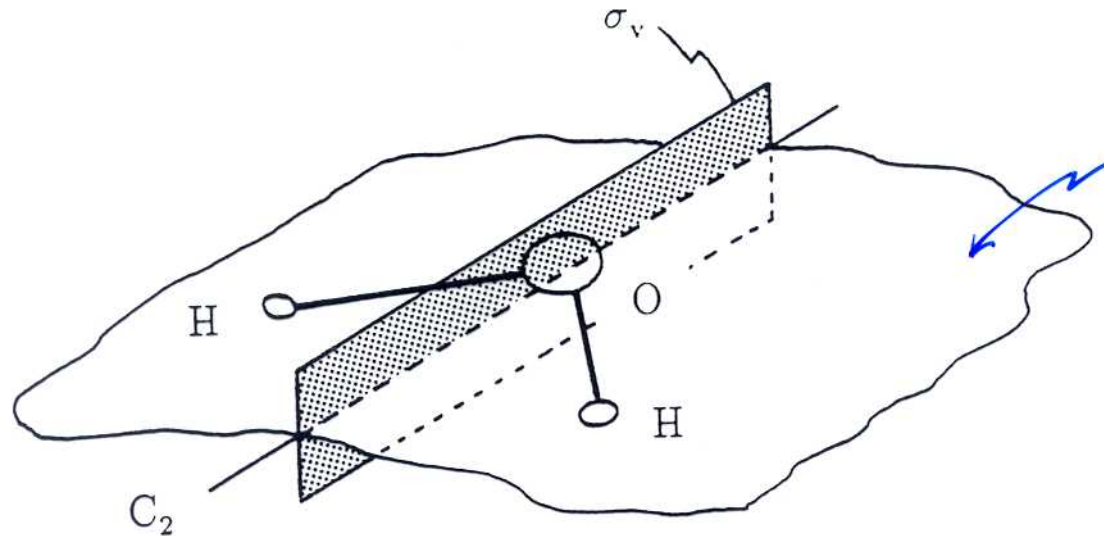
c)yclisch h)orizontal d)iagonal

v)ertikal S)piegel

SCHOENFLIES	HEXAGONAL	TETRAGONAL	TRIGONAL	ORTHO-RHOMBIC	MONOCLINIC	TRICLINIC
C_n	C_6  6	C_4  4	C_3  3		C_2  2	C_1  1
C_{nv}	C_{6v}  6mm	C_{4v}  4mm	C_{3v}  3m	C_{2v}  2mm		
C_{nh}	C_{6h}  6/m	C_{4h}  4/m			C_{2h}  2/m	
	C_{3h}  $\bar{6}$				C_{1h} ($\bar{2}$)  m	
S_n		S_4  $\bar{4}$	S_6  (C_{3i}) $\bar{3}$			S_3  (C_i) $\bar{1}$
D_n	D_6  622	D_4  422	D_3  32	D_2  (V) 222		
D_{nh}	D_{6h}  6/mmm	D_{4h}  4/mmm		D_{2h} (mmm)  (Vh) 2/mmm		
	D_{3h}  $\bar{6}2m$					
D_{nd}		D_{2d}  (Vd) $\bar{4}2m$	D_{3d} ($\bar{3}m$)  $\bar{3}2m$			

n.b.: International / Hermann-Mauguin





Punktgruppen

→ Symmetrie von Normalmoden

→ IR und Ramanaktivität

Üben: symmetry.otterbein.edu/gallery/

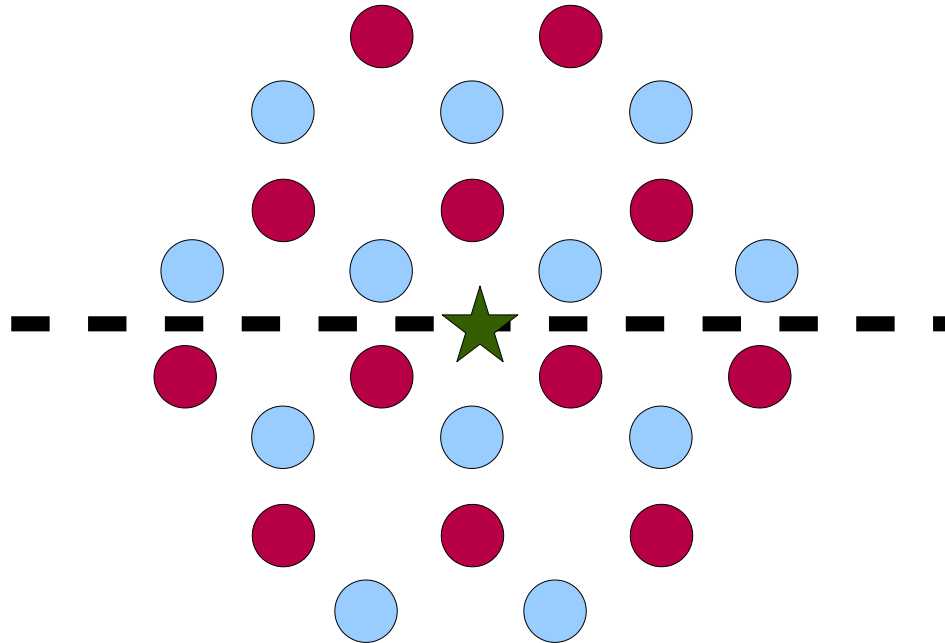
Professionelle Anwendung via Gruppentheorie, z. B. Vorlesung Prof. Pehlke

Das ist noch nicht alles:

Schraubenachsen, Gleitebenen

HCP structure viewed along c-axis

Lattice planes perpendicular to c-axis are separated by $c/2$
and contain, alternately, red and blue points



- Line parallel to c-axis passing through the dot is **screw axis**.

Structure invariant under $c/2$ translation along axis followed by 60° rotation
(but not invariant under either of them alone)

- Plane parallel to c-axis that intersects figure in dashed line is a **glide plane**.

Structure invariant under $c/2$ translation along c-axis followed by reflection
in glide plane (but not invariant under either of them alone)



Glück gehabt:

Die meisten Elemente & Verbindungshalbleiter sind:

fcc face-centered cubic

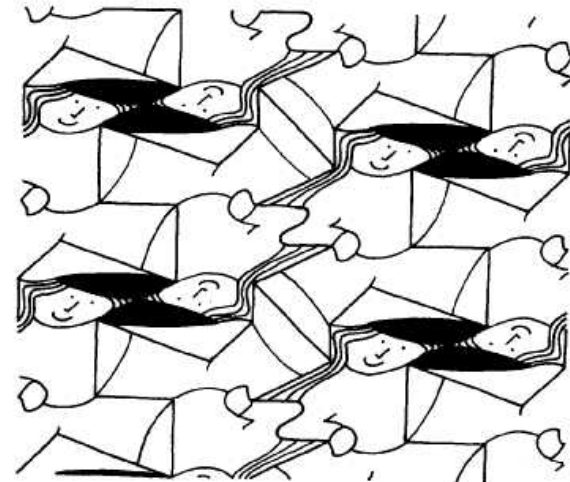
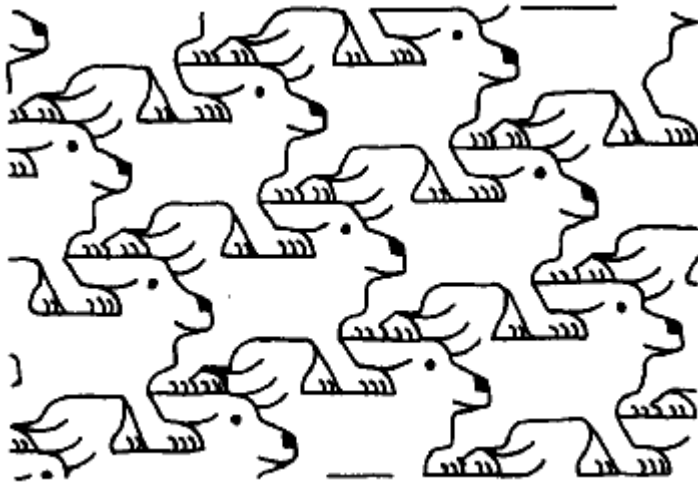
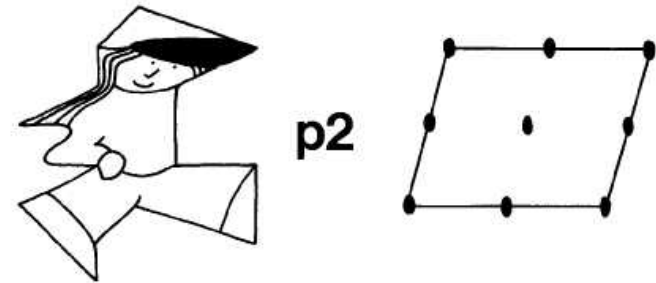
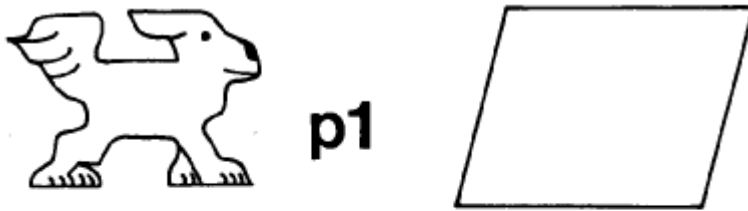
bcc body-centered cubic

Ein anderer Weg ins Glück:

werden Sie Oberflächenphysiker (und nicht 3d-Kristallograph) ...

In 2d gibt's nur 5 Bravaisgitter & 17 Raumgruppen

(außerdem sehen sie hübscher aus)



Konsequenzen fehlender Symmetrien:

Pyroelektrizität (z. B. Turmalin)

makroskopisches Dipolmoment

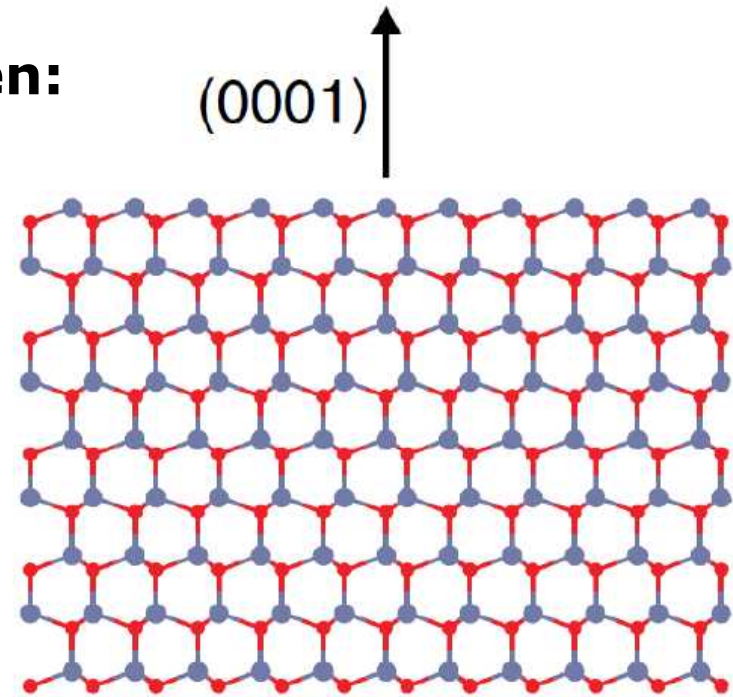
Piezoelektrizität (z. B. PZT)

verspannungsinduziertes Dipolmoment

Optische Aktivität (z. B. Quarz)

chirale Einheitszelle

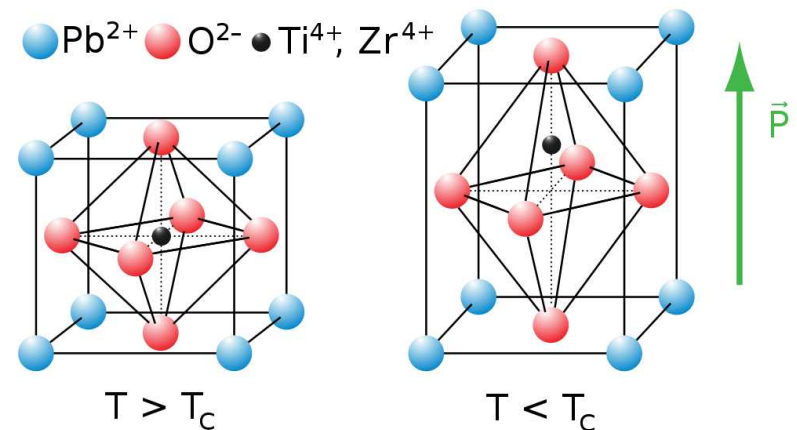
Blei-Zirkonat-Titanat
(Perowskit)

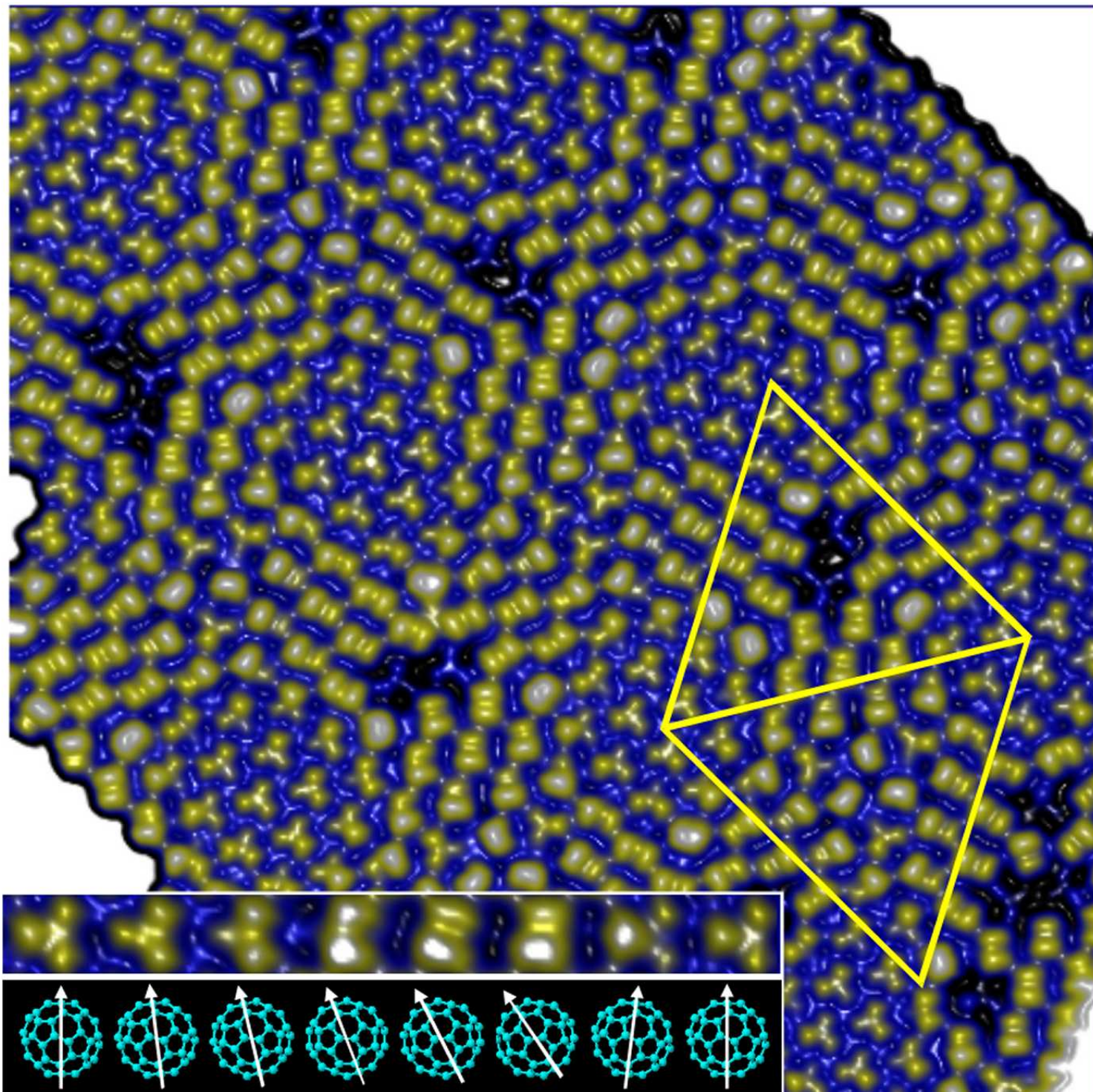


ZnO(0001): a polar surface

Wurtzite structure

$$a = 3.25 \text{ \AA} \quad c = 5.2 \text{ \AA}$$





Punktdefekte

• Wirtsatome

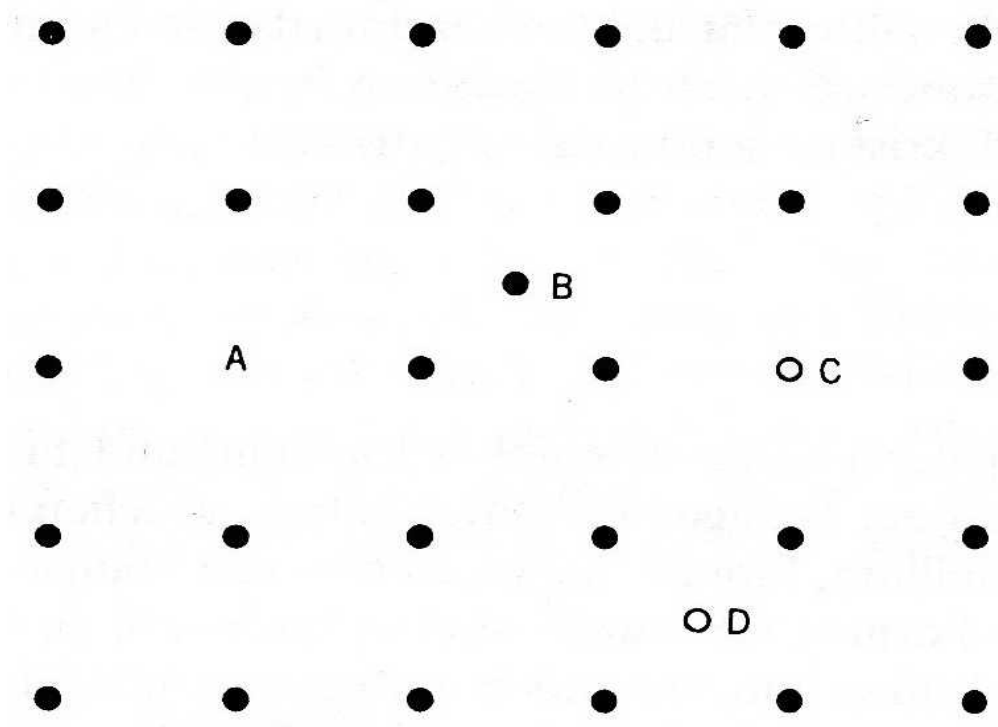
A Leerstelle

C substitutionelles Fremdatom

○ Fremdatom

B Zwischengitteratom

D interstitielles Fremdatom



Minimierung von ...

(helmholtzsche) freie Energie $F = U - T S$ ($T, V = \text{const}$)

freie Enthalpie (Gibbs-Energie) $G = H - T S$ ($T, p = \text{const}$)

"möchte", dass S groß ist (falls $T > 0$)

Konsequenz: Defekte sind i. A. notwendig.

Liniendefekte: Stufenversetzung

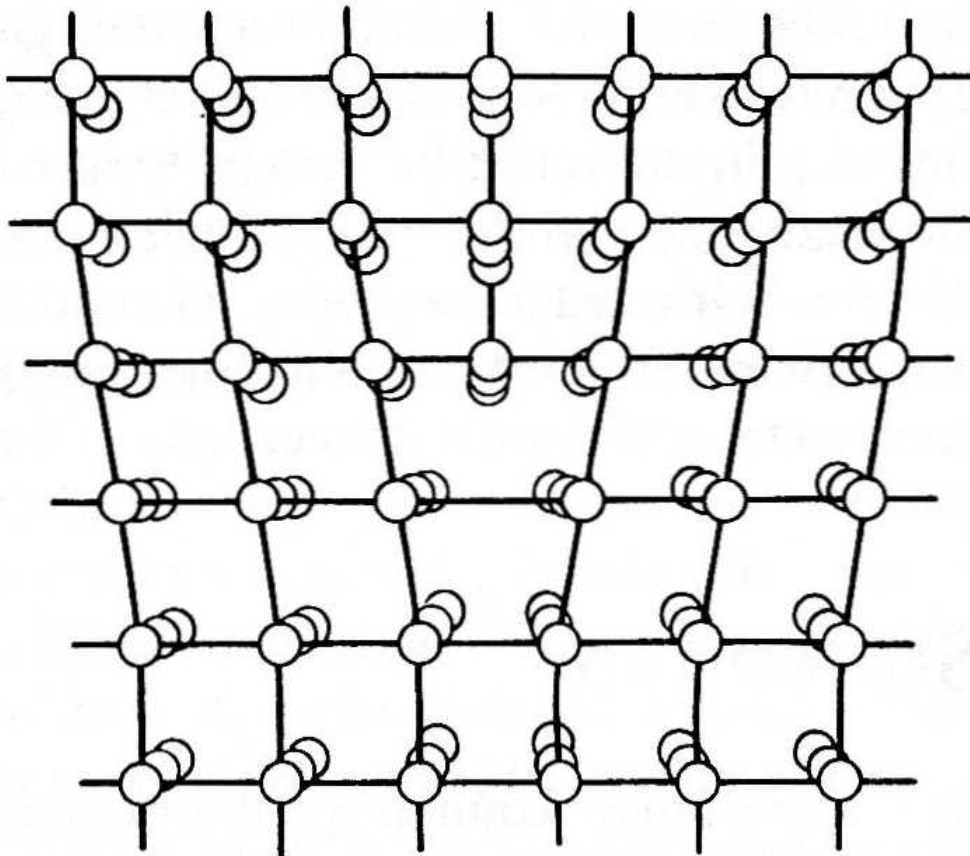


Versetzungen (dislocations)

Liniendefekt

Stufenversetzung

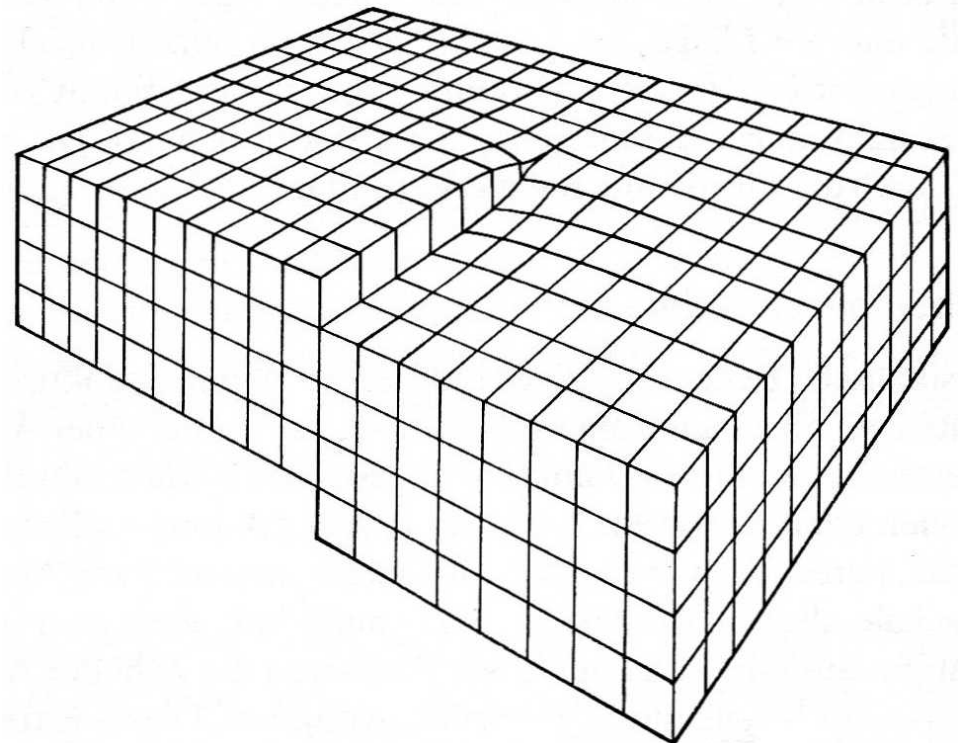
Zusätzliche Netzebene beginnt
in Bildmitte



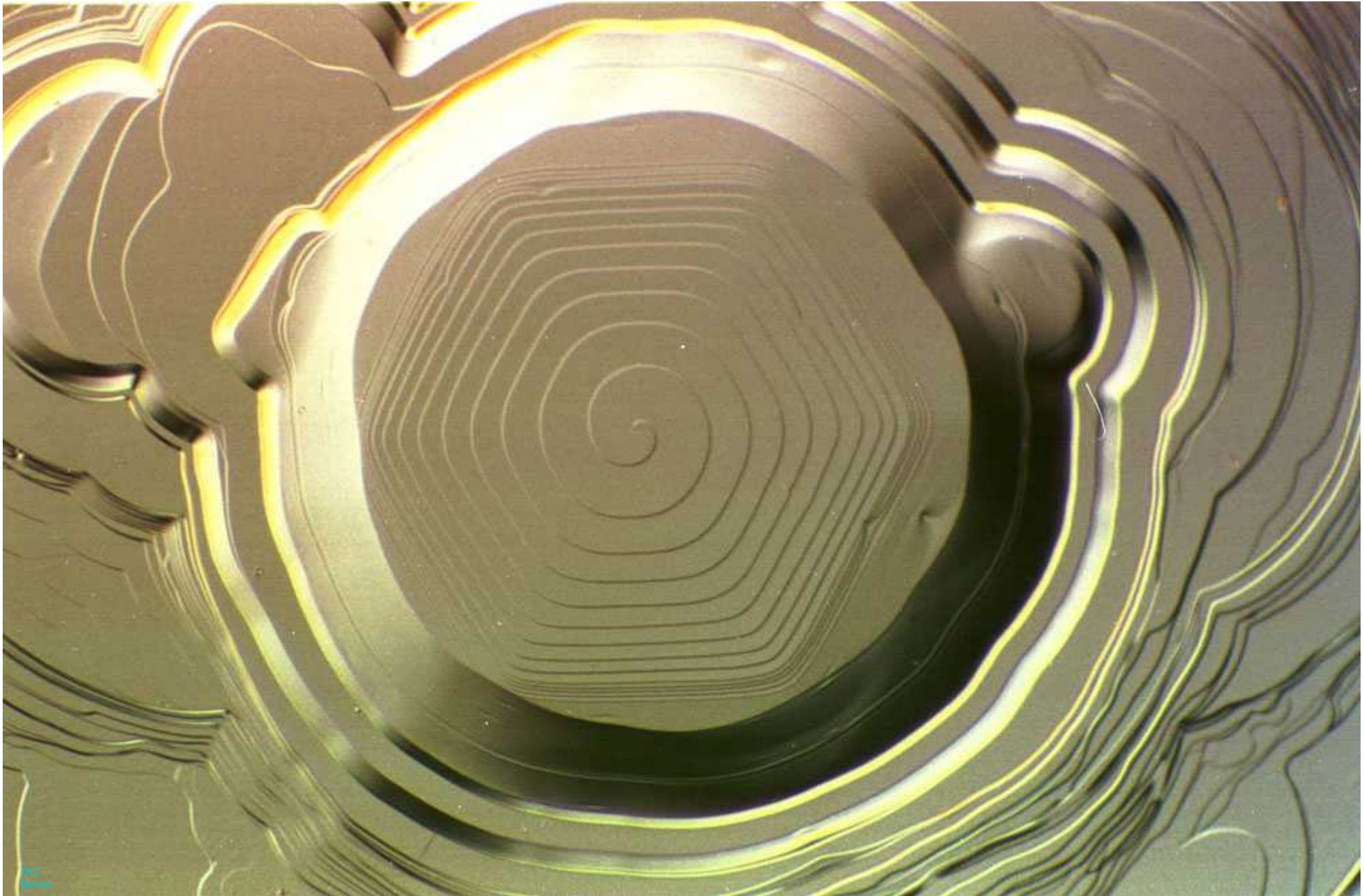
Schraubenversetzung

Versetzungsebene von vorn in
Kristallmitte

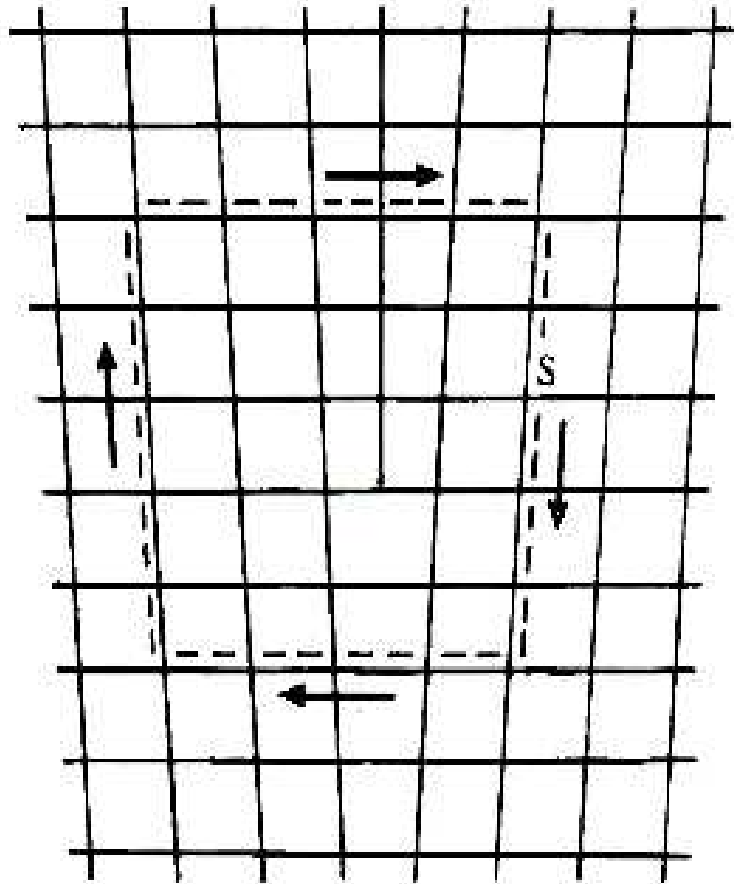
Atome links um Einheitszelle nach
oben verschoben



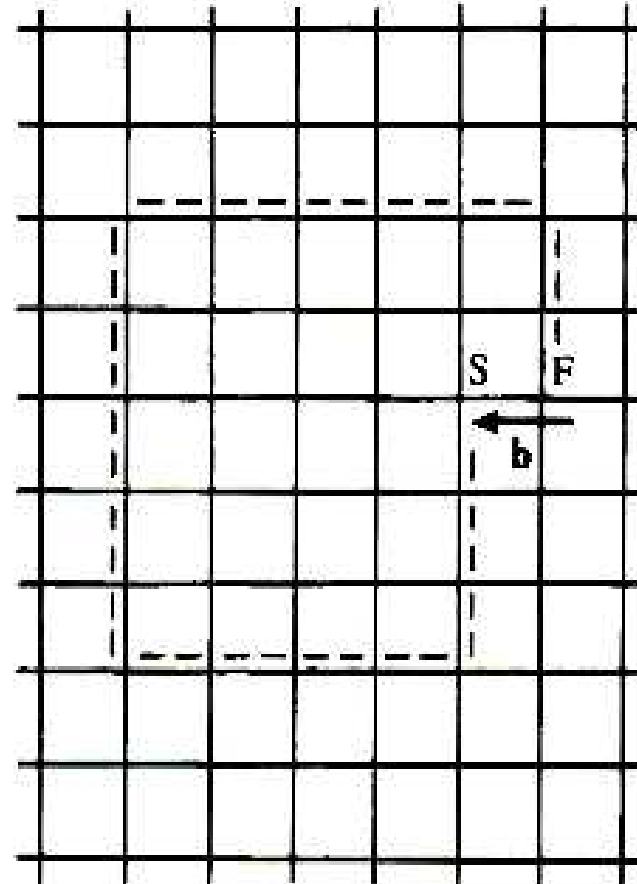
SiC



Burgersvektor b



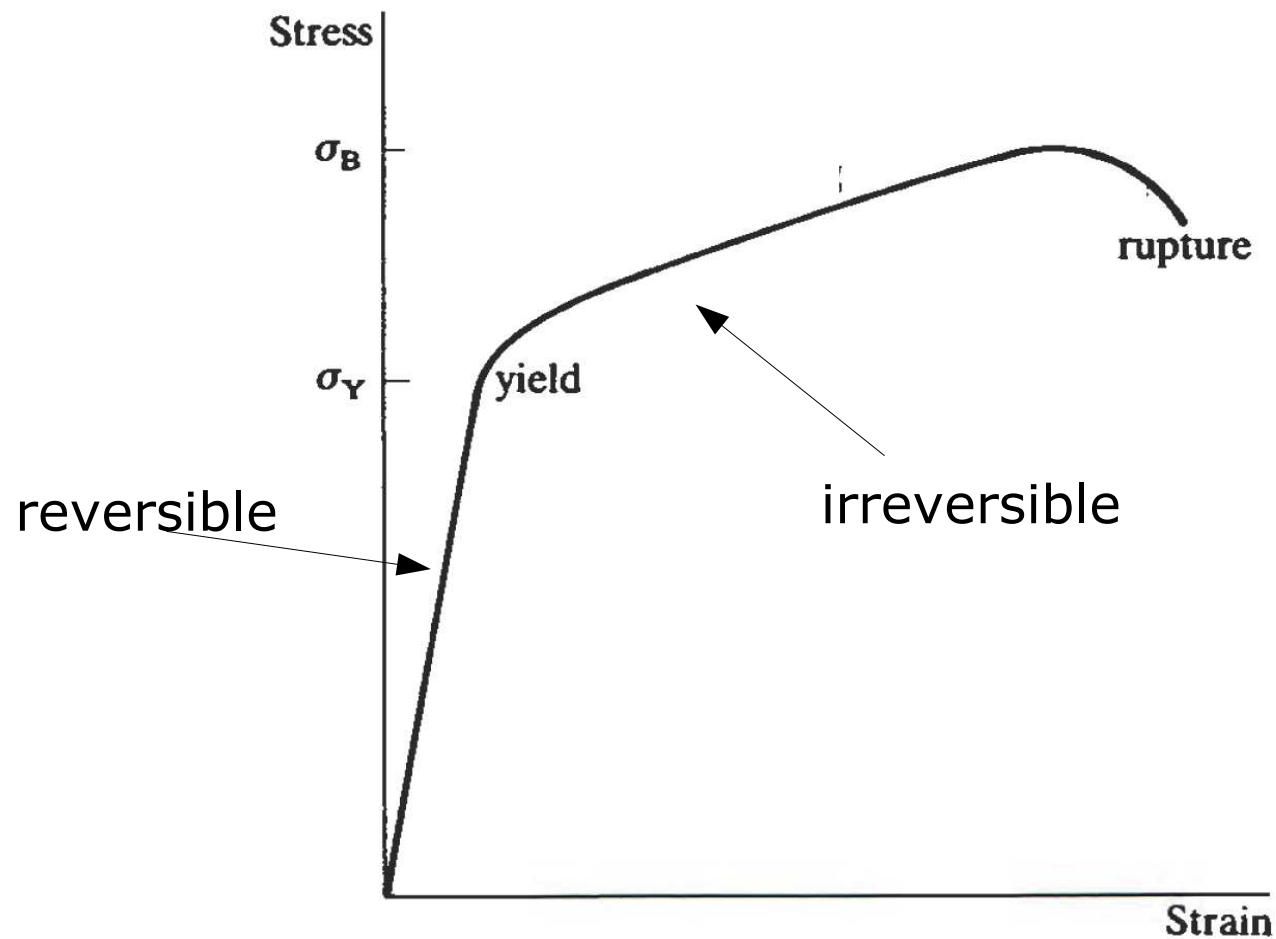
real crystal



ideal crystal

Spannungs-Dehnungs-Kurve

polykristallines Metall, sehr schematisch

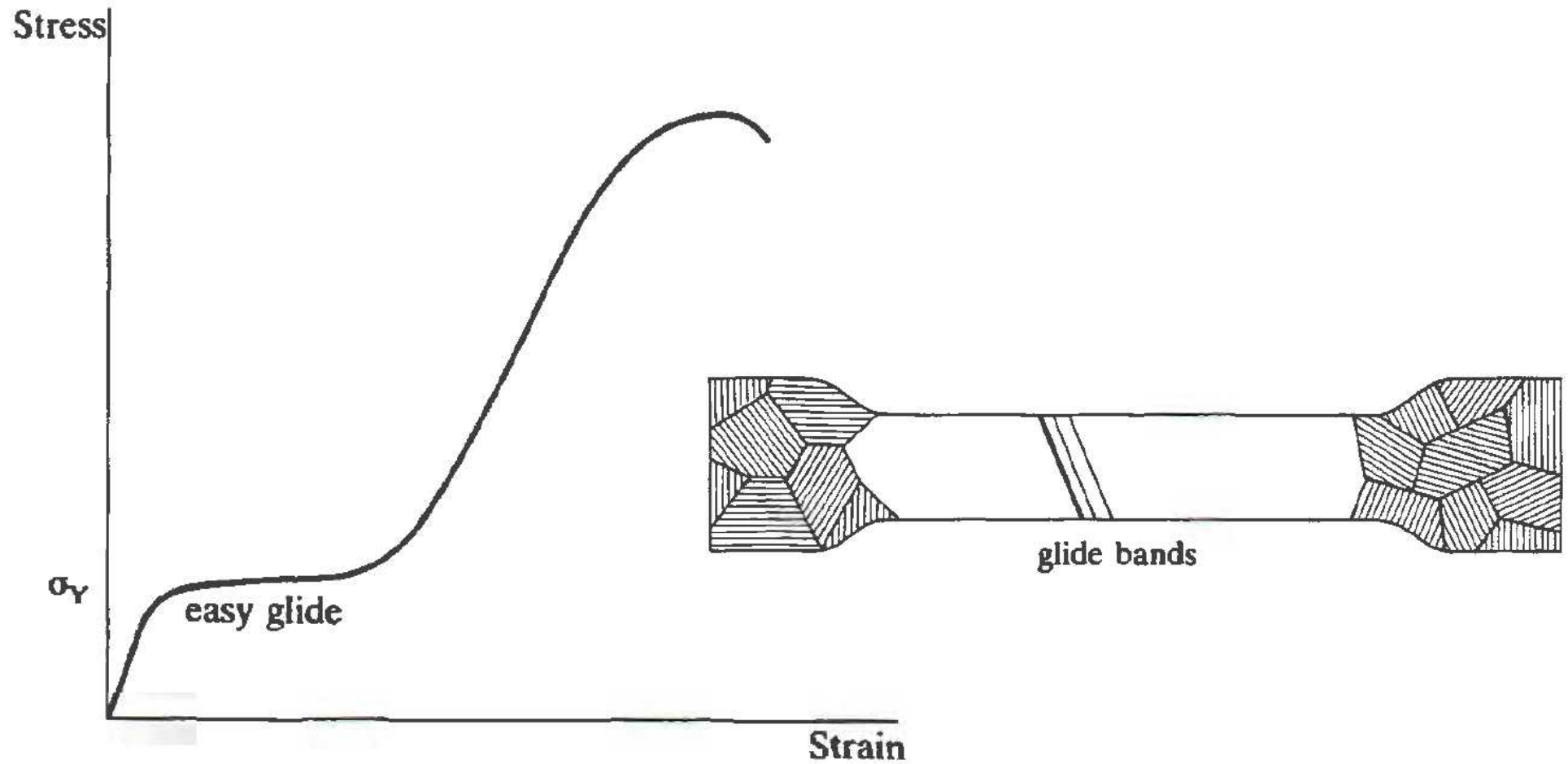


Young's modulus E

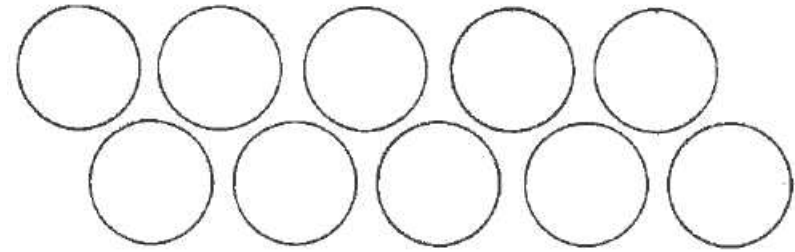
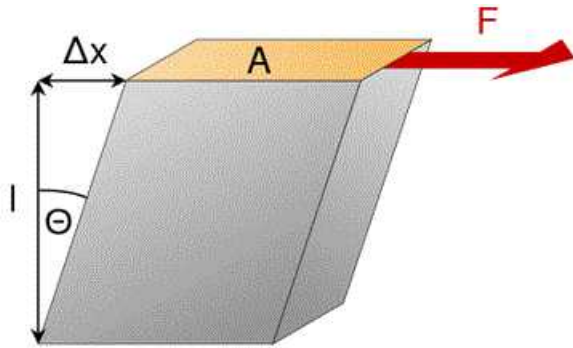
$$E = \frac{\text{stress}}{\text{strain}} = \frac{\text{force per unit area}}{\text{extension per unit length}}$$

Spannungs-Dehnungs-Kurve

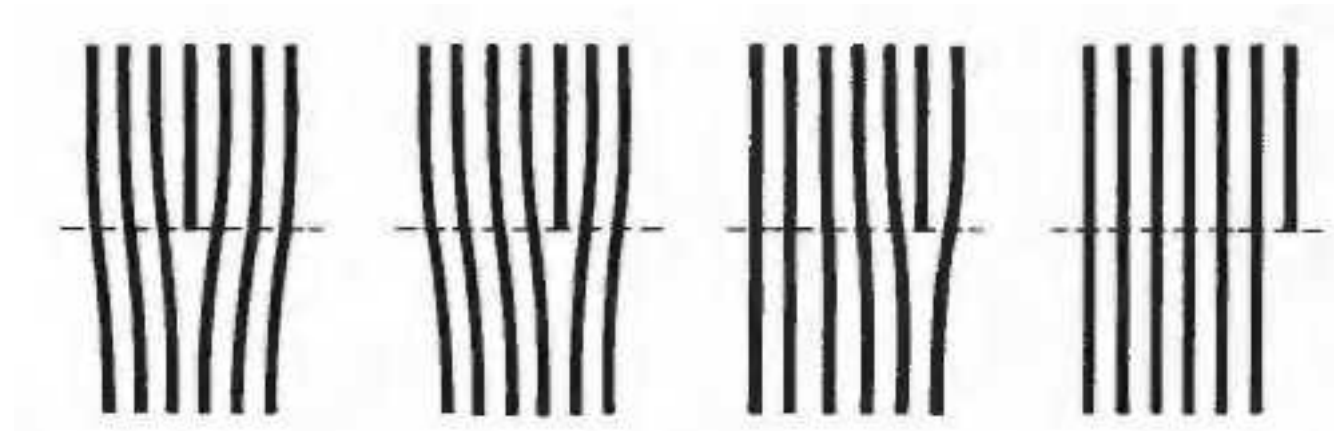
metallischer Einkristallstab



Versetzungen verringern Schermodul G drastisch



$$G = \frac{F/A}{\Delta x/l} = \frac{Fl}{A\Delta x}$$



Richtungen im Gitter

Eine Richtung $\mathbf{r} = x \mathbf{a}_1 + y \mathbf{a}_2 + z \mathbf{a}_3$ wird indiziert als $[x \ y \ z]$

$\langle x \ y \ z \rangle$ beschreibt alle zu $[x \ y \ z]$ symmetrie-äquivalenten Richtungen

$\langle 100 \rangle$ also in kubischen Gittern für $[100]$, $[010]$, $[001]$

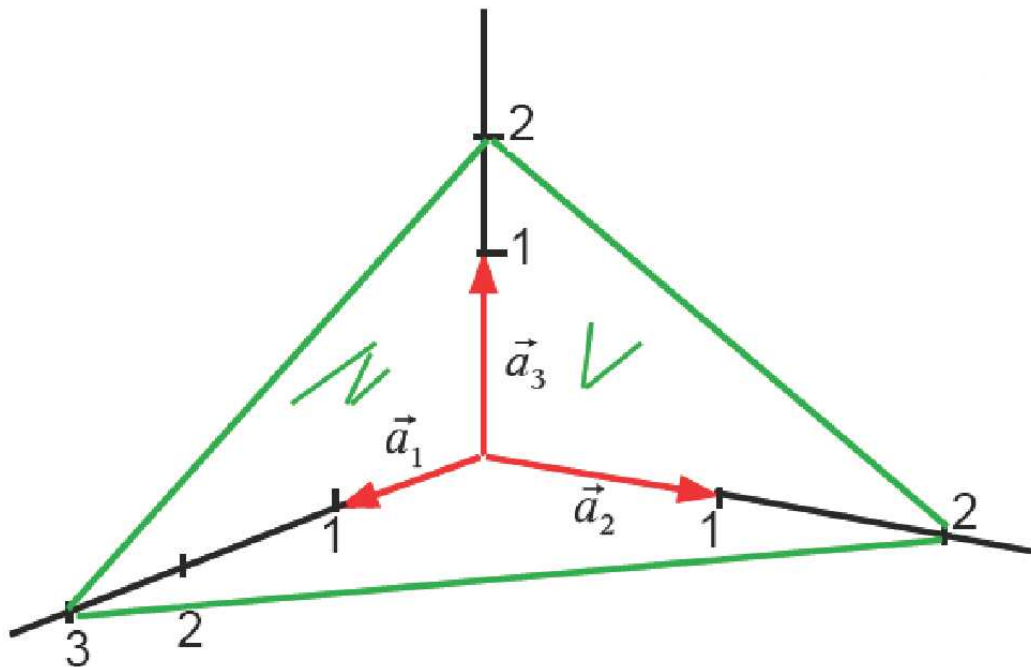
Miller Indizes: Gitterebenen

Ebene im Kristall durch Pkte $n_1 \vec{a}_1, n_2 \vec{a}_2, n_3 \vec{a}_3$

Indiziert durch Miller-Indizes $(h \ k \ l)$

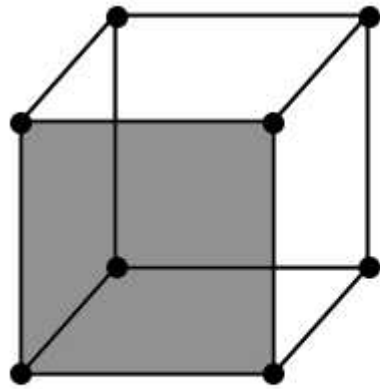
kleinste ganze Zahlen mit:

$$h : k : l = \frac{1}{n_1} : \frac{1}{n_2} : \frac{1}{n_3}$$

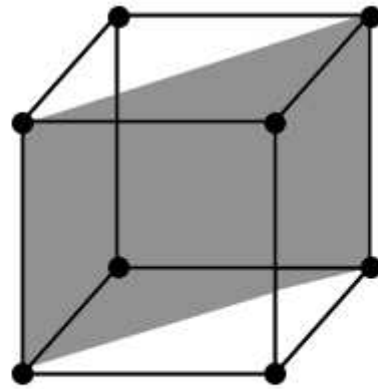


$$h : k : l = \frac{1}{3} : \frac{1}{2} : \frac{1}{2}$$

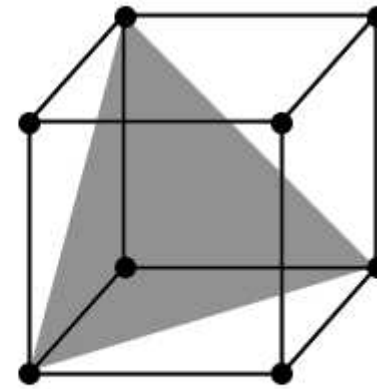
$$(2 \ 3 \ 3)$$



(100)



(110)



(111)

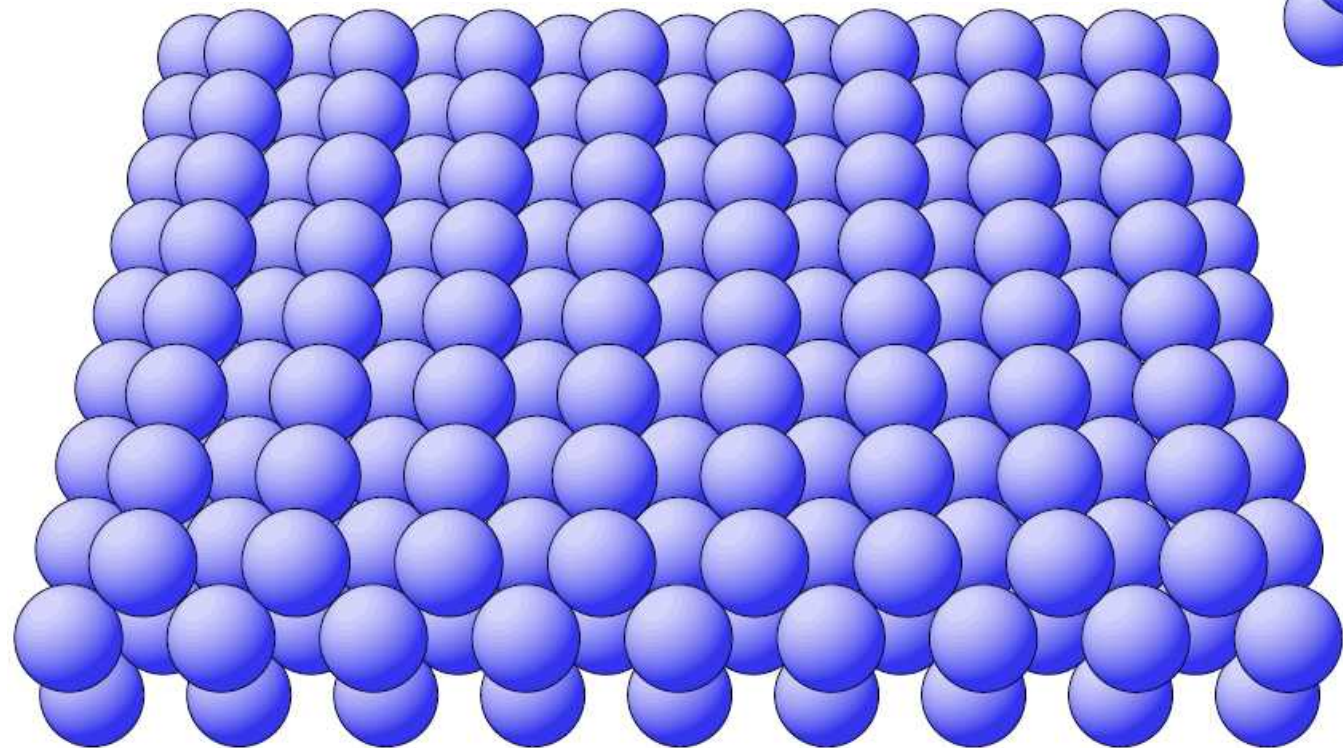
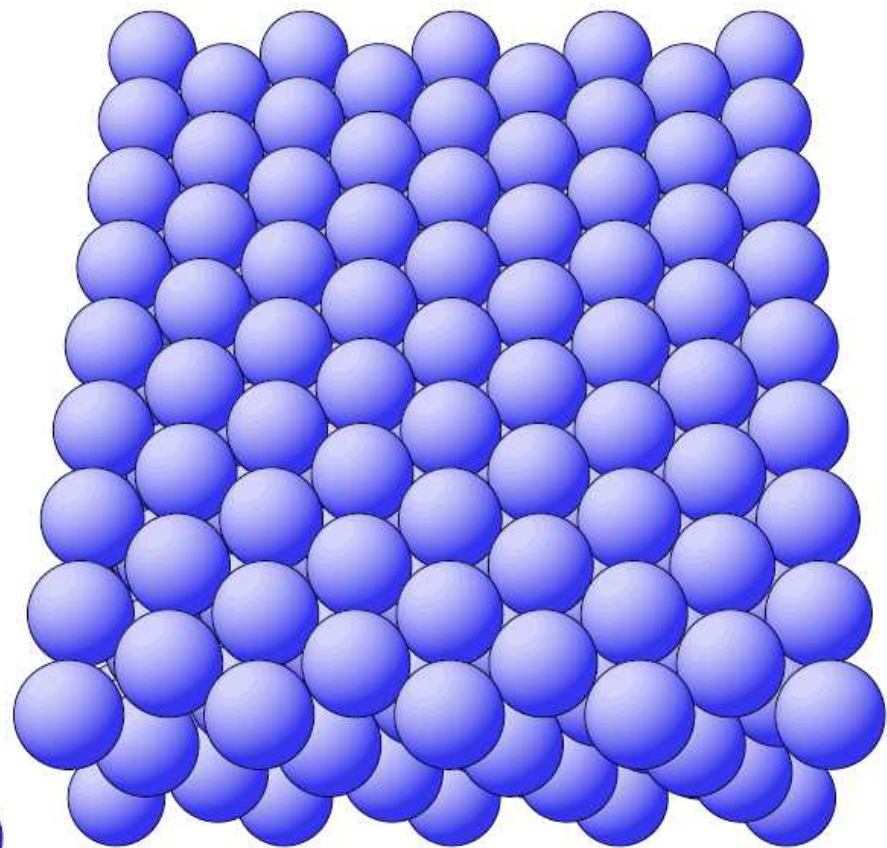
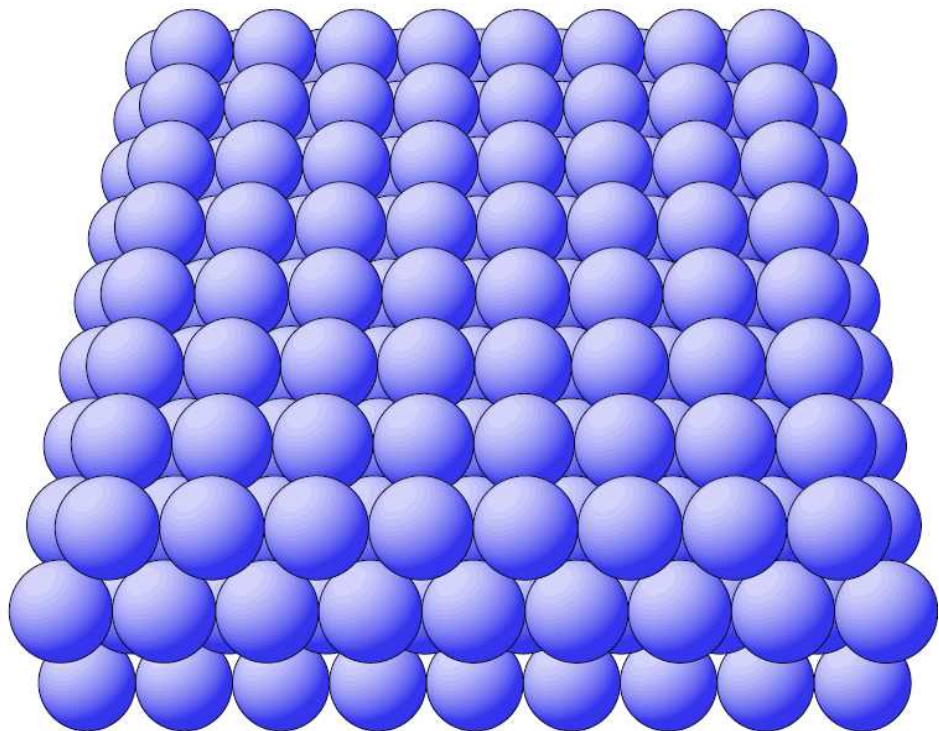
$$(100) = \frac{1}{1} : \frac{1}{\infty} : \frac{1}{\infty}$$

in kubischen Kristallen:

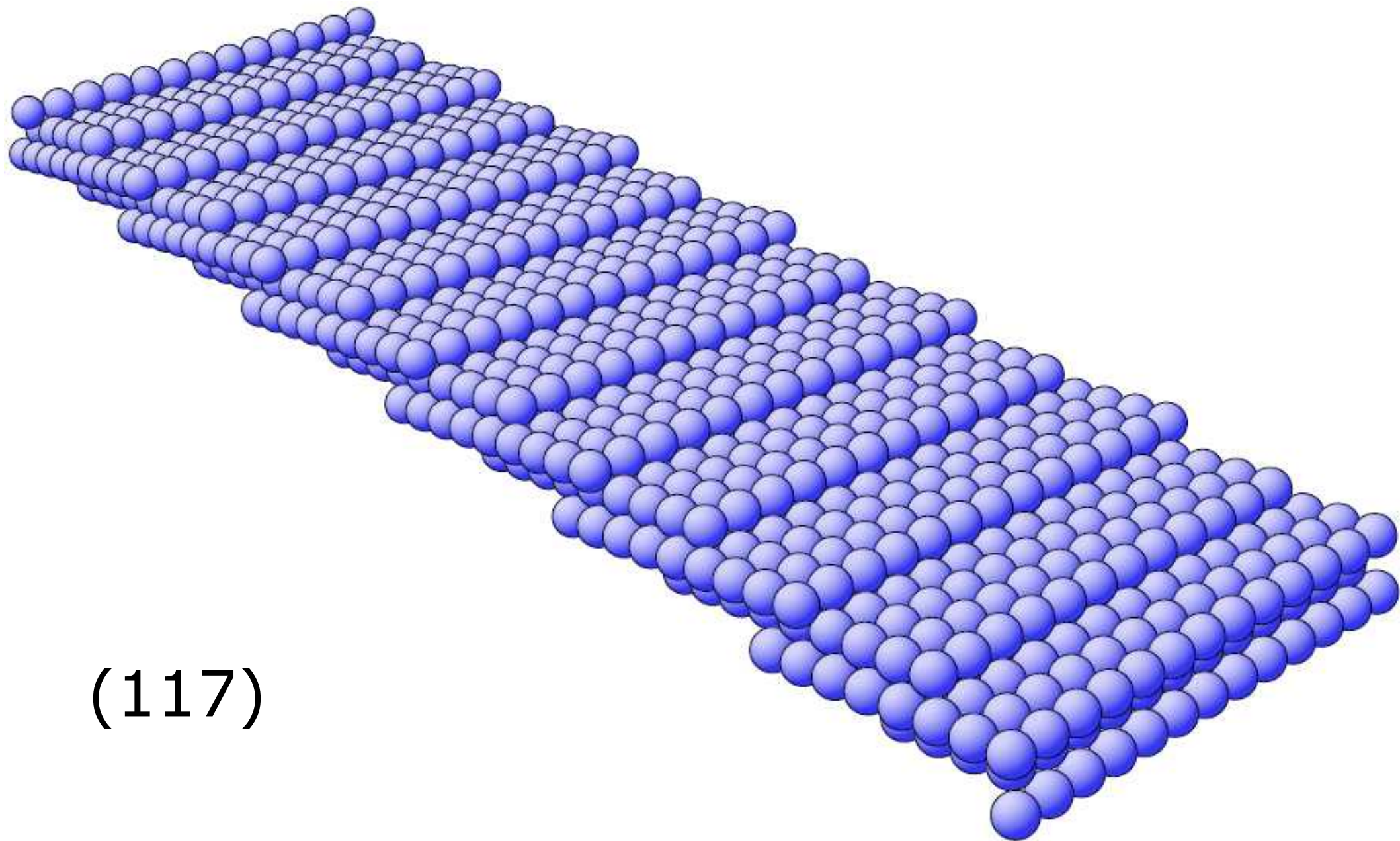
$(\bar{1}10)$

$$(h k l) \perp [h k l]$$

$\{100\}$ für (100), (010), (001)

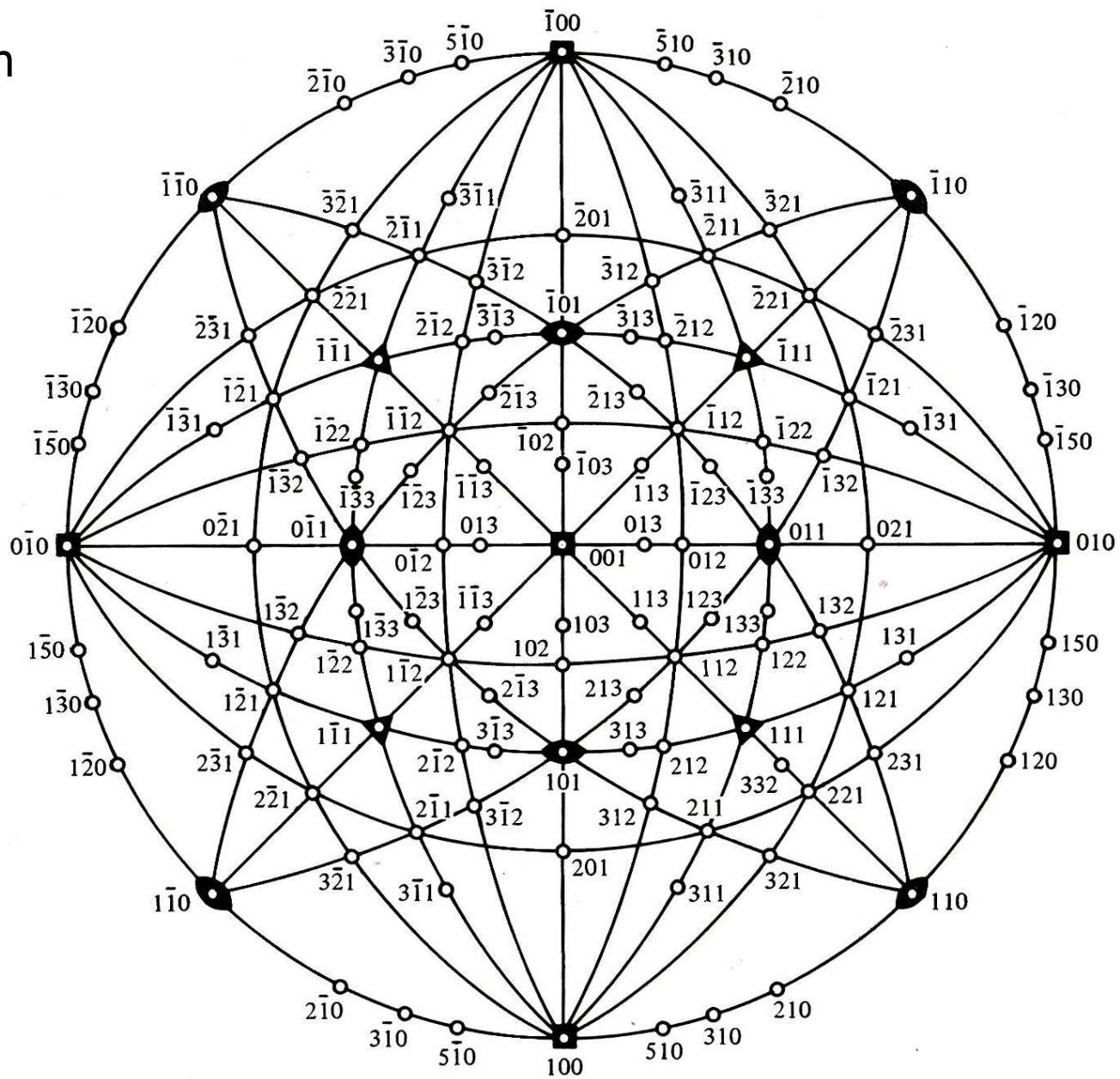


fcc



(117)

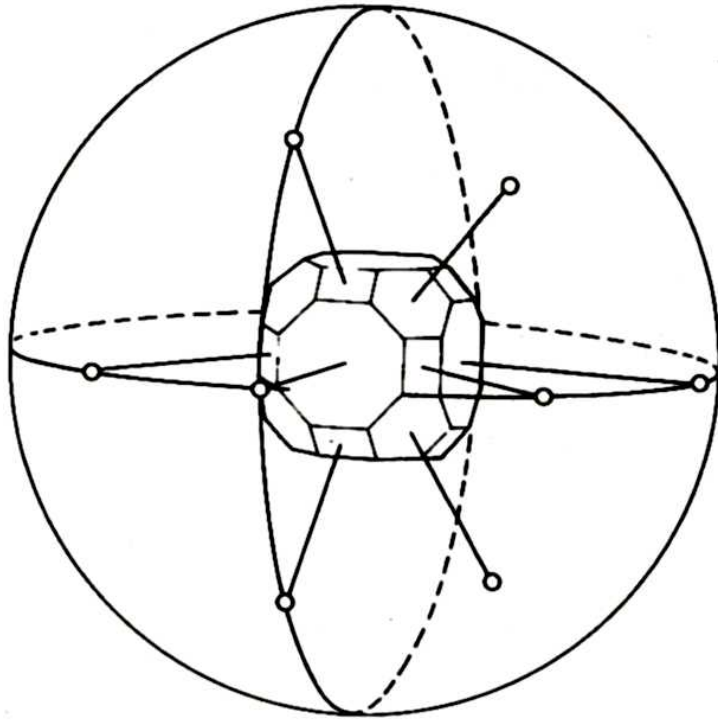
Stereogramm eines kubischen Kristalls



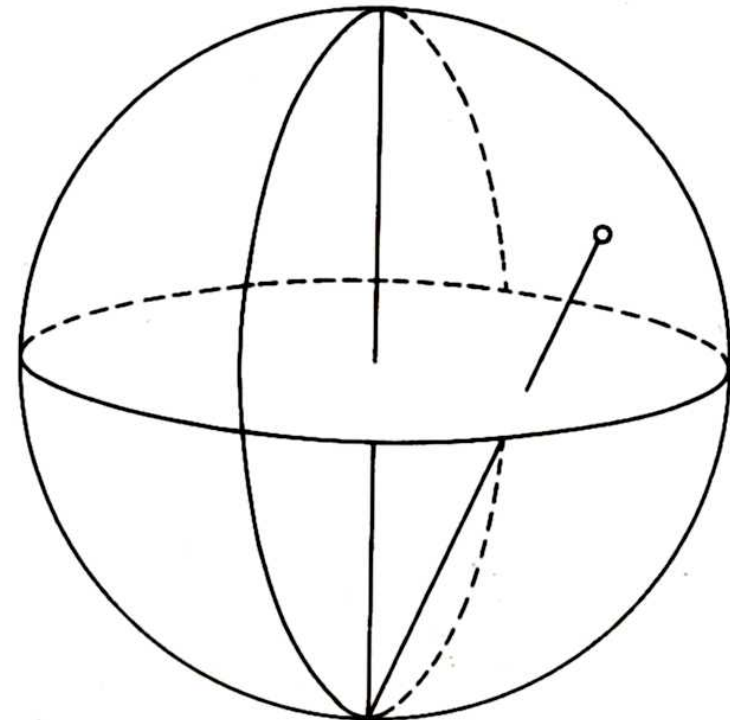
(aus Myers)

Part of a stereogram for a cubic crystal. The projection in question is made around the (001) plane, but any plane may be used. Certain groups of planes lie on 'great circles', i.e. diametral circles, and this facilitates the appreciation of angular relationships between crystal planes.

Konstruktion eines Stereogramms



(a)



P

(b)

Aufpunkt

(a) Imagine the crystal placed at the centre of a sphere. Each crystal plane is connected to the sphere by its normal. The points of intersection of the normals with the sphere produce the spherical projection.

(b) Now imagine an equatorial plane. Connect all points of the spherical projection in the 'northern hemisphere' to the 'south pole' P. The connecting lines cut the equatorial plane at points that form the stereographic projection of the upper half of the crystal. Only when the

(aus Myers)
crystal lacks a centre of symmetry need we project the upper and lower halves separately.