

Crystal Structure

- Translation vectors and unit cells

- Symmetry operations and Bravais lattices

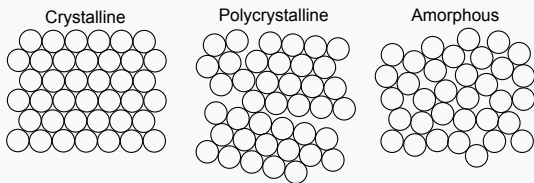
- Simple crystal structures

- Miller indices

Crystals, polycrystalline solids, and amorphous materials

Solid materials can be categorized according to the spatial arrangement of the constituting atoms:

- Crystalline solids (or, for short, crystals) are characterized by a strictly periodic arrangement of the constituting atoms in all three spatial dimensions. Crystals exhibit long-range order, i.e., the positions of the atoms in different parts of the crystal are correlated.
- Polycrystalline solids are composed of crystallites (small crystals) with varying size and orientation. Within each crystallite, the positions of the atoms are correlated. However, there is no long-range order between different crystallites.
- Amorphous solids are solids which do not possess long-range order.



Crystal Structure

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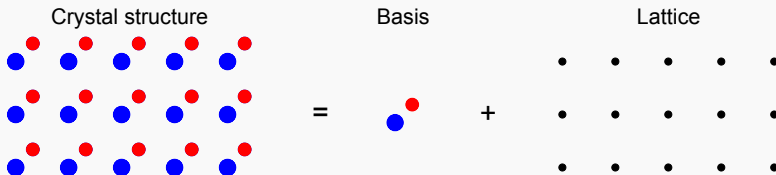
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Ideal crystals

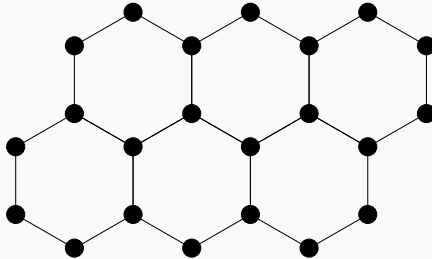
Solid materials can be categorized according to the spatial arrangement of the constituting atoms:

- An ideal crystal is composed of identical groups of atoms which are arranged in an infinite, periodic array.
- A set of equivalent points in the array defines the lattice of the crystal.
- A group of atoms that is attached to every point of the lattice is called a basis.



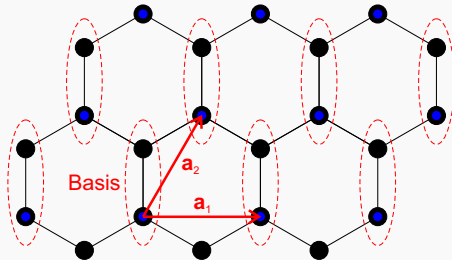
Example: Graphen

- Graphene consists of a single layer of carbon atoms arranged in a honeycomb structure.
- Each atom has three nearest neighbors with 120° bond angles resulting from sp^2 hybridization.
- Find the lattice and the basis!



Example: Graphen

- Graphene consists of a single layer of carbon atoms.
- Each atom has three nearest neighbors with 120° bond angles resulting from sp^2 hybridization.
- This honeycomb structure can be described by a triangular lattice with a two-atom basis.



Translation vectors

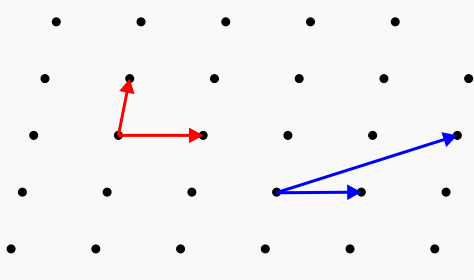
- A three-dimensional lattice can be characterized by a set of three primitive translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$.
- Two arbitrary points of the lattice, $\mathbf{R}$ and $\mathbf{R}'$, are connected through translation by suitable integer multiples m_j of the vectors $\mathbf{a}_j$:

$$\mathbf{R}' = \mathbf{R} + \sum_{j=1}^3 m_j \mathbf{a}_j.$$

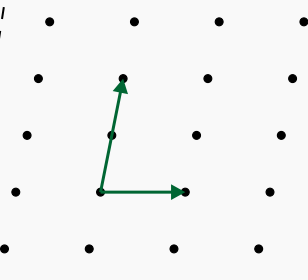
- For a given lattice, there is more than one set of primitive translation vectors. Moreover, not every set of vectors that connects a lattice point with three other lattice points defines a set of primitive translation vectors.

Example

Sets of primitive translation vectors



Not a set of primitive translation vectors



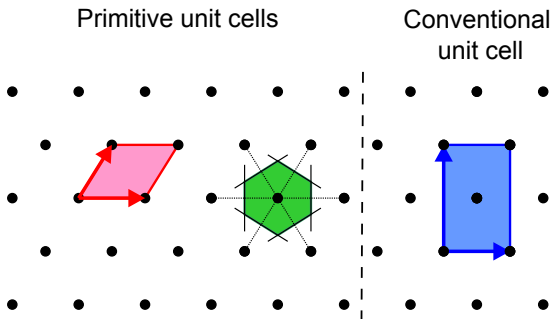
Unit cells

- A unit cell is a volume that fills all space without overlap or leaving voids when translated through a set of lattice vectors. If this set contains all lattice vectors, the unit cell is called a primitive cell or primitive unit cell.
- For a given lattice, there is no unique way of choosing a primitive cell. Each primitive cell contains one lattice point. Lattice points at the edges of the primitive cell are equally shared among the adjacent primitive cells.
- The parallelepiped spanned by three primitive translation vectors is a primitive cell. Its volume (and that of every other primitive cell) is given by

$$V_u = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3|.$$

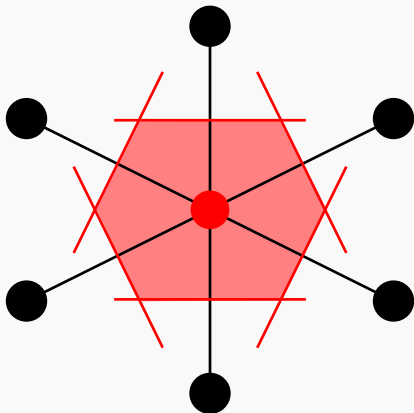
- It is often useful to choose a unit cell which is a parallelepiped with edges parallel to a suitable set of translation vectors and which displays the full symmetry of the lattice. This so-called conventional unit cell can contain more than one lattice point.

Example



Wigner-Seitz cell

The Wigner-Seitz cell is a primitive unit cell that contains all points in space that are closer to a particular lattice point than to any of the other lattice points.



Crystal Structure

Translation vectors and unit cells

Symmetry operations and Bravais lattices

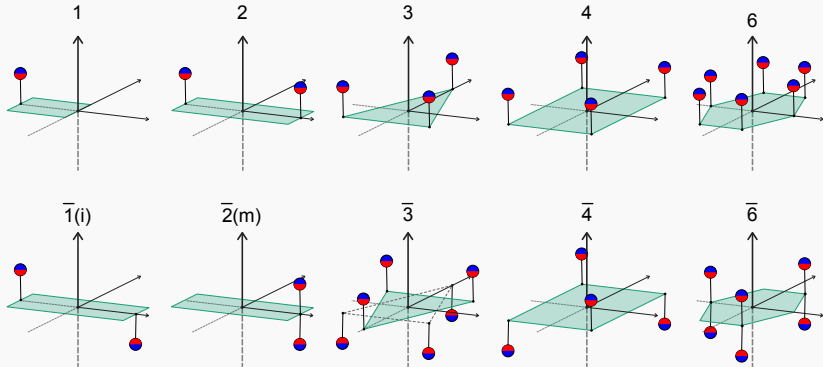
Simple crystal structures

Miller indices

Point groups and space groups

- The symmetry operations that transform a crystal into itself while leaving at least one point fixed form the so-called crystallographic point groups. In 3D, there are 32 distinct crystallographic point-groups.
- Possible symmetry operations of a point group are:
 - Rotations through multiples of $2\pi/n$ about some axis: The axis is called a n -fold axis. A Bravais lattice (see next section) can contain only 2-, 3-, 4-, or 6-fold axes.
 - Reflections: Reflection in a plane.
 - Inversions: Every point $\mathbf{r}$ is taken into $-\mathbf{r}$. The origin is the inversion center.
 - Rotation-reflection: Rotation through $2\pi/n$ followed by a reflection in a plane perpendicular to the rotation axis.
 - Rotation-inversion: Rotation through $2\pi/n$ followed by an inversion in a point of the rotation axis.
- The combination of these symmetry operations with translational symmetries forms the so-called space group. In 3D, there are 230 different space groups.

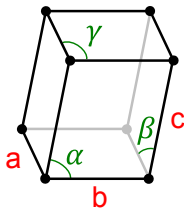
Symmetry operations of the point group



- 1: identity
- 2, 3, 4, 6: 2-, 3-, 4-, 6-fold rotation
- $\bar{1}(i)$: inversion
- $\bar{2}(m)$: reflection; 2-fold rotation followed by inversion
- $\bar{3}, \bar{4}, \bar{6}$: 3-, 4-, 6-fold rotation followed by inversion

- Often, we are only interested in the symmetry properties of the lattice of a crystal, i.e., translations, rotations, reflections, and inversions, that take the lattice into itself.
- In 3D, there are 14 distinct types of lattices, the so-called Bravais lattices.
- The 14 Bravais lattices are grouped into 7 lattice systems: triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, and cubic.

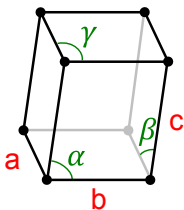
Triclinic lattice system



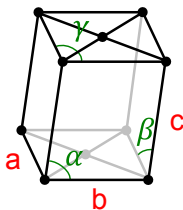
Lattice parameters: $a \neq b \neq c, \alpha \neq \beta \neq \gamma$.

Monoclinic lattice system

Simple
monoclinic

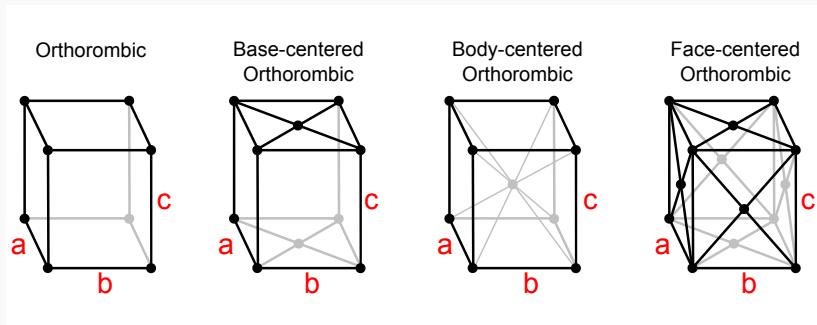


Base-centered
monoclinic



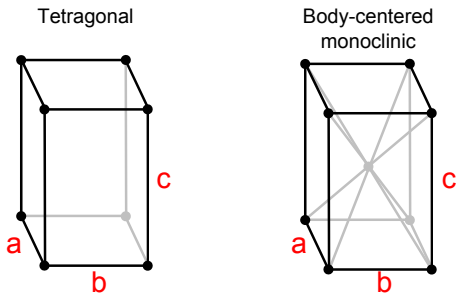
Lattice parameters: $a \neq b \neq c$, $\beta \neq 90^\circ$, $\alpha = \gamma = 90^\circ$.

Orthorhombic lattice system



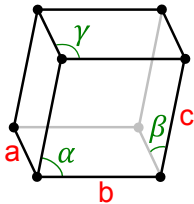
Lattice parameters: $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$.

Tetragonal lattice system



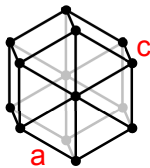
Lattice parameters: $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$.

Rhombohedral lattice system



Lattice parameters: $a = b = c$, $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$.

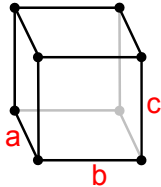
Hexagonal lattice system



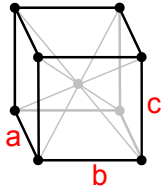
Lattice parameters: $a = b \neq c$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$.

Cubic lattice system

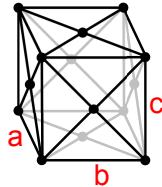
Simple cubic (sc)



Body-centered cubic (bcc)



Face-centered cubic (fcc)



Lattice parameters: $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$.

Crystal Structure

Translation vectors and unit cells

Symmetry operations and Bravais lattices

Simple crystal structures

Miller indices

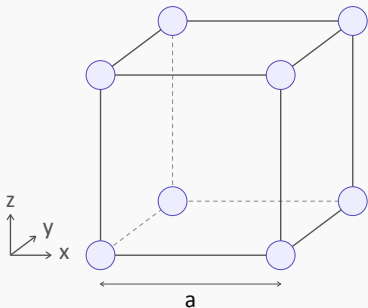
Crystal structure of elements in the periodic table

1 H																	2 He														
3 Li W	4 Be Mg											5 B β-B	6 C g-C	7 N	8 O	9 F	10 Ne														
11 Na W	12 Mg Mg											13 Al Cu	14 Si d-C	15 P b-P	16 S α-S	17 Cl	18 Ar														
19 K W	20 Ca Cu	21 Sc Mg	22 Ti Mg	23 V W	24 Cr W	25 Mn α-Mn	26 Fe W	27 Co Mg	28 Ni Cu	29 Cu Cu	30 Zn Mg	31 Ga α-Ga	32 Ge d-C	33 As α-As	34 Se γ-Se	35 Br	36 Kr														
37 Rb W	38 Sr Cu	39 Y Mg	40 Zr Mg	41 Nb W	42 Mo W	43 Tc Mg	44 Ru Mg	45 Rh Cu	46 Pd Cu	47 Ag Cu	48 Cd Mg	49 In In	50 Sn β-Sn	51 Sb α-As	52 Te γ-Se	53 I Cl	54 Xe														
55 Cs W	56 Ba W	71 Lu Mg	72 Hf Mg	73 Ta W	74 W W	75 Re Mg	76 Os Mg	77 Ir Cu	78 Pt Cu	79 Au Cu	80 Hg Cu	81 Tl Mg	82 Pb Cu	83 Bi α-Bi	84 Po α-Po	85 At	86 Rn														
87 Fr	88 Ra W	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og														
																		57 La α-La	58 Ce α-La	59 Pr α-La	60 Nd α-La	61 Pm α-La	62 Sm α-Sm	63 Eu W	64 Gd Mg	65 Tb Mg	66 Dy Mg	67 Ho Mg	68 Er Mg	69 Tm Mg	70 Yb Cu
																		89 Ac Cu	90 Th Cu	91 Pa α-La	92 U α-U	93 Np α-Np	94 Pu α-Pu	95 Am α-La	96 Cm α-La	97 Bk α-La	98 Cf α-La	99 Es Cu	100 Fm	101 Md	102 No

Legend:

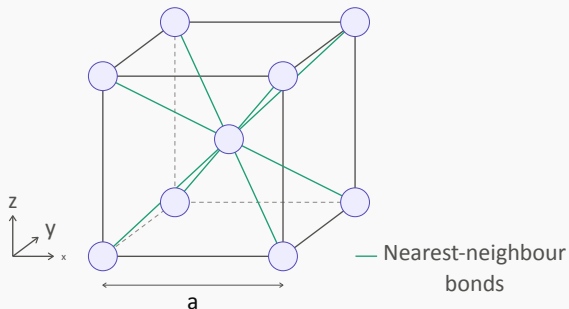
- Primitive monoclinic structures: α -Pu
- Orthorhombic structures: b-P, α -Ga, Cl, α -U, α -S, α -Np
- Body-centered tetragonal structures: In, β -Sn, α -Pa
- Rhombohedral structures: β -B, α -As, α -Sm
- Hexagonal structures: Mg, α -La, g-C, γ -Se
- Primitive cubic structures: α -Po
- Body-centered cubic structures: W, α -Mn
- Face-centered cubic structures: d-C, Cu
- Not solid at standard temperature and pressure or uncertain

Simple cubic



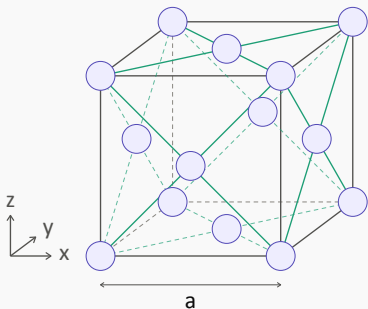
- Example: α -Po
- Packing fraction: 0.52
- Coordination number (# of nearest neighbors): 6
- Nearest-neighbor distance: a

Body-centered cubic



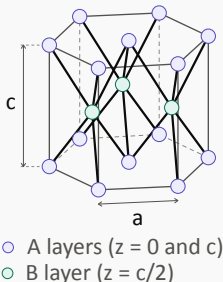
- Examples: W, α -Fe, Cr
- Packing fraction: 0.68
- Coordination number (# of nearest neighbors): 8
- Nearest-neighbor distance: $a\sqrt{3}/2$

Face-centered cubic



- Examples: Cu, Ag, Au, Al
- Packing fraction: 0.74
- Stacking sequence (layers): ABCABC
- Coordination number (# of nearest neighbors): 12
- Nearest-neighbor distance: $a/\sqrt{2}$

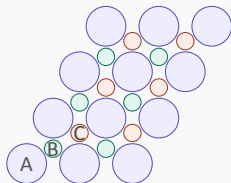
Hexagonal close-packed



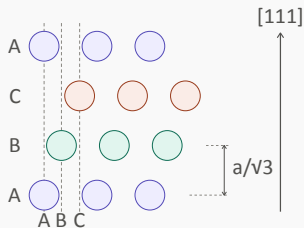
- Examples: Mg, Zn, Ti, Co
- Hexagonal lattice with 2-atom basis: $(0, 0, 0)$ and $(1/3, 2/3, 1/2)$
- Ratio $a/c = \sqrt{8/3} \approx 1.633$
- Packing fraction: 0.74
- Stacking sequence (layers): ABABAB

FCC vs HCP

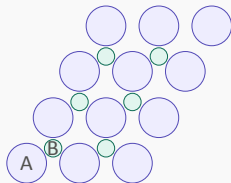
FCC: Top view



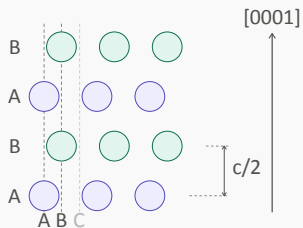
FCC: Side view



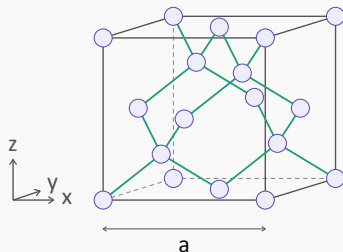
HCP: Top view



HCP: Side view

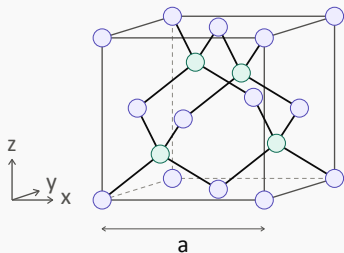


Diamond structure



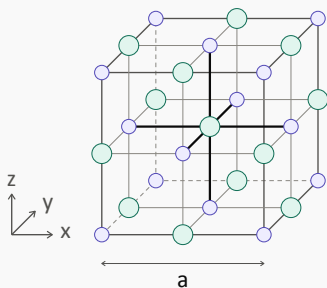
- Examples: C (diamond), Si, Ge
- fcc lattice with 2-atom basis: $(0,0,0)$ and $(1/4, 1/4, 1/4)$
- Packing fraction: 0.34
- Coordination number: 4
- Nearest-neighbor distance: $(\sqrt{3}/4)a$

Zincblende structure



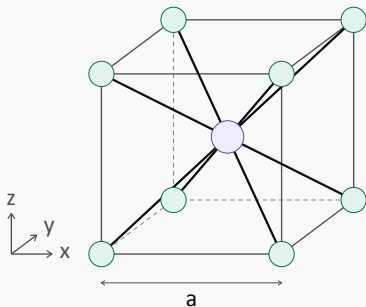
- Examples: GaAs, InP, ZnS
- fcc lattice with 2-atom basis: $(0,0,0)$ and $(1/4, 1/4, 1/4)$
- Coordination number: 4 : 4
- Nearest-neighbor distance: $(\sqrt{3}/4)a$

NaCl structure



- Examples: NaCl, KCl, MgO
- fcc lattice with 2-atom basis: $(0,0,0)$ and $(1/2, 1/2, 1/2)$
- Coordination number: 6 : 6
- Nearest-neighbor distance: $a/2$

CsCl structure



- Examples: CsCl, CsBr, CsI
- sc lattice with 2-atom basis: $(0,0,0)$ and $(1/2, 1/2, 1/2)$
- Coordination number: 8 : 8
- Nearest-neighbor distance: $a\sqrt{3}/2$

Crystal Structure

Translation vectors and unit cells

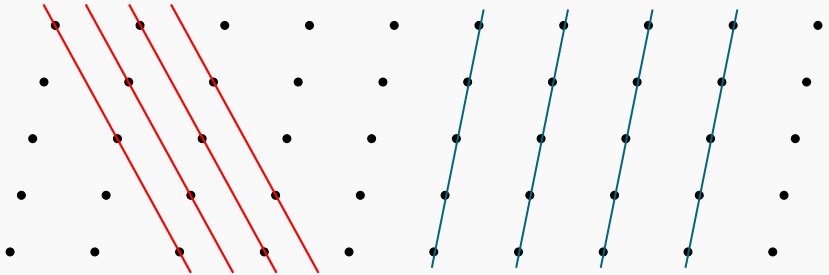
Symmetry operations and Bravais lattices

Simple crystal structures

Miller indices

Lattice planes and families of lattice planes

- A lattice plane of a Bravais lattice is defined by 3 noncollinear lattice points. Because of the translational symmetry of the Bravais lattice, the lattice plane will contain infinitely many lattice points.
- A family of lattice planes is a set of parallel and equally spaced lattice planes which together contain all lattice points of the Bravais lattice.



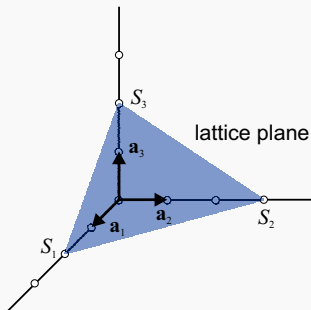
Families of lattice planes and Miller indices

- A family of lattice planes can be characterized by a set of three numbers (hkl). The so-called Miller indices h, k, l are determined in the following way:
 - The translation vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ define three crystal axes.
 - Determine the intercepts $S_1 = s_1|\mathbf{a}_1|$, $S_2 = s_2|\mathbf{a}_2|$, $S_3 = s_3|\mathbf{a}_3|$ of one of the lattice planes with the axes.
 - The Miller indices are the smallest three integers h, k, l with no common factor that satisfy

$$h : k : l = \frac{1}{s_1} : \frac{1}{s_2} : \frac{1}{s_3}.$$

- The Miller index is set to 0 if the lattice plane is parallel to the corresponding axis.
 - A negative Miller index is denoted by an overbar, e.g., $(h, -k, l) \rightarrow (h, \bar{k}, l)$.
- Note that the set of Miller indices depends on the choice of translation vectors.

Example: Miller indices



- Intercepts with axes: $s_1 = 2, s_2 = 3, s_3 = 2$.
- Miller indices: $h : k : l = \frac{1}{2} : \frac{1}{3} : \frac{1}{2} = 3 : 2 : 3$.
- Family of lattice planes: (323) .

(hkl) , $\{hkl\}$, and $[hkl]$

- In the case of hexagonal and rhombohedral lattice systems one often uses the Miller-Bravais system with four indices $(hkil)$ to characterize family of planes. Here, h , k and l are the corresponding Miller indices and the index i obeys the constraint $h + k + i = 0$. The advantage of the Miller-Bravais indices is that they make permutation symmetries apparent which are not obvious in the case of the Miller indices.
- The notation $\{hkl\}$ represents all families of planes that are equivalent to (hkl) by the symmetry of the lattice. For example, in a cubic crystal $\{100\}$ denotes the three families of planes (100) , (010) , and (001) .
- Directions in a lattice are denoted by square brackets. The $[hkl]$ -direction is parallel to the vector $h\mathbf{a}_1 + k\mathbf{a}_2 + l\mathbf{a}_3$.

Example: Miller-Bravais indices

