Lecture 2 - Crystal Lattices

R. Hielscher

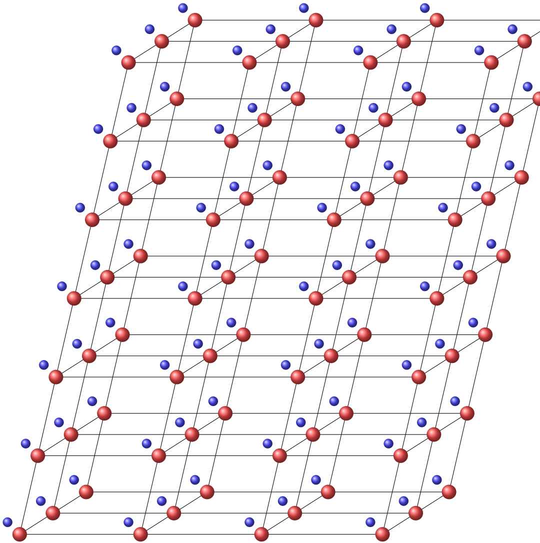
Faculty of Mathematics,
Chemnitz University of Technology, Germany

MTEX Workshop 2021

Crystals

Definition

A crystal is an anisotropic, homogenous body consisting of a three-dimensional periodic ordering of atoms, ions or molecules.



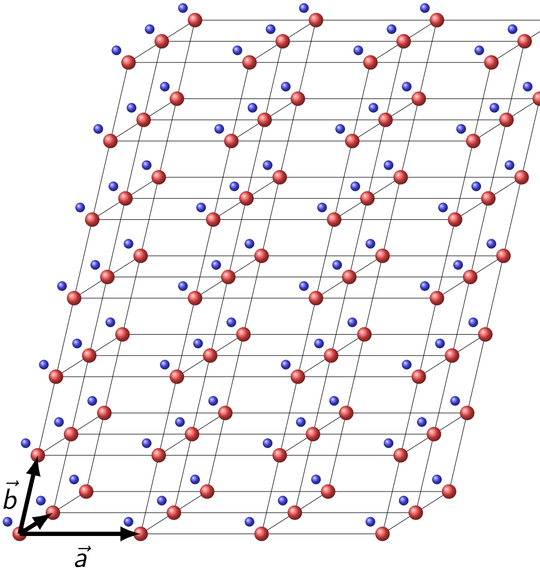
Crystals

Definition

A crystal is an anisotropic, homogenous body consisting of a three-dimensional periodic ordering of atoms, ions or molecules.

Consequence: There are linearly independent vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ such that the atomic structure is invariant with respect to translations about these vectors.

- The definition of periodicity assumes infinity of the atomic structure.
- The choice of the vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ is not unique



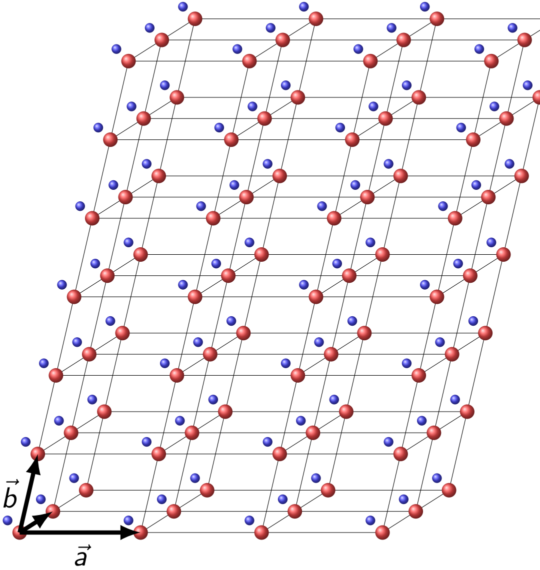
The Unit Cell

- is the parallelepiped spanned by $\vec{a}$, $\vec{b}$, $\vec{c}$.
- is the smallest region that constitutes a repeating pattern.
- is characterized by the length and angles

$$a = |\vec{a}|,\ b = |\vec{b}|,\ c = |\vec{c}|$$
$$\alpha = \measuredangle(\vec{b}, \vec{c}),\ \beta = \measuredangle(\vec{a}, \vec{c}),\ \gamma = \measuredangle(\vec{b}, \vec{a}).$$

```
abc = [5.2, 5.2, 5.3]
abg = [90 99.25 90] * degree;
cs = crystalSymmetry('1',abc,abg)
```

```
ans = crystalSymmetry
  symmetry             : 1
  a, b, c              : 5.2, 5.2, 5.3
  alpha, beta, gamma: 90, 99.25, 90
```



The Crystal Coordinate Systems

The vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ constitute a right handed but non orthogonal coordinate system.

Lattice points are given by coordinates u, v, w:

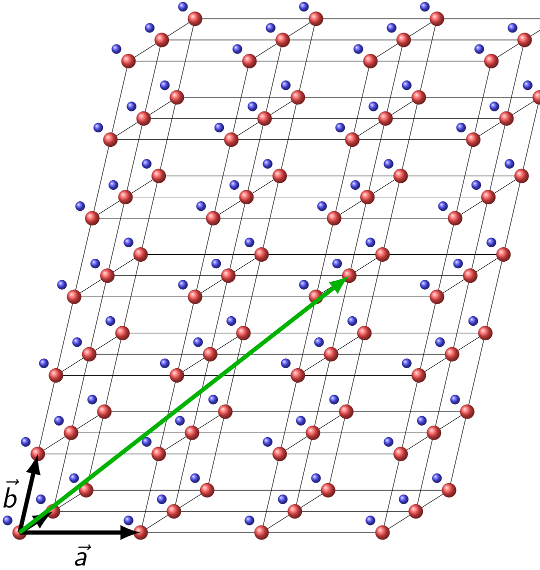
$$\cdot uvw \cdot = \vec{d} = u\vec{a} + v\vec{b} + w\vec{c}.$$

Usage: slip systems, dislocation systems

```
d = Miller(1,1,0,cs,'uvw')
```

```
d = Miller
 size: 1 x 1
 symmetry: 1
  u 1
  v 1
  w 0
```

Smaller integers u, v, w indicate higher density of lattice points on the line and larger distance between parallel lines.



The Crystal Coordinate Systems

The vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ constitute a right handed but non orthogonal coordinate system.

Lattice points are given by coordinates u, v, w:

$$\cdot uvw \cdot = \vec{d} = u\vec{a} + v\vec{b} + w\vec{c}.$$

Usage: slip systems, dislocation systems

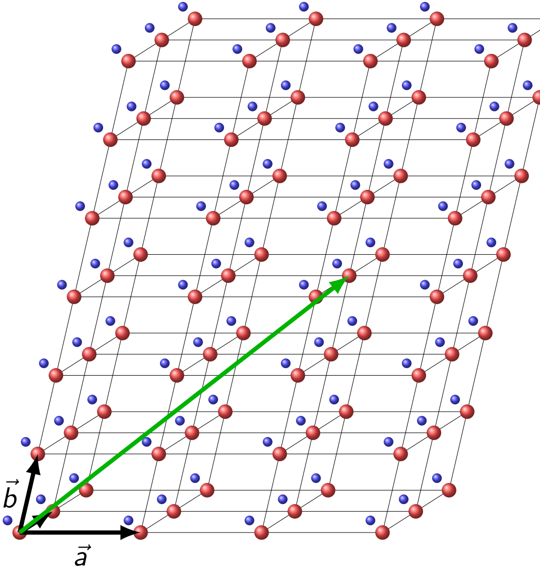
```
d = Miller(1,1,0,cs,'uvw')
```

Lattice directions $[uvw]$: all vectors parallel to $\vec{d}$

```
d == [2*d, -d]
```

```
ans =

   1    0
```



The Crystal Coordinate Systems

The vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ constitute a right handed but non orthogonal coordinate system.

Lattice points are given by coordinates u, v, w:

$$\cdot uvw \cdot = \vec{d} = u\vec{a} + v\vec{b} + w\vec{c}.$$

Usage: slip systems, dislocation systems

```
d = Miller(1,1,0,cs,'uvw')
```

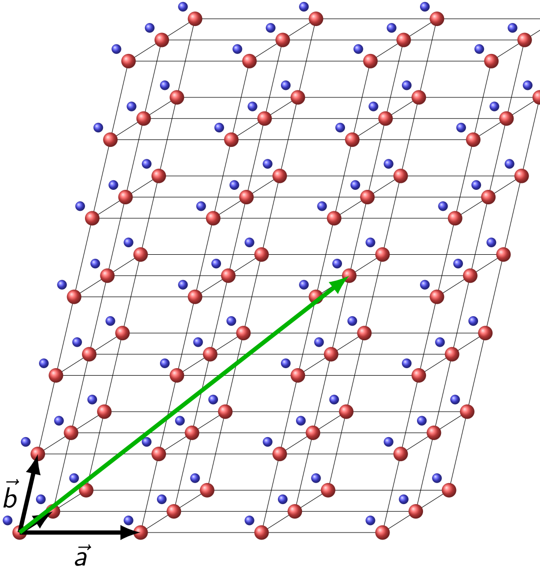
Lattice directions $[uvw]$: all vectors parallel to $\vec{d}$

```
d == [2*d, -d]
```

```
[abs(d), norm(2*d)]
```

```
ans =

    1.4142    2.8284
```



The Crystal Coordinate Systems

The vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ constitute a right handed but non orthogonal coordinate system.

Lattice points are given by coordinates u, v, w:

$$\cdot uvw \cdot = \vec{d} = u\vec{a} + v\vec{b} + w\vec{c}.$$

Usage: slip systems, dislocation systems

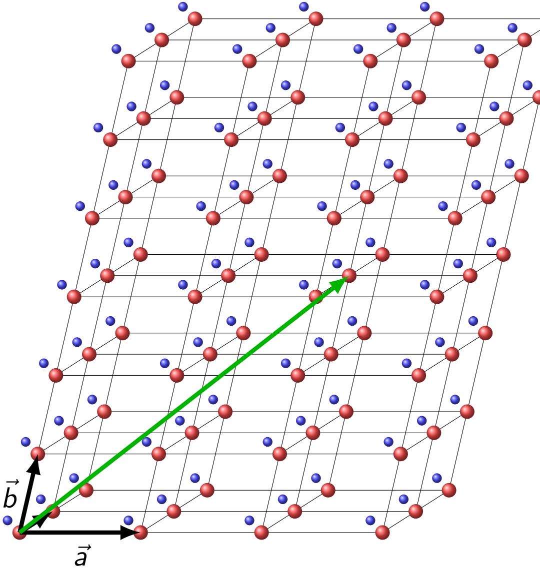
```
d = Miller(1,1,0,cs,'uvw')
```

Lattice directions $[uvw]$: all vectors parallel to $\vec{d}$

```
d == [2*d, -d]
```

```
[abs(d), norm(2*d)]
```

Examples: $[100]$, $[1\bar{1}0] = [2\bar{2}0] \neq [\bar{1}10]$



The Reciprocal Coordinate System

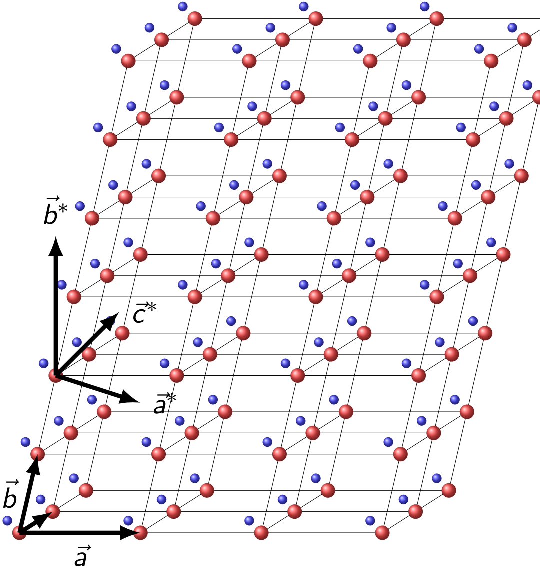
The reciprocal axes are orthogonal to $\vec{a}, \vec{b}, \vec{c}$,

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V}, \ \vec{b}^* = \frac{\vec{c} \times \vec{a}}{V}, \ \vec{c}^* = \frac{\vec{a} \times \vec{b}}{V}$$

- $V = \vec{a} \cdot (\vec{b} \times \vec{c})$ is the volume of the unit cell
- $\vec{a} \cdot \vec{a}^* = 1, \ \vec{b} \cdot \vec{b}^* = 1, \ \vec{c} \cdot \vec{c}^* = 1$
- units of $\vec{a}^*$, $\vec{b}^*$, $\vec{c}^*$ are reciprocal to $\vec{a}, \vec{b}, \vec{c}$
- for cubic lattices $\vec{a} || \vec{a}^*$, $\vec{b} || \vec{b}^*$, $\vec{c} || \vec{c}^*$,

Directions with respect to the $\vec{a}^*, \vec{b}^*, \vec{c}^*$ are given by integers coordinates h, k, ℓ

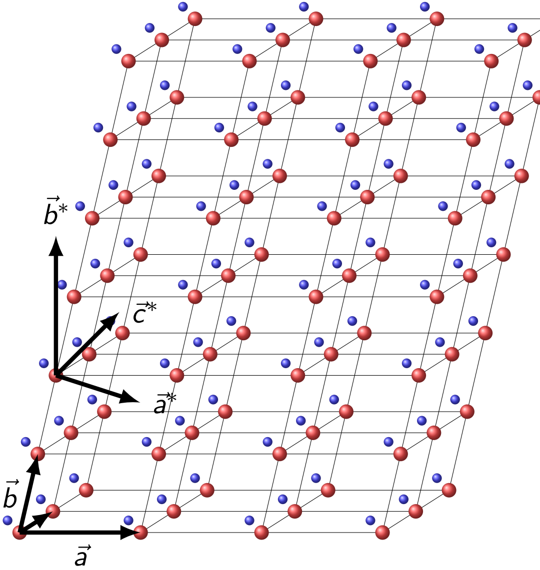
$$\vec{n} = h\vec{a}^* + k\vec{b}^* + \ell c^*$$



The Reciprocal Coordinate System

```
n = Miller(1,1,0,cs,'hkl')
```

```
d = Miller
 symmetry: 1
  h 1
  k 1
  l 0
```

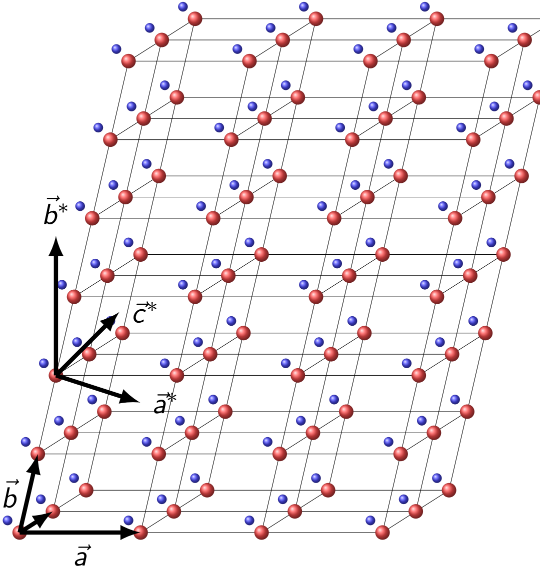


The Reciprocal Coordinate System

```
n = Miller(1,1,0,cs,'hkl')
```

```
Miller({1,1,0},{0,1,1},cs,'hkl')
```

```
ans = Miller
 symmetry: 1
  h  1
  k  1
  l  0
```

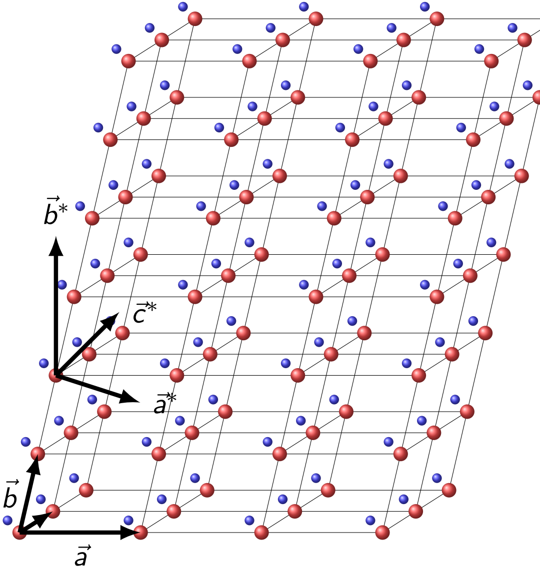


The Reciprocal Coordinate System

```
n = Miller(1,1,0,cs,'hkl')
```

```
Miller({1,1,0},{0,1,1},cs,'hkl')
```

```
rec = [cs.aAxisRec,cs.bAxisRec,...
       cs.cAxisRec]
```



The Reciprocal Coordinate System

```
n = Miller(1,1,0,cs,'hkl')
```

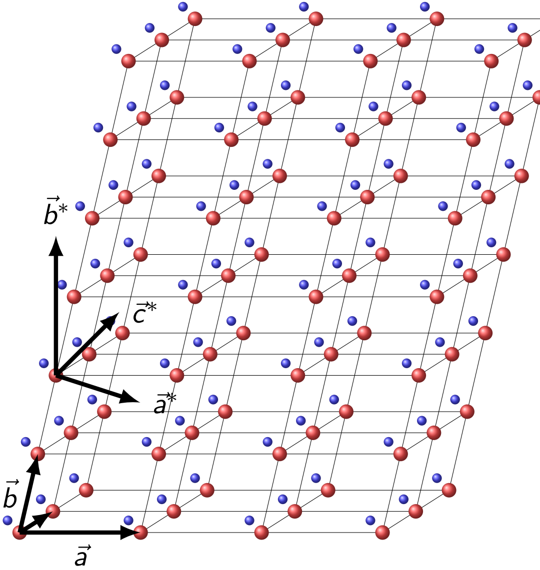
```
Miller({1,1,0},{0,1,1},cs,'hkl')
```

```
rec = [cs.aAxisRec,cs.bAxisRec,...
       cs.cAxisRec]
```

```
dot(rec,cs.aAxis)
```

```
ans =

     1     0     0
```



The Reciprocal Coordinate System

```
n = Miller(1,1,0,cs,'hkl')
```

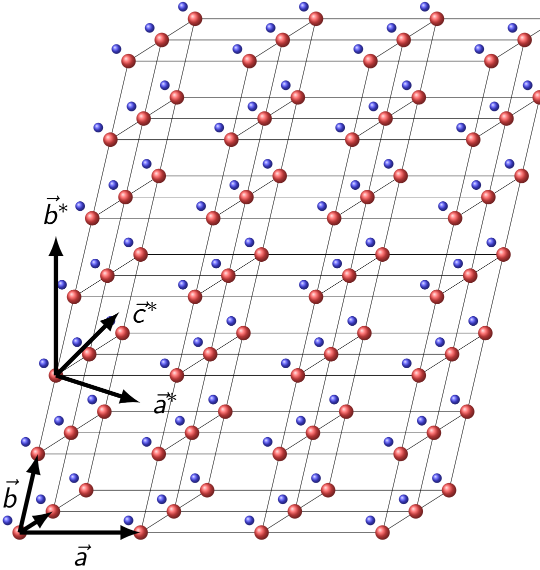
```
Miller({1,1,0},{0,1,1},cs,'hkl')
```

```
rec = [cs.aAxisRec,cs.bAxisRec,...
       cs.cAxisRec]
```

```
dot(rec,cs.aAxis)
```

```
cross(cs.aAxisRec,cs.bAxisRec)
```

```
ans = Miller
 symmetry: 1
  u        0
  v        0
  w        1
```



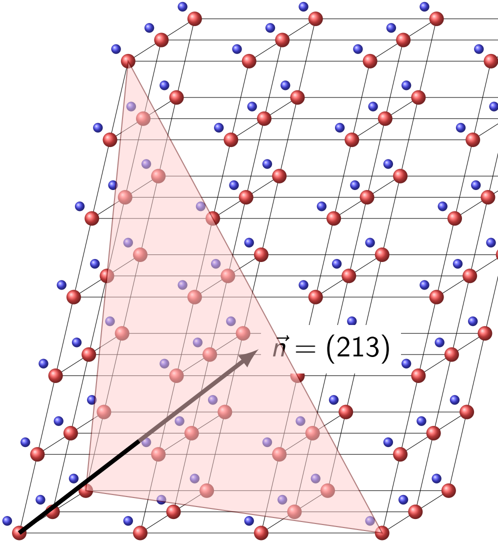
Crystal Lattice Planes

The plane P normal to $\vec{n} = h\vec{a}^* + k\vec{b}^* + \ell c^*$ is

$$P = \{\vec{x} \mid \vec{x} \cdot \vec{n} = d\} = (hk\ell).$$

It intersects the $\vec{a}$-axis in $\cdot u00 \cdot$ if

$$d = u\vec{a} \cdot n = u\vec{a} \cdot (h\vec{a}^* + k\vec{b}^* + \ell c^*) = uh.$$



Crystal Lattice Planes

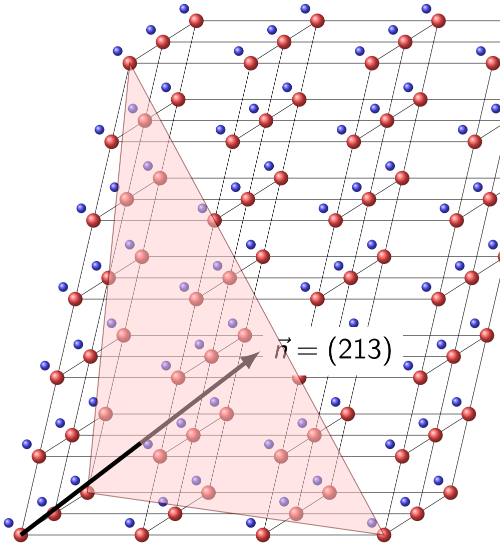
The plane P normal to $\vec{n} = h\vec{a}^* + k\vec{b}^* + \ell c^*$ is

$$P = \{\vec{x} \mid \vec{x} \cdot \vec{n} = d\} = (hk\ell).$$

It intersects the $\vec{a}$-axis in $\cdot u00\cdot$ if

$$d = u\vec{a} \cdot n = u\vec{a} \cdot (h\vec{a}^* + k\vec{b}^* + \ell c^*) = uh.$$

Hence, $(hk\ell)$ intersects $\vec{a}$, $\vec{b}$ and $\vec{c}$ in $\frac{d}{h}, \frac{d}{k}, \frac{d}{\ell}$.



Crystal Lattice Planes

The plane P normal to $\vec{n} = h\vec{a}^* + k\vec{b}^* + \ell c^*$ is

$$P = \{\vec{x} \mid \vec{x} \cdot \vec{n} = d\} = (hk\ell).$$

It intersects the $\vec{a}$-axis in $\cdot u00\cdot$ if

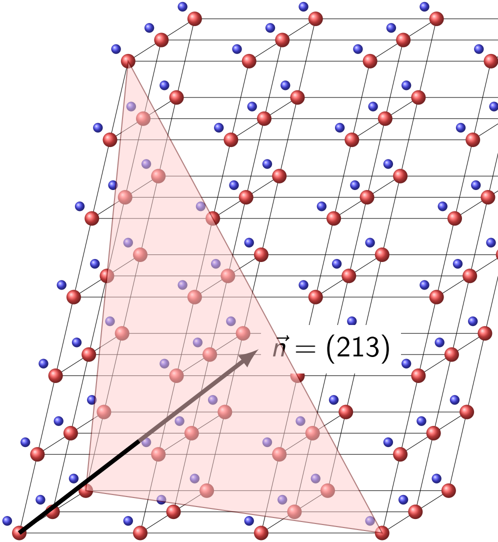
$$d = u\vec{a} \cdot n = u\vec{a} \cdot (h\vec{a}^* + k\vec{b}^* + \ell c^*) = uh.$$

Hence, $(hk\ell)$ intersects $\vec{a}$, $\vec{b}$ and $\vec{c}$ in $\frac{d}{h}, \frac{d}{k}, \frac{d}{\ell}$.

Given axes intersections $m, n, p \in \mathbb{N}$. The corresponding normal vector is

$$\vec{n} = \frac{d}{m}\vec{a}^* + \frac{d}{n}\vec{b}^* + \frac{d}{p}\vec{c}^*$$

with $d = \mathrm{LCM}(m, n, p)$.



Crystal Lattice Planes

The plane P normal to $\vec{n} = h\vec{a}^* + k\vec{b}^* + \ell c^*$ is

$$P = \{\vec{x} \mid \vec{x} \cdot \vec{n} = d\} = (hk\ell).$$

It intersects the $\vec{a}$-axis in $\cdot u00 \cdot$ if

$$d = u\vec{a} \cdot n = u\vec{a} \cdot (h\vec{a}^* + k\vec{b}^* + \ell c^*) = uh.$$

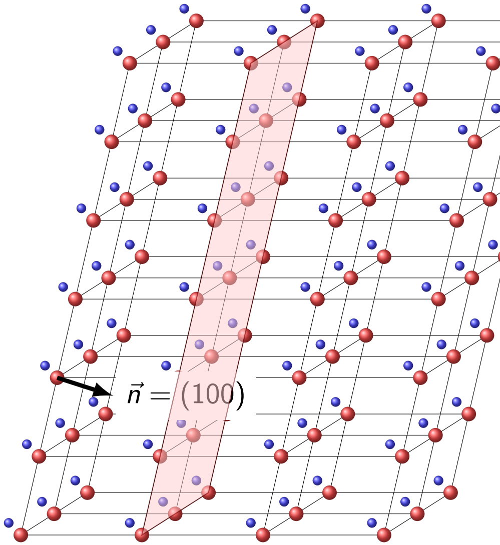
Hence, $(hk\ell)$ intersects $\vec{a}$, $\vec{b}$ and $\vec{c}$ in $\frac{d}{h}, \frac{d}{k}, \frac{d}{\ell}$.

Given axes intersections $m, n, p \in \mathbb{N}$. The corresponding normal vector is

$$\vec{n} = \frac{d}{m}\vec{a}^* + \frac{d}{n}\vec{b}^* + \frac{d}{p}\vec{c}^*$$

with $d = \mathrm{LCM}(m, n, p)$.

$k = 0 \iff \frac{1}{0} = \infty \iff (hkl)$ is parallel to $\vec{b}$



Crystal Lattice Planes

The plane P normal to $\vec{n} = h\vec{a}^* + k\vec{b}^* + \ell c^*$ is

$$P = \{\vec{x} \mid \vec{x} \cdot \vec{n} = d\} = (hk\ell).$$

It intersects the $\vec{a}$-axis in $\cdot u00 \cdot$ if

$$d = u\vec{a} \cdot n = u\vec{a} \cdot (h\vec{a}^* + k\vec{b}^* + \ell c^*) = uh.$$

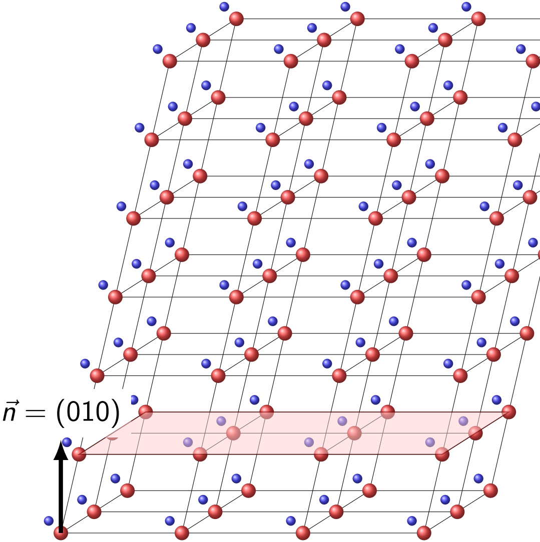
Hence, $(hk\ell)$ intersects $\vec{a}$, $\vec{b}$ and $\vec{c}$ in $\frac{d}{h}, \frac{d}{k}, \frac{d}{\ell}$.

Given axes intersections $m, n, p \in \mathbb{N}$. The corresponding normal vector is

$$\vec{n} = \frac{d}{m}\vec{a}^* + \frac{d}{n}\vec{b}^* + \frac{d}{p}\vec{c}^*$$

with $d = \mathrm{LCM}(m, n, p)$.

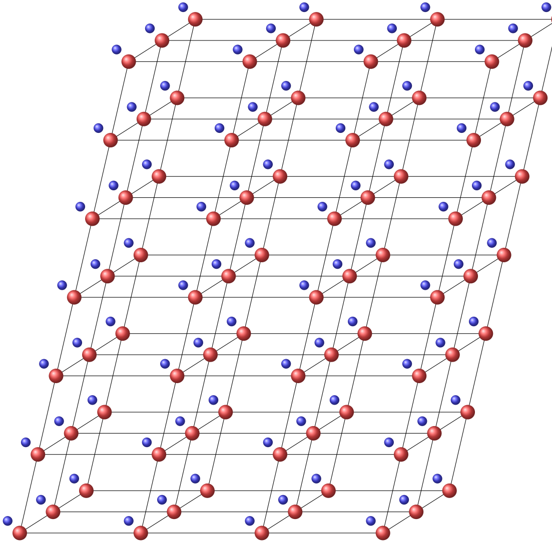
$k = 0 \iff \frac{1}{0} = \infty \iff (hkl)$ is parallel to $\vec{b}$



Miller Indices

The lattice plane (123) perpendicular to $\vec{n} = \vec{a}^* + 2\vec{b}^* + 3\vec{c}^*$ which intersects the direct lattice axes $\vec{a}$, $\vec{b}$ and $\vec{c}$ at 1, $\frac{1}{2}$ and $\frac{1}{3}$.

- The coordinates h, k, ℓ are the Miller indices of the plane P.
- planes $(hk\ell)$ parallel to $\vec{a}$ have interception point $\frac{1}{\infty}$ and hence $h = 0$
- planes $(h00)$ perpendicular to $\vec{a}^*$ have interception points $(\frac{d}{h}, \frac{1}{\infty}, \frac{1}{\infty})$



The Zone Equation

A direction $[uvw]$ is parallel to a plane $(hk\ell)$ if

$$hu + kv + \ell w = 0.$$

```
d1 = Miller(1,-1,2,cs,'uvw')
n1 = Miller(1,1,0,cs,'hkl')
dot(d1,n1)
```

```
ans =

   7.7716e-16
```

The Zone Equation

A direction $[uvw]$ is parallel to a plane $(hk\ell)$ if

$$hu + kv + \ell w = 0.$$

```
d1 = Miller(1,-1,2,cs,'uvw')
n1 = Miller(1,1,0,cs,'hkl')
dot(d1,n1)
```

```
angle(n1,d2) ./ degree
```

```
ans =

   90.0000
```

The Zone Equation

A direction $[uvw]$ is parallel to a plane $(hk\ell)$ if

$$hu + kv + \ell w = 0.$$

```
d1 = Miller(1,-1,2,cs,'uvw')
n1 = Miller(1,1,0,cs,'hkl')
dot(d1,n1)
```

```
angle(n1,d2) ./ degree
```

The plane (hkl) spanned by the directions $[u_1 v_1 w_1]$ and $[u_2 v_2 w_2]$:

$$(hkl) = [u_1 v_1 w_1] \times [u_2 v_2 w_2]$$

```
d2 = Miller(1,0,0,cs,'uvw')
cross(d1,d2)
```

```
ans = Miller
 symmetry: 1
  h  0
  k  2
  l  1
```

The Zone Equation

A direction $[uvw]$ is parallel to a plane $(hk\ell)$ if

$$hu + kv + \ell w = 0.$$

```
d1 = Miller(1,-1,2,cs,'uvw')
n1 = Miller(1,1,0,cs,'hkl')
dot(d1,n1)
```

```
angle(n1,d2) ./ degree
```

The plane (hkl) spanned by the directions $[u_1 v_1 w_1]$ and $[u_2 v_2 w_2]$:

$$(hkl) = [u_1 v_1 w_1] \times [u_2 v_2 w_2]$$

```
d2 = Miller(1,0,0,cs,'uvw')
cross(d1,d2)
```

The common direction $[uvw]$ of two planes $(h_1 k_1 \ell_1)$ and $(h_2 k_2 \ell_2)$

$$[uvw] = (h_1 k_1 \ell_1) \times (h_2 k_2 \ell_2)$$

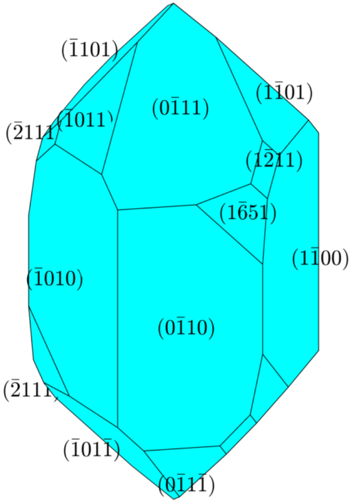
```
n2 = Miller(1,0,0,cs,'hkl')
cross(n1,n2)
```

```
ans = Miller
 symmetry: 1
  u   0
  v   0
  w  -1
```

Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

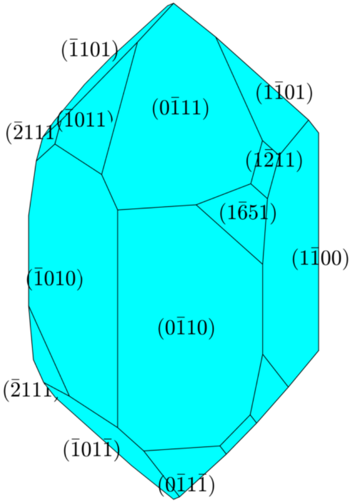
- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

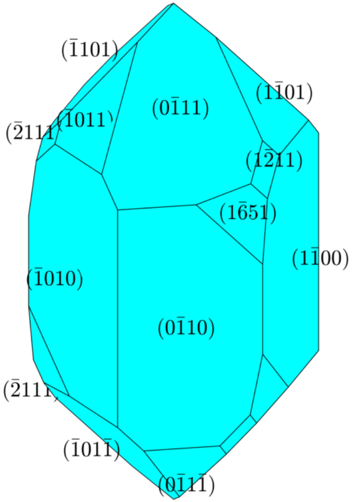
- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

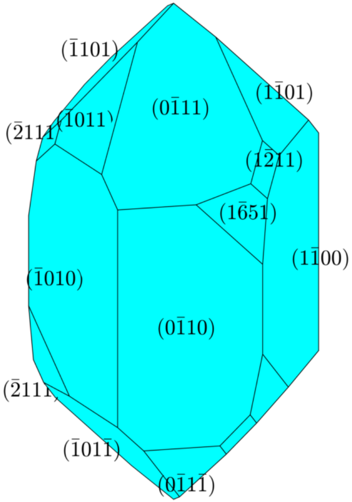
- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

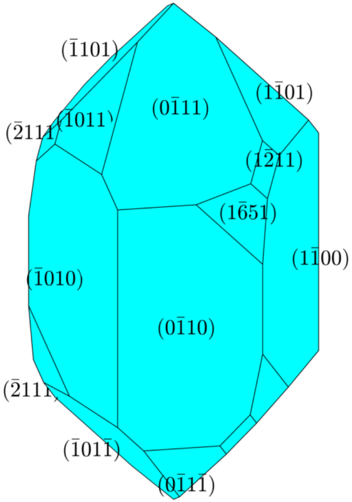
- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

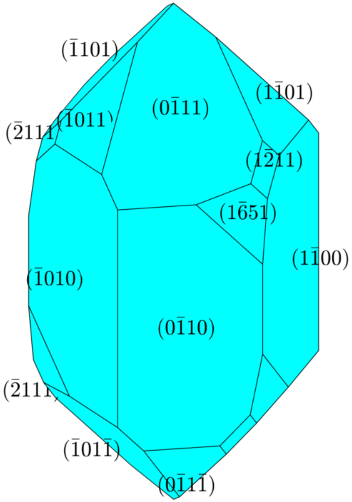
- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

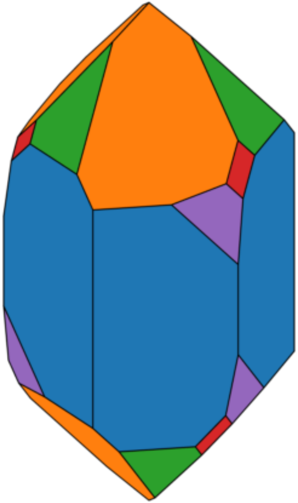
- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



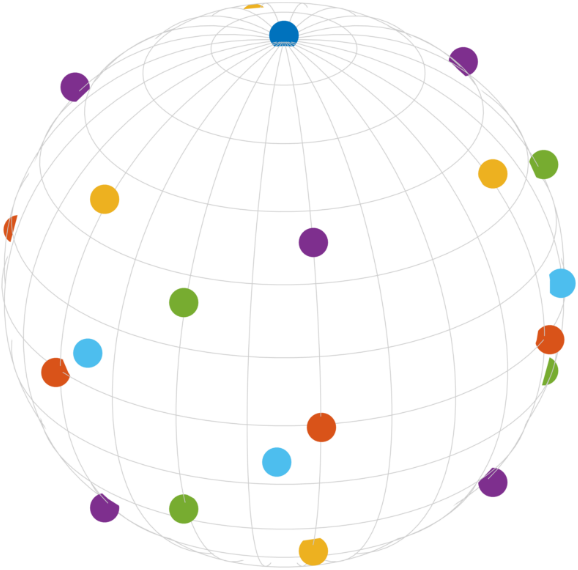
Morphology

Crystals are formed by crystallization from a solution or a melt.
the two steps of crystallization: nucleation and growth

- the grow rate is an anisotropic property
- lattice planes with high grow rate get smaller
- lattice planes with low grow rate become larger
- lattice planes $(hk\ell)$ with small Miller indices usually have high density and grow slowly
- the shape of a crystal is formed by its low index lattice planes
- law of constant dihedral angles



The Crystal Planes of Quartz in a Stereographic Projection



c c-axis:
(0001), $(000\bar{1})$

m hexagonal prism:
$(10\bar{1}0)$, $(01\bar{1}0)$,$(1\bar{1}00)$
$(\bar{1}010)$, $(0\bar{1}10)$,$(\bar{1}100)$

r positive rhomboeder:
$(10\bar{1}1$, $(\bar{1}101)$, $(0\bar{1}11)$

z negative rhomboder:
$(1\bar{1}01)$,$(01\bar{1}1)$,$(\bar{1}011)$

s trigonal bipyramid:
$(11\bar{2}1)$, $(1\bar{2}11)$, $(\bar{2}111)$

x positive trapezohedron:
$(51\bar{6}1)$, $(\bar{6}511)$, $(1\bar{6}51)$

Defining Crystal Shapes

Show this live!