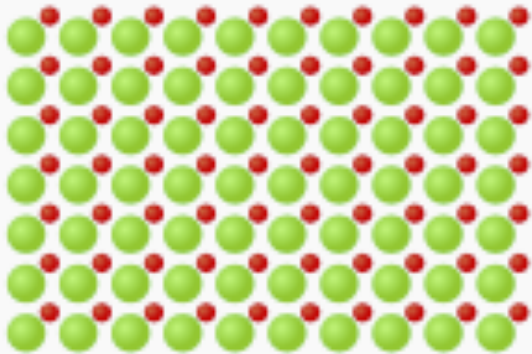


ChE 430

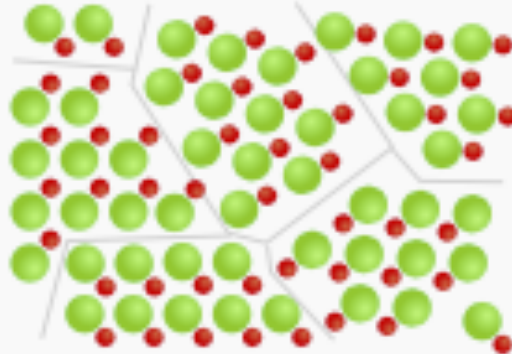
Nanomaterials for Chemical Engineering Applications

Appendix: Bravais lattices and Miller Indices

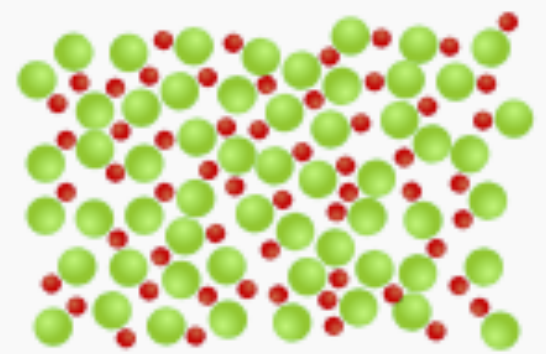
Classification of solids



crystalline



polycrystalline



amorphous

Unit cells

In a crystal we can identify repetitive units. This repetitive units are called “unit cells”

For a given crystal there are always quite a few possible unit cells:

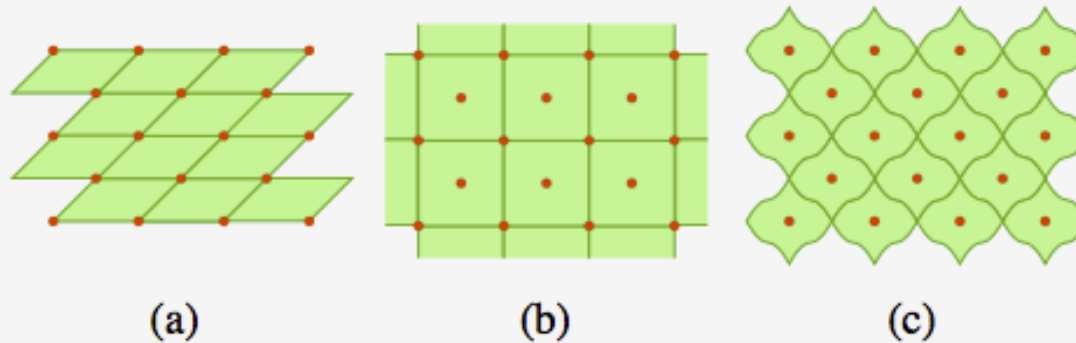


Fig. 1 - For a certain lattice there are many different possible unit cells. Here are some examples for a two-dimensional lattice.

Often it is convenient to choose the one with the highest level of inner symmetry.

Bravais lattices

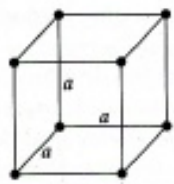
FIRST STEP: 7 CRYSTAL SYSTEMS BASED ON THE SYMMETRY OF THE UNIT CELL

In a first step one divides the Bravais lattices into 7 **crystal systems** which are defined by the lengths a , b , c and angles α , β , γ between the primitive translation vectors. The resulting crystal systems are listed and visualised below.^{[2] [3] [4]}

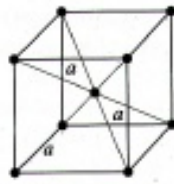
Crystal System	Lengths	Angles
cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
trigonal	$a = b = c$	$\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$
tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$
triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$

Fig. 1 - Overview over the 7 crystal systems: They are defined by the lengths and angles of the primitive translation vectors and exhibit different levels of symmetry.

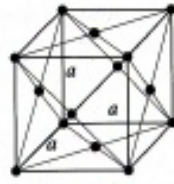
Bravais lattices



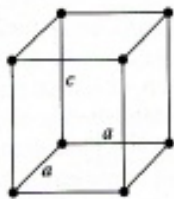
SIMPLE
CUBIC (*P*)



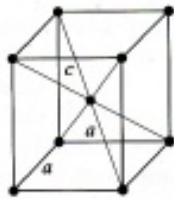
BODY-CENTERED
CUBIC (*I*)



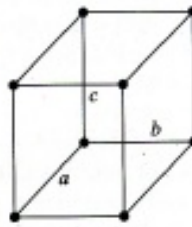
FACE-CENTERED
CUBIC (*F*)



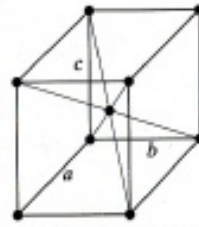
SIMPLE
TETRAGONAL
(*P*)



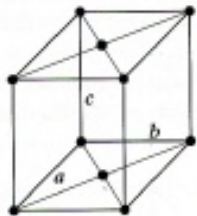
BODY-CENTERED
TETRAGONAL
(*I*)



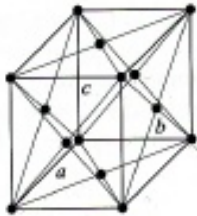
SIMPLE
ORTHORHOMBIC
(*P*)



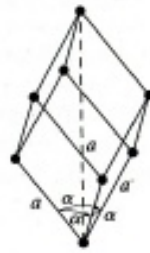
BODY-CENTERED
ORTHORHOMBIC
(*I*)



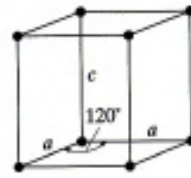
BASE-CENTERED
ORTHORHOMBIC
(*C*)



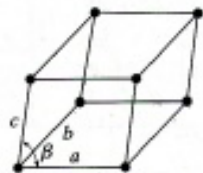
FACE-CENTERED
ORTHORHOMBIC
(*F*)



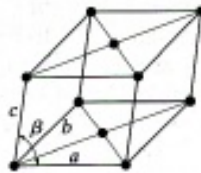
RHOMBOHEDRAL
(*R*)



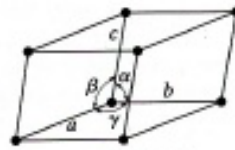
HEXAGONAL
(*P*)



SIMPLE
MONOCLINIC (*P*)



BASE-CENTERED
MONOCLINIC (*C*)



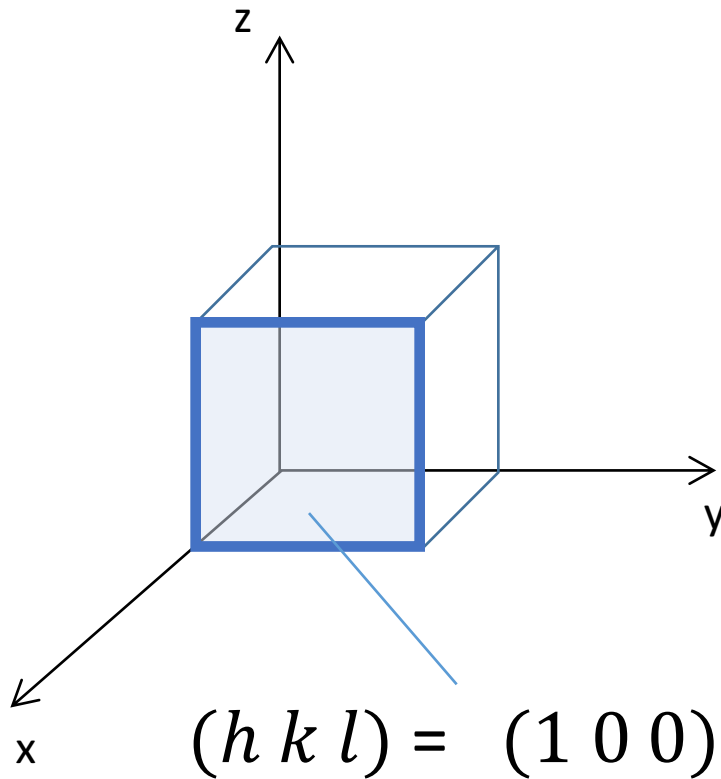
TRICLINIC (*P*)

SECOND STEP:

The 14
Bravais
lattices

The Miller Indices

Miller indices are used to refer to specific lattice planes



Intercepts

$$x = 1$$

$$y \rightarrow \infty$$

$$z \rightarrow \infty$$

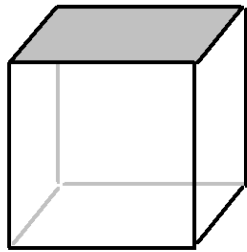
Reciprocal

$$\frac{1}{1} = 1 \quad h$$

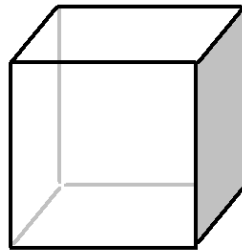
$$\frac{1}{\infty} = 0 \quad k$$

$$\frac{1}{\infty} = 0 \quad l$$

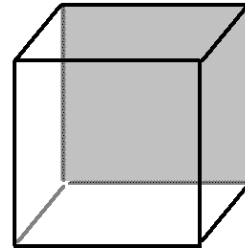
The Miller Indices for the cubic cell



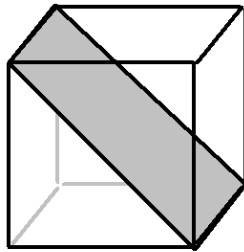
(001)



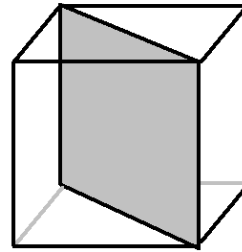
(100)



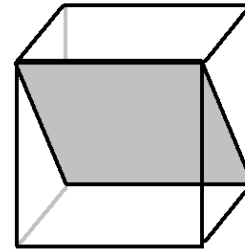
(010)



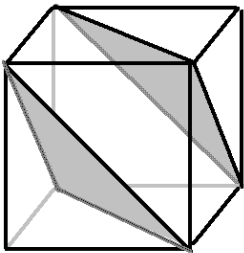
(101)



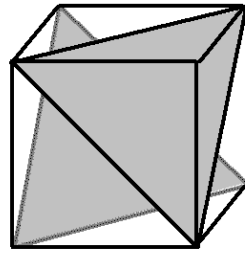
(110)



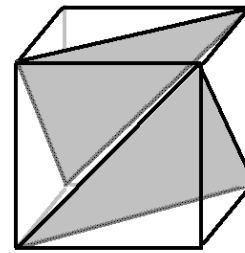
(011)



(111)



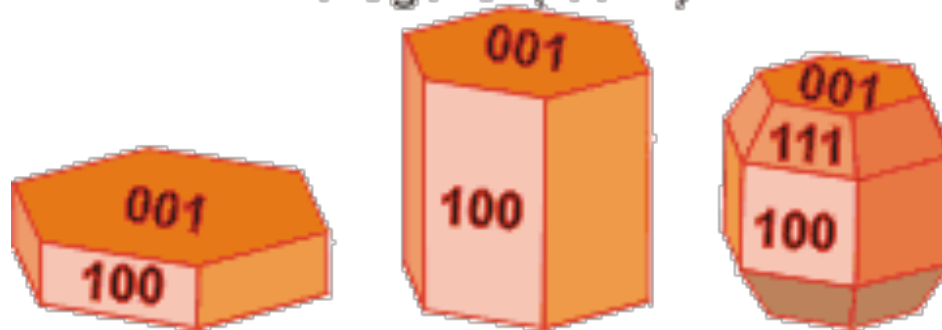
$(\bar{1}\bar{1}1)$



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

Naming crystal facets

Hexagonal (Ice Ih)



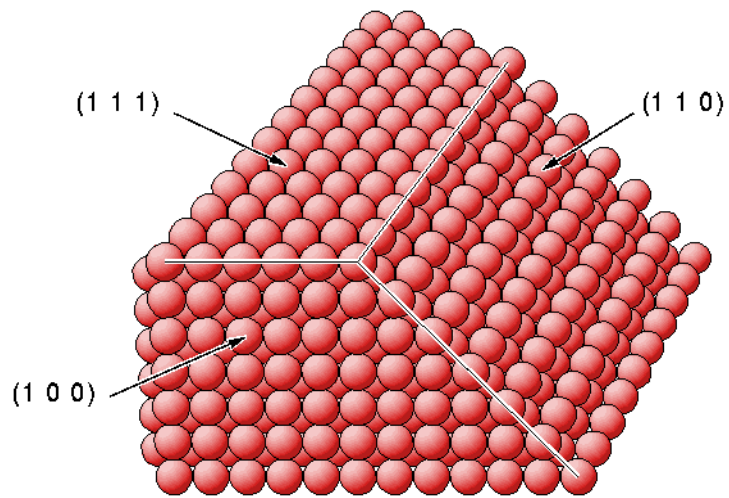
Cubic (Ice Ic)



Trigonal (Ice Isd)

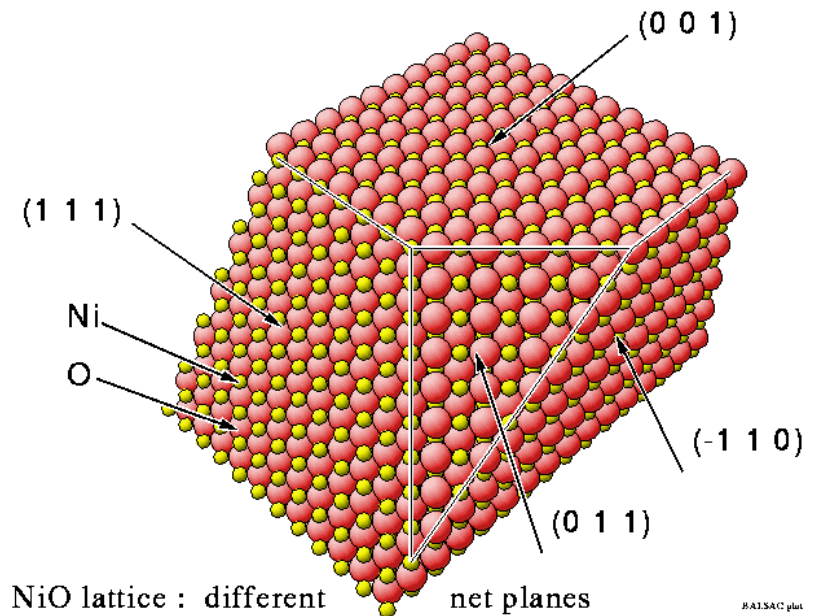


Different arrangement of atoms on different facets



fcc lattice : different net planes

BALSAO plot



NiO lattice : different net planes

BALSAO plot