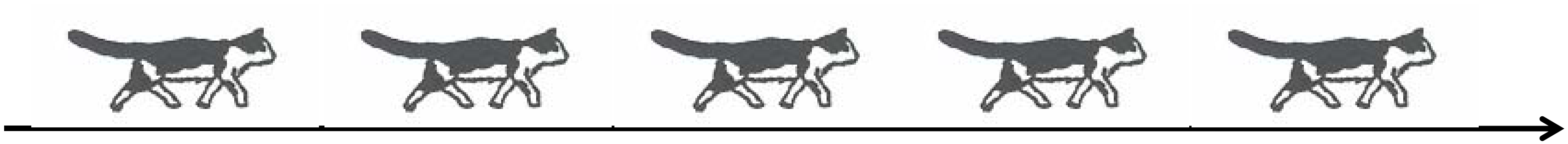
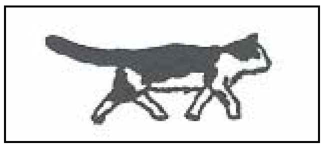
Dr Semën Gorfman
Department of Physics, University of SIegen

Lecture course on crystallography, 2015

Lectures 3-4: Properties of crystal lattice, lattice planes

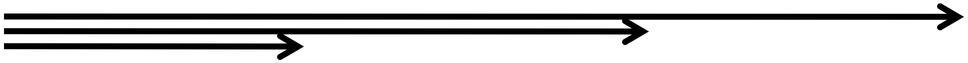
1 Dimensional crystal (1D periodic structures)





Unit cell

Crystal lattice

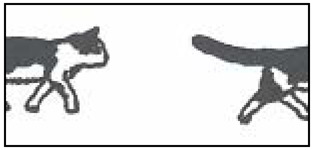


A=*na*

Lattice vectors

To obtain the whole crystal structure one has to translate the UNIT CELL to each LATTICE POINT

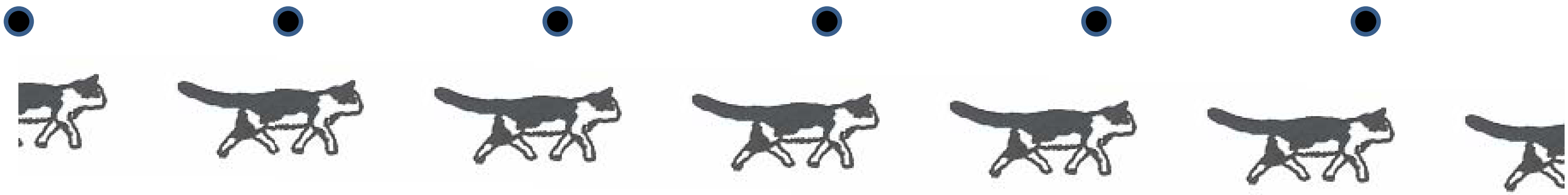
Different choices of unit cell

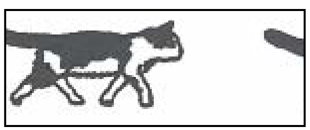


Unit cell

+

Crystal lattice

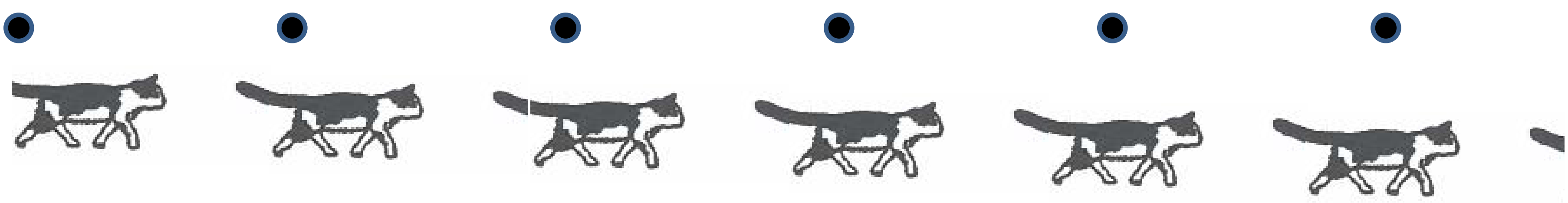




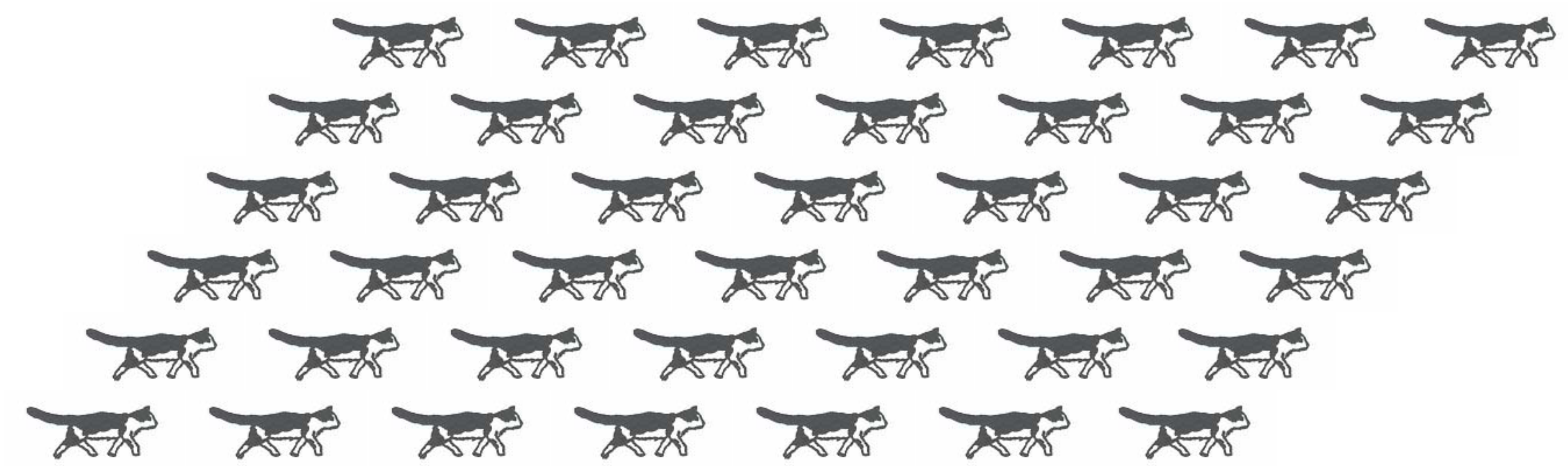
Unit cell

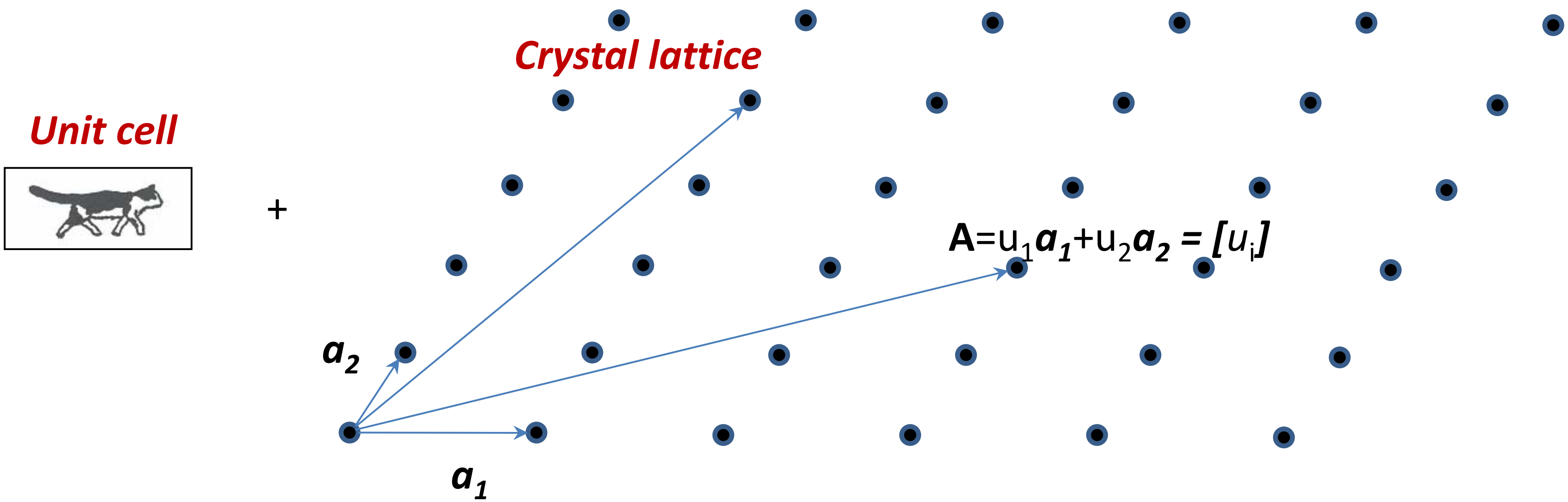
+

Crystal lattice



2 Dimensional crystal (2D periodic structures)





IMPORTANT MESSAGES!!!

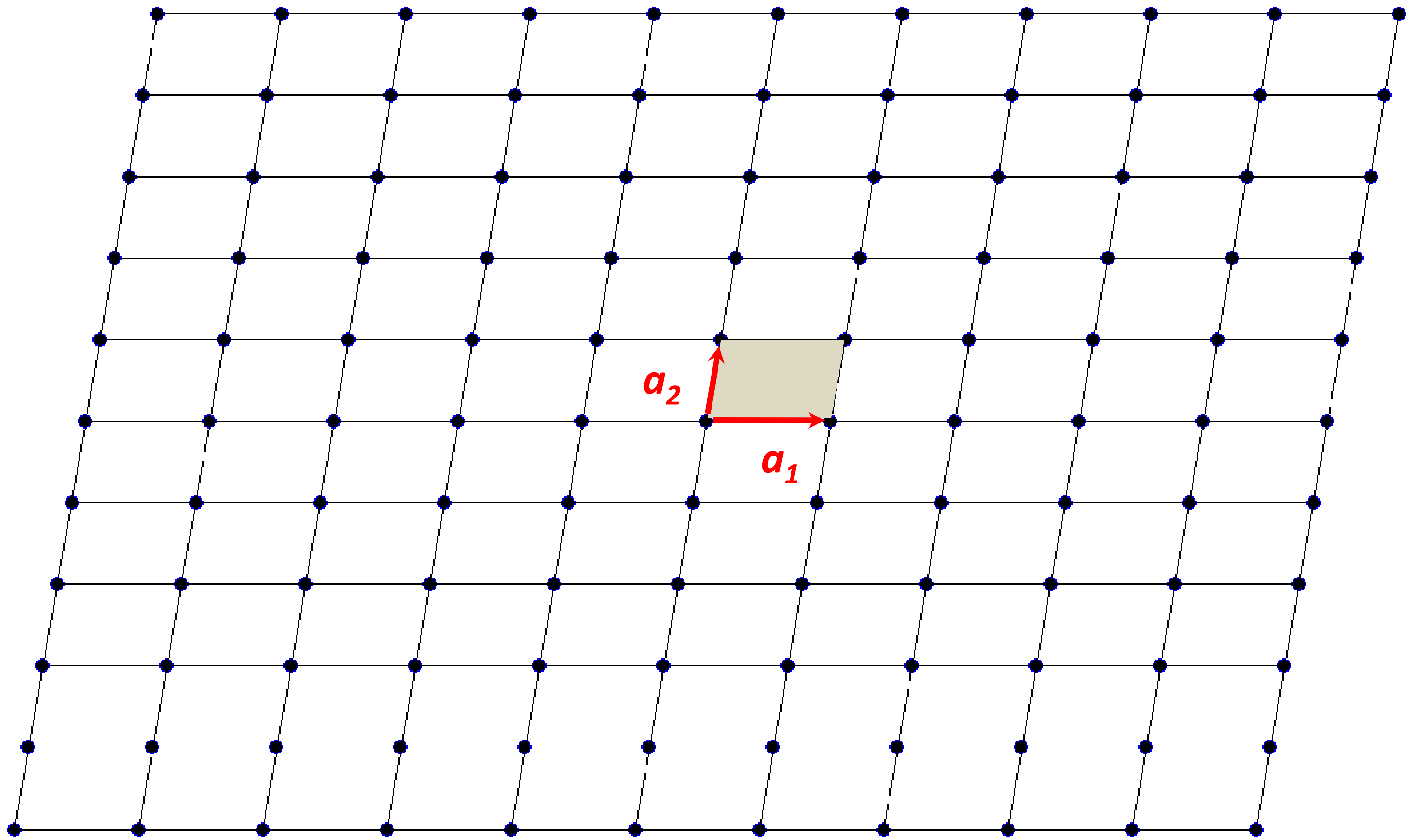
- **Crystal lattice is the mathematical object, describing the periodicity of crystal structure.**

- **Do not confuse crystal lattice with crystal structure**

- **Crystal structure is UNIT CELL * CRYSTAL LATTICE**

- **In order to get the whole crystal structure one has to translate the unit cell to the all lattice points**

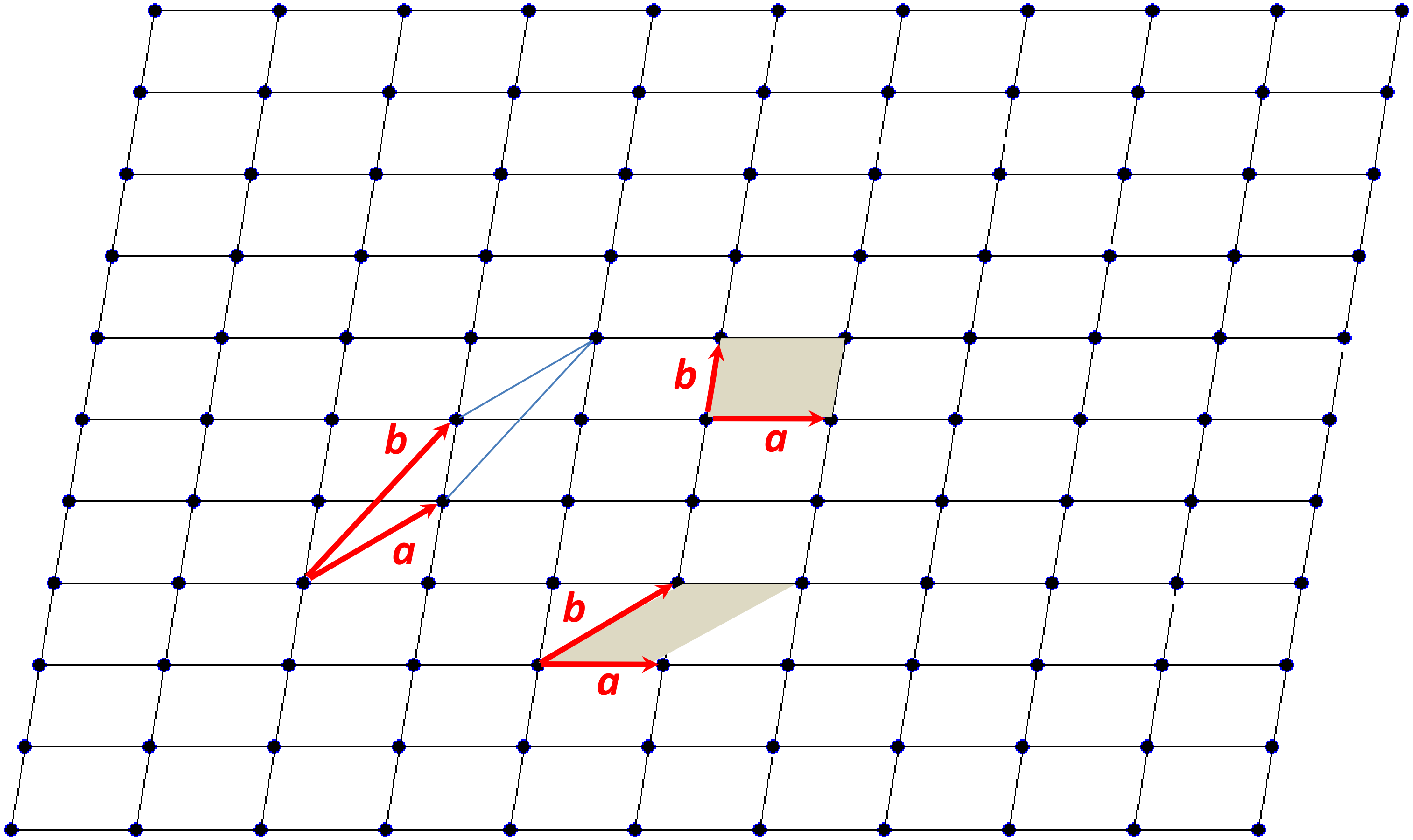
BASIS VECTORS and CRYSTAL LATTICE PARAMETERS



Lattice parameters for two dimensional case: $a=|\boldsymbol{a}|$, $b=|\boldsymbol{b}|$, $\alpha=\angle(\boldsymbol{a},\boldsymbol{b})$

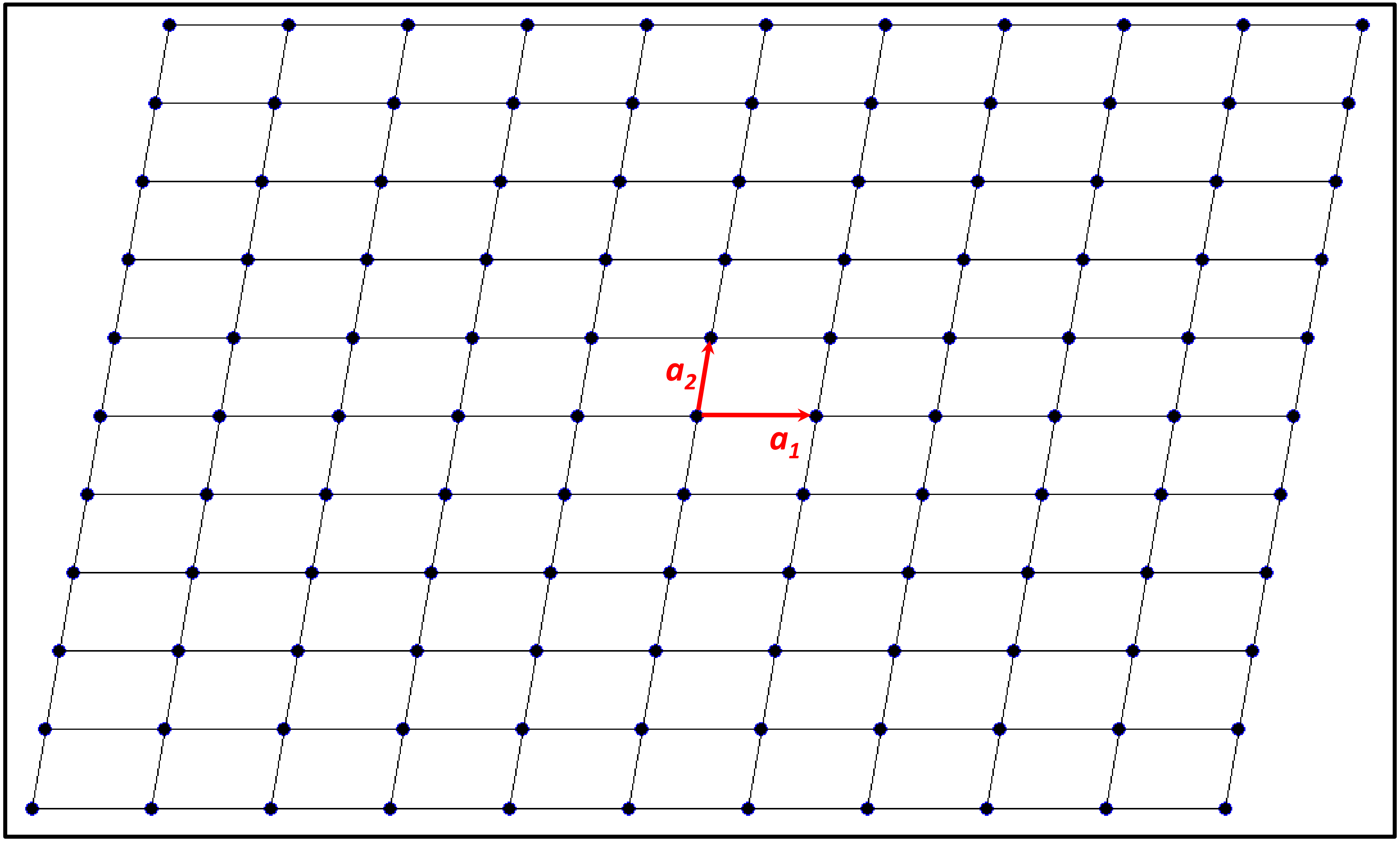
For the given example: a=1.5, b=1, α=80 deg

Different choices of basis vectors and lattice parameters

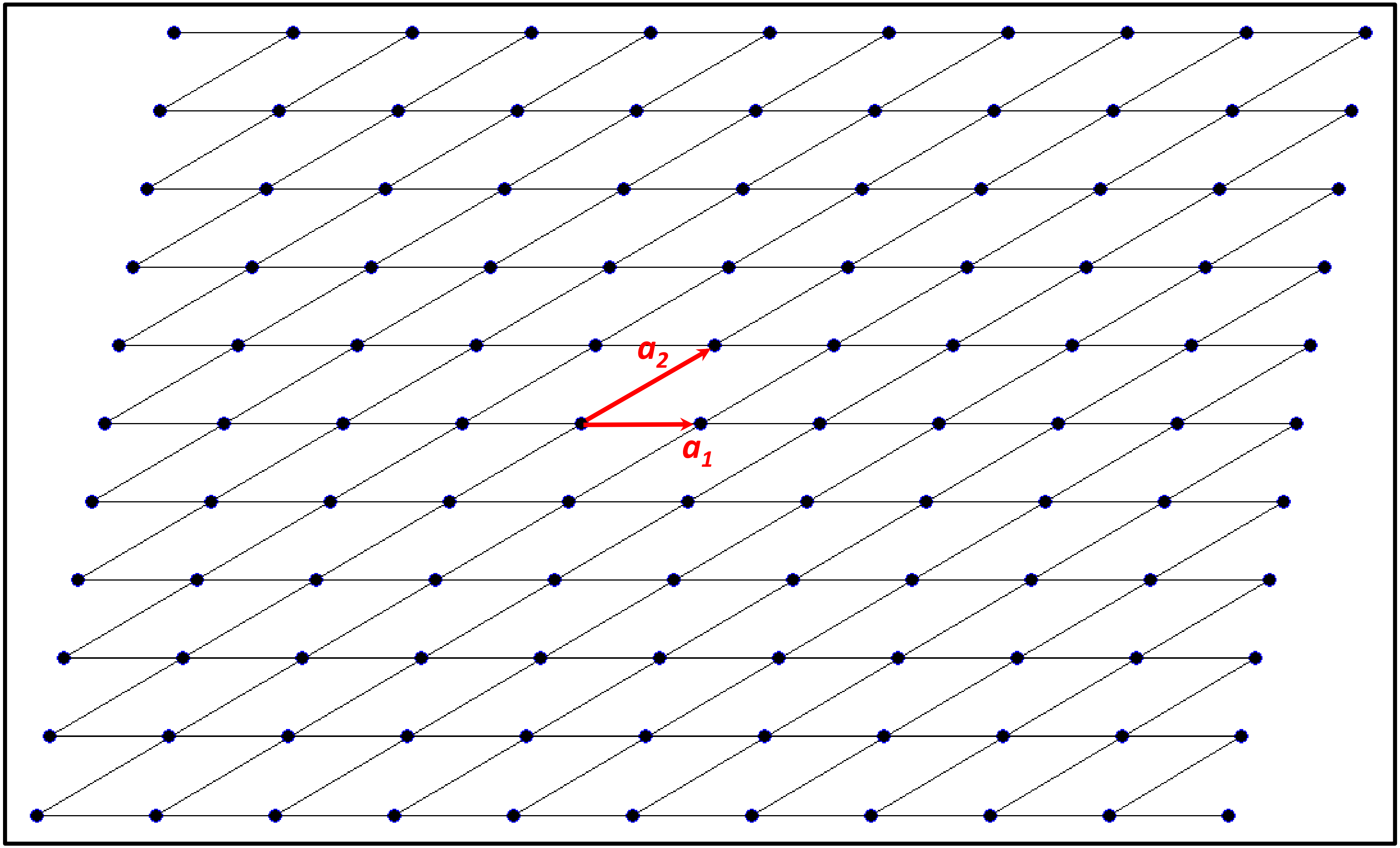


There is a freedom of choice of the lattice basis vectors and therefore lattice parameters

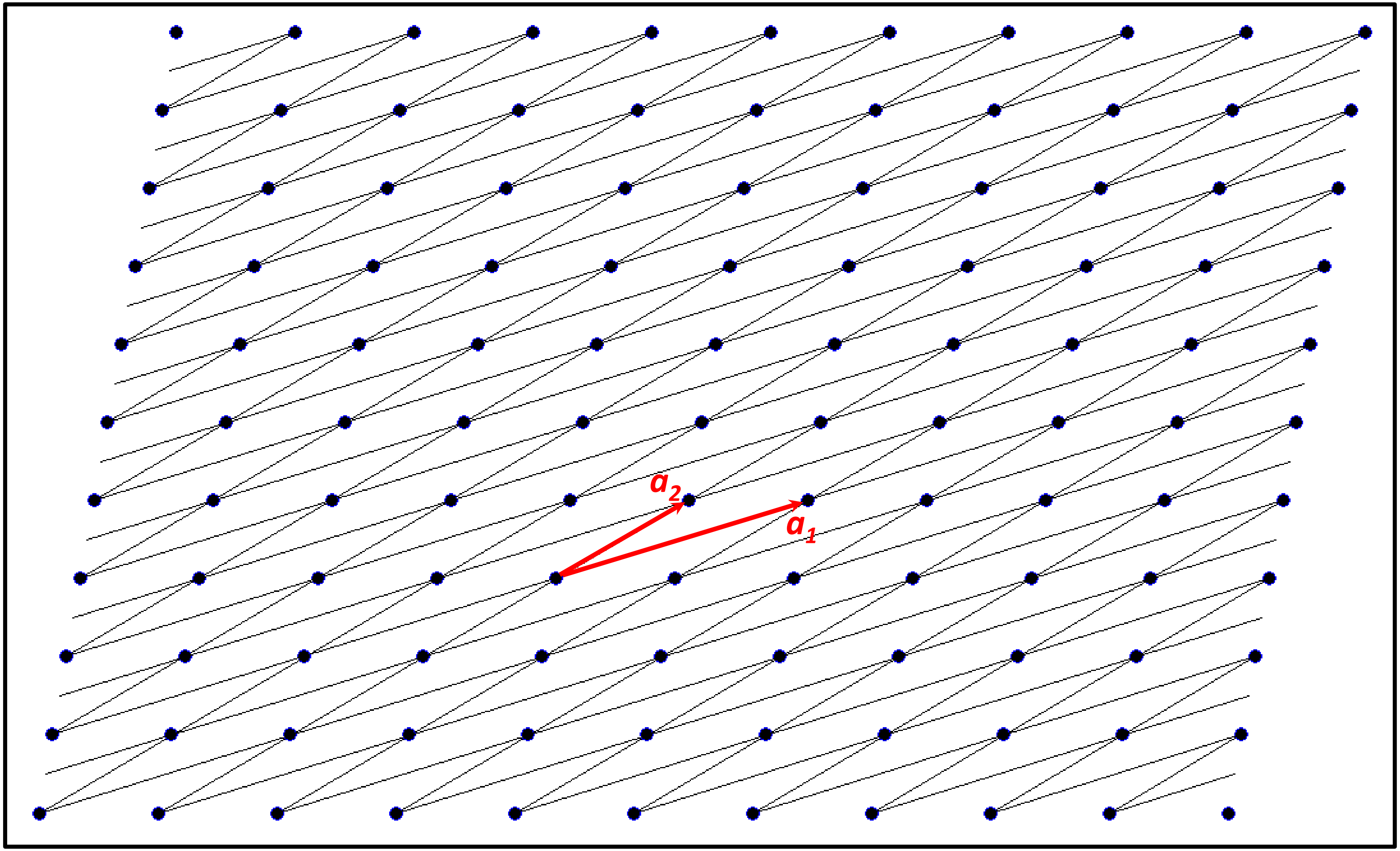
Building a lattice : choice of basis vectors 1



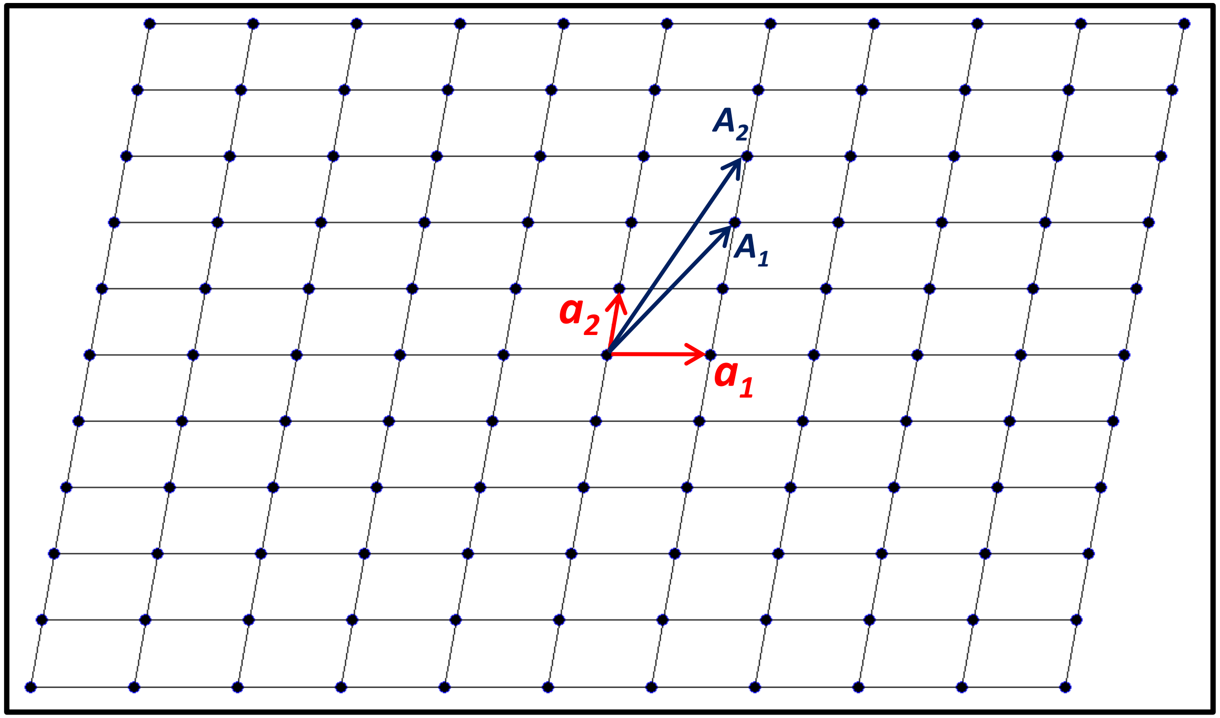
Building a lattice : choice of basis vectors 2



Building a lattice : choice of basis vectors 3



Theorem about the choice of basis vectors



Consider the lattice built with two basis vectors, $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$

Take two other lattice vectors

$A_1=[u_{1i}]=u_{11}\boldsymbol{a_1}+u_{12}\boldsymbol{a_2}$

$A_2=[u_{2i}]=u_{21}\boldsymbol{a_1}+u_{22}\boldsymbol{a_2}$

u_{ij} are integer

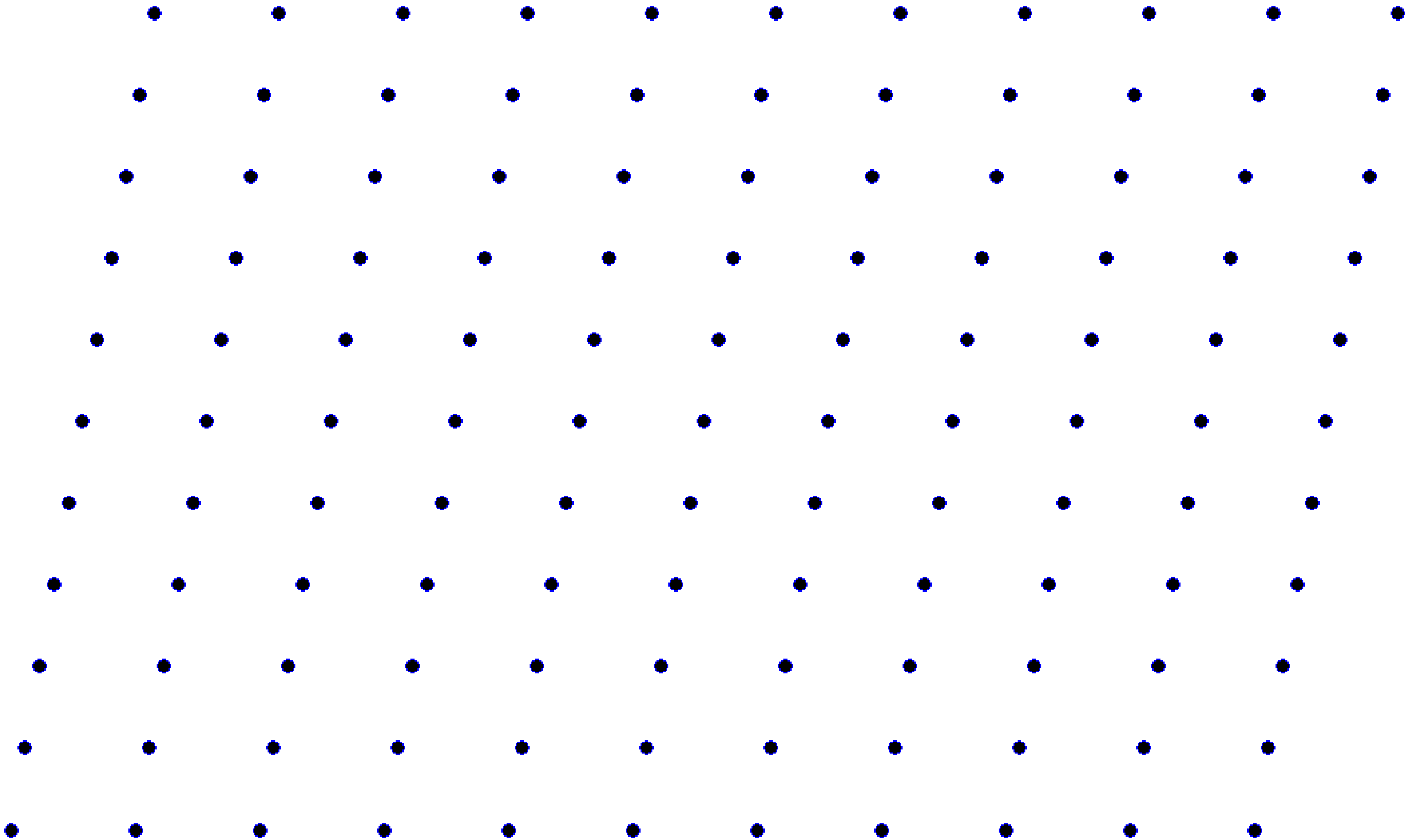
Does this new pair of vectors build the same lattice???

It is necessary to provide that the area, ***S*** of the parallelogram built on $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$ is the same as the area of parallelogram built on A_1 and A_2

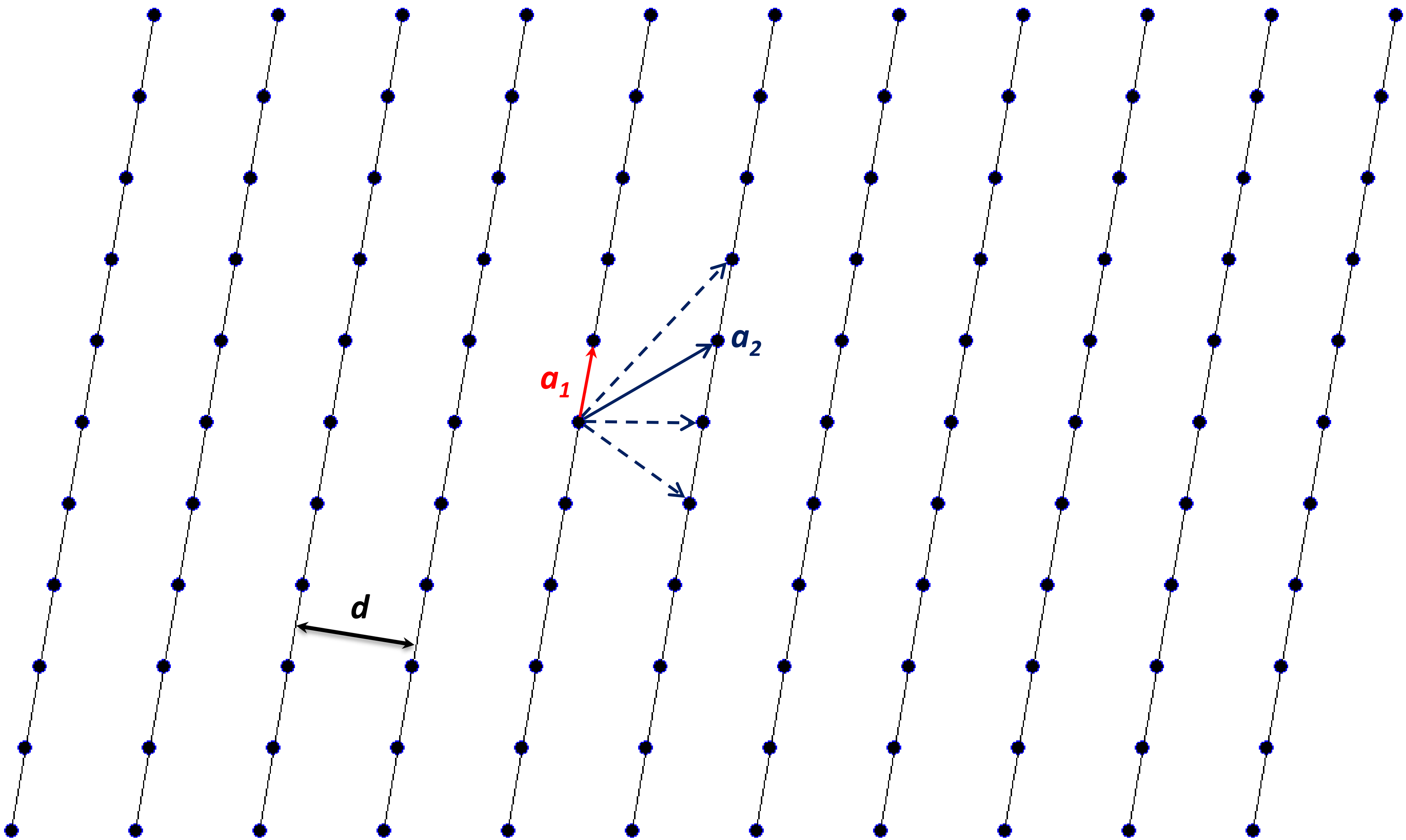
$$S(\boldsymbol{A_1},\boldsymbol{A_2}) = \pm\begin{vmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{vmatrix} S(\boldsymbol{a_1},\boldsymbol{a_2}) \qquad \begin{vmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{vmatrix} = \pm 1$$

If the last equation is fulfilled the pair of vectors A_1 and A_2 can be chosen as basis vectors for the SAME LATTICE

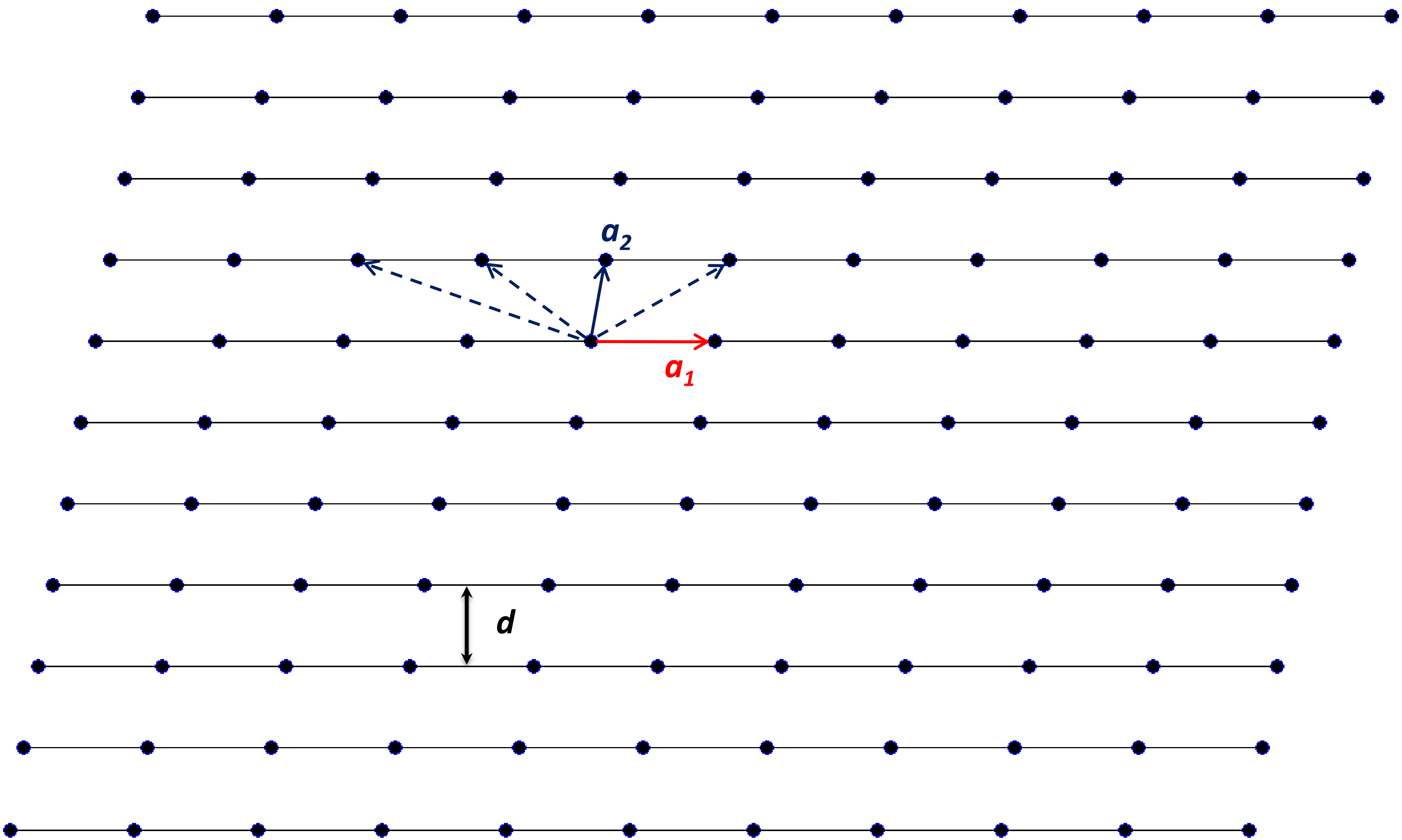
Lattice rows (2D) / Lattice planes (3D)



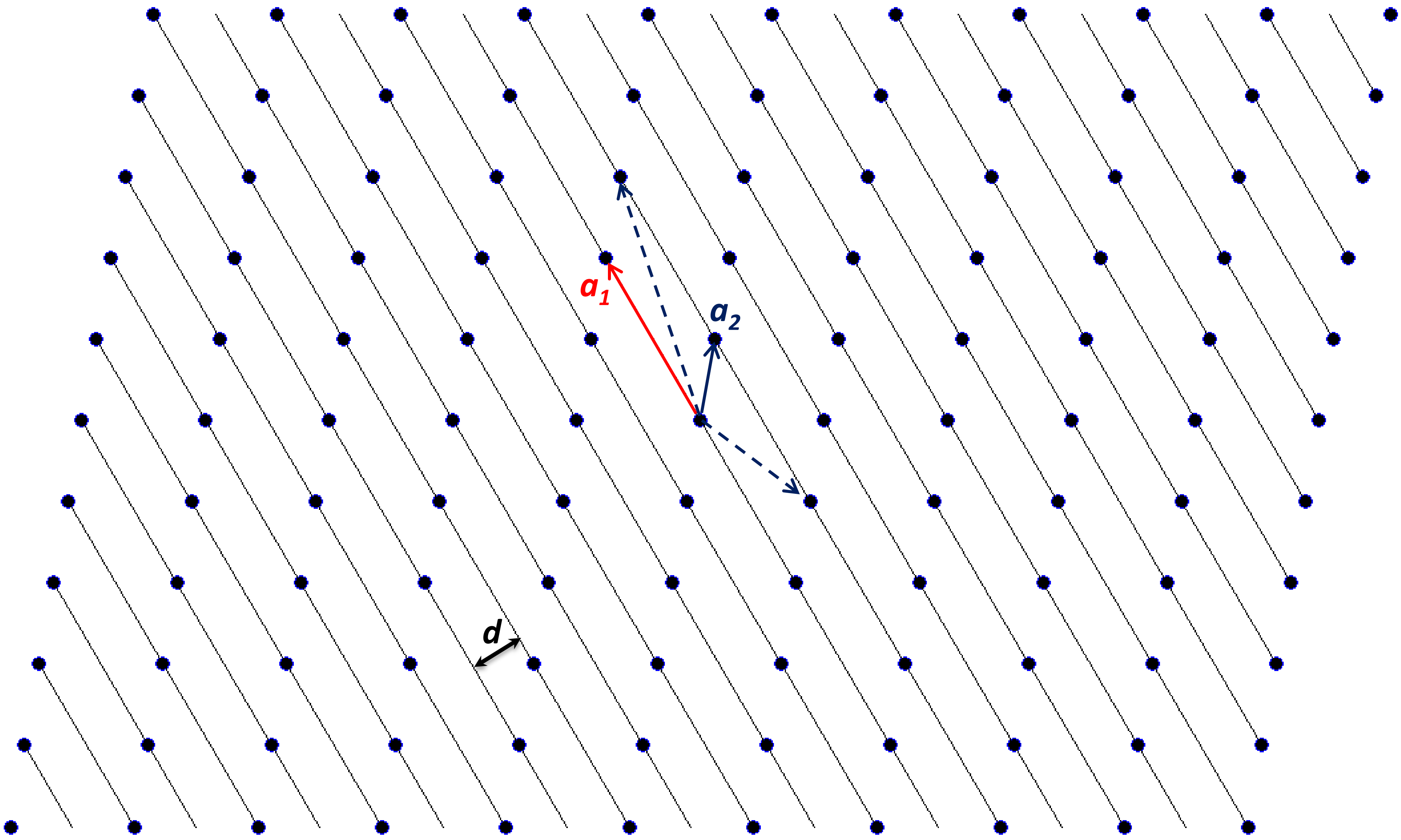
Lattice rows (2D) / Lattice planes (3D)



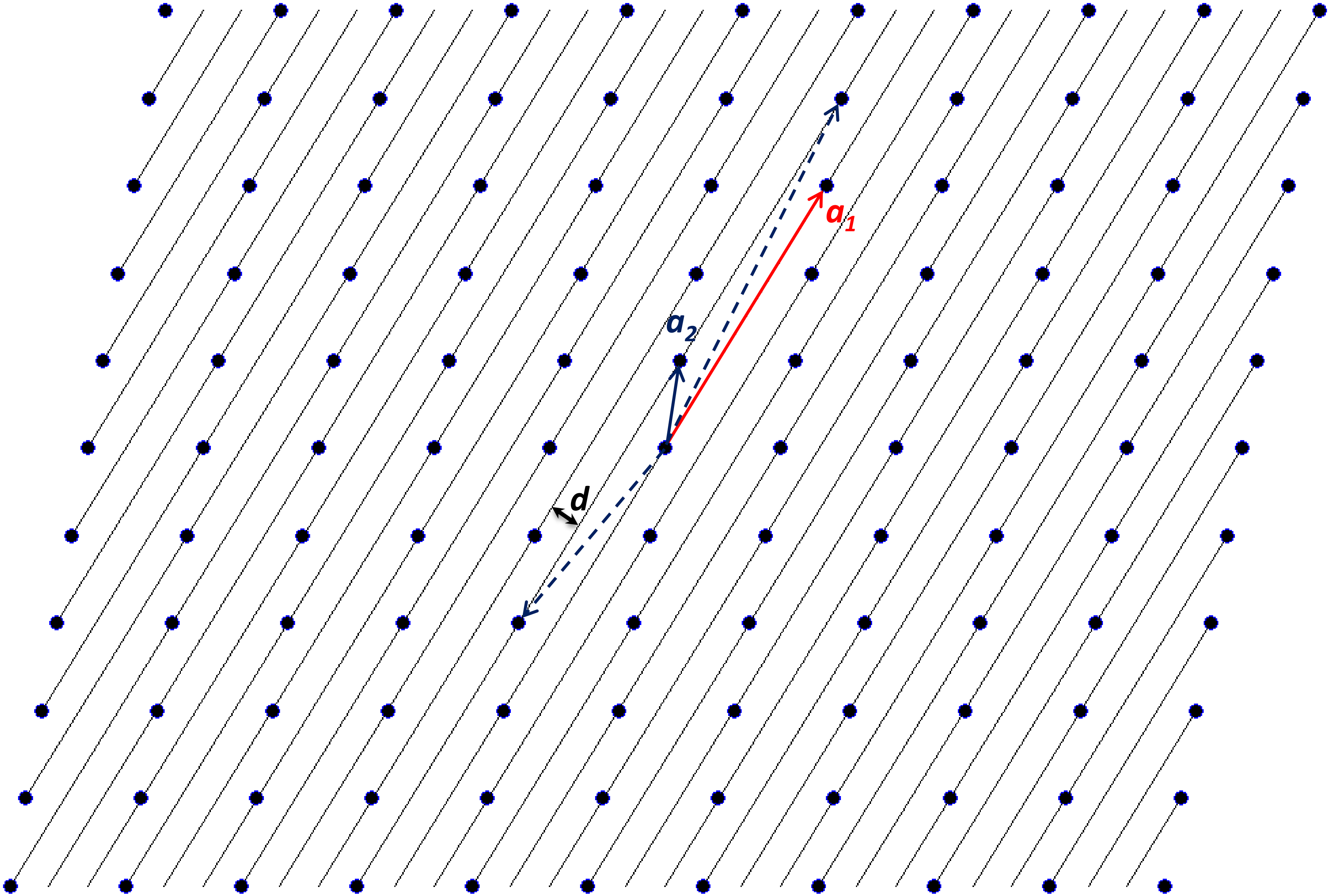
Lattice rows (2D) / Lattice planes (3D)



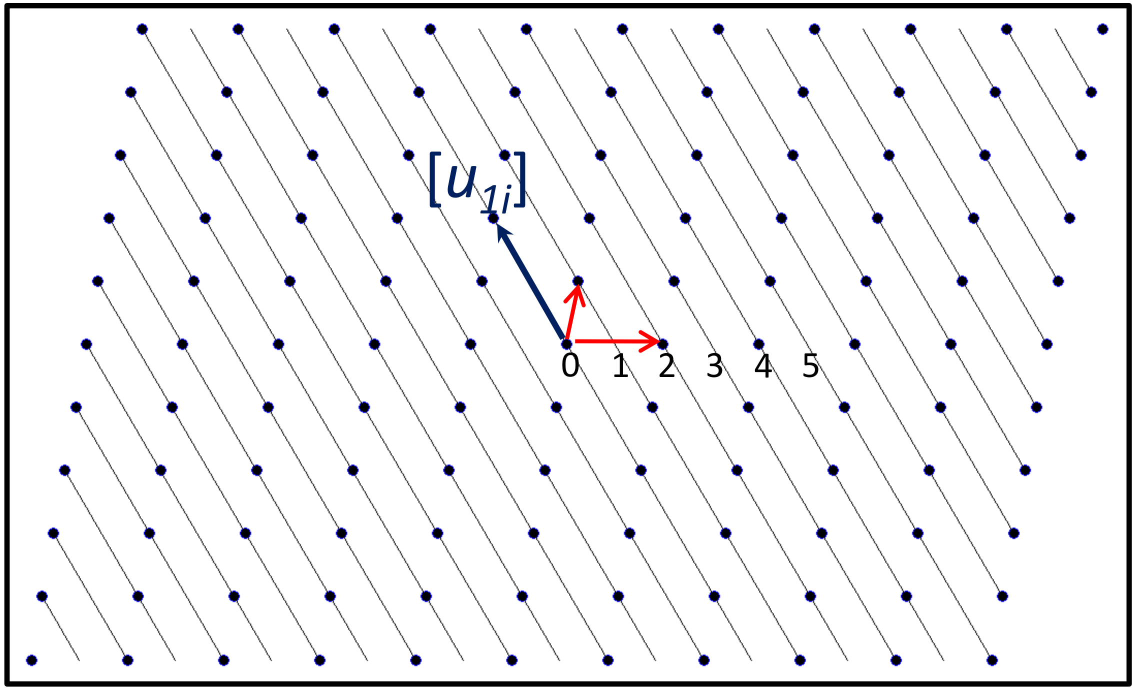
Lattice rows (2D) / Lattice planes (3D)



Lattice rows (2D) / Lattice planes (3D)



Description of the lattice planes



Suppose the pair of basis vectors, $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$ is chosen and the lattice is built.

We split the lattice into the system of rows parallel to the lattice vectors A_1=[u_{11} u_{12}]. We aim to formulate the equation for the point within row N

Row number 0

$$\begin{vmatrix} x_1 & x_2 \\ u_{11} & u_{12} \end{vmatrix} = 0$$

Row number 1

$$\begin{vmatrix} x_1 & x_2 \\ u_{11} & u_{12} \end{vmatrix} = 1$$

Row number 2

$$\begin{vmatrix} x_1 & x_2 \\ u_{11} & u_{12} \end{vmatrix} = 2$$

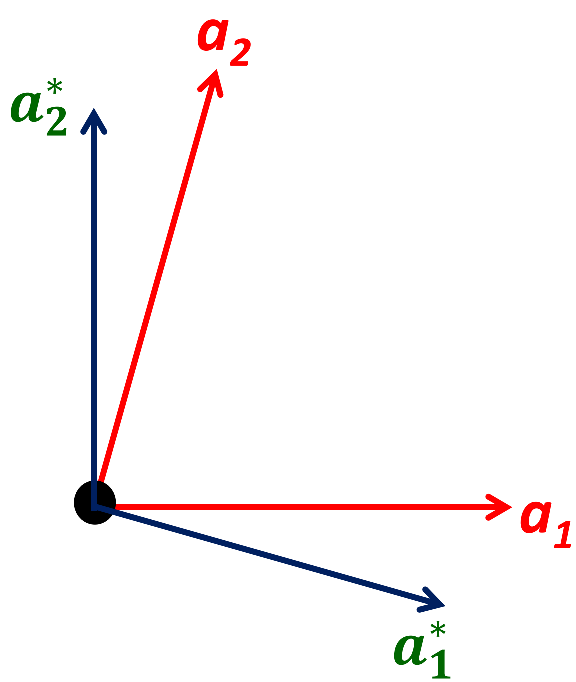
The equation of the row number N

$$h_1 x_1 + h_2 x_2 = N$$

with $h=u_{12}$ *and* $k=-u_{11}$

Reciprocal basis vectors

Consider a lattice built on the pair of vectors, $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$. The pair of reciprocal basis vectors, $\boldsymbol{a}_1^*$ and $\boldsymbol{a}_2^*$ is introduced according to the following dot products



$$\boldsymbol{a}_1 \cdot \boldsymbol{a}_1^* = 1 \quad \boldsymbol{a}_1 \cdot \boldsymbol{a}_2^* = 0$$
$$\boldsymbol{a}_2 \cdot \boldsymbol{a}_1^* = 0 \quad \boldsymbol{a}_2 \cdot \boldsymbol{a}_2^* = 1$$

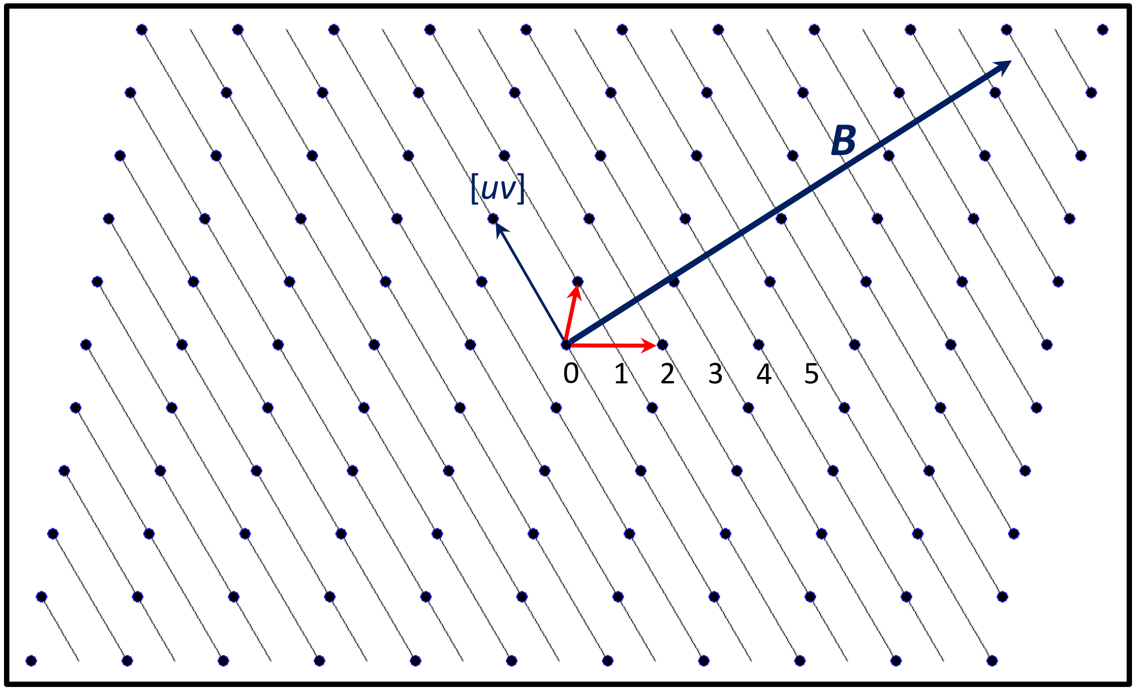
is perpendicular to **a**

is perpendicular to **b**

$$\boldsymbol{A} = u_i \boldsymbol{a_i}$$
$$\boldsymbol{B} = h_j \boldsymbol{a}_{\boldsymbol{j}}^*$$
$$\boldsymbol{A} \cdot \boldsymbol{B} = u_i h_i = u_1 h_1 + u_2 h_2$$

The lattice based on the vectors $\boldsymbol{a}_1^*$ and $\boldsymbol{a}_2^*$ is a RECIPROCAL LATTICE

Equation of planes in terms of reciprocal basis vectors



The equation of the lattice rows:

$$h_1 x_1 + h_2 x_2 = N$$

can now be rewritten as simply with the dot product

$$(\boldsymbol{B}\ \boldsymbol{R}) = N$$

with $\boldsymbol{R} = x_i \boldsymbol{a_i}$ $\quad \boldsymbol{B} = h_i \boldsymbol{a}_i^*$

For the row number 0 (plane going through the origin) we get

$$(\boldsymbol{B}\ \boldsymbol{R}) = 0$$

i.e. the row is perpendicular to the vector ***B.***

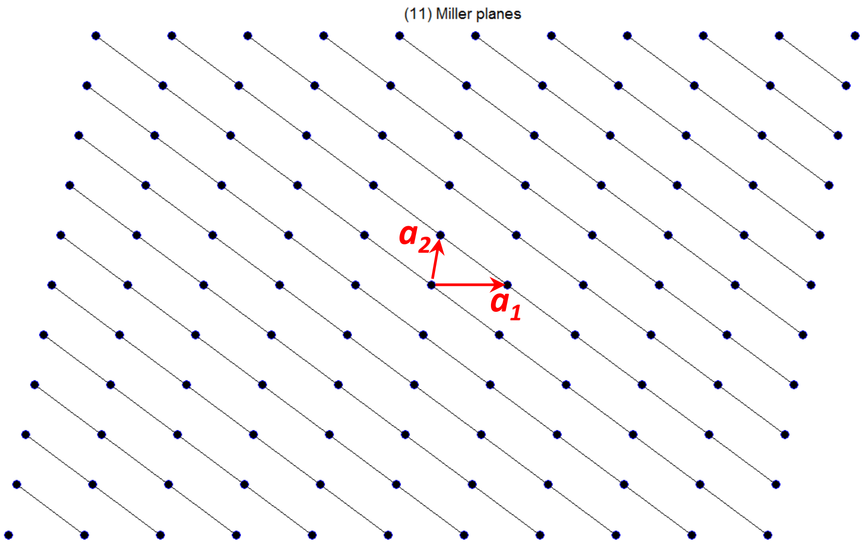
For the first plane ($\boldsymbol{B}\ \boldsymbol{R}$) = 1.

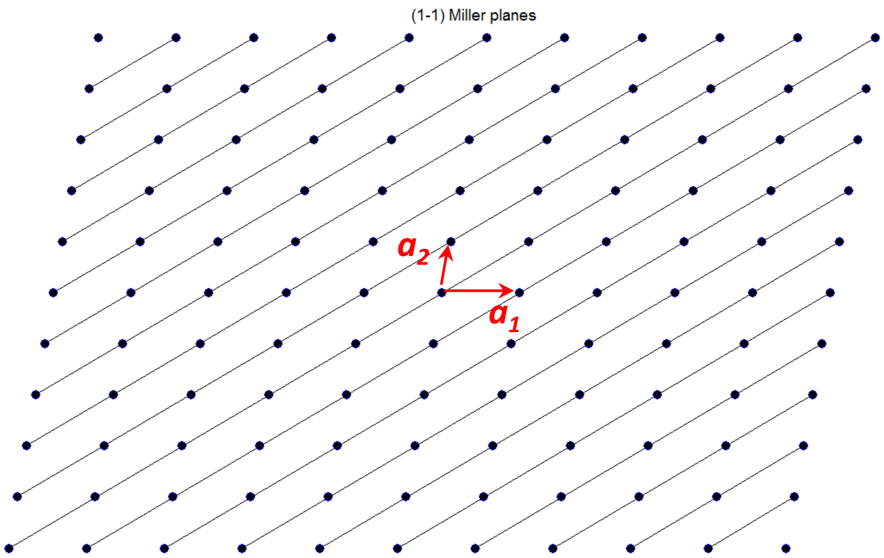
Each set of lattice rows is described by the INTEGER NUMBERS (typically called *h* and *k*) known as **MILLER INDICES**

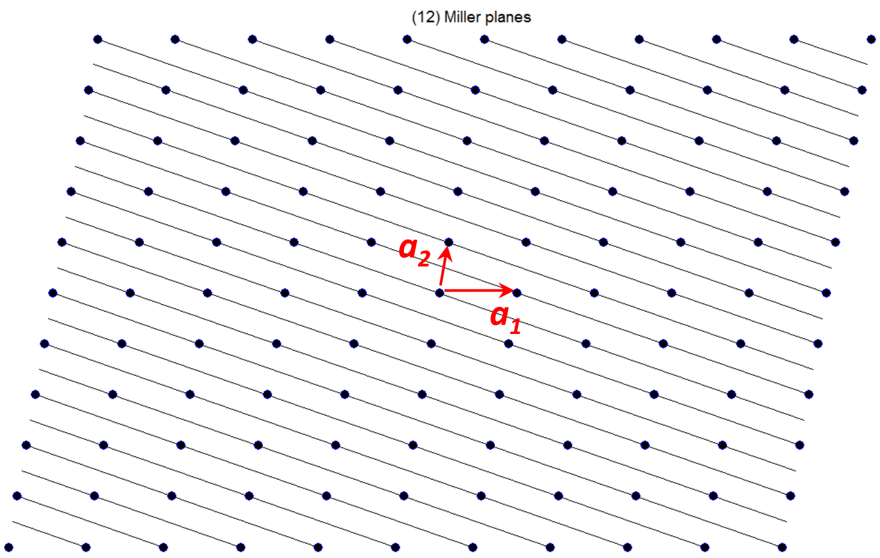
The properties of lattice planes with MILLER INDICES h_1 and h_2 (NB!!! These indices are commonly written as h and k)

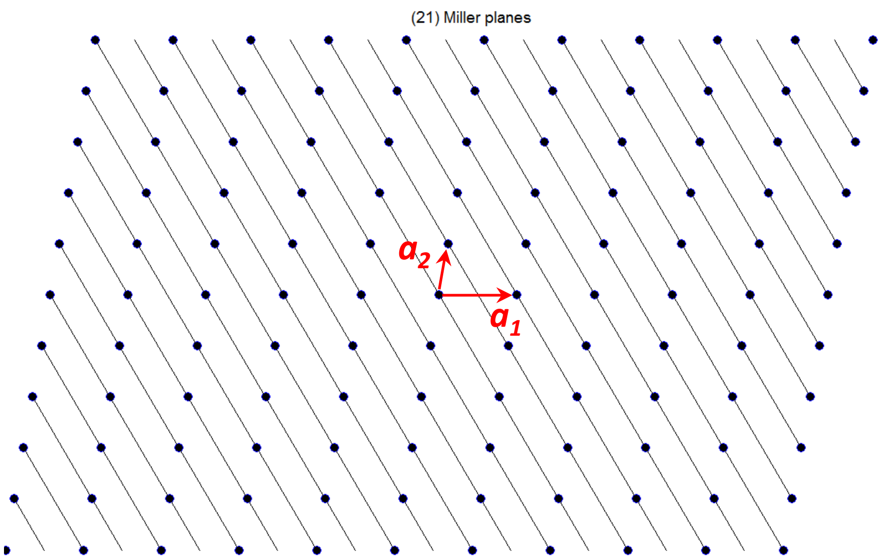
1. *The equation of planes are* $h_1 x_1 + h_2 y_2 = N$ (with *N* integer)
2. According to the definition the numbers h_1 *(h)* and h_2 *(k)* are mutually prime integers
3. The set of planes is perpendicular to the reciprocal lattice vector $\boldsymbol{B} = h_1 \boldsymbol{a}_1^* + h_2 \boldsymbol{a}_2^*$
4. The distance between the neighbouring planes is given by $d = 1 / |B|$
5. The plane intersect the lattice basis vectors in the points [N/h, 0] and [0, N/k]
6. The distance between two lattice point within single plane is $l_{hk} = |B| * S(\boldsymbol{a},\boldsymbol{b})$

Examples. MILLER INDICES AND LATTICE PLANES

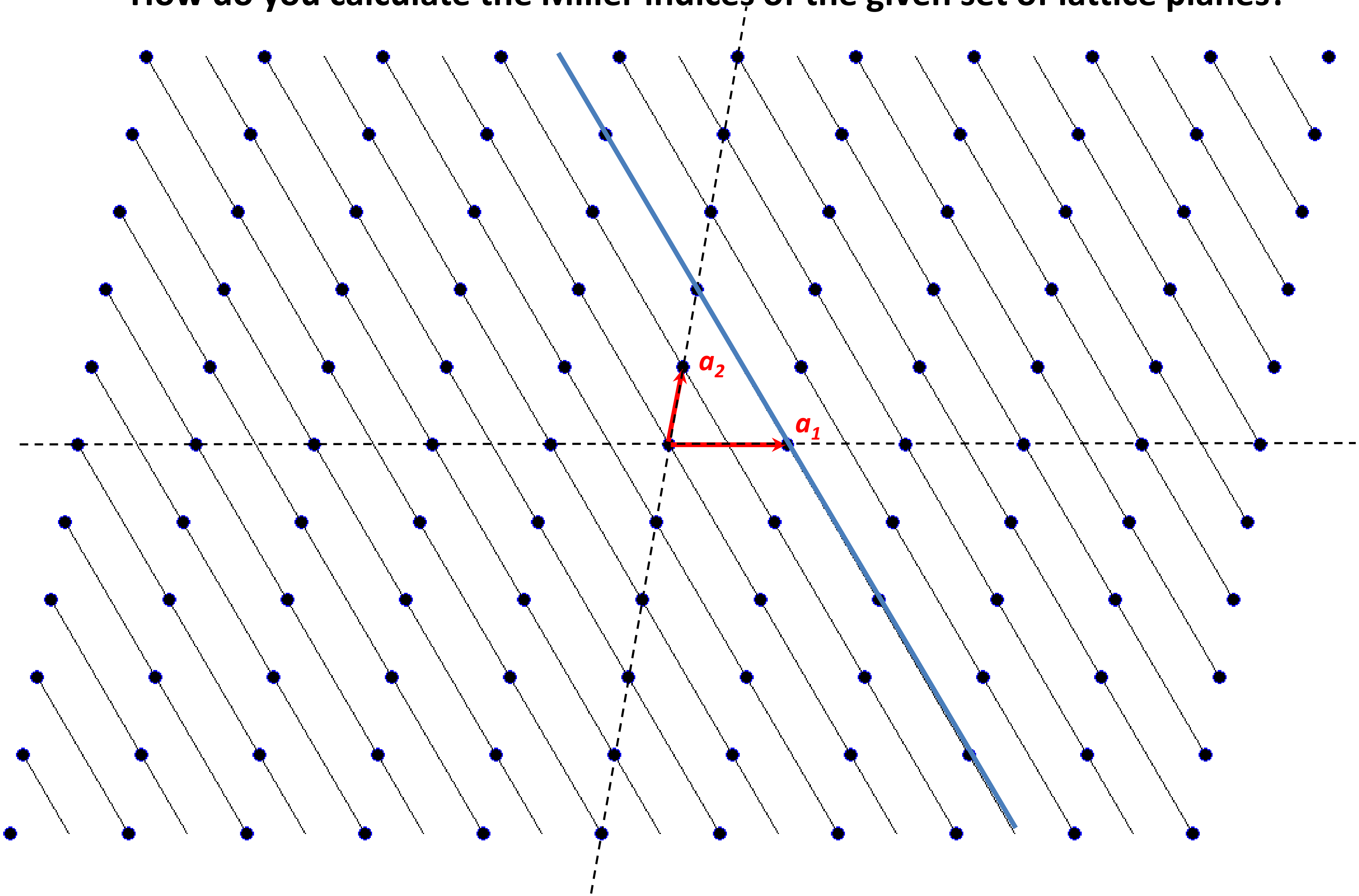








How do you calculate the Miller indices of the given set of lattice planes?

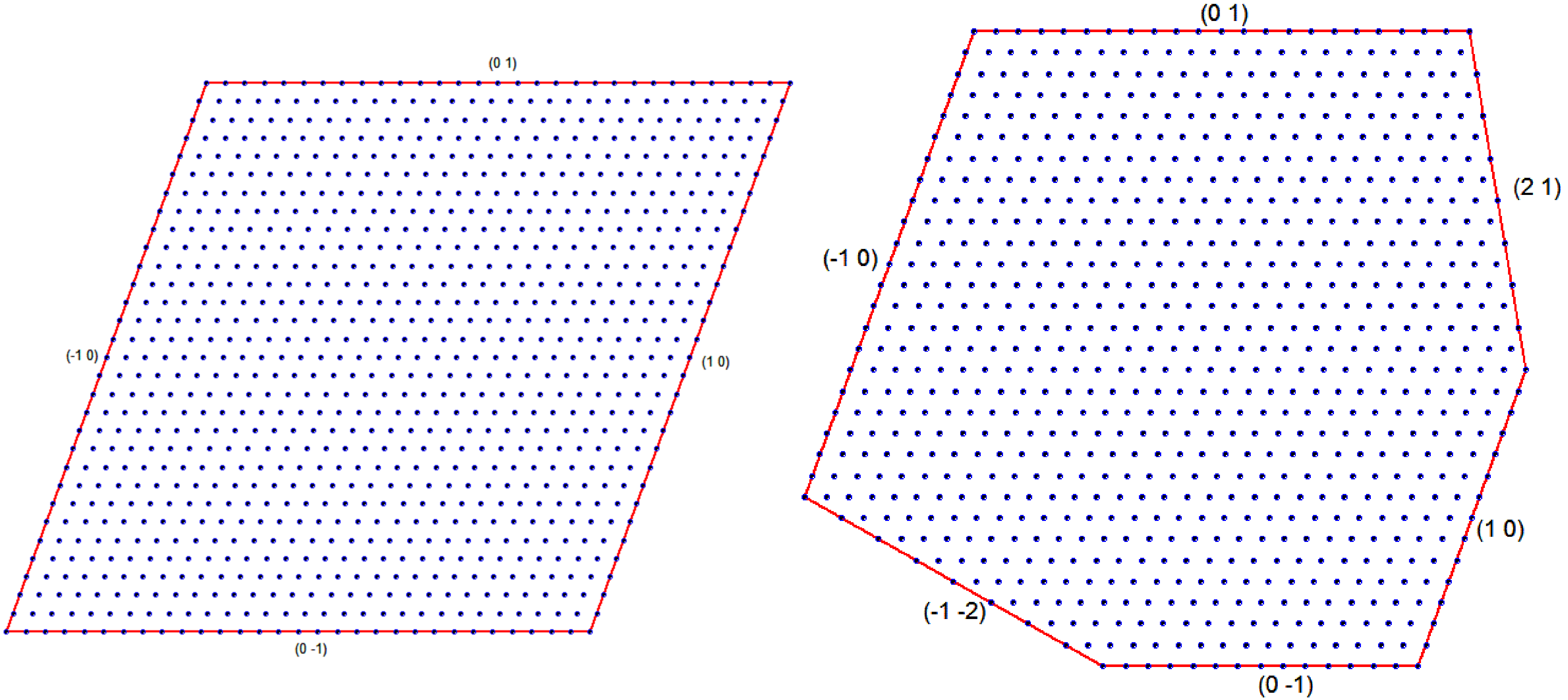


1. There is a plane (number N) intersecting the main axes ***a*** and ***b*** in points [1,0] and [0,2].
2. According to equation of this plane h=N and k=N/2.
3. The mutually prime h and k are obtained by taking N=2. We get h=2 and k=1.

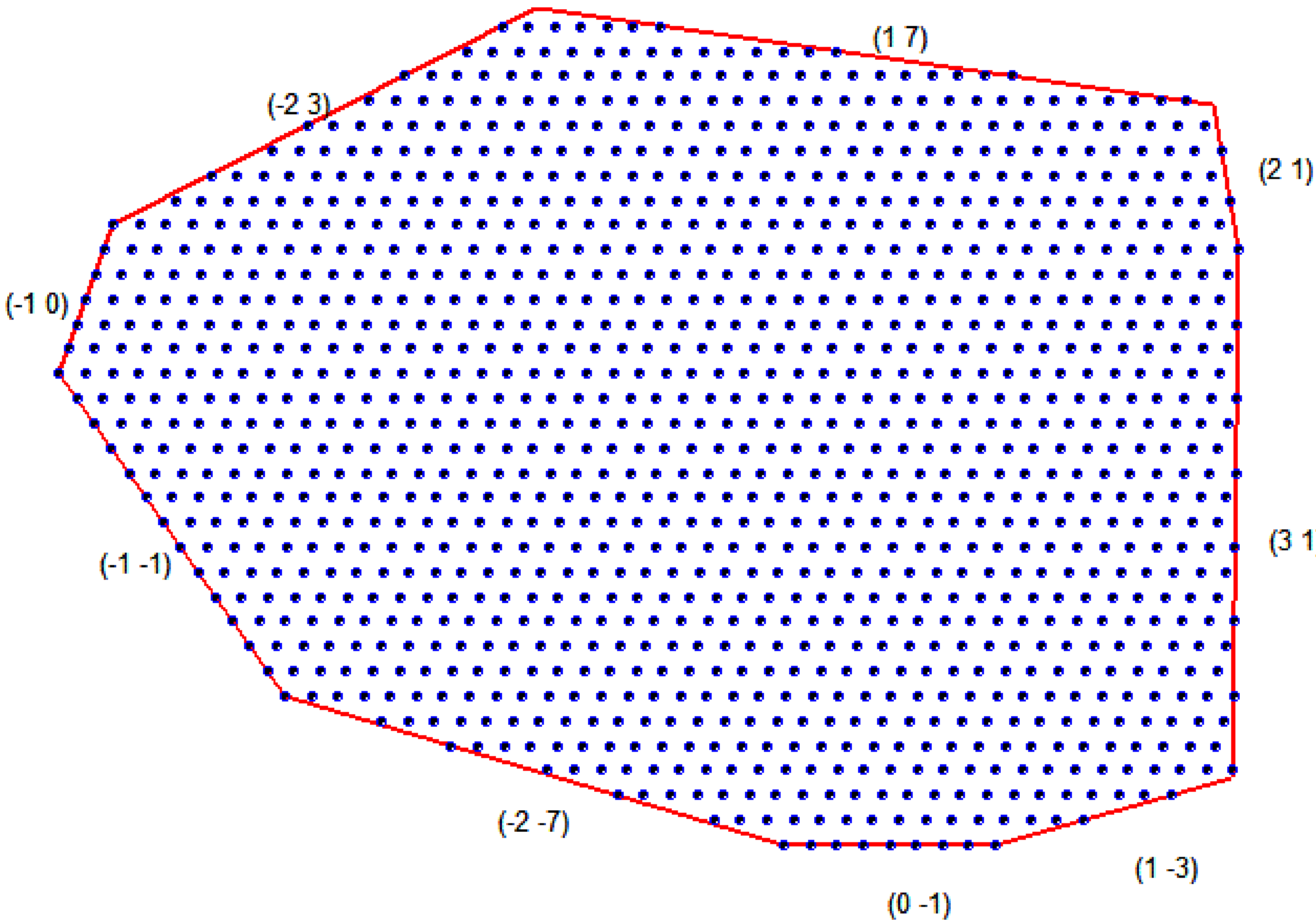
Examples. MILLER INDICES AND CRYSTAL MORPHOLOGY

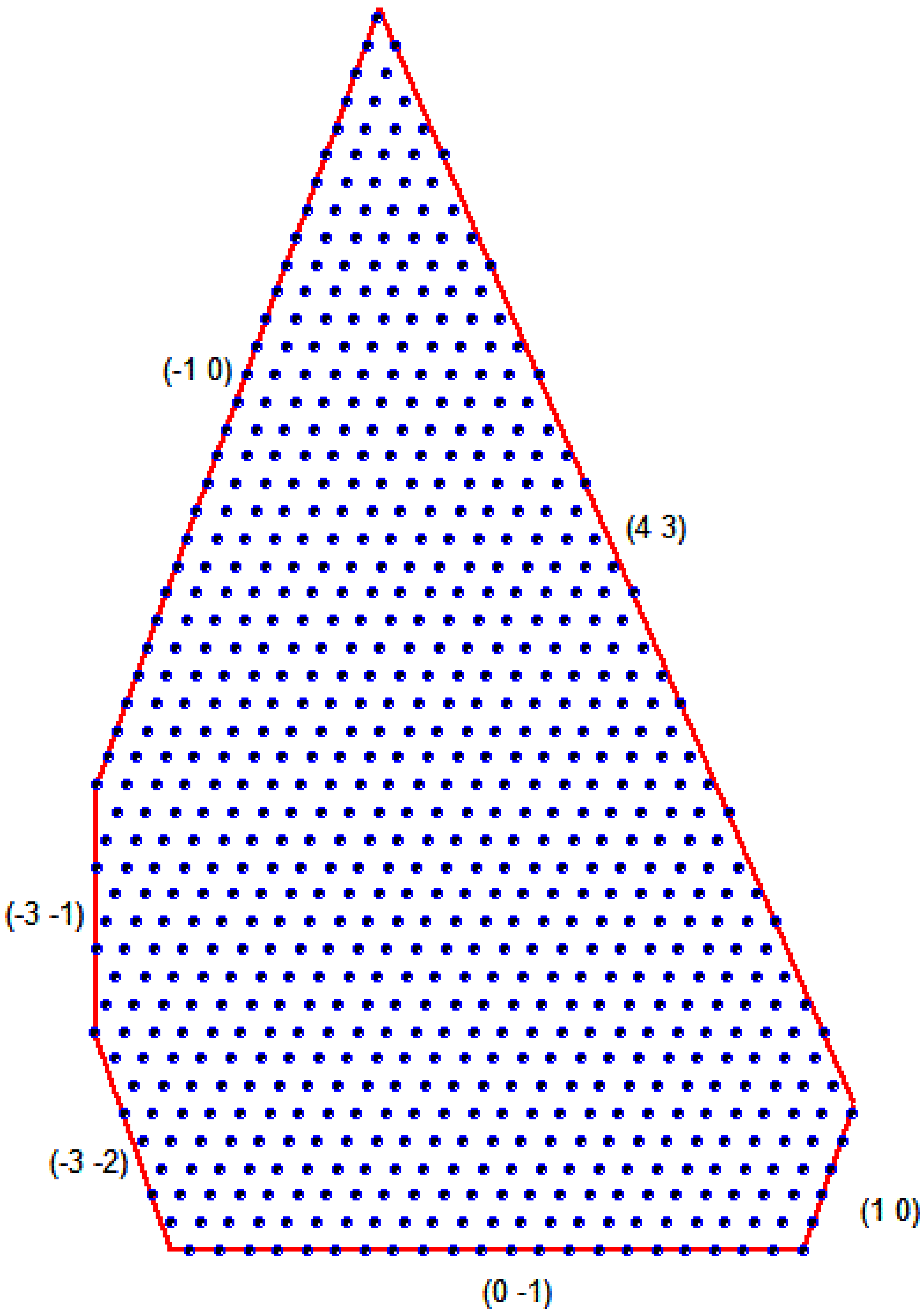
According to the original idea of ***Haüy*** the faces of a crystal are parallel to the lattice planes. Now we can characterize the crystal faces in terms of the Miller indices.

We take a lattice and construct a polyhedron from the different number of faces

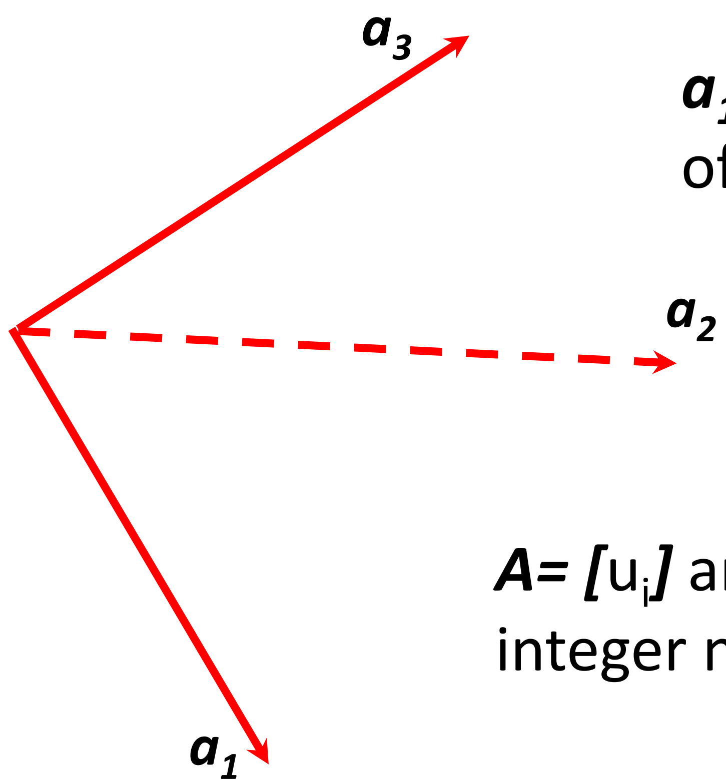


Examples. MILLER INDICES AND CRYSTAL MORPHOLOGY




(-1 0)
(4 3)
(-3 -1)
(-3 -2)
(1 0)
(0 -1)

BASIS VECTORS and CRYSTAL LATTICE PARAMETERS in 3D



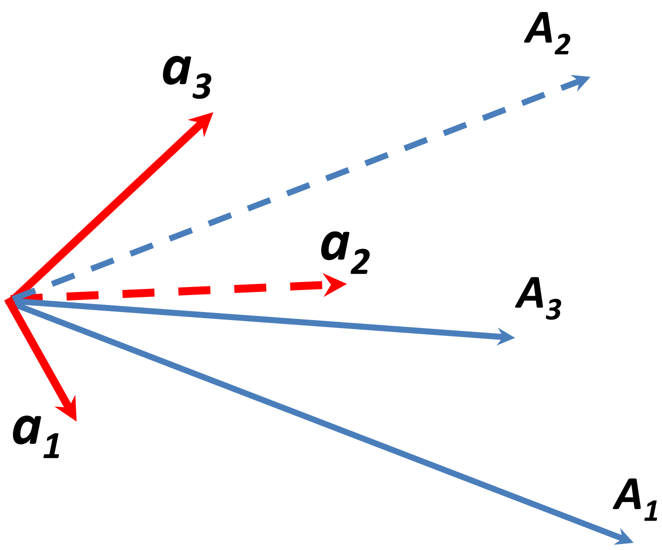
$\boldsymbol{a_1}$,$\boldsymbol{a_2}$ and $\boldsymbol{a_3}$ are the BASIS VECTORS of a crystal lattice

A= [u_i***]*** are the set of LATTICE POINTS (u_i are integer numbers)

The set of lattice parameters for the 3D lattice

$a=|\boldsymbol{a}|$, $b=|\boldsymbol{b}|$, $c=|\boldsymbol{c}|$, $\alpha=\angle(\boldsymbol{b},\boldsymbol{c})$, $\beta=\angle(\boldsymbol{a},\boldsymbol{c})$, $\gamma=\angle(\boldsymbol{a},\boldsymbol{b})$

Theorem about the choice of basis vectors, 3D case



Consider the lattice built with three basis vectors, $\boldsymbol{a_1}$ and $\boldsymbol{a_2}$ and $\boldsymbol{a_3}$

Take three other lattice vectors

$A_1=[u_{1i}]=u_{11}\,\boldsymbol{a_1}+u_{12}\,\boldsymbol{a_2}+u_{13}\,\boldsymbol{a_3}$
$A_2=[u_{2i}]=u_{21}\,\boldsymbol{a_1}+u_{22}\,\boldsymbol{a_2}+u_{23}\,\boldsymbol{a_3}$
$A_3=[u_{3i}]=u_{31}\,\boldsymbol{a_1}+u_{32}\,\boldsymbol{a_2}+u_{33}\,\boldsymbol{a_3}$

u_{ij} are integer numbers

Does this new triple of vectors build the same lattice???

It is necessary to provide that the volume of the parallelepiped built on **a**, **b** and **c** is the same as the area of parallelogram built on A_1, A_2 and A_3

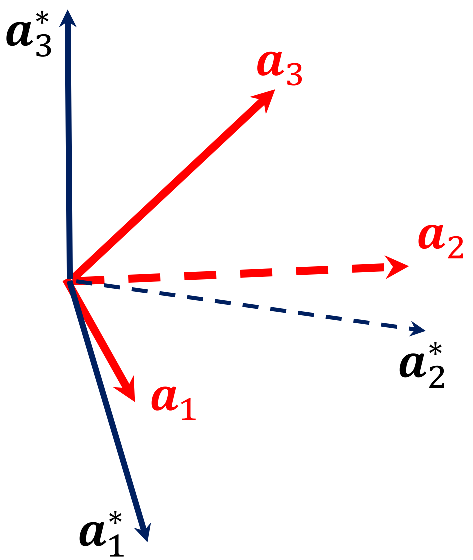
$$V(\boldsymbol{A}_1,\boldsymbol{A}_2,\boldsymbol{A}_3)=\pm\begin{vmatrix}u_{11} & u_{12} & u_{13}\\ u_{21} & u_{22} & u_{23}\\ u_{31} & u_{32} & u_{33}\end{vmatrix}V(\boldsymbol{a}_1,\boldsymbol{a}_2,\boldsymbol{a}_3)$$

$$\begin{vmatrix}u_{11} & u_{12} & u_{13}\\ u_{21} & u_{22} & u_{23}\\ u_{31} & u_{32} & u_{33}\end{vmatrix}=\pm 1 \qquad (*)$$

If equation (*) is fulfilled if the vectors A_1, A_2 and A_3 can be chosen as basis vectors for the SAME LATTICE

Reciprocal basis vectors (3D case)

Consider the crystal lattice and the pair of lattice basis vectors ***a***, ***b*** ***and*** ***c***. The pair of reciprocal basis vectors, ***a**** **,** ***b**** and ***c**** is introduced according to the following dot products

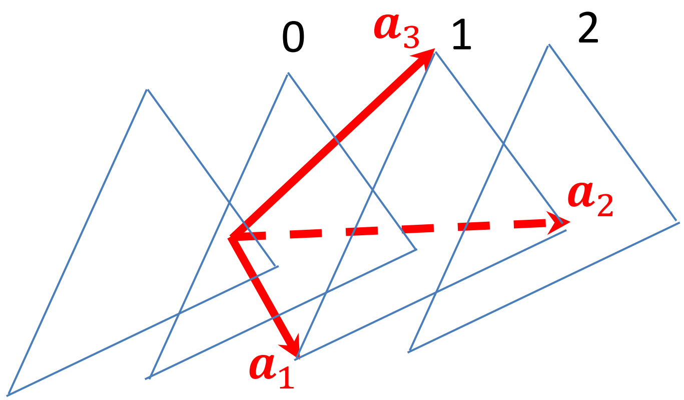


$$\boldsymbol{a}_1 \cdot \boldsymbol{a}_1^* = 1 \quad \boldsymbol{a}_1 \cdot \boldsymbol{a}_2^* = 0 \quad \boldsymbol{a}_1 \cdot \boldsymbol{a}_3^* = 0$$
$$\boldsymbol{a}_2 \cdot \boldsymbol{a}_1^* = 0 \quad \boldsymbol{a}_2 \cdot \boldsymbol{a}_2^* = 1 \quad \boldsymbol{a}_2 \cdot \boldsymbol{a}_3^* = 0$$
$$\boldsymbol{a}_3 \cdot \boldsymbol{a}_1^* = 0 \quad \boldsymbol{a}_3 \cdot \boldsymbol{a}_2^* = 0 \quad \boldsymbol{a}_3 \cdot \boldsymbol{a}_3^* = 1$$

That means $\boldsymbol{a}_1^*$ is perpendicular to the $(\boldsymbol{a}_2\boldsymbol{a}_3)$ plane
That means $\boldsymbol{a}_2^*$ is perpendicular to the $(\boldsymbol{a}_3\boldsymbol{a}_1)$ plane
That means $\boldsymbol{a}_3^*$ is perpendicular to the $(\boldsymbol{a}_1\boldsymbol{a}_2)$ plane

$$\boldsymbol{A} = u_i\boldsymbol{a_i}$$
$$\boldsymbol{B} = h_j\boldsymbol{a_j^*}$$
$$\boldsymbol{A} \cdot \boldsymbol{B} = u_i h_i = u_1 h_1 + u_2 h_2 + u_3 h_3$$

Mathematical description of lattice planes (3D case)



Suppose the triple of main basis vectors, $\boldsymbol{a_1}$, $\boldsymbol{a_2}$ and $\boldsymbol{a_3}$ is chosen and the lattice is built

We split the lattice into the system of planes so that the plane is defined by the lattice vectors $\boldsymbol{A_1}=[u_{1i}]$ and $\boldsymbol{A_2}=[u_{2i}]$. Similar to the 2D case we can use the theorem about the choice of basis vectors to construct the equations of planes

Plane number 0

$$\begin{vmatrix} x_1 & x_2 & x_3 \\ u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \end{vmatrix} = 0$$

Plane number 1

$$\begin{vmatrix} x_1 & x_2 & x_3 \\ u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \end{vmatrix} = 1$$

Plane number 2

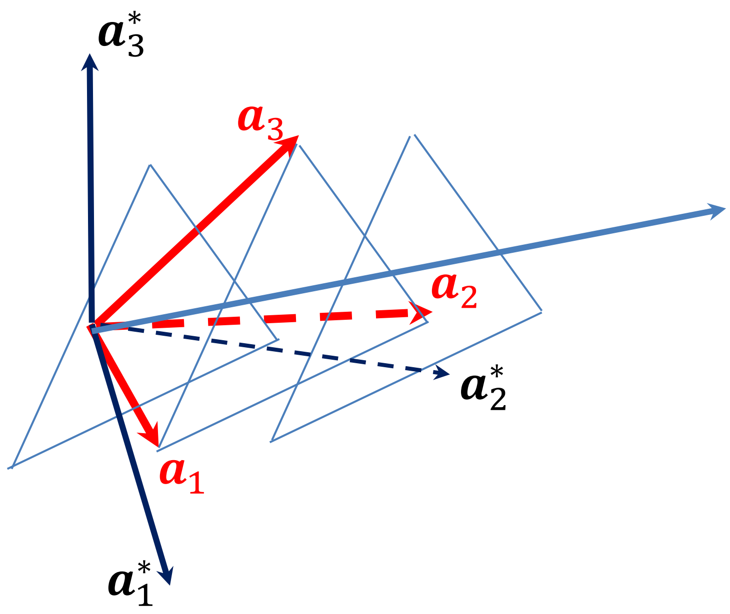
$$\begin{vmatrix} x_1 & x_2 & x_3 \\ u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \end{vmatrix} = 2$$

In general the equation of the plane number N from the origin

$$h_1x_1 + h_2x_2 + h_3x_3 = N$$

with $h_1 = \begin{vmatrix} u_{12} & u_{13} \\ u_{22} & u_{23} \end{vmatrix}$ $h_2 = -\begin{vmatrix} u_{11} & u_{13} \\ u_{21} & u_{23} \end{vmatrix}$ $h_3 = \begin{vmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{vmatrix}$

Equation of planes in terms of reciprocal basis vectors (3D)



The equation for the lattice planes:

$$h_1 x_1 + h_2 x_2 + h_3 x_3 = N$$

can now be rewritten as simply with the dot product

(***B*** ***R***) = N

$$\boldsymbol{R} = x_i \boldsymbol{a_i} \qquad \boldsymbol{B} = h_i \boldsymbol{a}_i^*$$

For the plane number 0 (plane going through the origin) we get (***B R) = 0,*** that means the plane is perpendicular to the vector ***B.*** For the first plane (***B R***) = 1.

Each set of lattice rows is described by the INTEGER NUMBERS (typically called *h, k and l*) known as **MILLER INDICES**

The properties of lattice planes with MILLER INDICES h k l

1. *The equation of planes are* $h\,x + k\,y + lz = N$ (with N integer)

2. According to the definition h, k and l are MUTUALLY PRIME

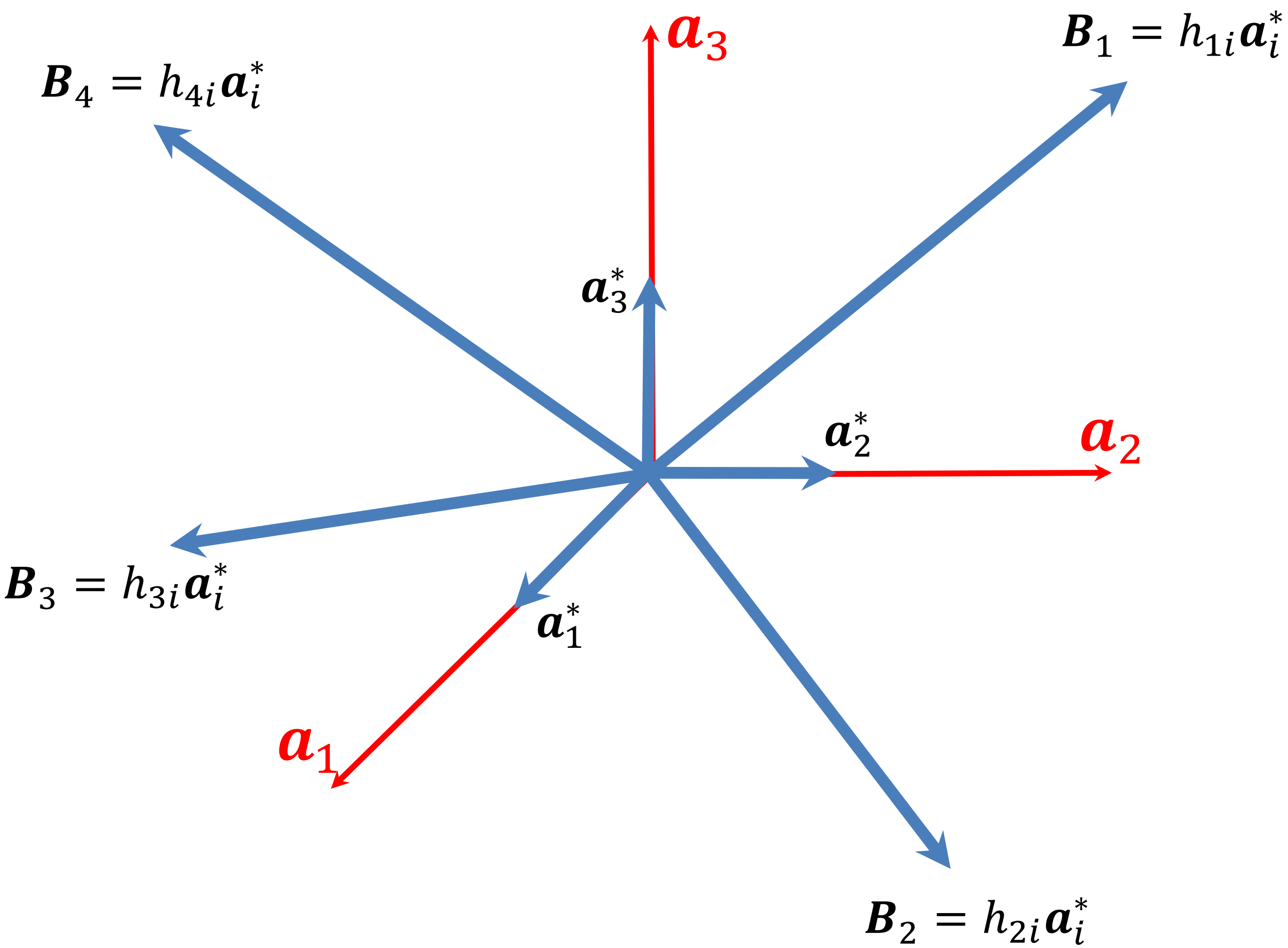
3. The set of planes is perpendicular to the reciprocal lattice vector
   $B = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$

4. The distance between the neighbouring planes is given by $d = 1 / |B|$

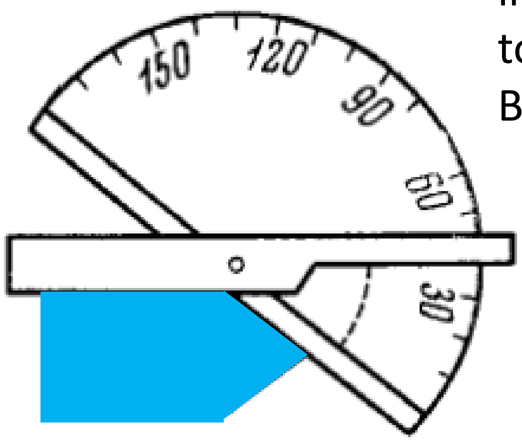
5. The plane intersect the lattice basis vectors in the points [N/h, 0, 0], [0, N/k,0], [0,0,N/*l*]

6. The area of 2D lattice between four lattice point within single plane is $S_{hk} = |B| * V(\boldsymbol{a},\boldsymbol{b},\boldsymbol{c})$

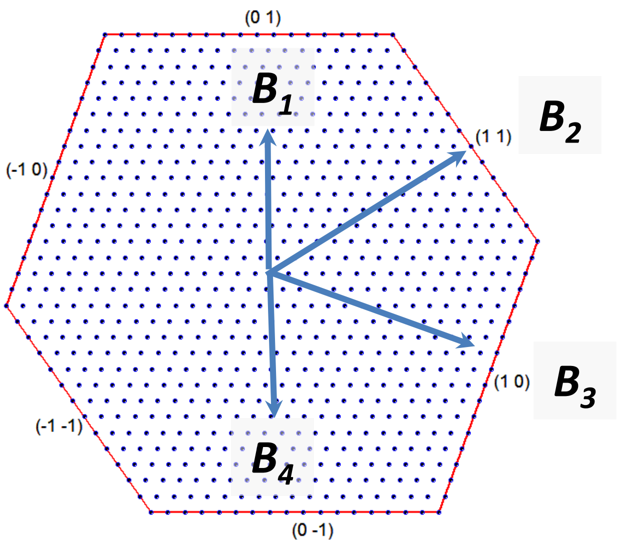
3D crystal morphologies. Crystal shapes corresponding to the cubic lattice (lattice constants a=b=c, $\alpha = \beta = \gamma$ =90 deg)



The angles between faces: how do they depend on the crystal lattice



The face with the Miller indices (hkl) is perpendicular to the reciprocal lattice vector B=[hkl]*=h***a****+k***b****+l***c****



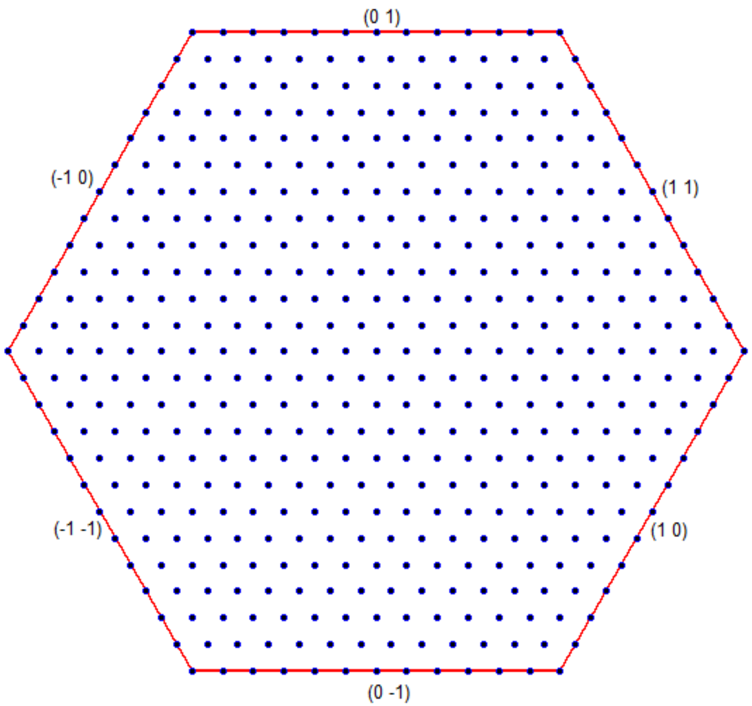
The angle between faces $\alpha_{IJ} = \angle(\boldsymbol{B}_I, \boldsymbol{B}_J)$

$$cos\alpha_{IJ} = \frac{(\boldsymbol{B}_I \cdot \boldsymbol{B}_J)}{B_I B_J}$$

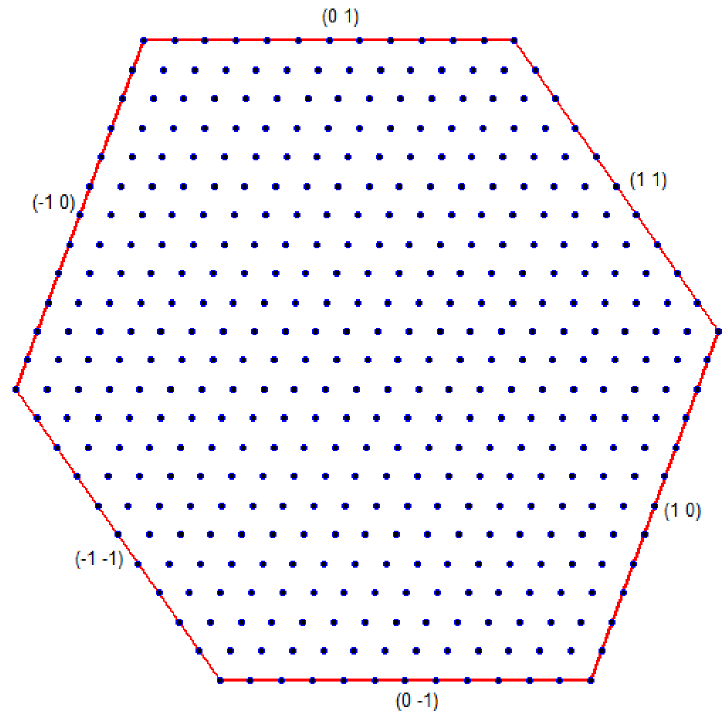
$$(\boldsymbol{B}_I \cdot \boldsymbol{B}_J) = h_{Ii} h_{Jj} G^*_{ij}$$

Example: the polyhedral shape of a 2D for two different crystal lattices

a=1, b=1, α=60 deg



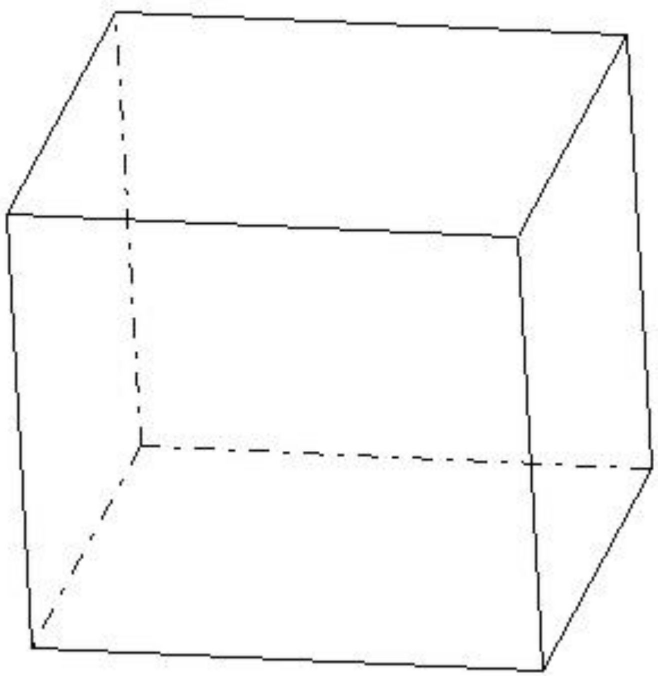
a=1, b=1, α=70 deg



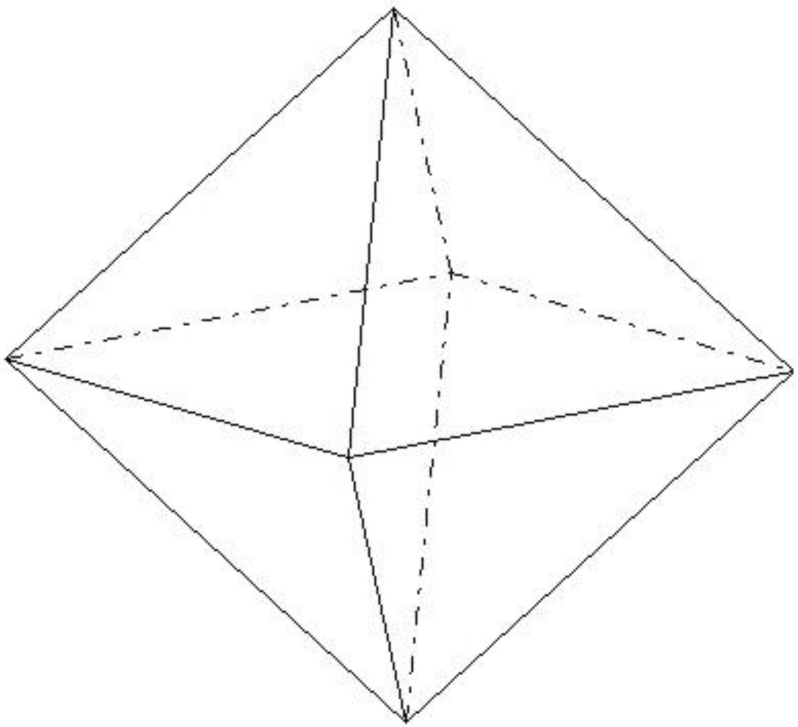
The angles between the natural faces of a crystals are defined by the crystal lattice parameters. This is the background for the law of constancy of the interfacial angles

Simple shapes corresponding to the cubic lattice (lattice constants a=b=c, $\alpha = \beta = \gamma$ =90 deg)

Cube



Octahedron



The list of faces for a cube:

(100) (010) (001)

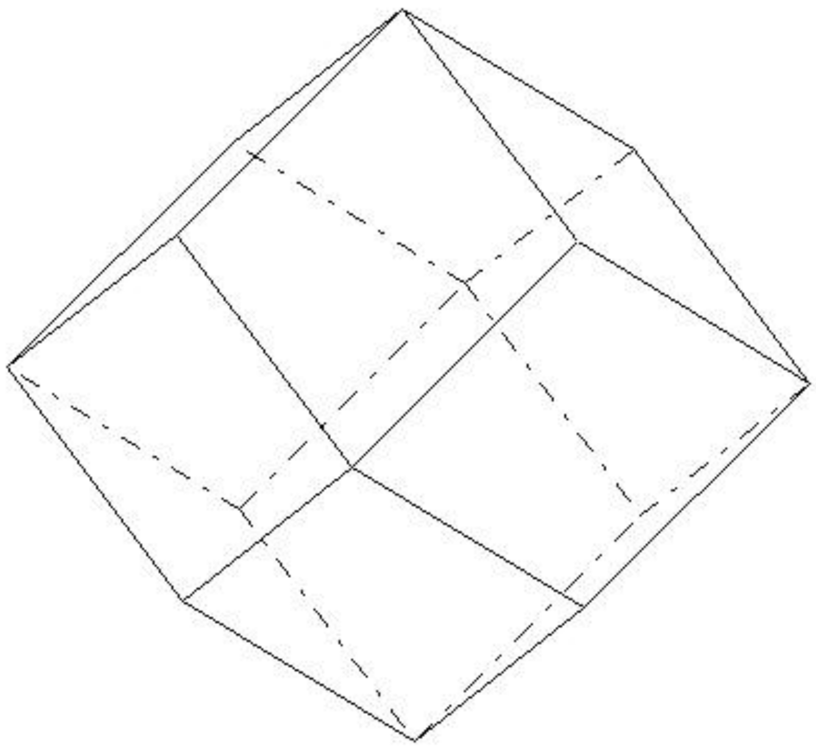
$(\bar{1}00)$ $(0\bar{1}0)$ $(00\bar{1})$

The list of faces for an octahedron:

(111) $(\bar{1}11)$ $(1\bar{1}1)$ $(\bar{1}\bar{1}1)$

$(11\bar{1})$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ $(\bar{1}\bar{1}\bar{1})$

Rhombododecahedron



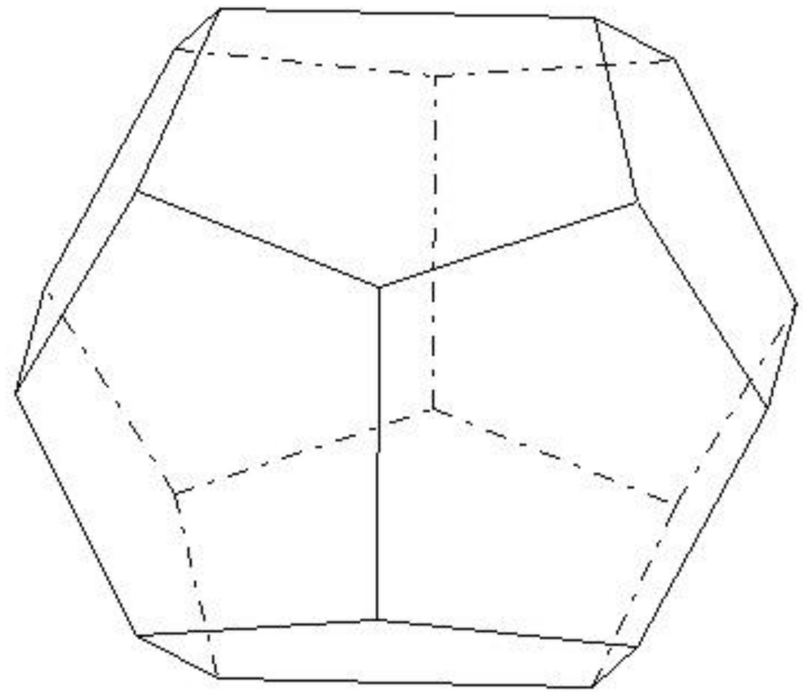
The list of faces :

(110) $(1\bar{1}0)$ $(\bar{1}10)$ $(\bar{1}\bar{1}0)$

(101) $(10\bar{1})$ $(\bar{1}01)$ $(\bar{1}0\bar{1})$

(011) $(01\bar{1})$ $(0\bar{1}1)$ $(0\bar{1}\bar{1})$

Pentagondodecahedron

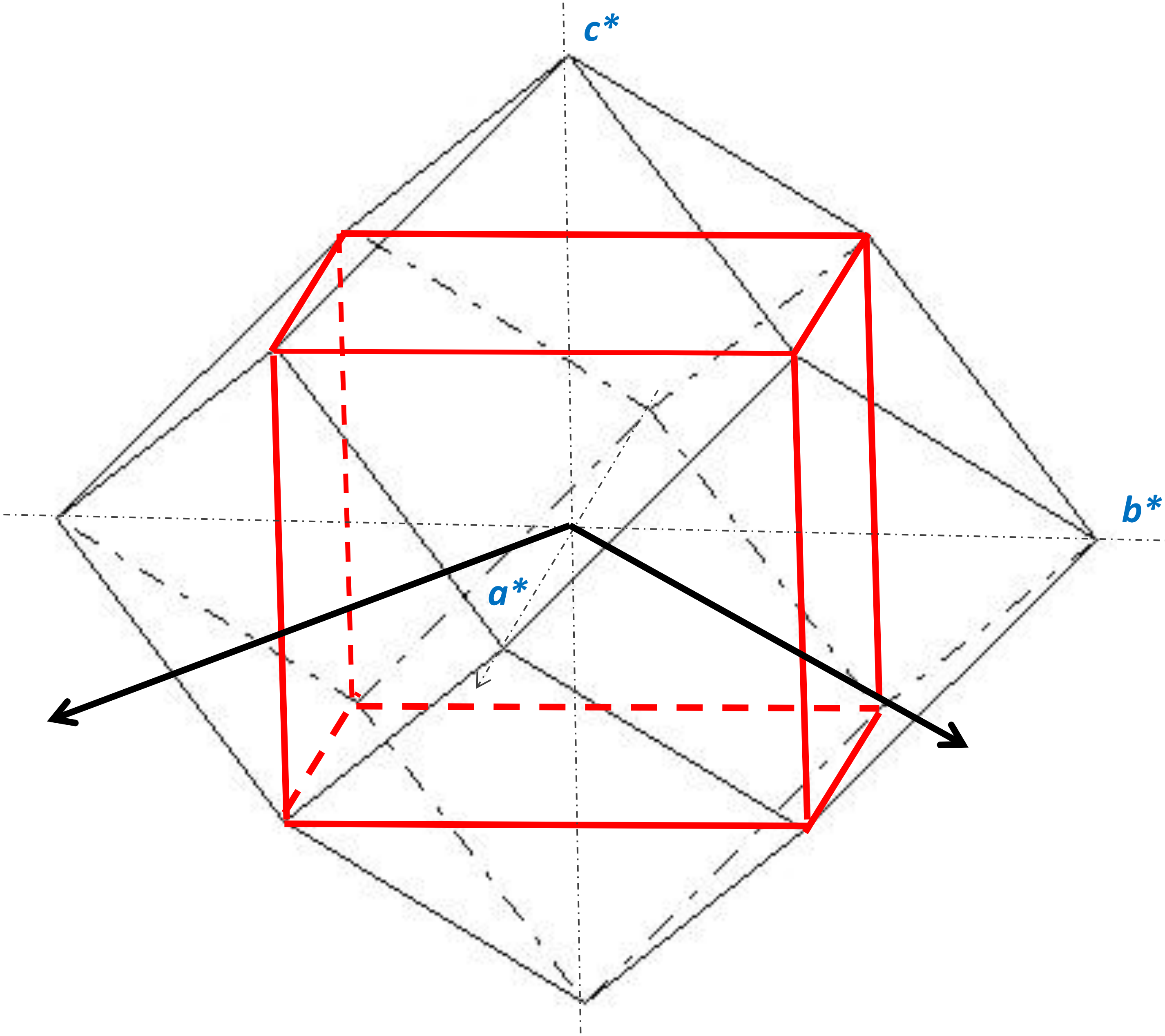


The list of faces :

(120) $(1\bar{2}0)$ $(\bar{1}20)$ $(\bar{1}\bar{2}0)$

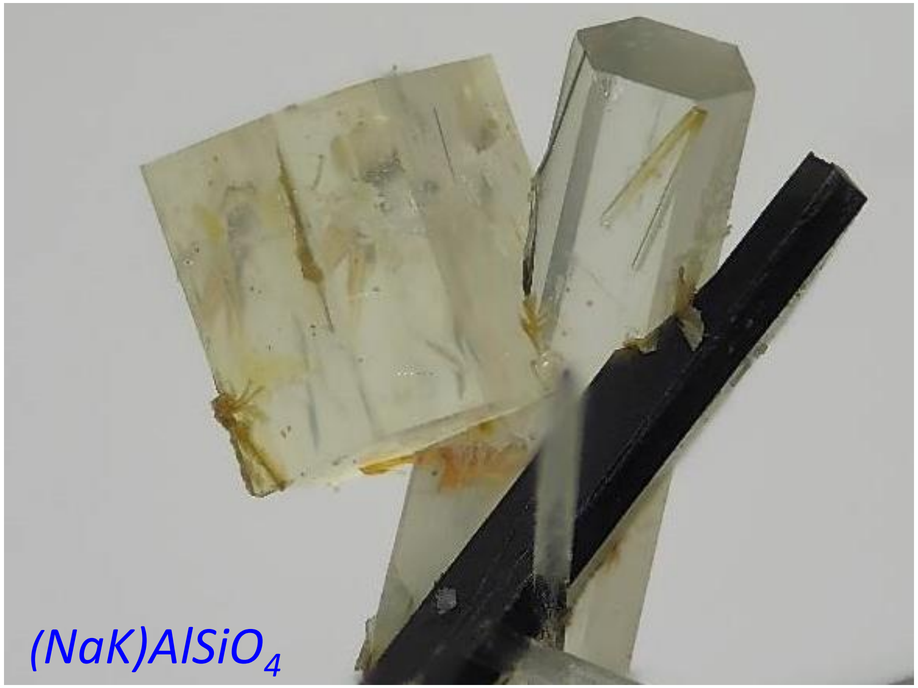
(201) $(20\bar{1})$ $(\bar{2}01)$ $(\bar{2}0\bar{1})$

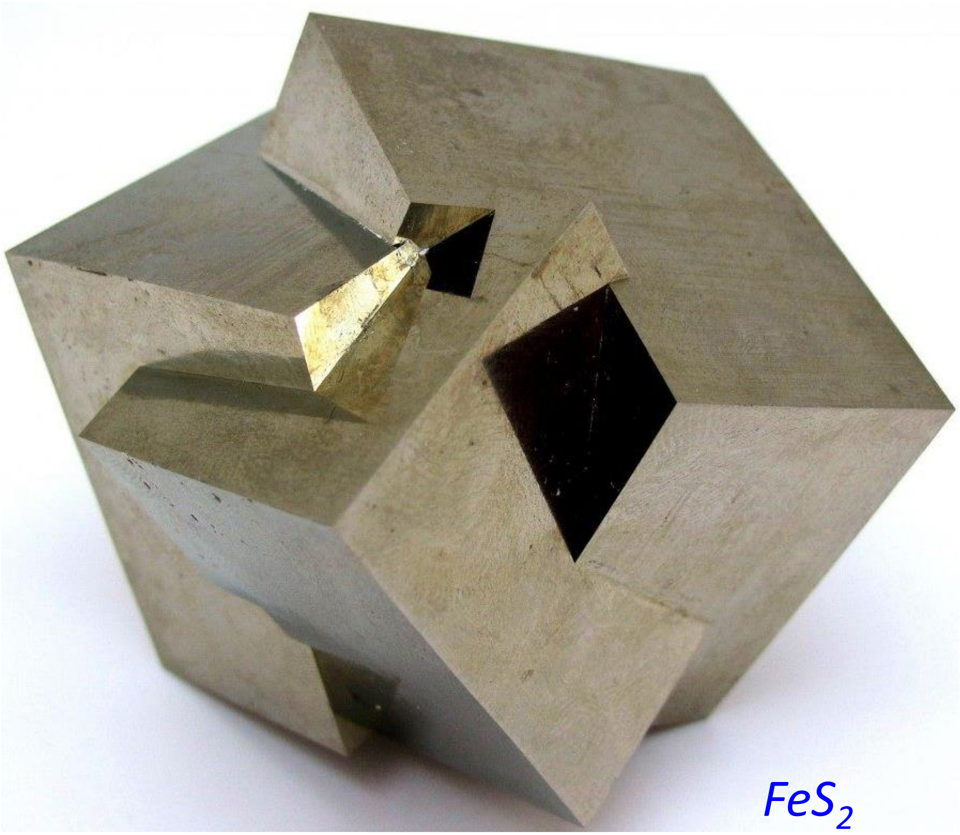
(012) $(01\bar{2})$ $(0\bar{1}2)$ $(0\bar{1}\bar{2})$


c*
b*
a*

Crystal morphologies

http://www.geologypage.com/p/minerals.html



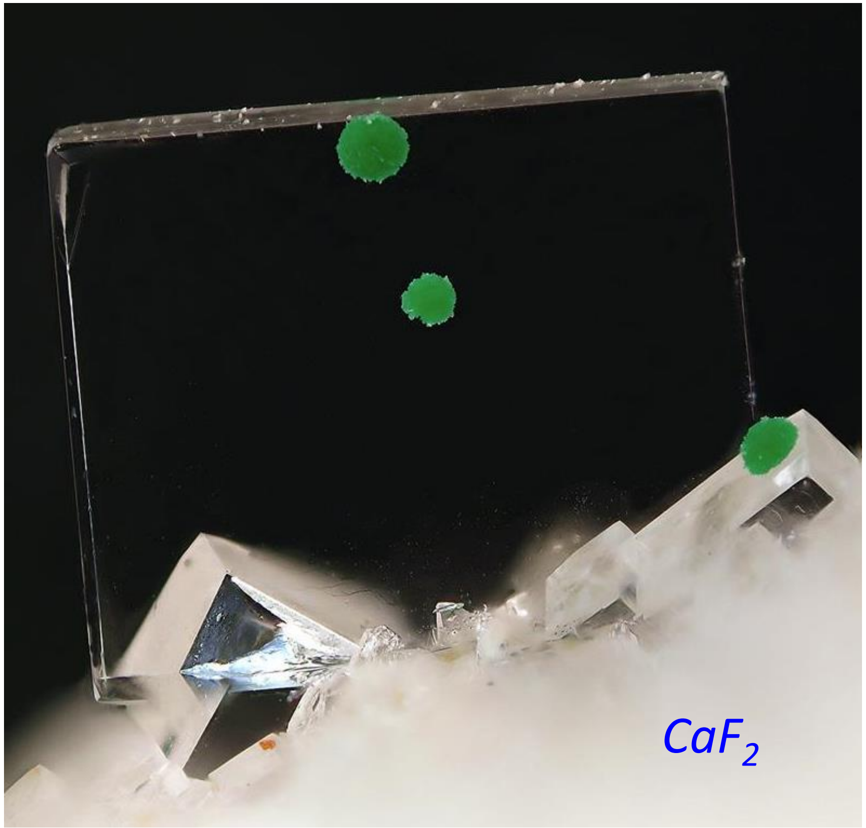


Crystal morphologies

http://www.geologypage.com/p/minerals.html

Crystal morphologies

http://www.geologypage.com/p/minerals.html



Crystal morphologies

http://www.geologypage.com/p/minerals.html

Crystal morphologies

http://www.geologypage.com/p/minerals.html