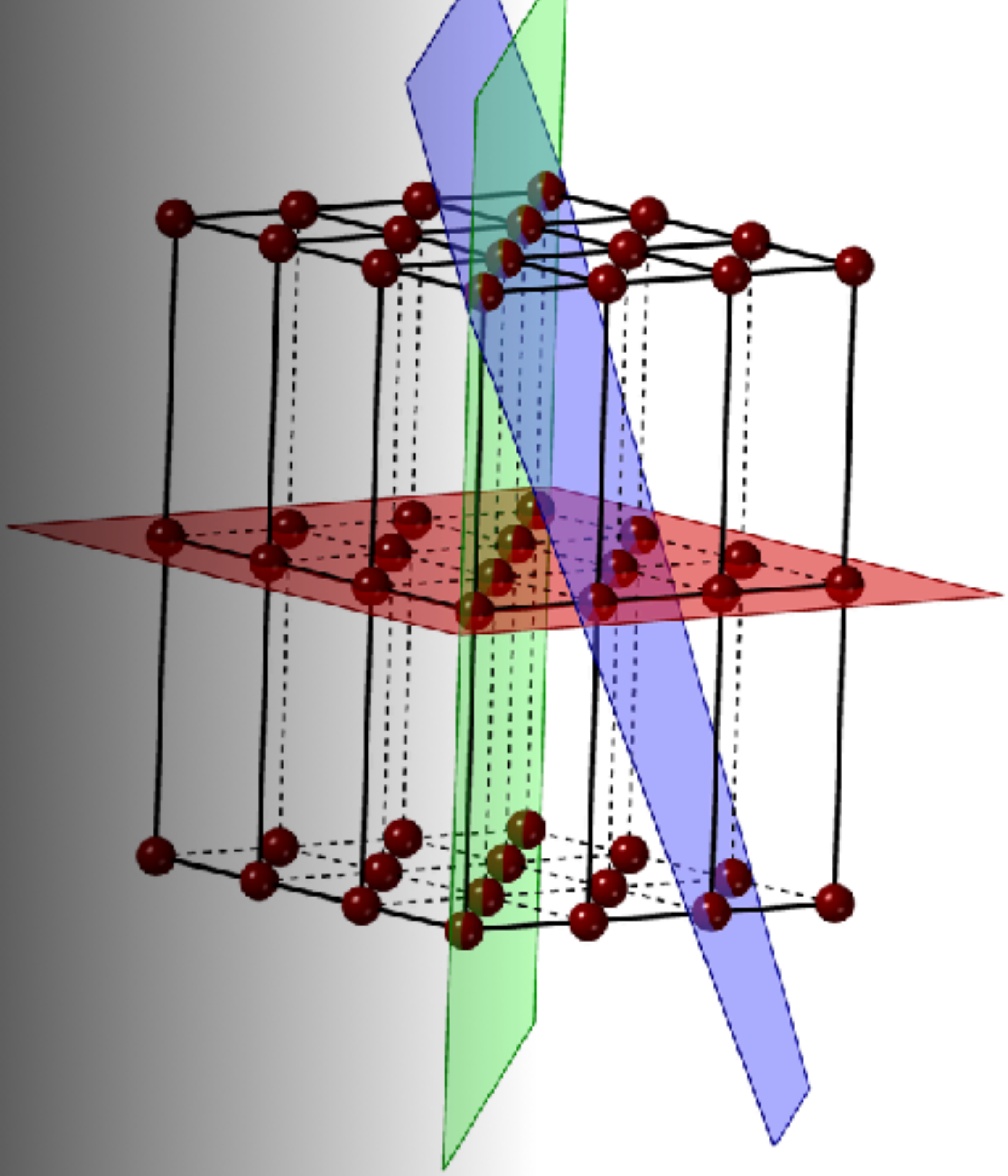
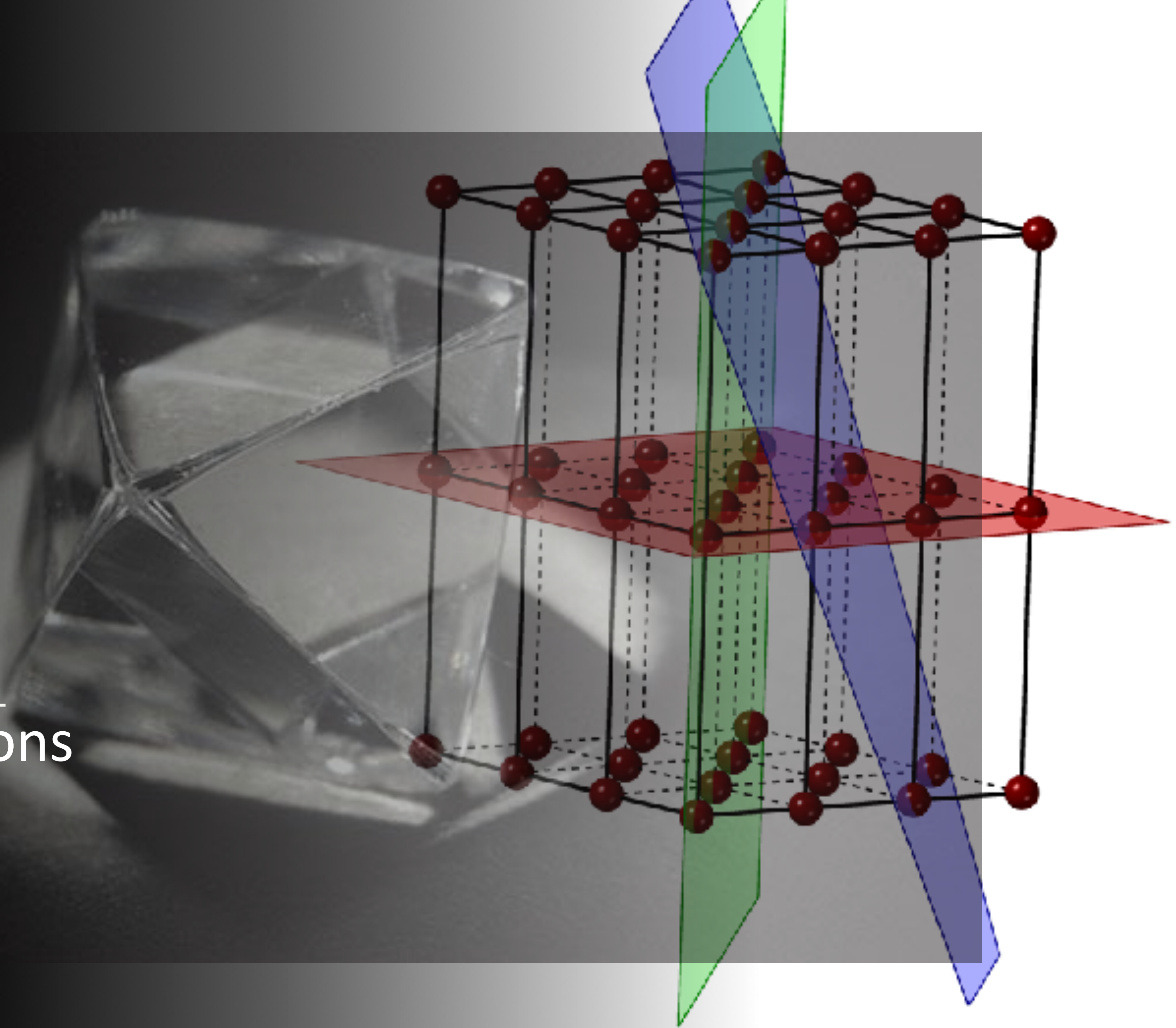
Lattice planes

Geometry and Computations



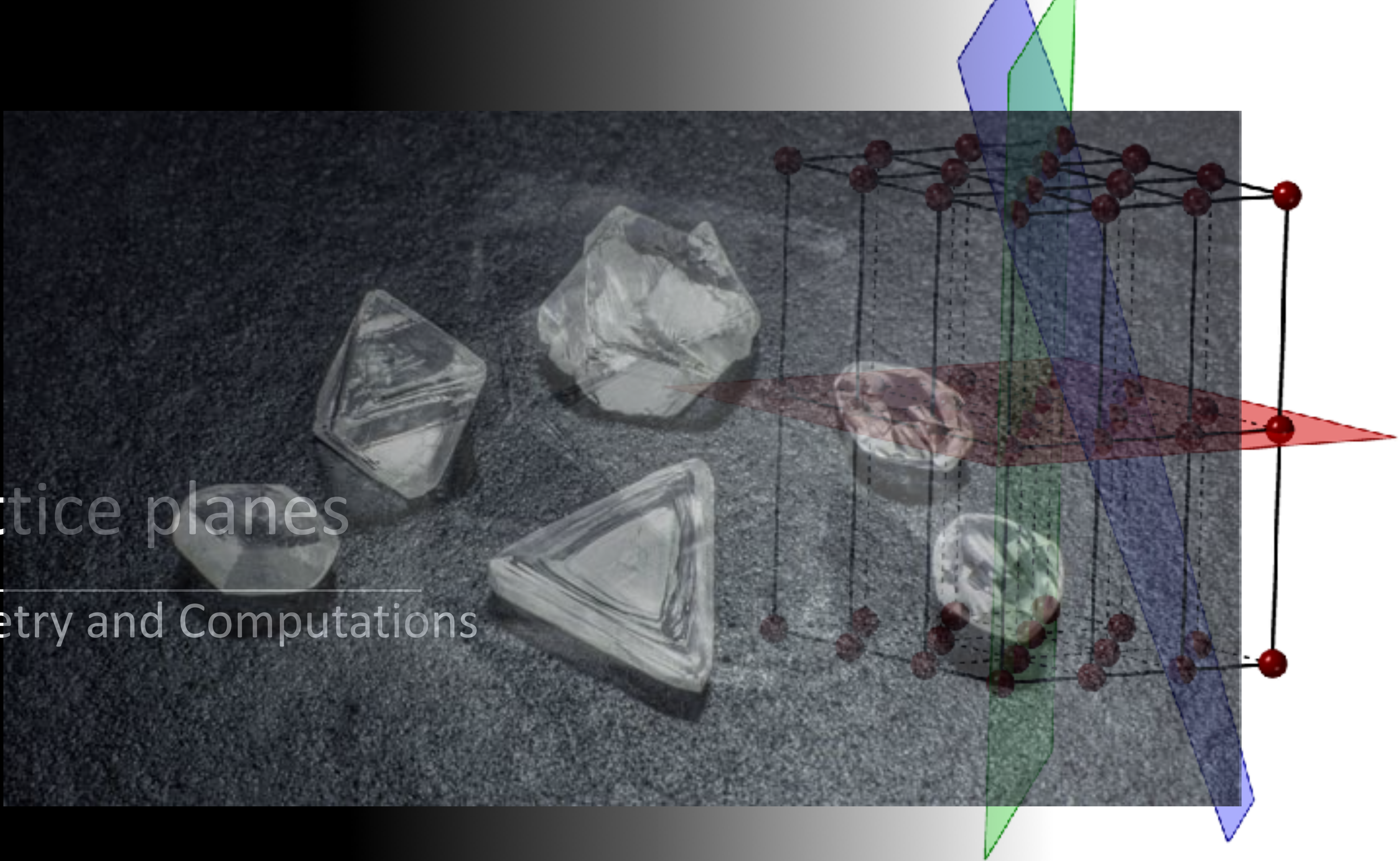
Lattice planes

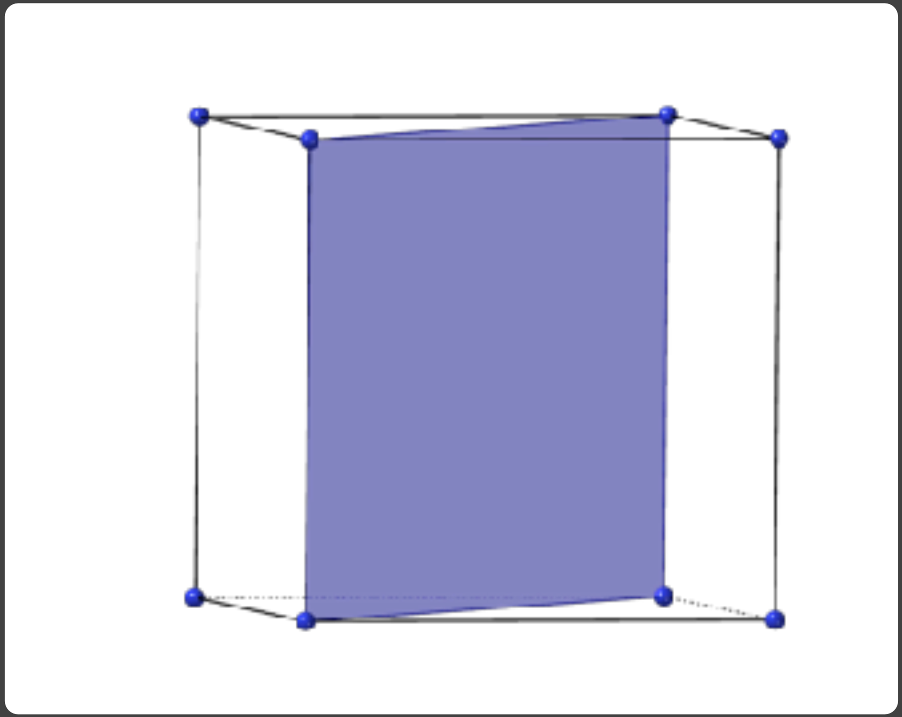
Geometry and Computations

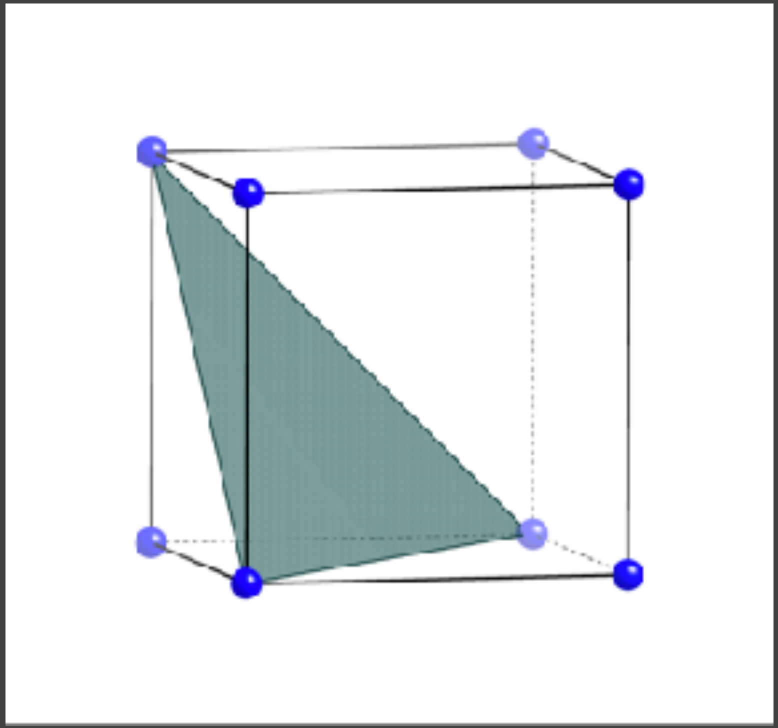


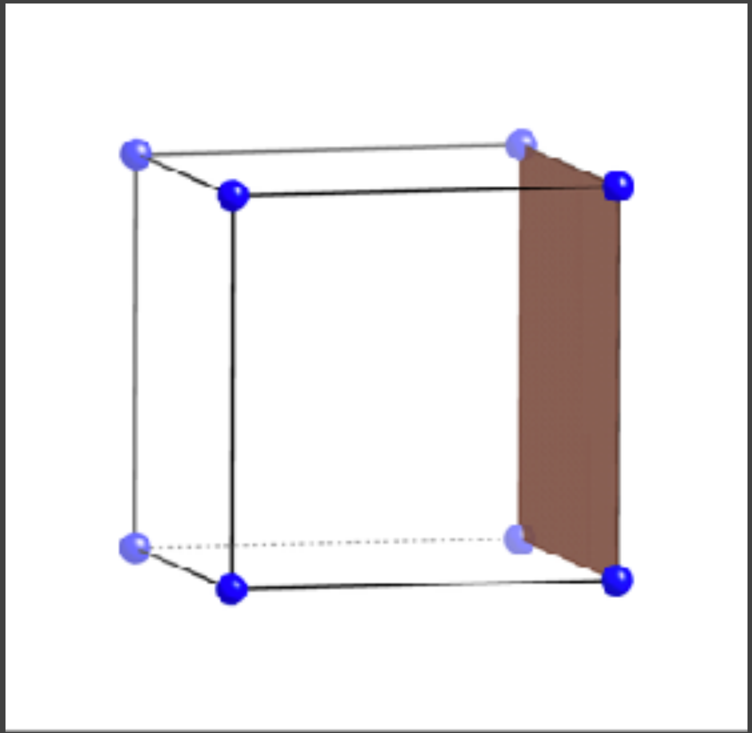
Lattice planes

Geometry and Computations









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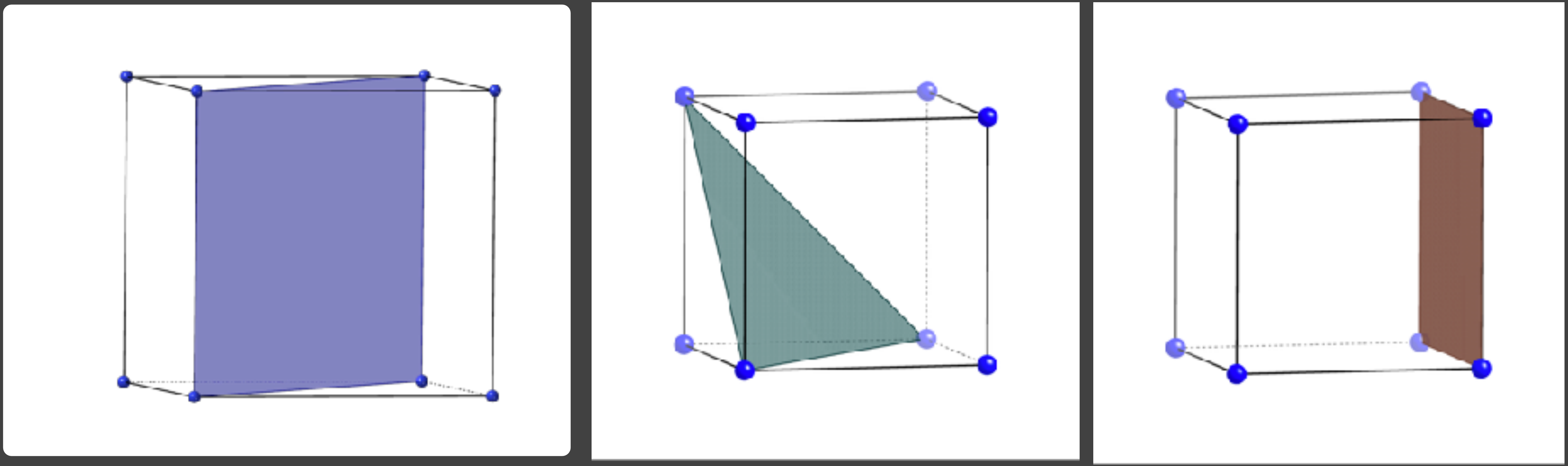

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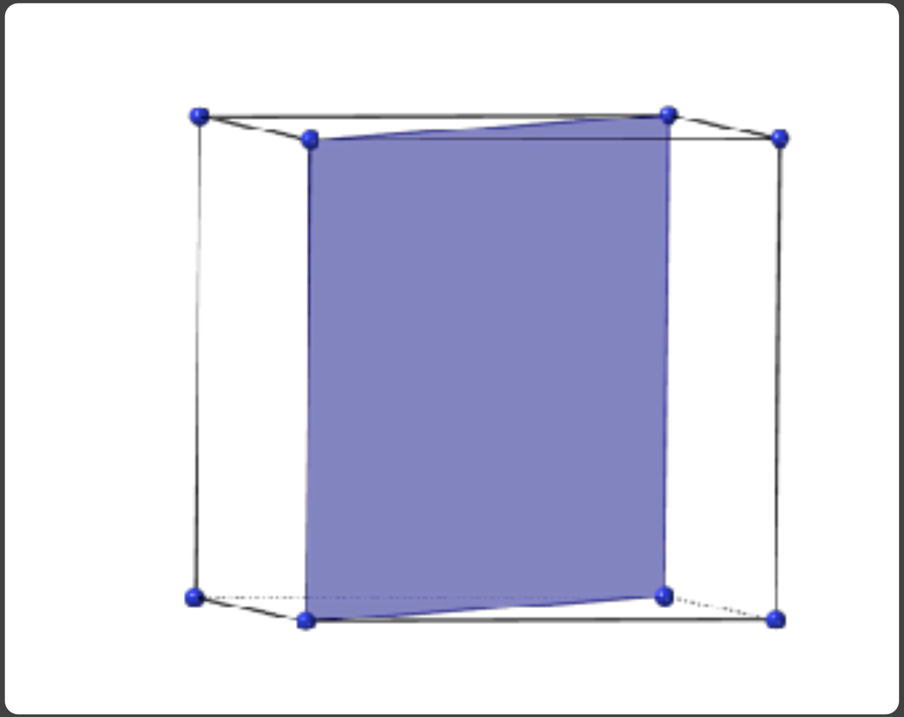
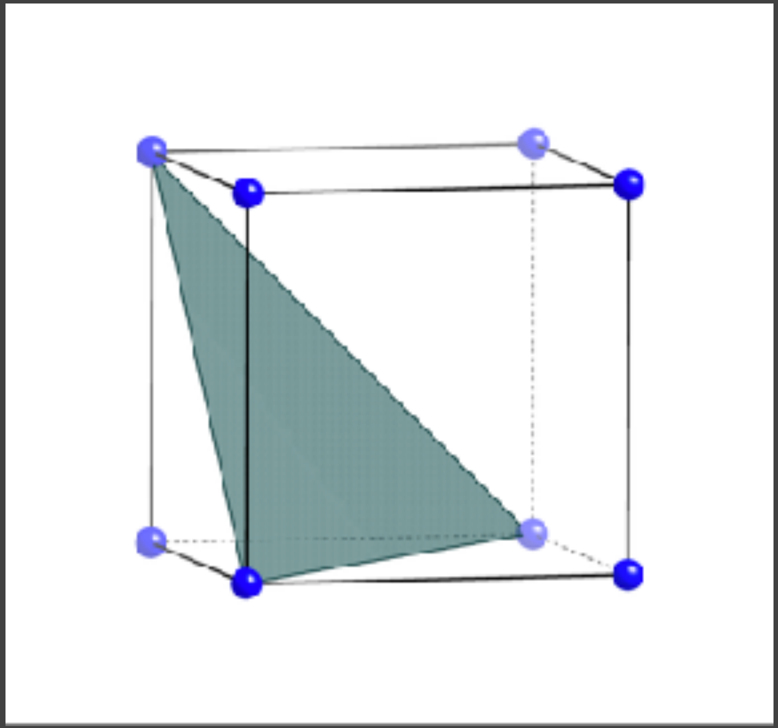
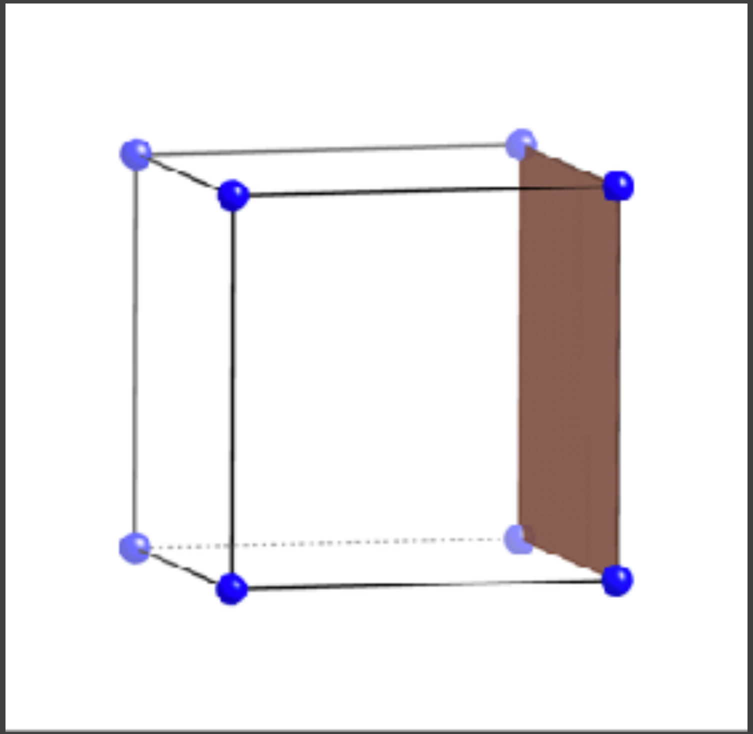
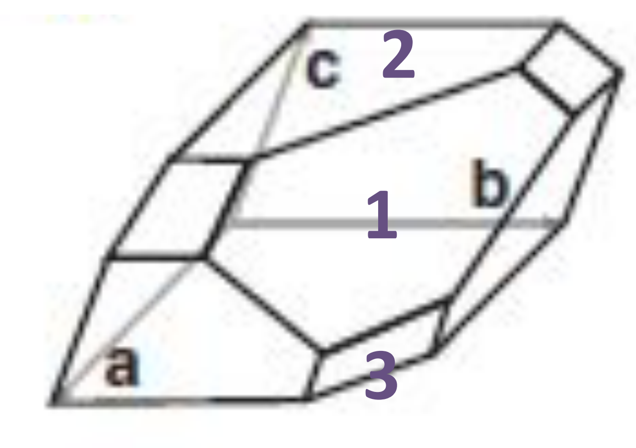




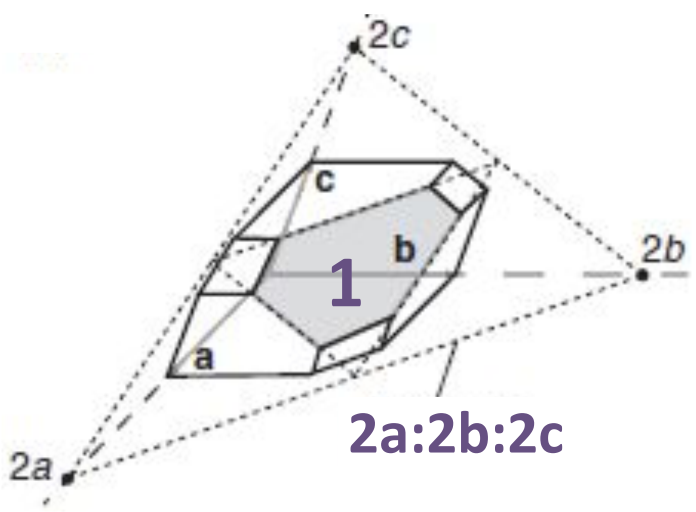


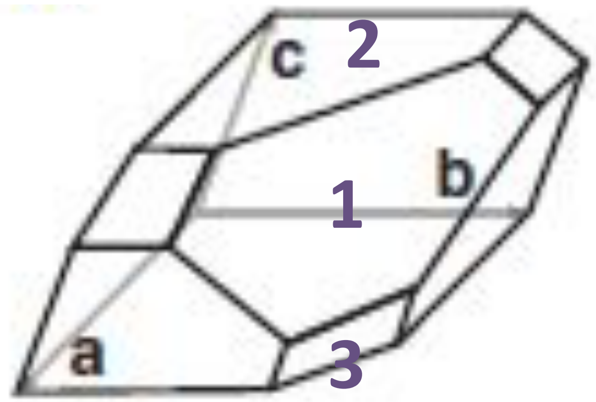
Lattice planes



Lattice plane nomenclature:

Miller Indices





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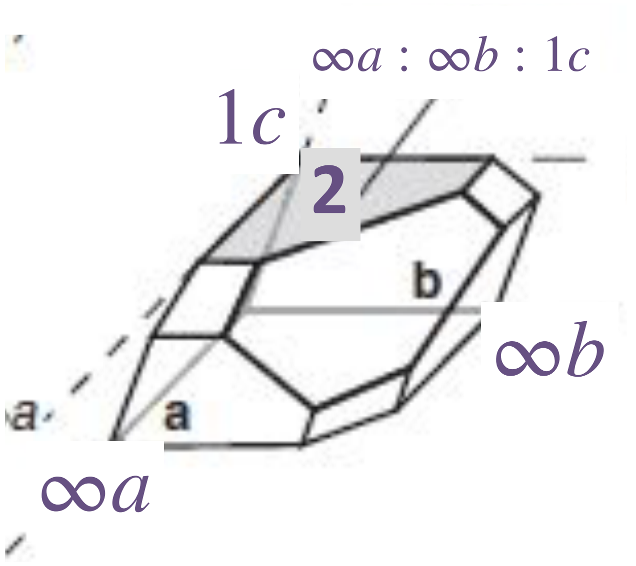

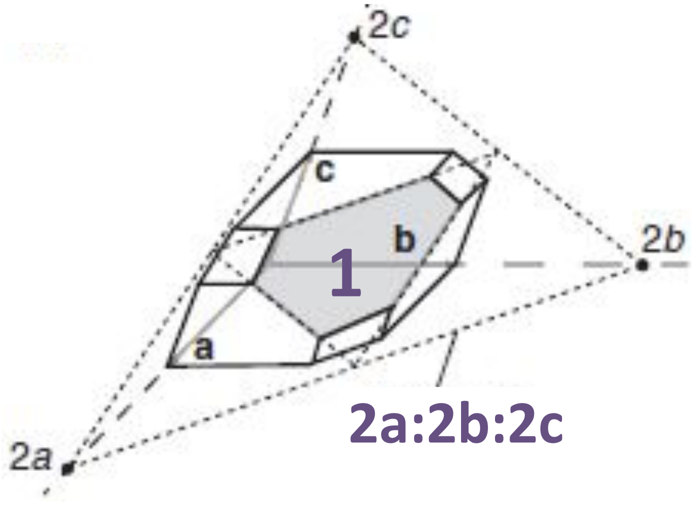

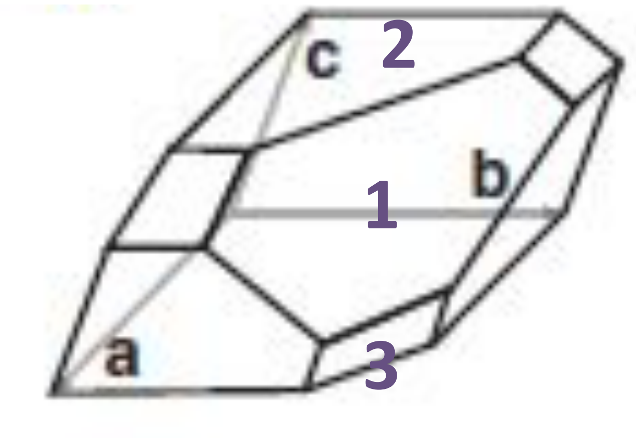

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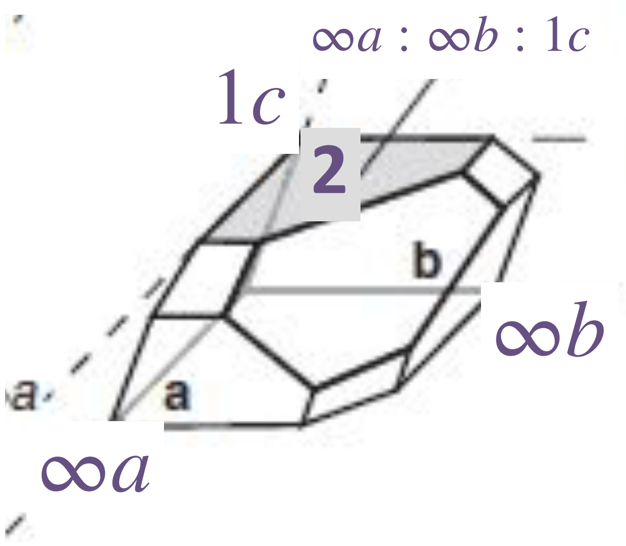
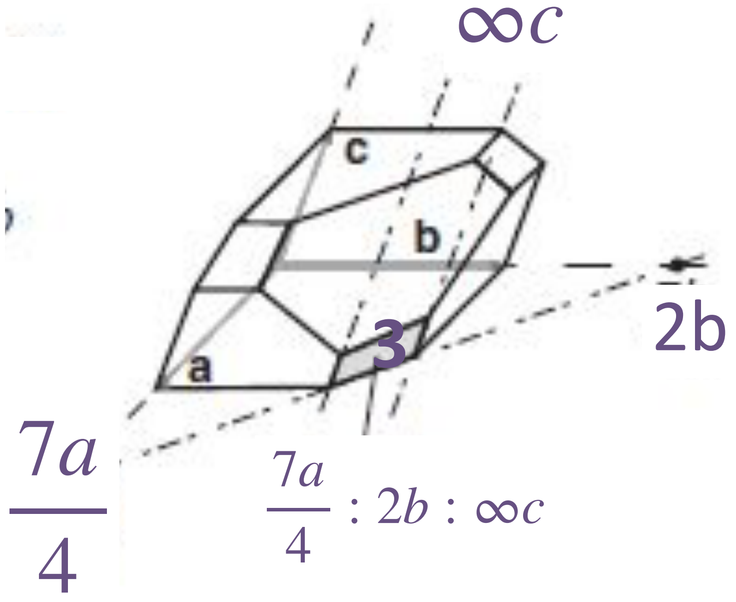
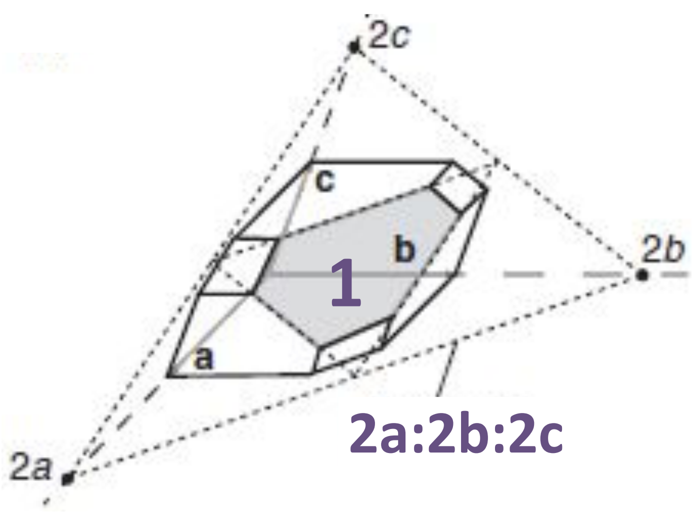
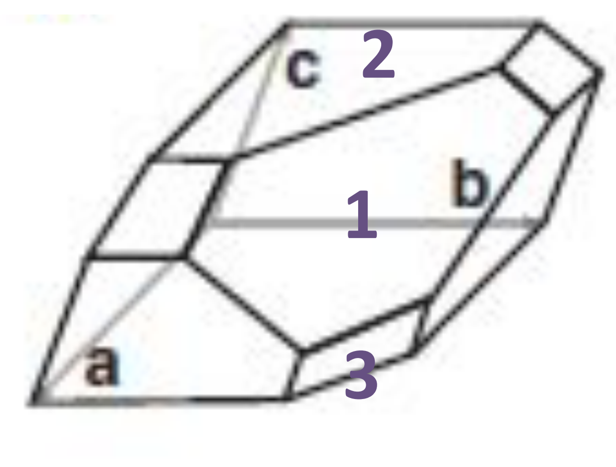






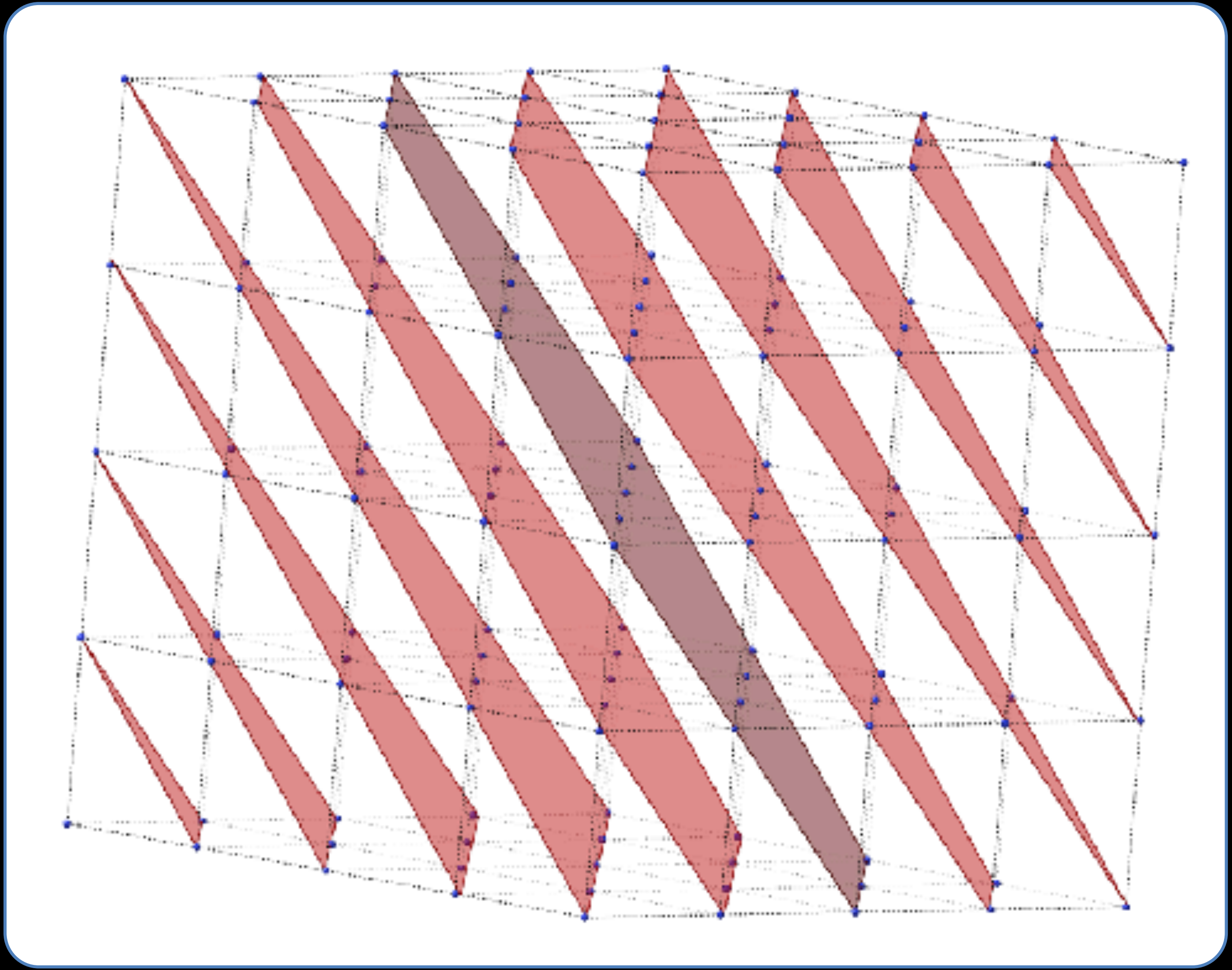


Lattice plane nomenclature:

Miller Indices

Set of planes

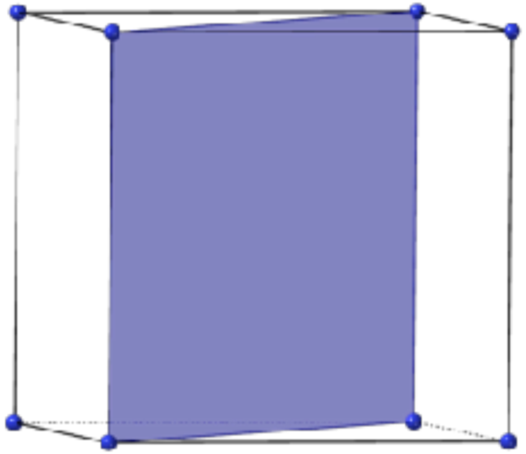
Set of planes



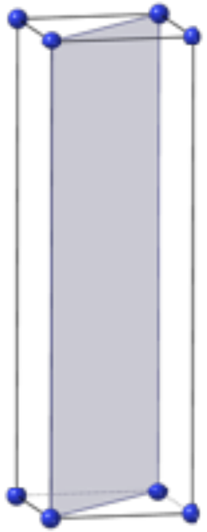
Symmetry related

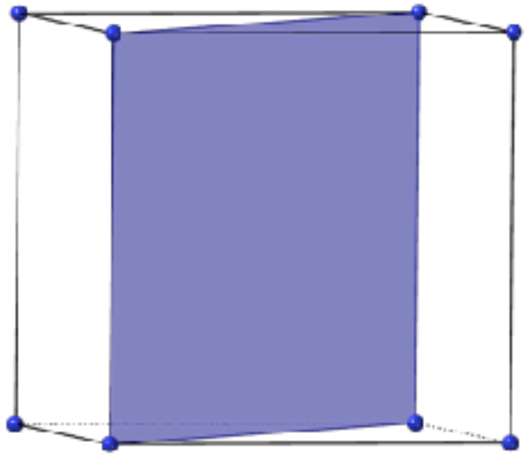
or

Family of planes



Symmetry related or Family of planes

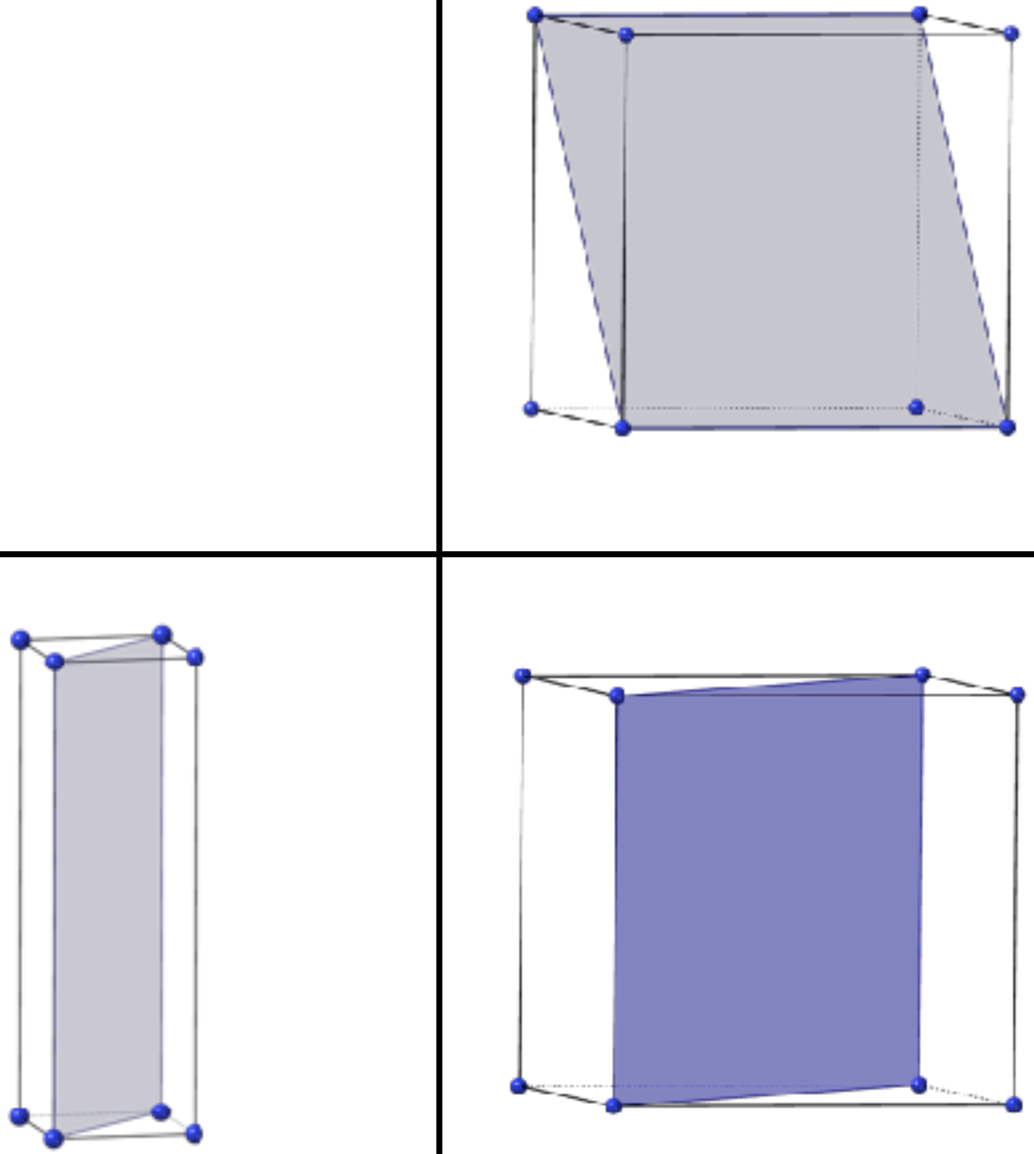




Symmetry related

or

Family of planes

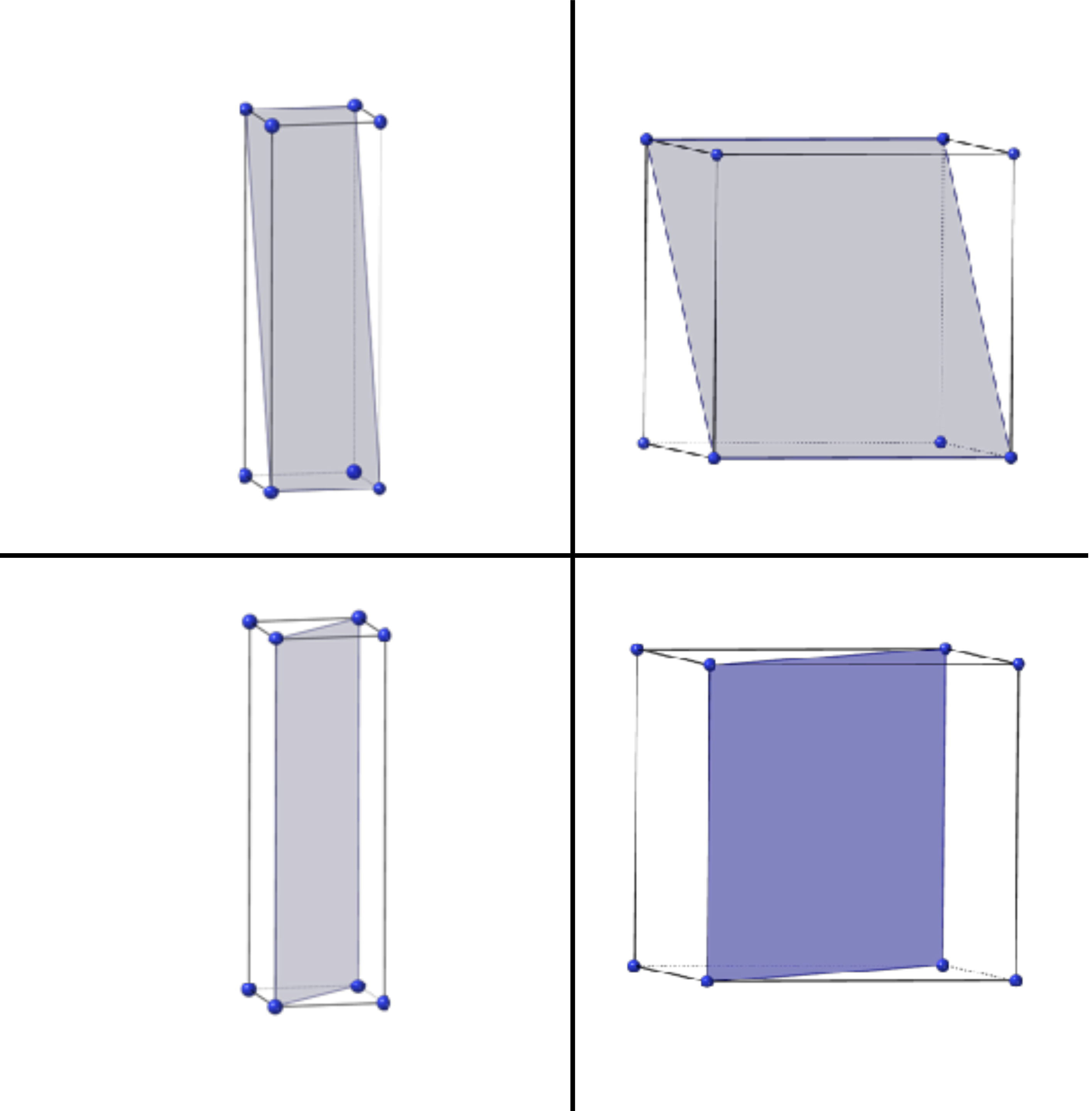


Symmetry related

or

Family of

planes

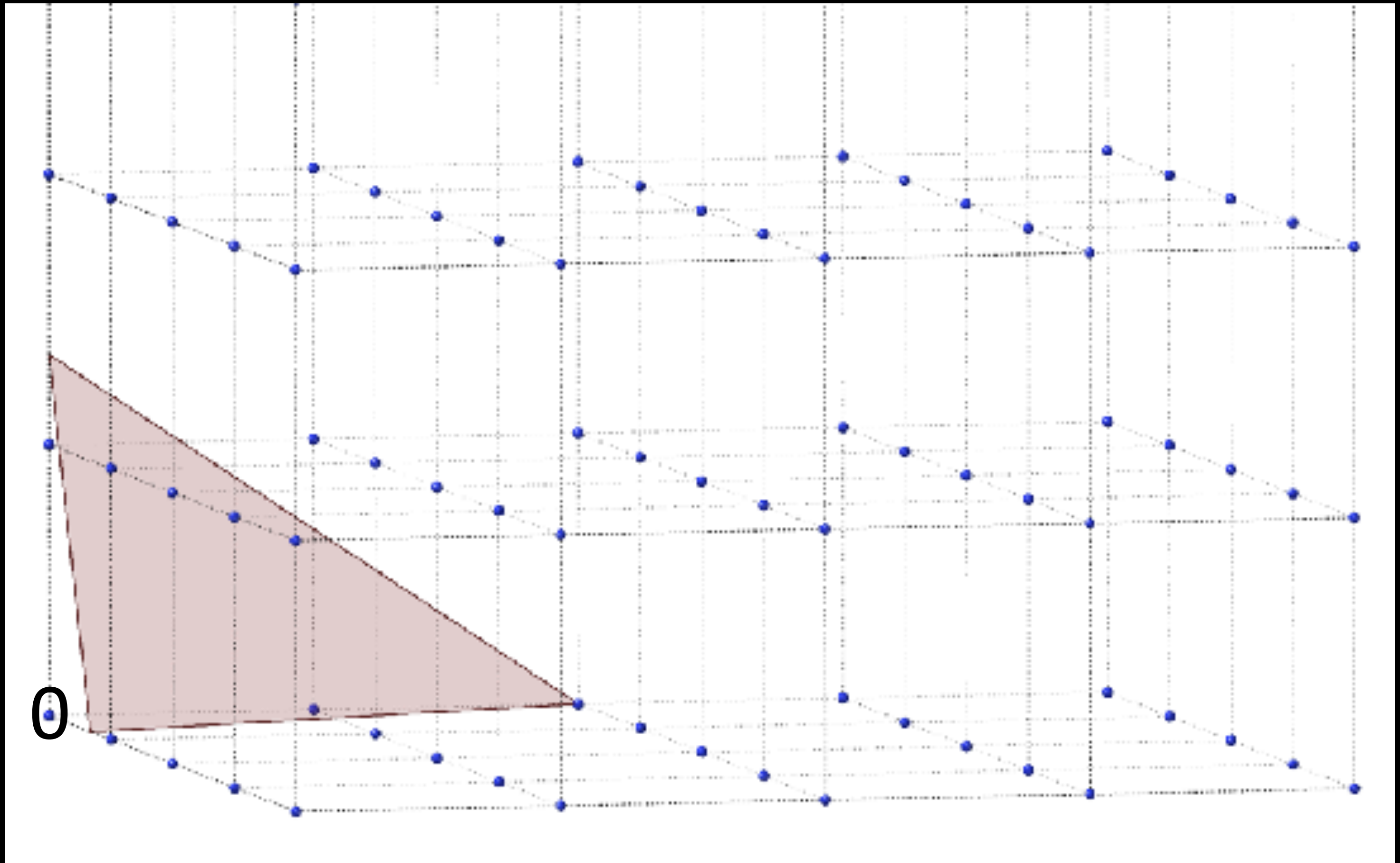


Symmetry related

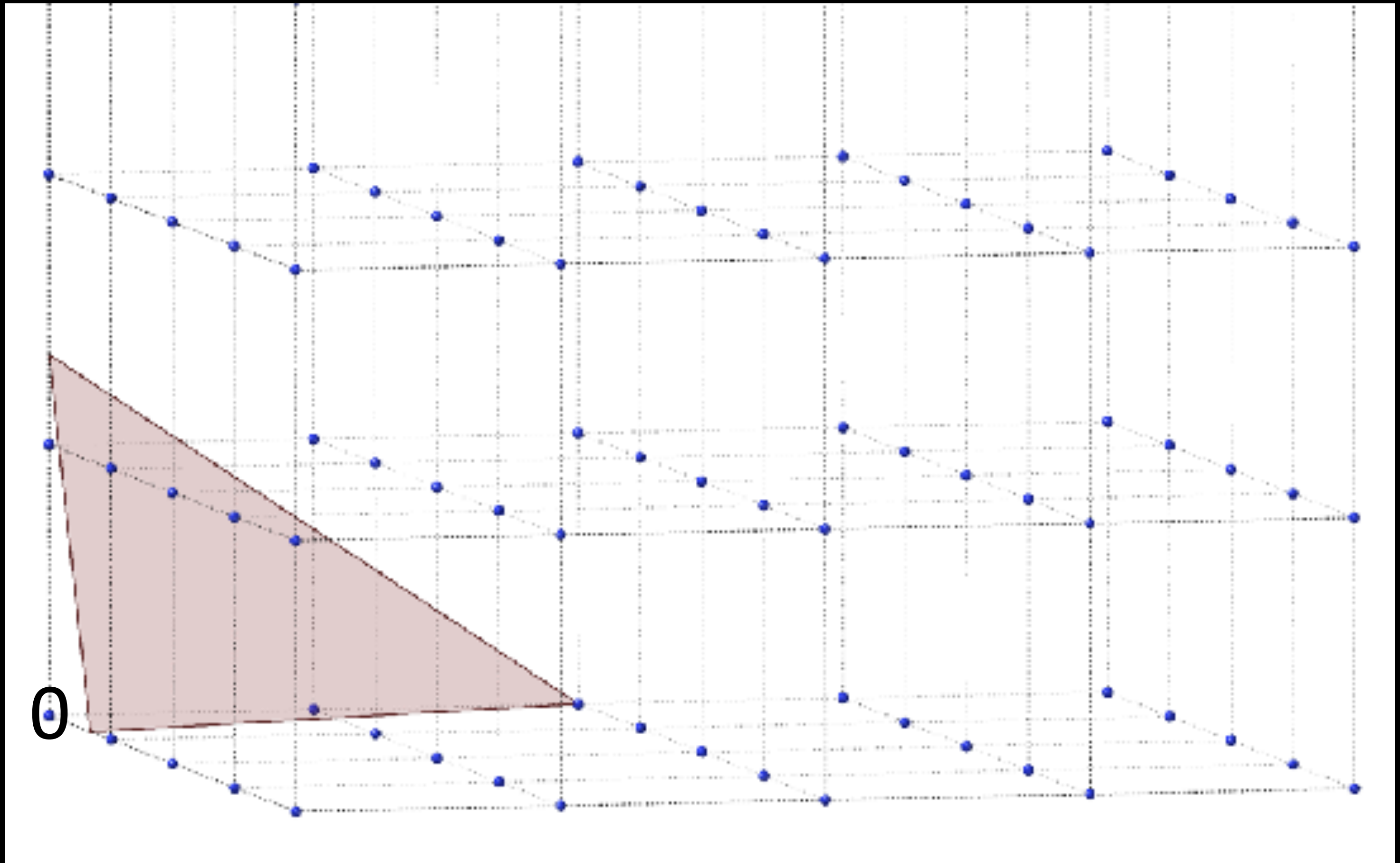
or

Family of planes

The intercept equation of a plane



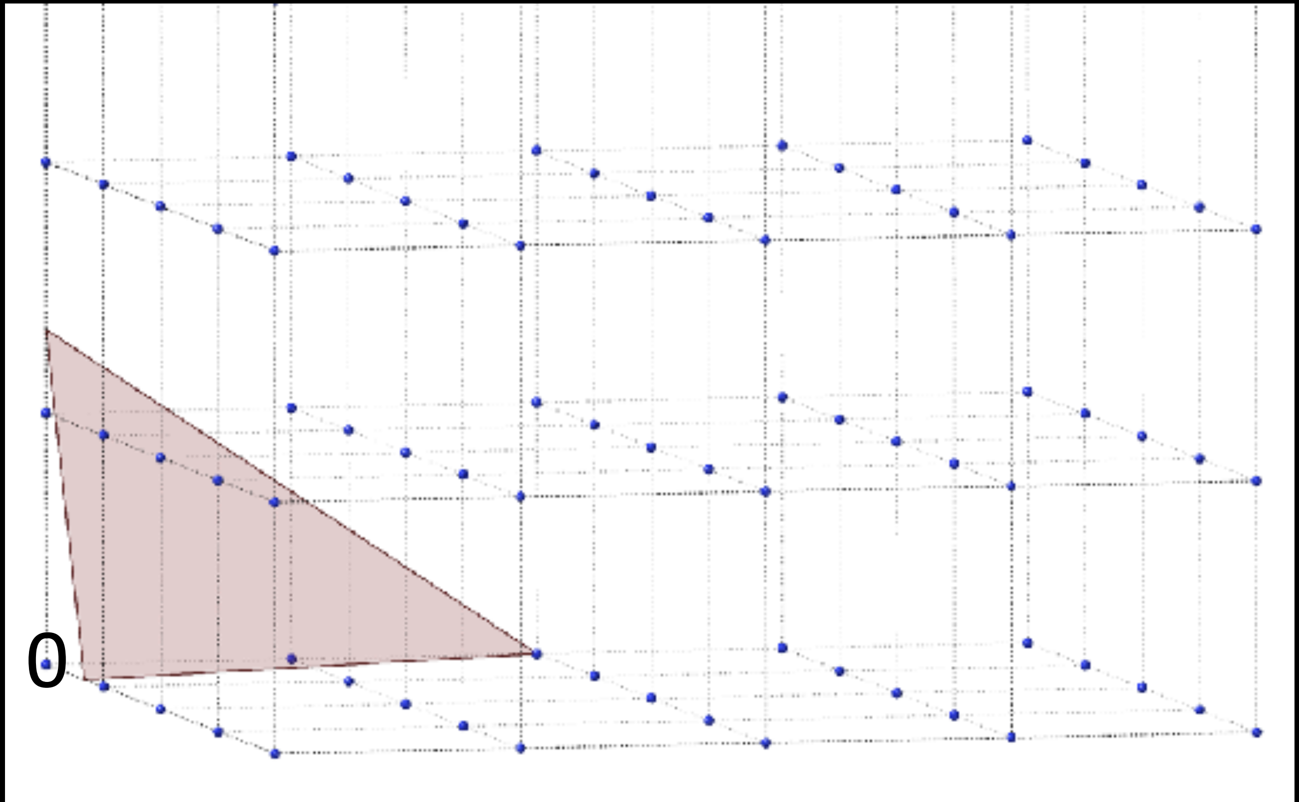
The intercept equation of a plane



If a plane intersects the basis vectors at intercepts s_i then equation of plane is:

$$\frac{x}{s_1} + \frac{y}{s_2} + \frac{z}{s_3} = 1$$

Plane and its' normal



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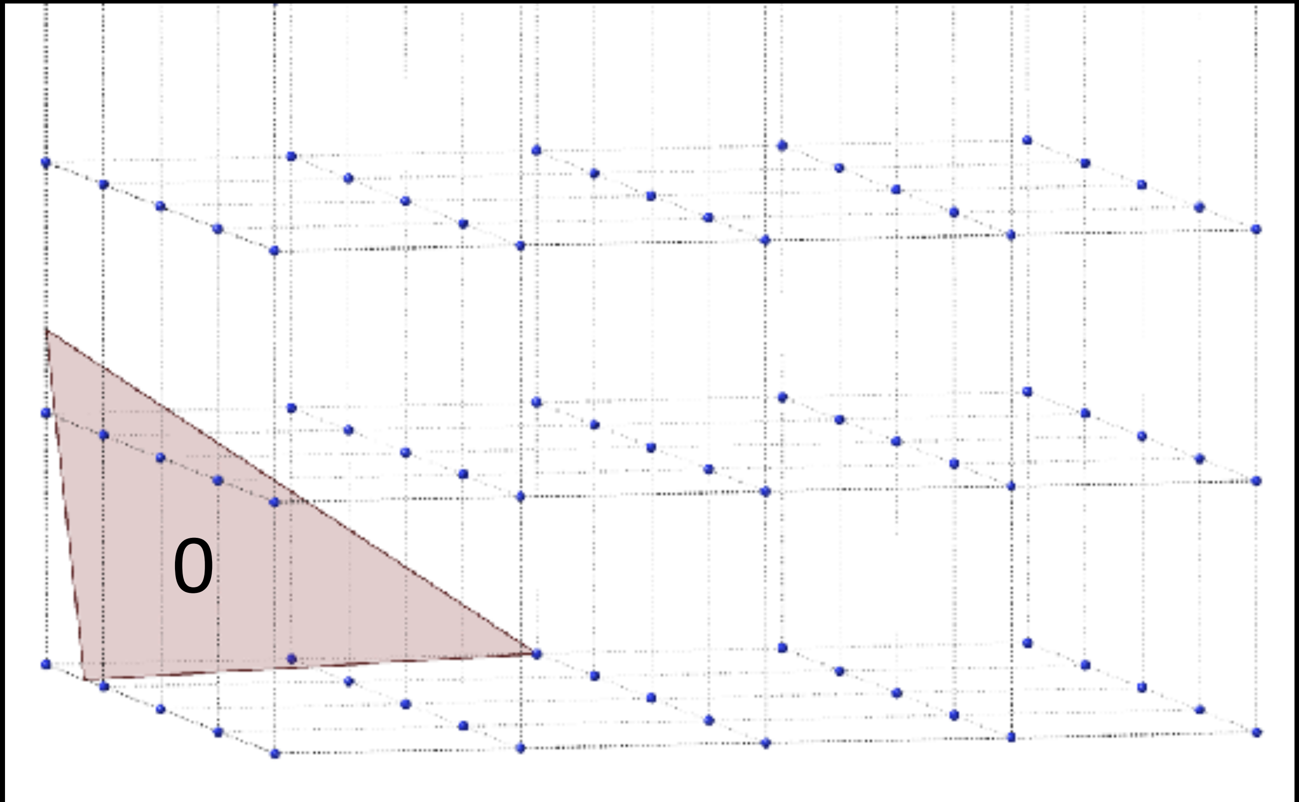
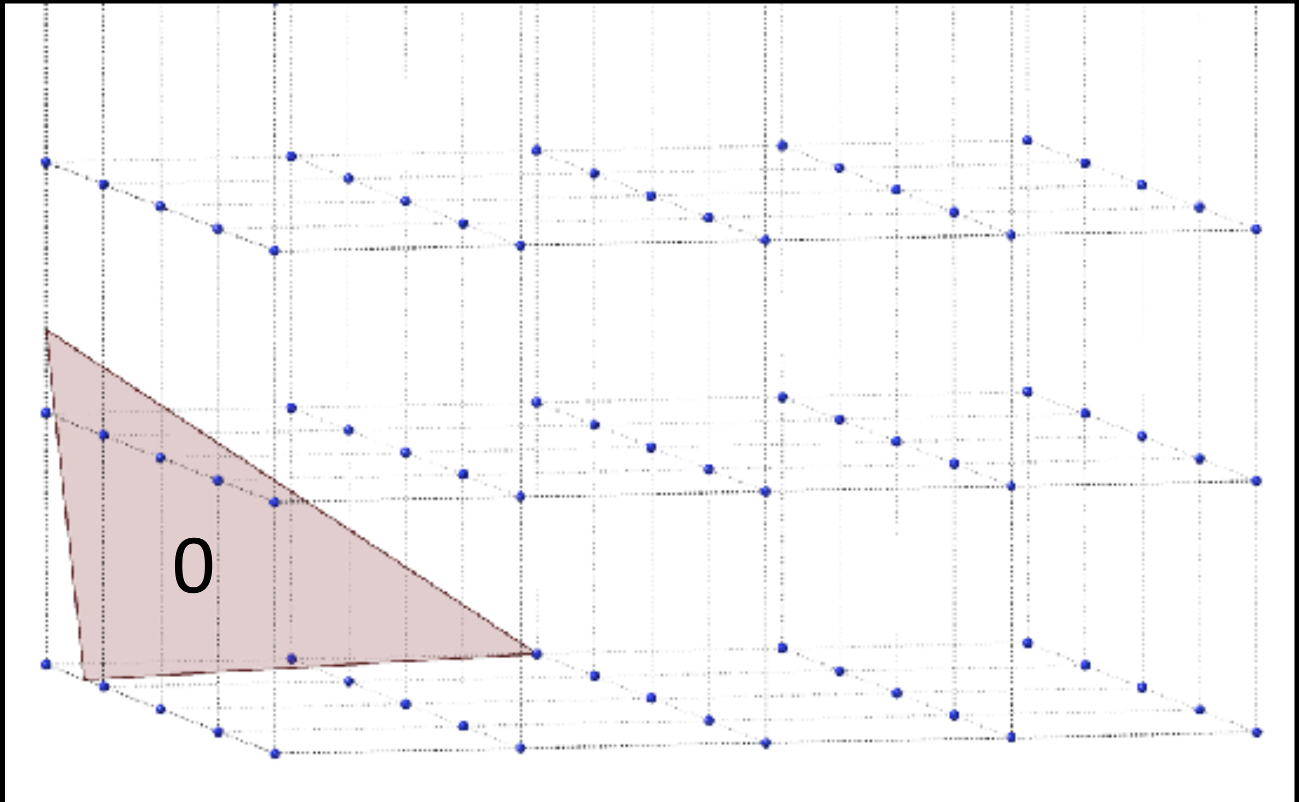


Plane and its’ normal

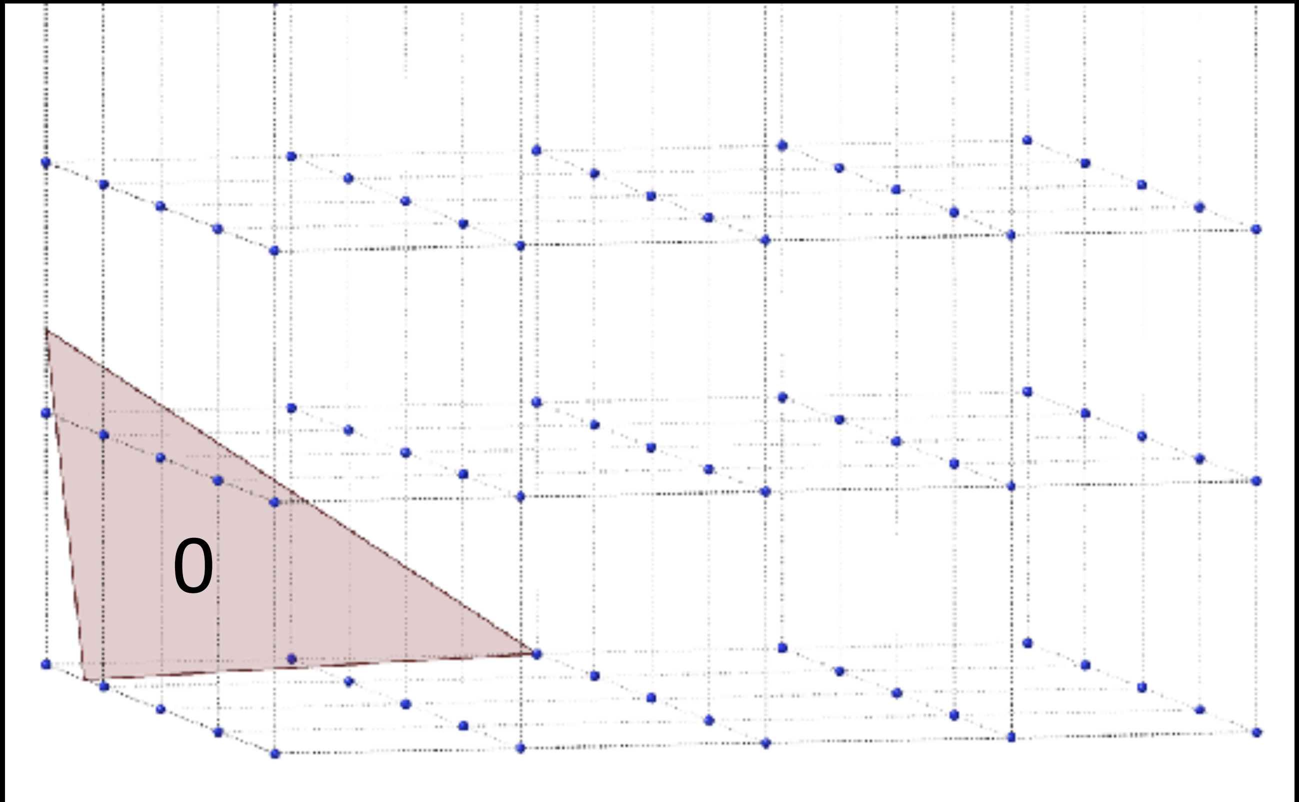


Translation of plane along its’ perpendicular:

- changes the value of the R.H.S.
- does not change its’ normal

For plane through origin:

Plane and its' normal



Translation of plane along its' perpendicular:

- changes the value of the R.H.S.
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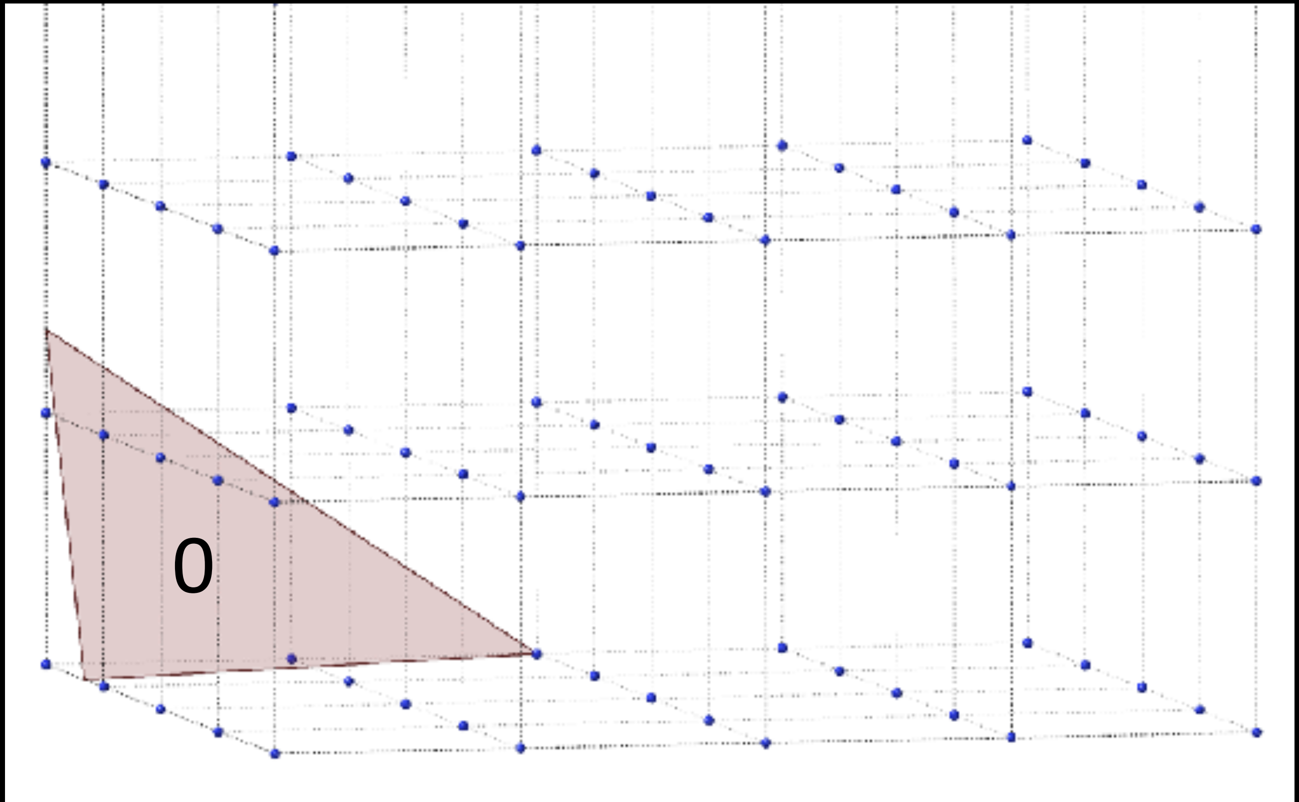
For plane through origin:

$$\frac{x}{s_1} + \frac{y}{s_2} + \frac{z}{s_3} = 0$$

Plane and its' normal



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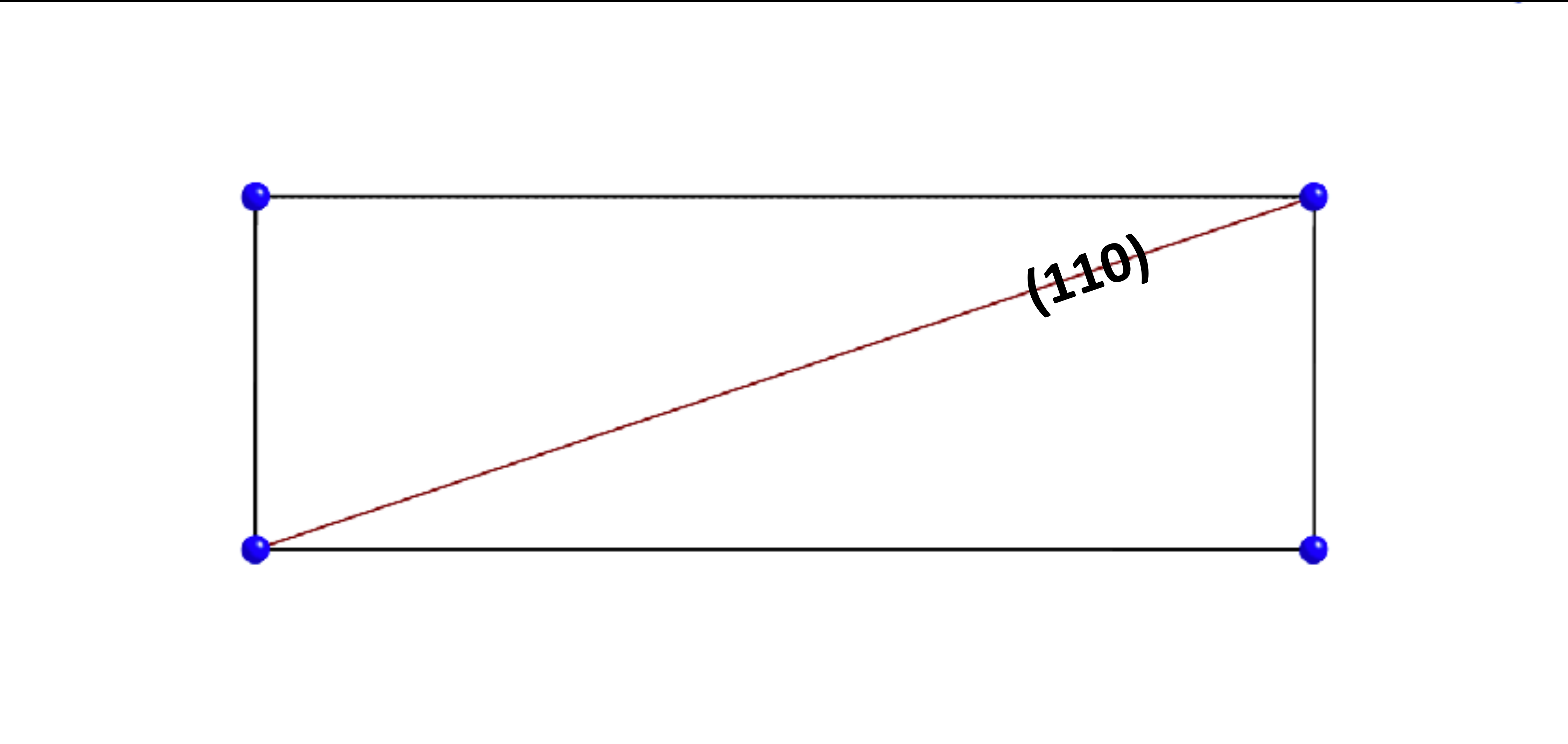
- changes the value of the R.H.S.
- does not change its' normal

For plane through origin:

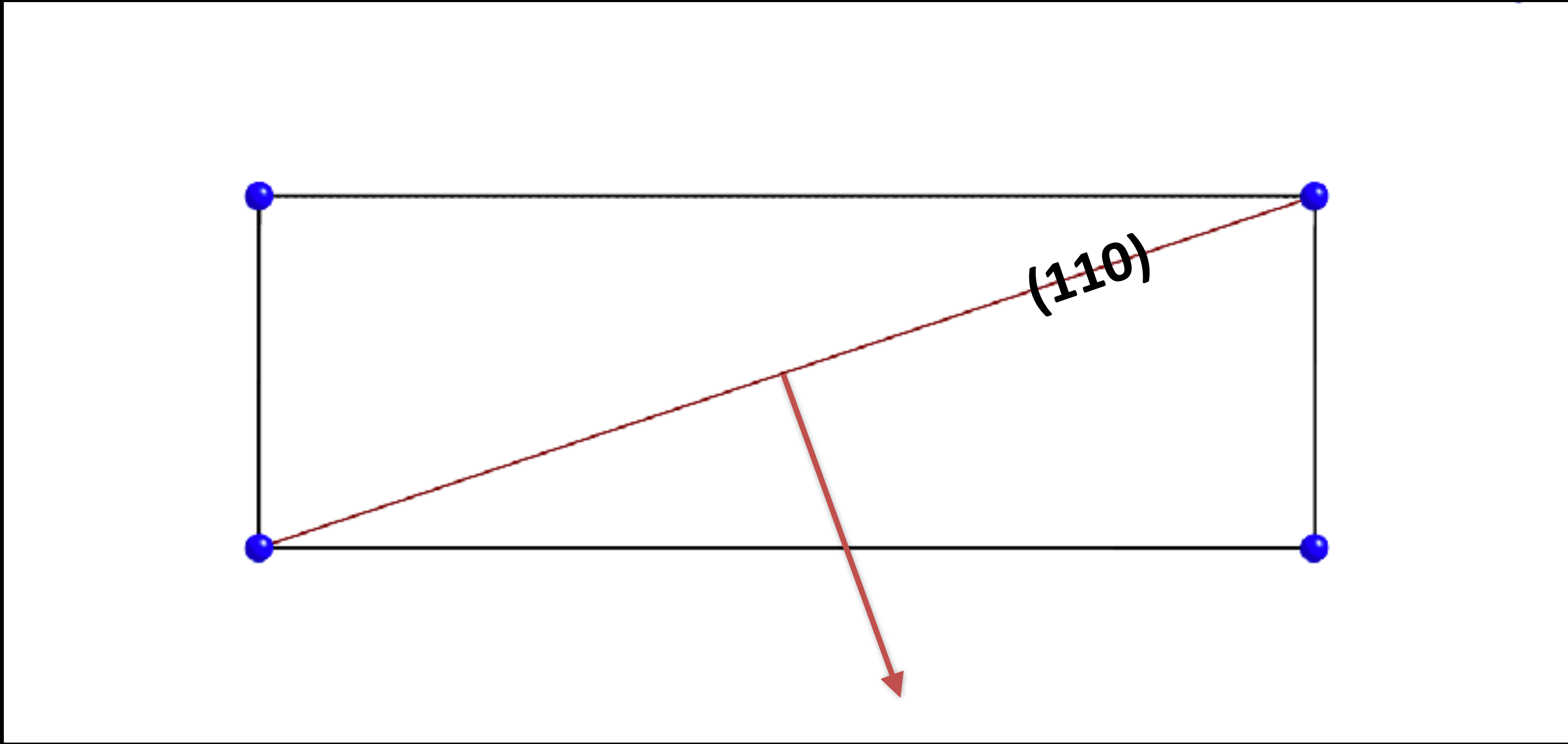
$$\frac{x}{s_1} + \frac{y}{s_2} + \frac{z}{s_3} = 0$$

$$hx + ky + lz = 0$$

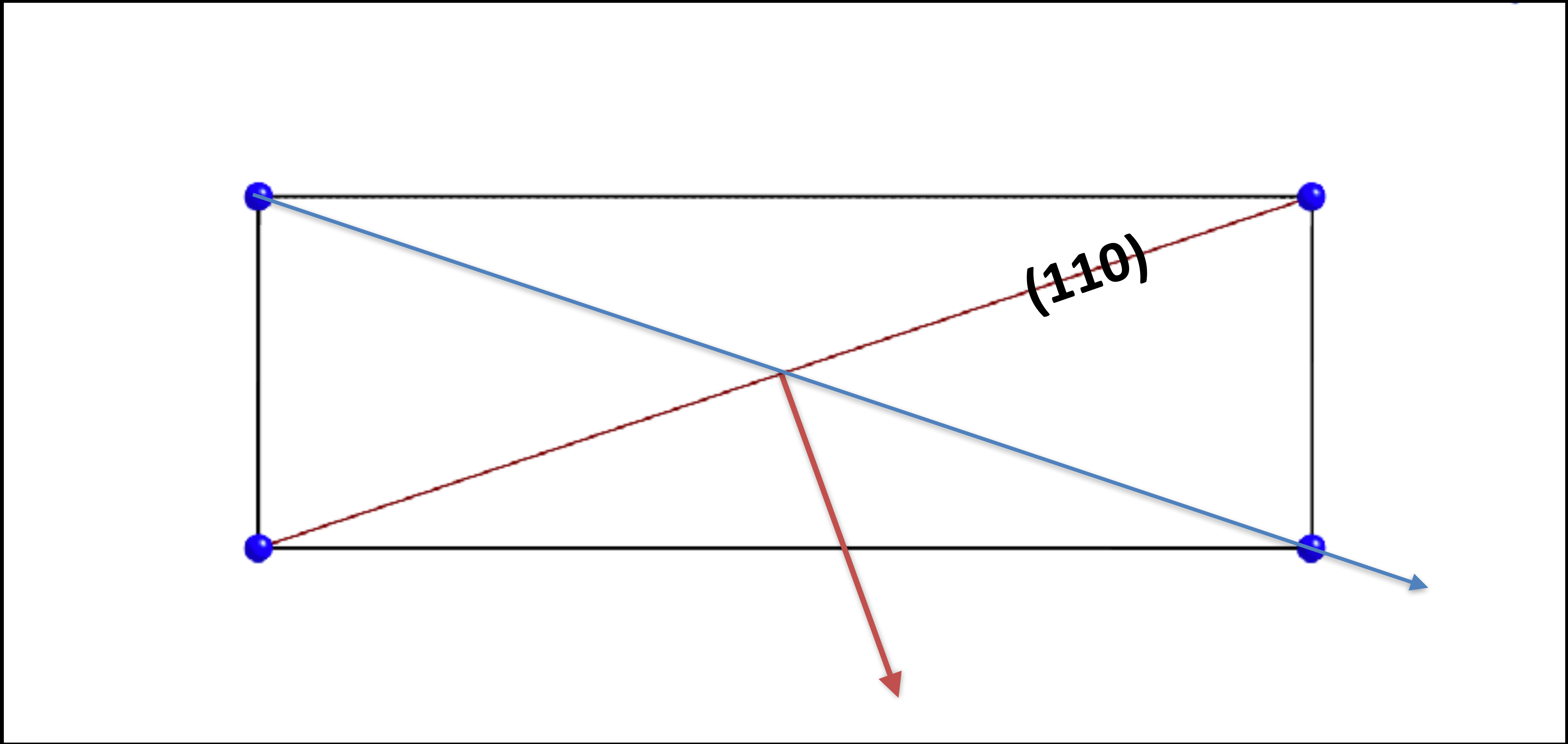
Normal vector to a plane



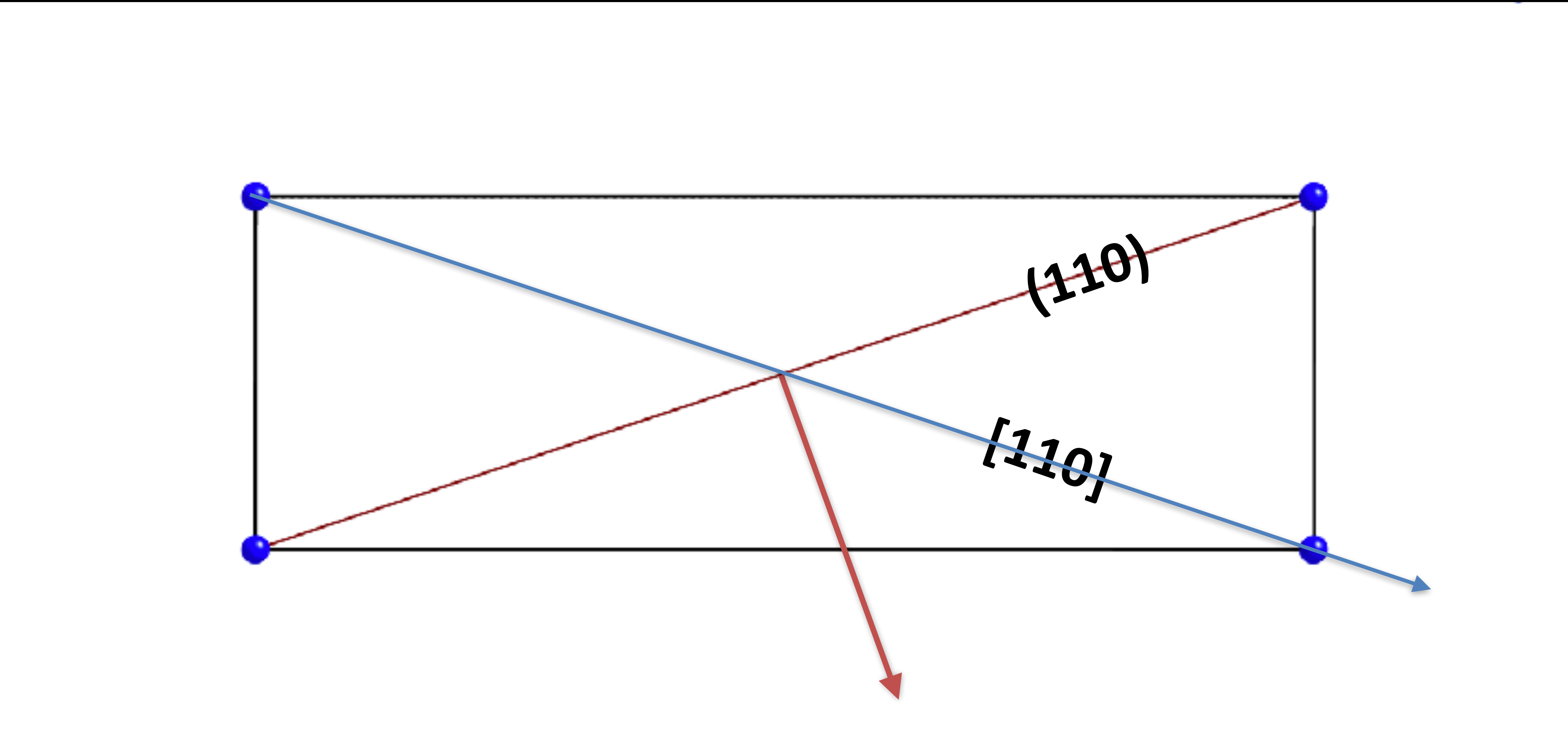
Normal vector to a plane



Normal vector to a plane



Normal vector to a plane



Reciprocal Space

Defining a new set of vectors

$$\mathbf{a_i} \bullet \mathbf{a_j^*} = 2\pi\delta_{ij}$$

reciprocal space vectors

Kronecker delta

Defining a new set of vectors

$$\mathbf{a_i} \bullet \mathbf{a_j^*} = \cancel{2\pi}\,\delta_{ij}$$

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reciprocal space vectors

Kronecker delta

New set of basis vectors

Defining a new set of vectors

$$\mathbf{a_i} \bullet \mathbf{a_j^*} = \cancel{2\pi}\delta_{ij}$$

reciprocal space vectors

Kronecker delta

$$\begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{bmatrix} \bullet \begin{bmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* \end{bmatrix}$$

New set of basis vectors

Form of the new basis vectors

$$\begin{pmatrix} \mathbf{a_1} \cdot \mathbf{a_1^*} & \mathbf{a_1} \cdot \mathbf{a_2^*} & \mathbf{a_1} \cdot \mathbf{a_3^*} \\ \mathbf{a_2} \cdot \mathbf{a_1^*} & \mathbf{a_2} \cdot \mathbf{a_2^*} & \mathbf{a_2} \cdot \mathbf{a_3^*} \\ \mathbf{a_3} \cdot \mathbf{a_1^*} & \mathbf{a_3} \cdot \mathbf{a_2^*} & \mathbf{a_3} \cdot \mathbf{a_3^*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Form of the new basis vectors

$$\begin{pmatrix} \mathbf{a_1} \cdot \mathbf{a_1^*} & \mathbf{a_1} \cdot \mathbf{a_2^*} & \mathbf{a_1} \cdot \mathbf{a_3^*} \\ \mathbf{a_2} \cdot \mathbf{a_1^*} & \mathbf{a_2} \cdot \mathbf{a_2^*} & \mathbf{a_2} \cdot \mathbf{a_3^*} \\ \mathbf{a_3} \cdot \mathbf{a_1^*} & \mathbf{a_3} \cdot \mathbf{a_2^*} & \mathbf{a_3} \cdot \mathbf{a_3^*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Form of the new basis vectors

Off-diagonal terms

$$\begin{pmatrix} \mathbf{a_1} \cdot \mathbf{a_1^*} & \mathbf{a_1} \cdot \mathbf{a_2^*} & \mathbf{a_1} \cdot \mathbf{a_3^*} \\ \mathbf{a_2} \cdot \mathbf{a_1^*} & \mathbf{a_2} \cdot \mathbf{a_2^*} & \mathbf{a_2} \cdot \mathbf{a_3^*} \\ \mathbf{a_3} \cdot \mathbf{a_1^*} & \mathbf{a_3} \cdot \mathbf{a_2^*} & \mathbf{a_3} \cdot \mathbf{a_3^*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\Rightarrow \mathbf{a_1^*} \perp \mathbf{a_2}$ and $\mathbf{a_3}$

$\Rightarrow \mathbf{a_1^*} = K\left(\mathbf{a_2} \times \mathbf{a_3}\right)$

Form of the new basis vectors

Off-diagonal terms

$$\begin{pmatrix} \mathbf{a}_1 \cdot \mathbf{a}_1^* & \mathbf{a}_1 \cdot \mathbf{a}_2^* & \mathbf{a}_1 \cdot \mathbf{a}_3^* \\ \mathbf{a}_2 \cdot \mathbf{a}_1^* & \mathbf{a}_2 \cdot \mathbf{a}_2^* & \mathbf{a}_2 \cdot \mathbf{a}_3^* \\ \mathbf{a}_3 \cdot \mathbf{a}_1^* & \mathbf{a}_3 \cdot \mathbf{a}_2^* & \mathbf{a}_3 \cdot \mathbf{a}_3^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\Rightarrow \mathbf{a}_1^* \perp \mathbf{a}_2 \text{ and } \mathbf{a}_3$$

$$\Rightarrow \mathbf{a}_1^* = K\left(\mathbf{a}_2 \times \mathbf{a}_3\right)$$

Also, $\mathbf{a}_2^* = L\left(\mathbf{a}_3 \times \mathbf{a}_1\right)$

$$\mathbf{a}_3^* = M\left(\mathbf{a}_1 \times \mathbf{a}_2\right)$$

Form of the new basis vectors

Off-diagonal terms

Form of the new basis vectors

Form of the new basis vectors

$$\begin{pmatrix} \mathbf{a_1} \cdot \mathbf{a_1^*} & \mathbf{a_1} \cdot \mathbf{a_2^*} & \mathbf{a_1} \cdot \mathbf{a_3^*} \\ \mathbf{a_2} \cdot \mathbf{a_1^*} & \mathbf{a_2} \cdot \mathbf{a_2^*} & \mathbf{a_2} \cdot \mathbf{a_3^*} \\ \mathbf{a_3} \cdot \mathbf{a_1^*} & \mathbf{a_3} \cdot \mathbf{a_2^*} & \mathbf{a_3} \cdot \mathbf{a_3^*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Form of the new basis vectors

Diagonal terms

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Form of the new basis vectors

Diagonal terms

$$\mathbf{a_1} \cdot \mathbf{a_1^*} = K\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3}) = 1$$

$$\mathbf{a_2} \cdot \mathbf{a_2^*} = L\mathbf{a_2} \cdot (\mathbf{a_3} \times \mathbf{a_1}) = 1$$

$$\mathbf{a_3} \cdot \mathbf{a_3^*} = M\mathbf{a_3} \cdot (\mathbf{a_1} \times \mathbf{a_2}) = 1$$

$$\begin{pmatrix} \mathbf{a_1} \cdot \mathbf{a_1^*} & \mathbf{a_1} \cdot \mathbf{a_2^*} & \mathbf{a_1} \cdot \mathbf{a_3^*} \\ \mathbf{a_2} \cdot \mathbf{a_1^*} & \mathbf{a_2} \cdot \mathbf{a_2^*} & \mathbf{a_2} \cdot \mathbf{a_3^*} \\ \mathbf{a_3} \cdot \mathbf{a_1^*} & \mathbf{a_3} \cdot \mathbf{a_2^*} & \mathbf{a_3} \cdot \mathbf{a_3^*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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$$\mathbf{a_2} \cdot \mathbf{a_2^*} = L\mathbf{a_2} \cdot (\mathbf{a_3} \times \mathbf{a_1}) = 1$$

$$\mathbf{a_3} \cdot \mathbf{a_3^*} = M\mathbf{a_3} \cdot (\mathbf{a_1} \times \mathbf{a_2}) = 1$$

$$\begin{pmatrix} \mathbf{a_1} \cdot \mathbf{a_1^*} & \mathbf{a_1} \cdot \mathbf{a_2^*} & \mathbf{a_1} \cdot \mathbf{a_3^*} \\ \mathbf{a_2} \cdot \mathbf{a_1^*} & \mathbf{a_2} \cdot \mathbf{a_2^*} & \mathbf{a_2} \cdot \mathbf{a_3^*} \\ \mathbf{a_3} \cdot \mathbf{a_1^*} & \mathbf{a_3} \cdot \mathbf{a_2^*} & \mathbf{a_3} \cdot \mathbf{a_3^*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\therefore \; K = L = M = \frac{1}{\mathbf{a_1} \cdot (\mathbf{a_2} \times \mathbf{a_3})} = \frac{1}{V}$$

Reciprocal basis vectors

$$\mathbf{a_1^*} = \frac{1}{V}\left(\mathbf{a_2} \times \mathbf{a_3}\right)$$

$$\mathbf{a_2^*} = \frac{1}{V}\left(\mathbf{a_3} \times \mathbf{a_1}\right)$$

$$\mathbf{a_3^*} = \frac{1}{V}\left(\mathbf{a_1} \times \mathbf{a_2}\right)$$

The reciprocal space metric tensor

$$g^*_{ij} = \begin{pmatrix} \mathbf{a_1^*} \cdot \mathbf{a_1^*} & \mathbf{a_1^*} \cdot \mathbf{a_2^*} & \mathbf{a_1^*} \cdot \mathbf{a_3^*} \\ \mathbf{a_2^*} \cdot \mathbf{a_1^*} & \mathbf{a_2^*} \cdot \mathbf{a_2^*} & \mathbf{a_2^*} \cdot \mathbf{a_3^*} \\ \mathbf{a_3^*} \cdot \mathbf{a_1^*} & \mathbf{a_3^*} \cdot \mathbf{a_2^*} & \mathbf{a_3^*} \cdot \mathbf{a_3^*} \end{pmatrix}$$

15

Real - reciprocal space and vice-versa

15

Real - reciprocal space and vice-versa

Reciprocal space basis vectors:

$$Real\ space:\ \{\overrightarrow{a_1}, \overrightarrow{a_2}, \overrightarrow{a_3}\}$$

$$Reciprocal\ space:\ \overrightarrow{a_m^*} = g_{mi}^{-1}\,\overrightarrow{a_i}$$

15

Real - reciprocal space and vice-versa

Reciprocal space basis vectors:

$$Real\ space : \{\overrightarrow{a_1}, \overrightarrow{a_2}, \overrightarrow{a_3}\}$$

$$Reciprocal\ space : \overrightarrow{a_m^*} = g_{mi}^{-1}\,\overrightarrow{a_i}$$

Components of a vector:

$$\vec{p} = \{p_1\, p_2\, p_3\}$$

$$p_m^* = p_i\, g_{im}$$

$$\vec{p} = \{p_1^*\, p_2^*\, p_3^*\}$$

Real - reciprocal space and vice-versa

Reciprocal space basis vectors:

$$Real\ space : \{\overrightarrow{a_1}, \overrightarrow{a_2}, \overrightarrow{a_3}\}$$

$$Reciprocal\ space : \overrightarrow{a_m^*} = g_{mi}^{-1}\,\overrightarrow{a_i}$$

Components of a vector:

$$\vec{p} = \{p_1\, p_2\, p_3\}$$

$$p_m^* = p_i\, g_{im}$$

$$\vec{p} = \{p_1^*\, p_2^*\, p_3^*\}$$

Metric Tensor:

$$g_{mk}^* = g_{im}^{-1}$$

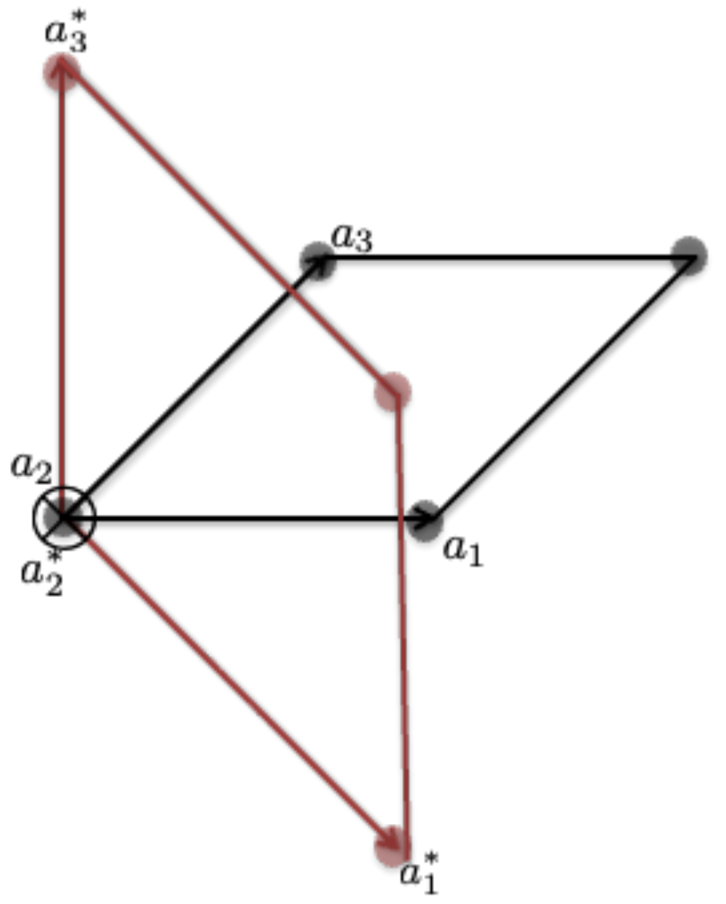
Determining reciprocal space

1. Given: Real space lattice parameters
2. Compute real space metric tensor
3. Invert it to get reciprocal space metric tensor
4. Post-multiply with the real space column vector

Reciprocal Lattice

Lattice vector in reciprocal space: $\mathbf{g} = g_i^* \mathbf{a}_\mathbf{i}^*$

If $g_i^* \in \mathbb{Z}$



The meaning of a reciprocal lattice vector

The meaning of a reciprocal lattice vector

Consider a particular reciprocal space lattice vector: $\mathbf{g} = g_i^* \mathbf{a}_\mathbf{i}^*, g_i^* \in \mathbb{Z}$

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Question: Which real space vectors, $\mathbf{X}_\mathbf{j} = x_{jk}\mathbf{a}_\mathbf{k}, x_{jk} \in \mathbb{R}$ are perpendicular to **g?**

The meaning of a reciprocal lattice vector

Consider a particular reciprocal space lattice vector: $\mathbf{g} = g_i^* \mathbf{a}_\mathbf{i}^*, g_i^* \in \mathbb{Z}$

Question: Which real space vectors, $\mathbf{X_j} = x_{jk}\mathbf{a_k}, x_{jk} \in \mathbb{R}$ are perpendicular to **g?**

$$\{\mathbf{X_j}\} \mid \mathbf{X_j} \bullet \mathbf{g} = 0$$

The meaning of a reciprocal lattice vector

Consider a particular reciprocal space lattice vector: $\mathbf{g} = g_i^* \mathbf{a}_\mathbf{i}^*, g_i^* \in \mathbb{Z}$

Question: Which real space vectors, $\mathbf{X}_\mathbf{j} = x_{jk} \mathbf{a}_\mathbf{k}, x_{jk} \in \mathbb{R}$ are perpendicular to **g?**

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$$\Longrightarrow \quad x_{11} \cdot g_1^* + x_{12} \cdot g_2^* + x_{13} \cdot g_3^* = 0$$

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$\implies g_1^* \equiv h, g_2^* \equiv k, g_3^* \equiv l$ $\quad \therefore \mathbf{g} \equiv \mathbf{g_{hkl}} = h\mathbf{a_1^*} + k\mathbf{a_2^*} + l\mathbf{a_3^*}$

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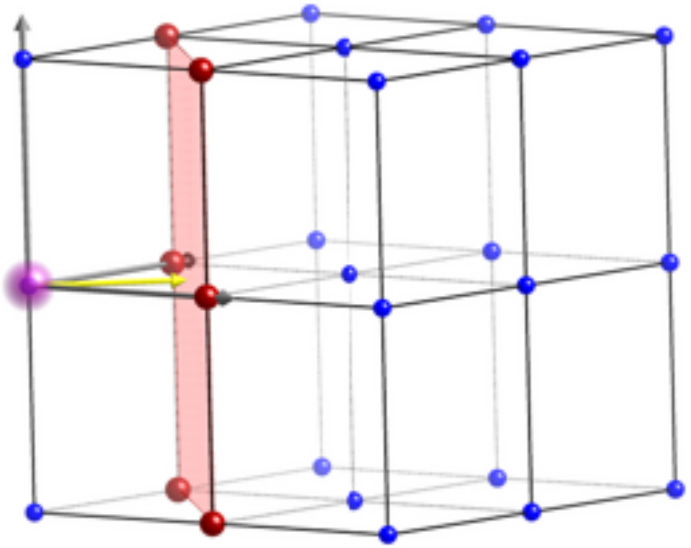

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Inter-planar spacing of the *(hkl)* plane
Length of the vector from origin to a point on the plane along the plane normal

Reciprocal basis vectors - Geometry

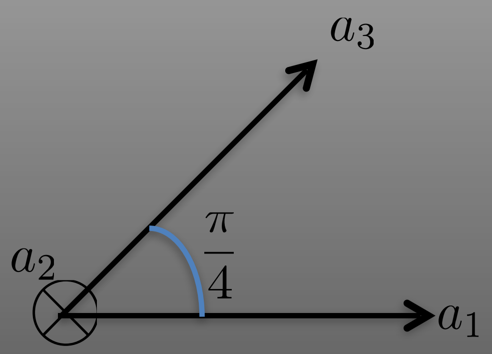
Consider a lattice with the following lattice parameters:

$$\{1, 1, 1, 90, 45, 90\}$$

- Determine the reciprocal basis vectors
- Reciprocal space components of: $\mathbf{p} = \frac{\mathbf{a_1}}{4} + \frac{\mathbf{a_3}}{2}$

21

Geometric Procedure



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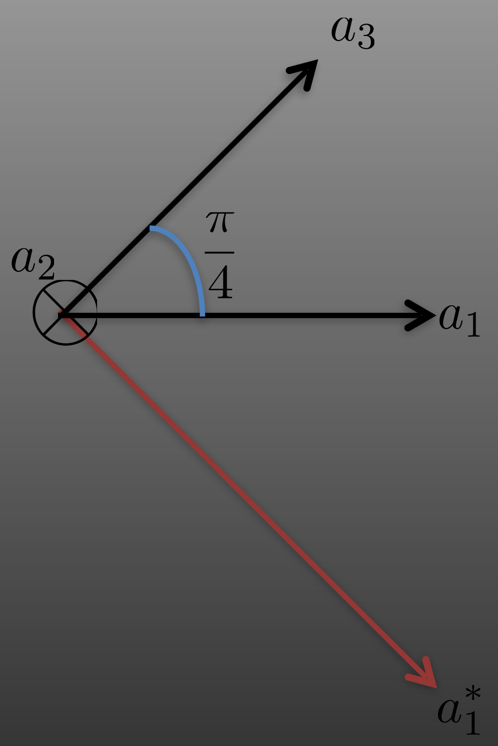

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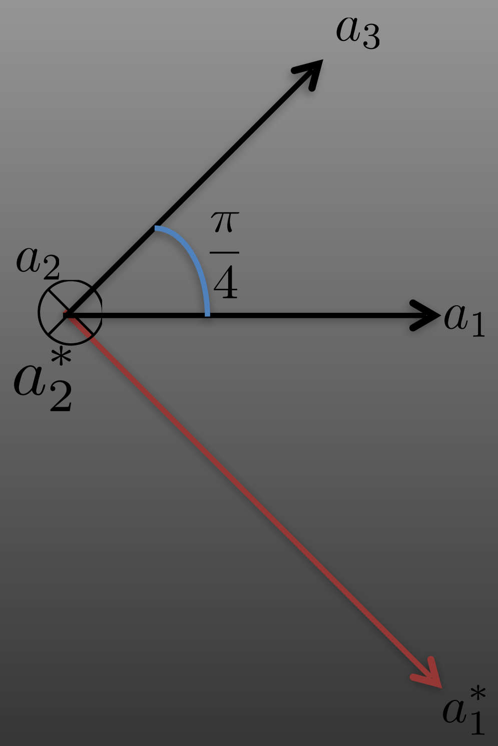

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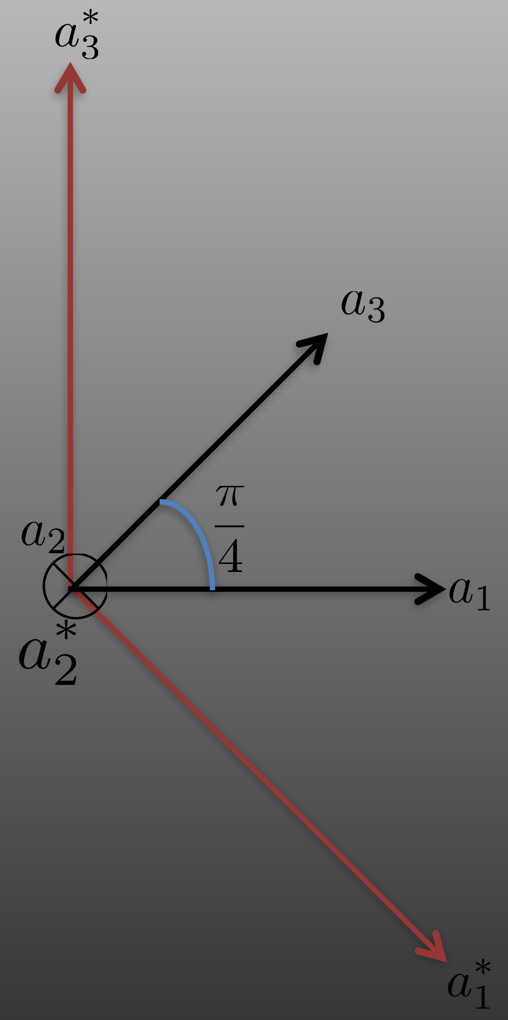

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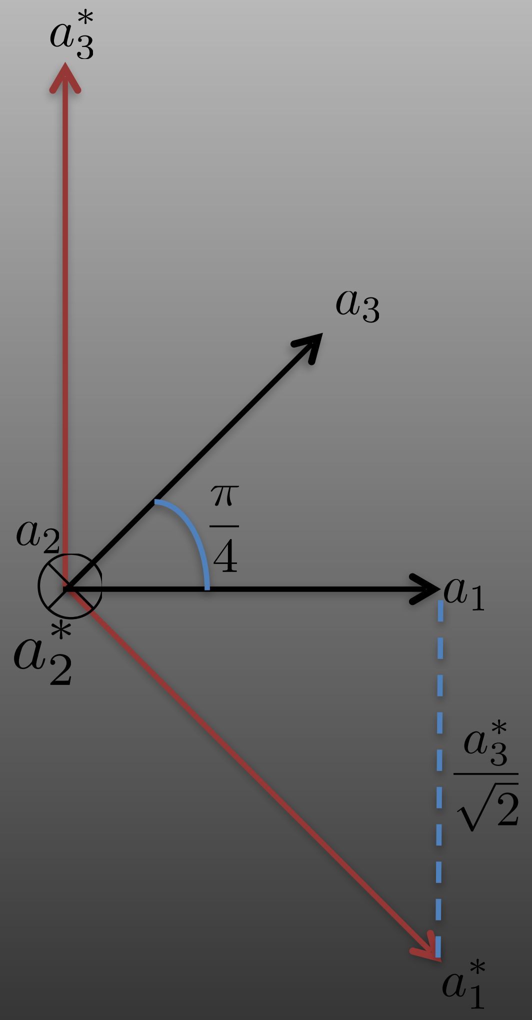

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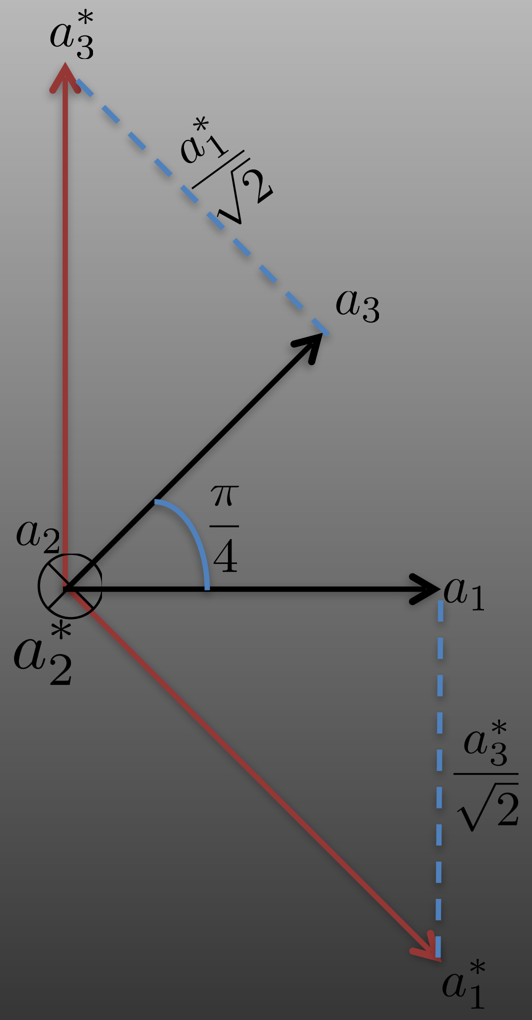

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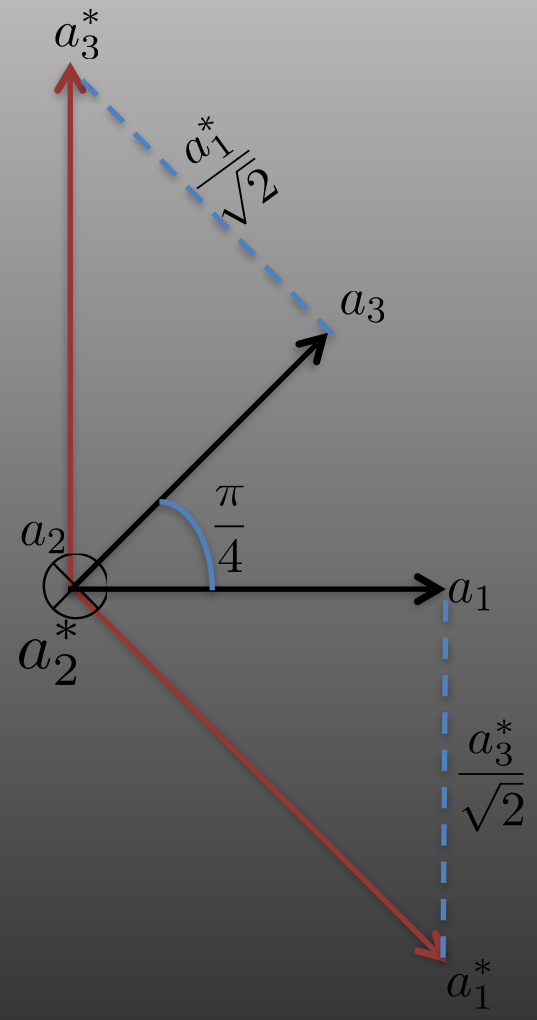

Geometric Procedure

$$\mathbf{a_1} = \mathbf{a_1^*} + \frac{\mathbf{a_3^*}}{\sqrt{2}}$$

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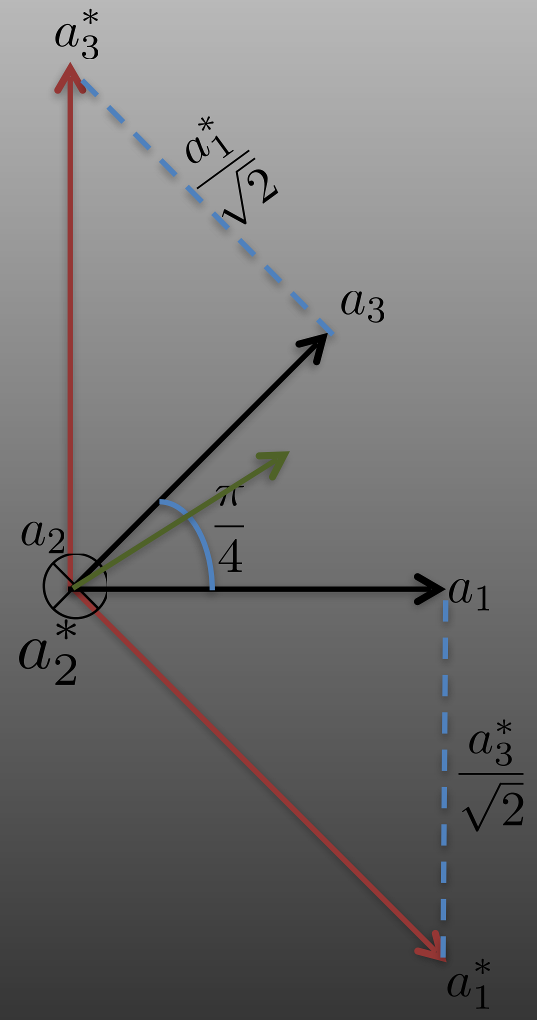

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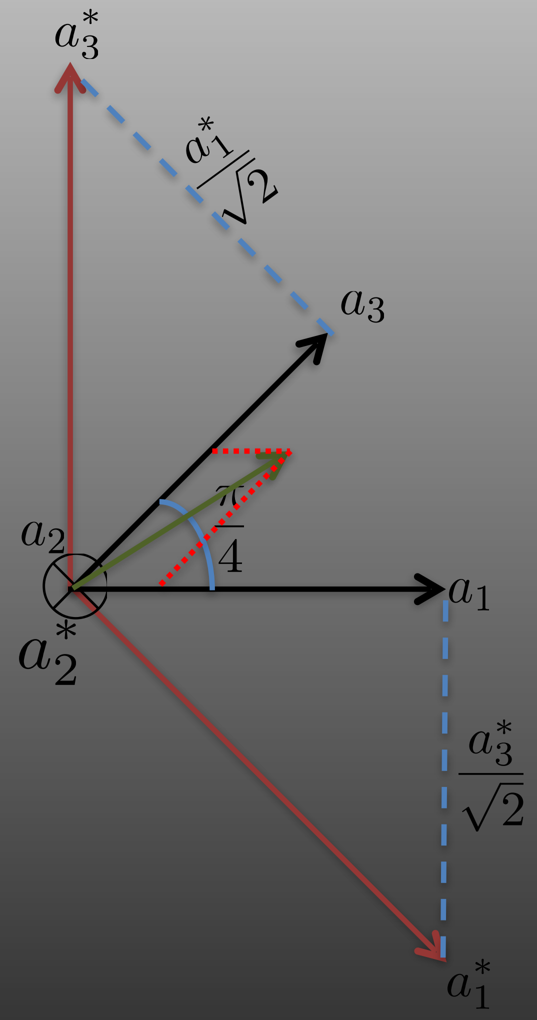

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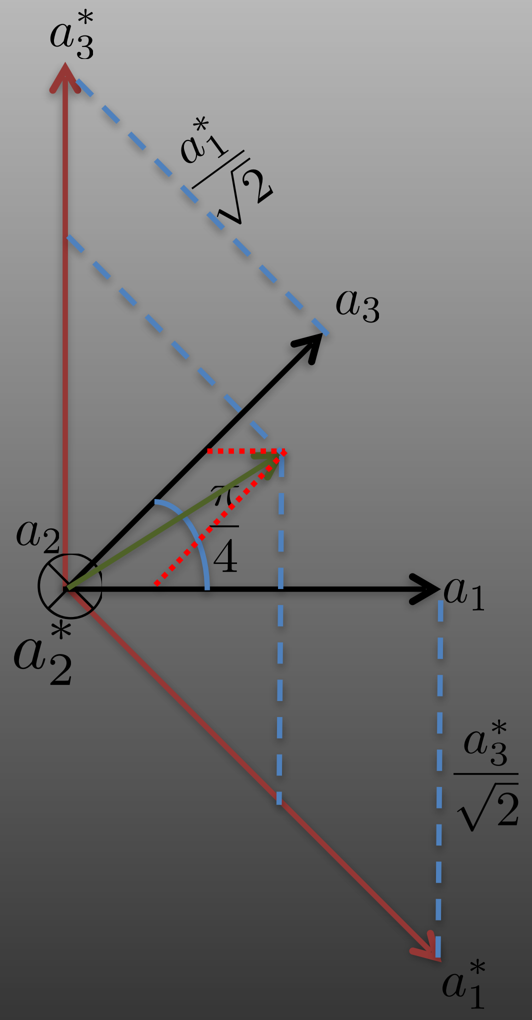

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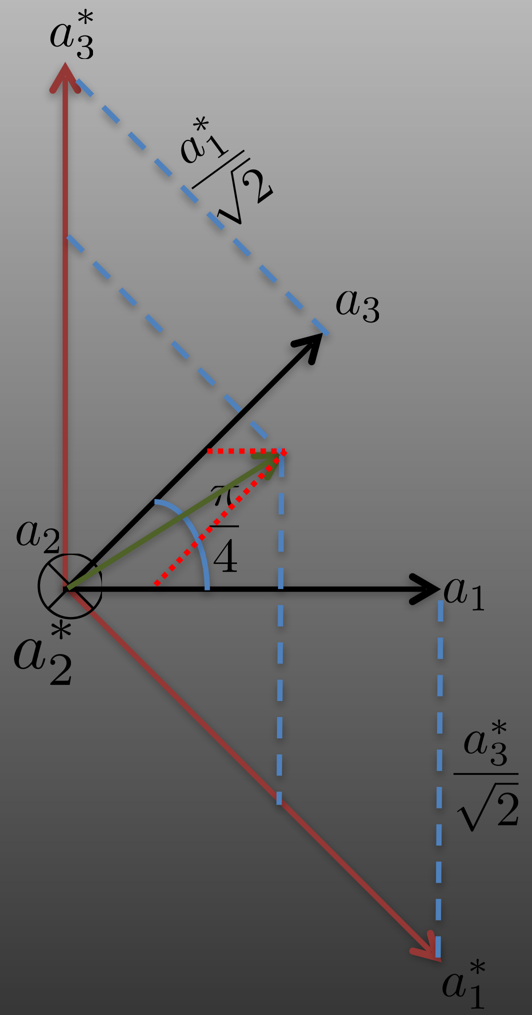

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$$\therefore \ \mathbf{p} = \frac{1}{4}(1+\sqrt{2})\mathbf{a_1^*} + \frac{1}{8}(4+\sqrt{2})\mathbf{a_3^*}$$

$$= 0.604\,\mathbf{a_1^*} + 0.677\,\mathbf{a_3^*}$$

Real to reciprocal and *vice versa*

A vector **exists** irrespective of its' reference frame

$$\therefore\ \mathbf{p} = p_i \mathbf{a_i} = p_j^* \mathbf{a_j^*}$$

Dot product both sides by real basis vectors, $\mathbf{a_m}$

$$p_i \mathbf{a_i} \cdot \mathbf{a_m} = p_j^* \mathbf{a_j^*} \cdot \mathbf{a_m}$$

$$\Rightarrow p_i g_{im} = p_j^* \delta_{jm} = p_m^*$$

Real space vector to reciprocal space vector

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$$\Downarrow$$

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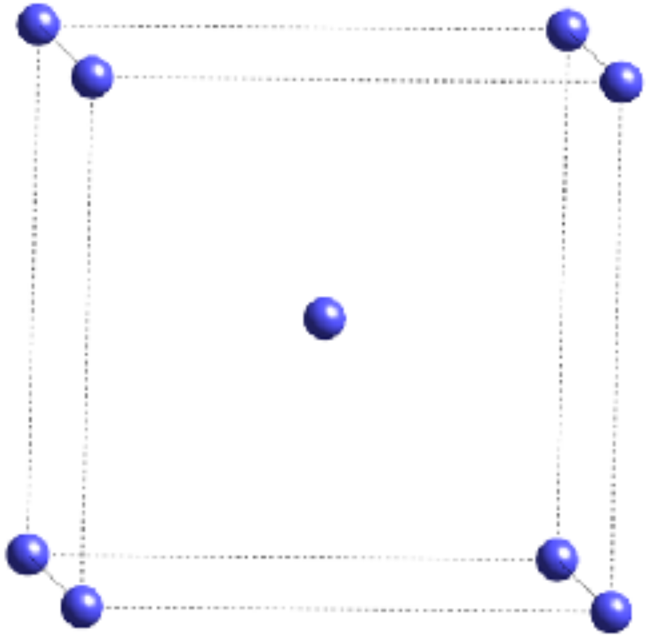
$$= \left[\frac{1}{4}\left(1+\sqrt{2}\right)\ 0\ \frac{1}{8}\left(4+\sqrt{2}\right)\right]$$

Reciprocal Lattice - cI



24

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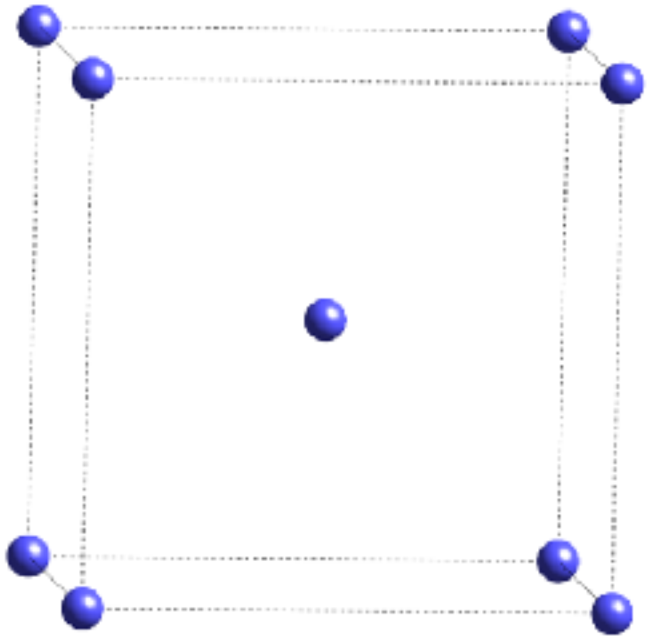

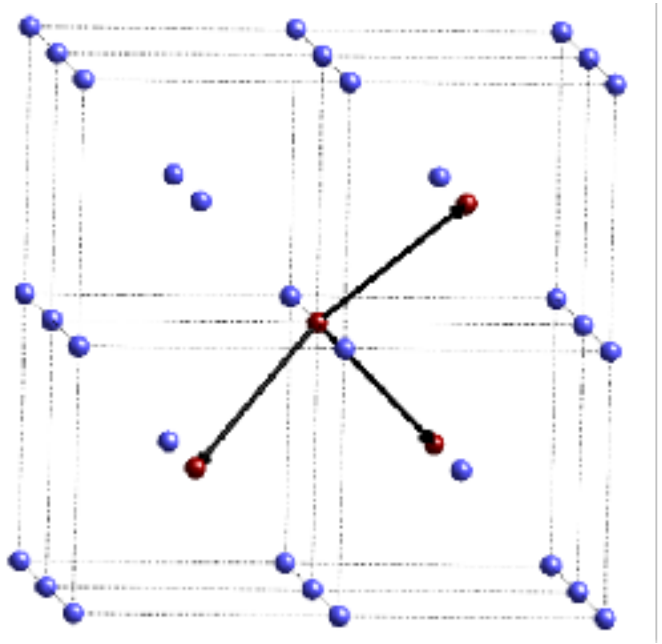

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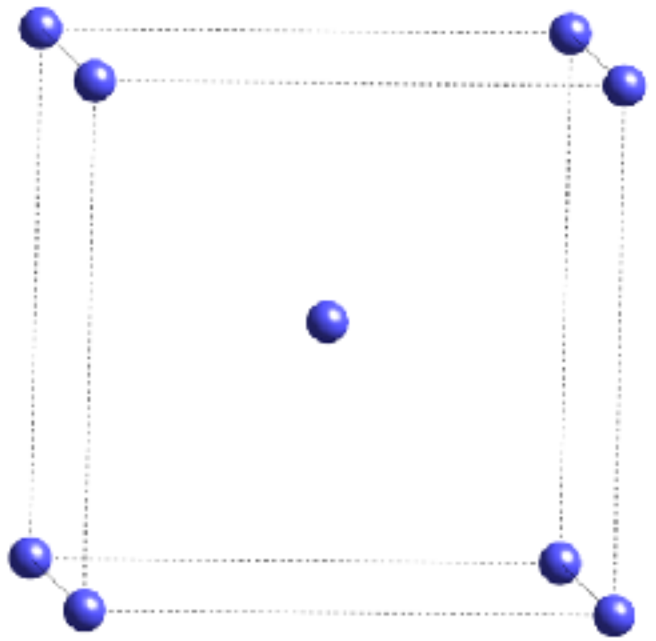
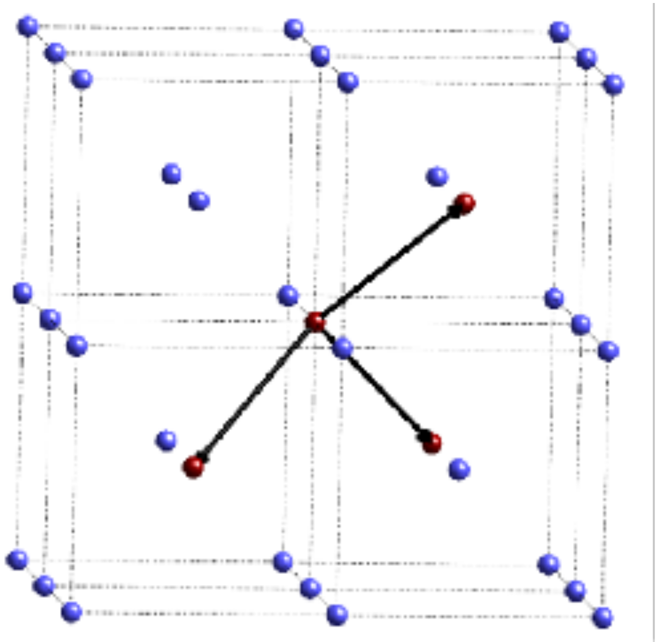




1

Choose primitive cell

2

Compute real space metric tensor

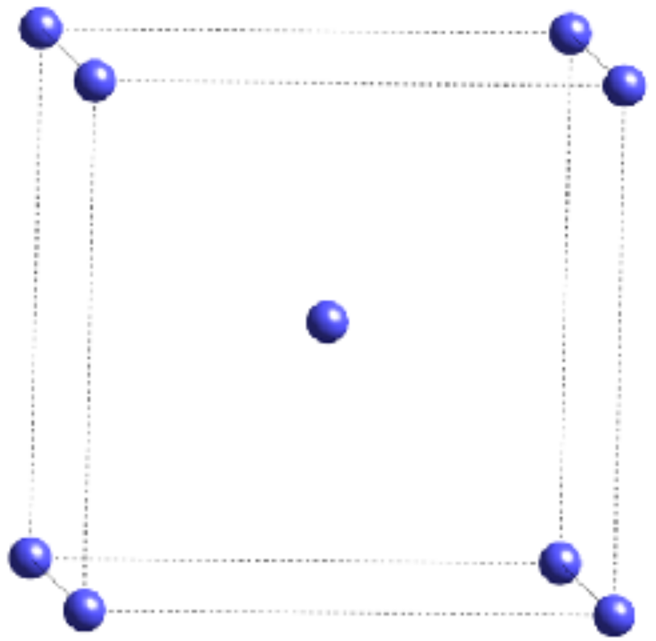
3

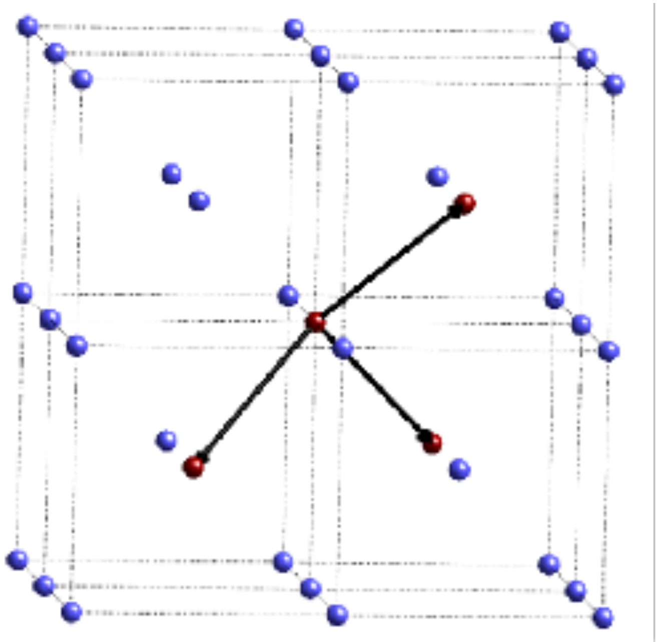
Invert it to get reciprocal space metric tensor

4

Post-multiply with the real space column vector

24 Reciprocal Lattice - cI





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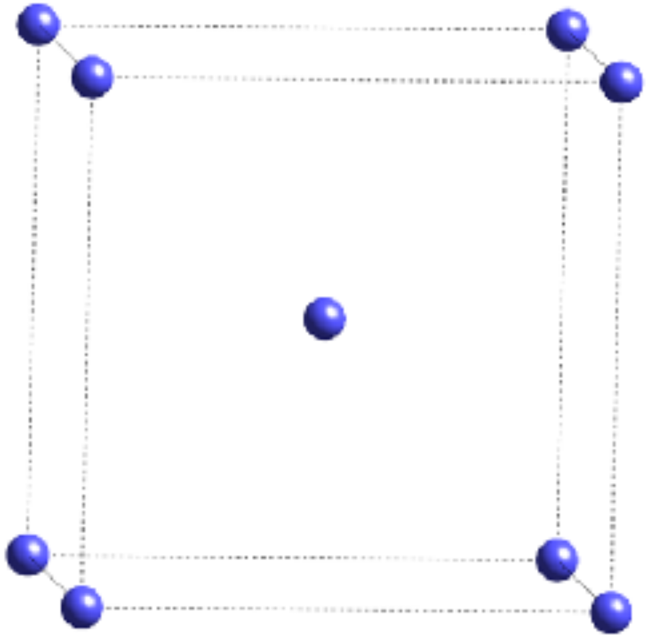

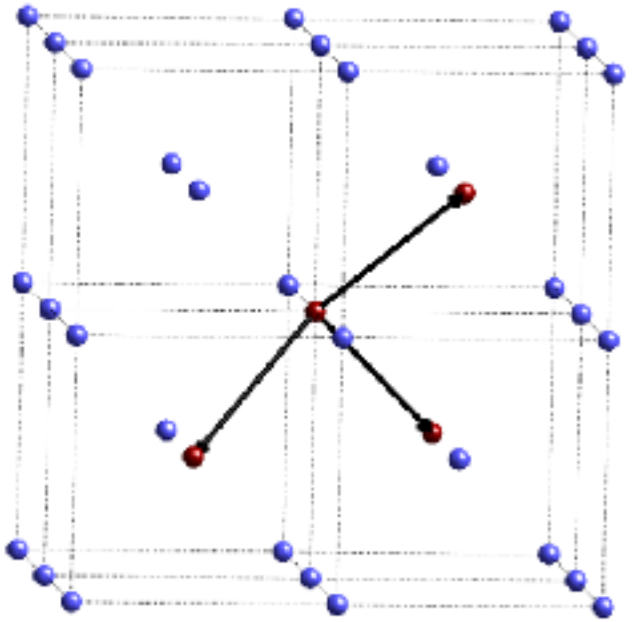

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$$g_{ij} = \frac{a^2}{4}\begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}$$

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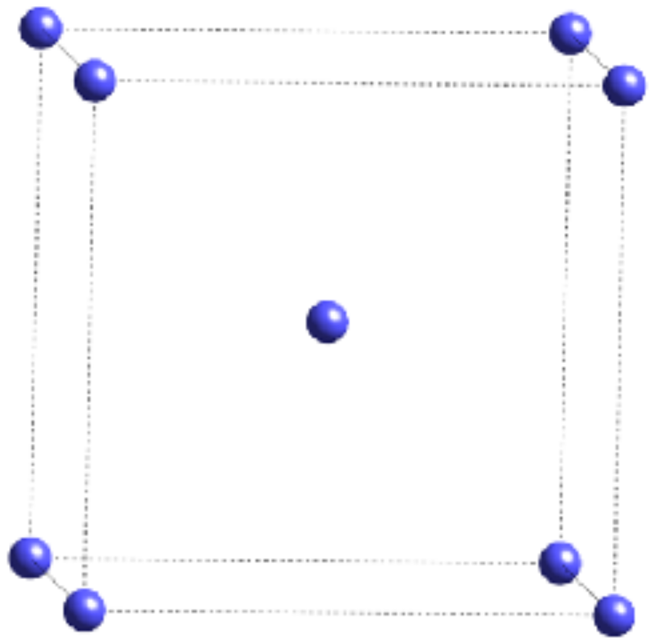

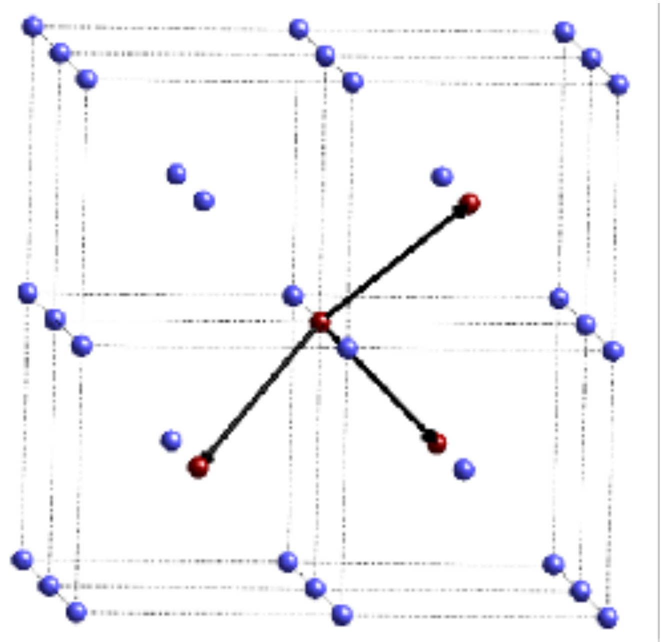

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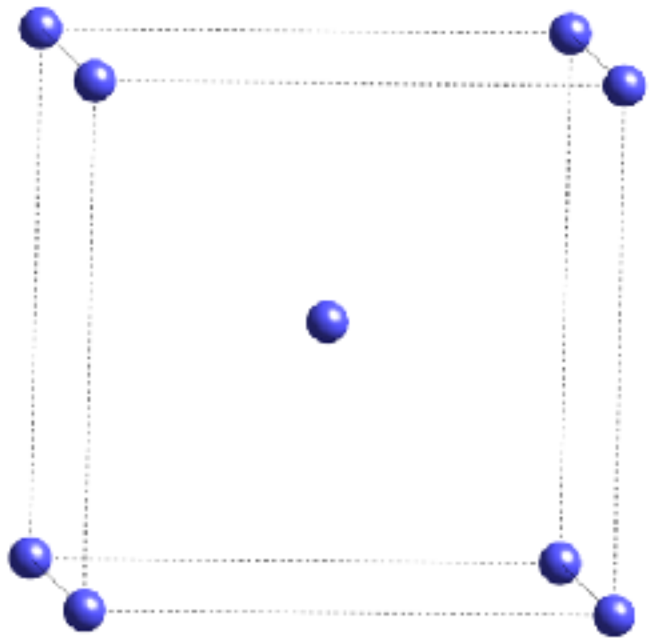

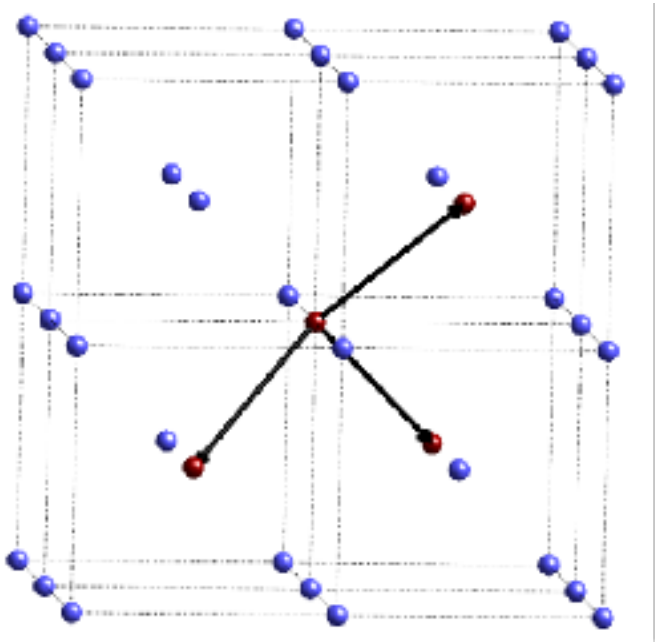

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