NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS -- DEPARTMENT OF INFORMATICS AND TELECOMMUNICATIONS

INFORMATION TECHNOLOGIES
IN MEDICINE AND BIOLOGY

ACADEMY OF ATHENS

BRFAA

A web based crystallographic tool for the construction of nanoparticles

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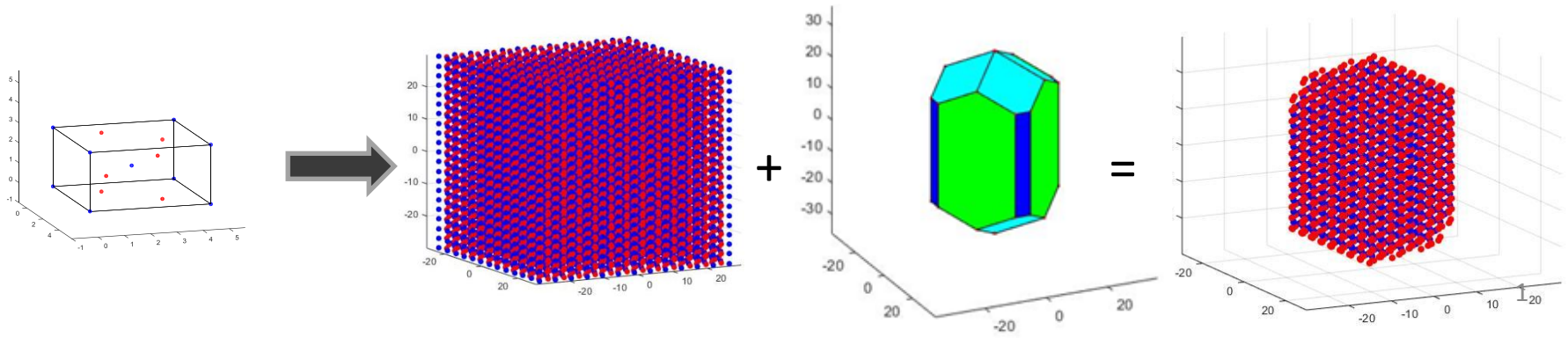
16/5/2018

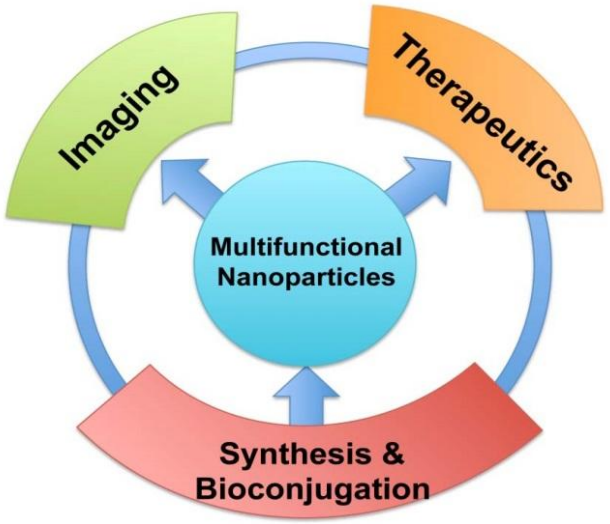


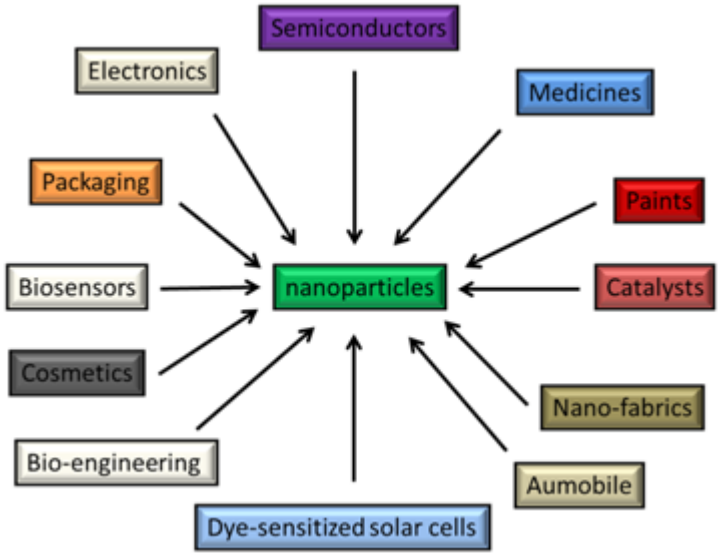
Outline

- Introduction
- Motivation
- Crystallography theory
- Creation of a web based crystallographic tool
- Conclusions

Introduction

- Nanoparticles are nano-engineered structures, 1-100 nm in size





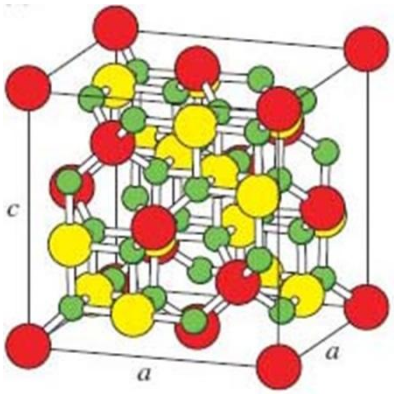
Nanoparticle applications

- Drug delivery systems
- Quantum computers
- Textiles (Technical, Medical, Electrocontucting, Anti-stain)
- Industrial catalysts
- Food packaging

Motivation

- Nanoparticles are formed by crystals of materials such as magnetite
- Individual crystals grow based on crystal habits, which give the characteristic external shape of a crystal
- Provide an easily accessible web based crystallographic tool which can produce nanoparticles for simulation from any material as they grow in nature of any type, any size and any shape

Magnetite (Fe3O4) unit cell



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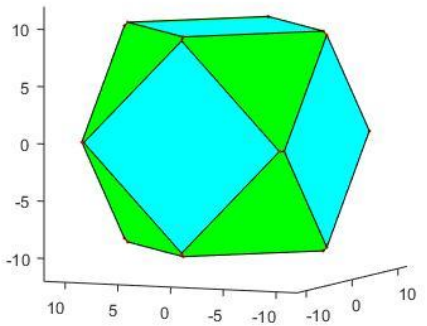
Magnetite (Fe3O4) crystal shape



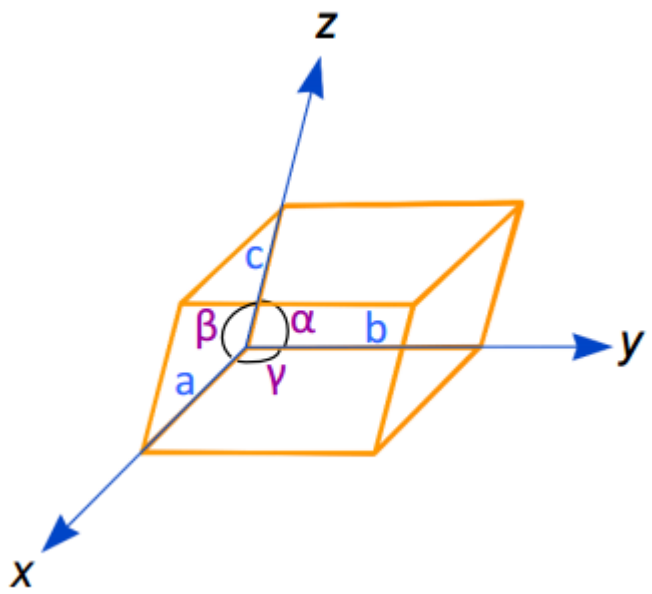
Unit Cell & Crystal Lattice

- The unit cell is the smallest group of particles in the material, which builds up the whole crystal structure

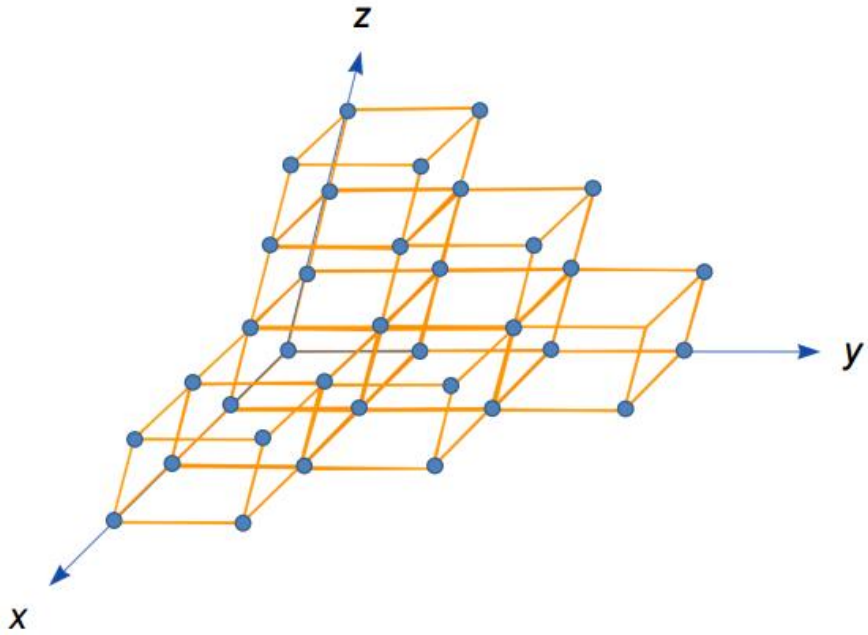
- The crystal lattice is built up by repetitive translation of the unit cell and its the symmetry and structure is completely defined by it

- The connection points between the unit cells form the crystal lattice

Unit cell

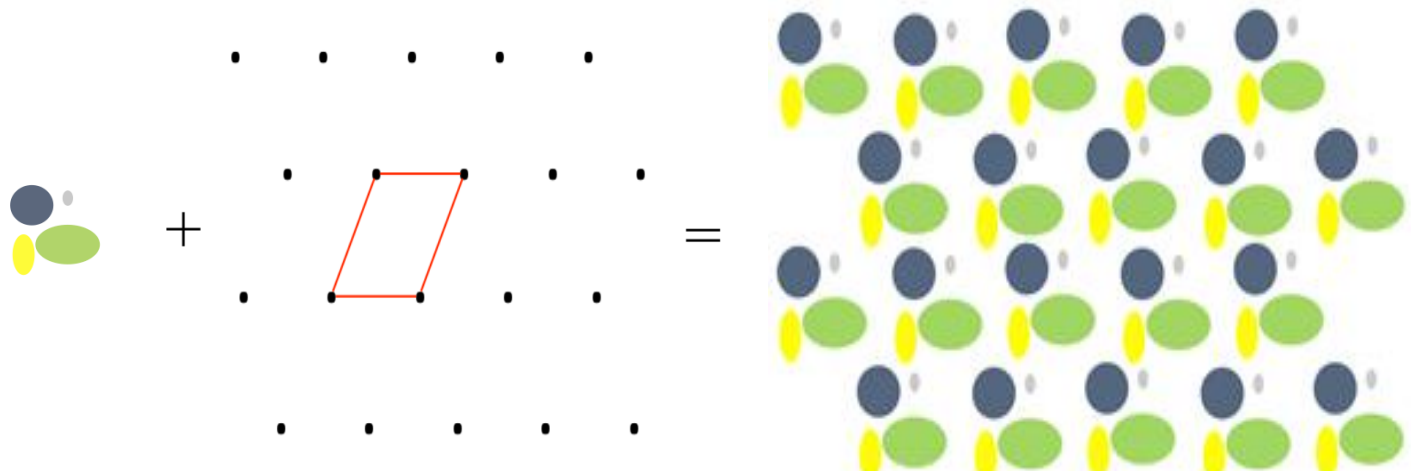


Crystal lattice



Crystal Structure = Lattice + Basis

- The basis consists of the arrangement of the building blocks (atoms, molecules) of a unit cell
- The basis is represented by a lattice point
- All building blocks of a crystal structure are subject to the same translation principle



Basis Lattice Crystal Structure

Crystal systems and Centering types

- Every imaginable crystal structure of the world belongs to one of altogether 7 possible crystal systems each one having 4 centering types

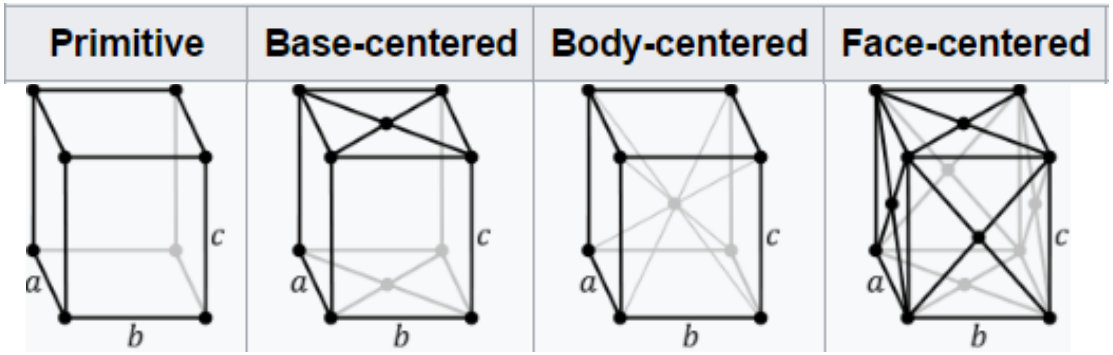
The 7 Crystal systems

symmetry

restrictions for	*cell constants*	*cell angles*
triclinic	none	none
monoclinic	none	$\alpha = \gamma = 90°$
orthorhombic	none	$\alpha = \beta = \gamma = 90°$
tetragonal	a = b	$\alpha = \beta = \gamma = 90°$
trigonal	a = b	$\alpha = \beta = 90°; \gamma = 120°$
hexagonal	a = b	$\alpha = \beta = 90°; \gamma = 120°$
cubic	a = b = c	$\alpha = \beta = \gamma = 90°$

hexagonal crystal *family*

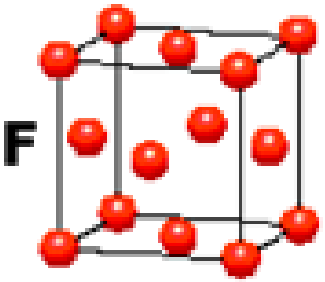
The 4 Centering types



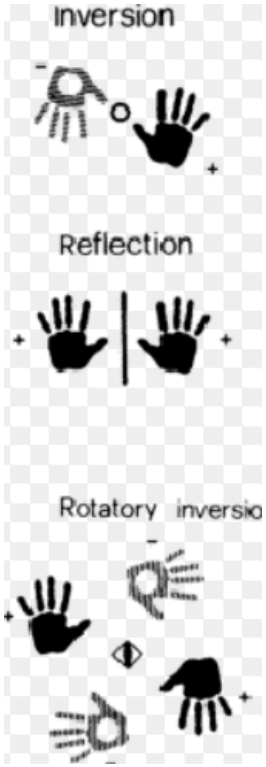
Centering type (Bravais) & Symmetry (Point groups) applied to crystal systems

7 Crystal systems

Add points & "centering" → 14 Bravais lattices



Rotation Reflection Inversion → 32 Point groups



Bravais lattices

restrictions for	*cell constants*	*cell angles*
triclinic	none	none
monoclinic	none	$\alpha = \gamma = 90°$
orthorhombic	none	$\alpha = \beta = \gamma = 90°$
tetragonal	a = b	$\alpha = \beta = \gamma = 90°$
trigonal	a = b	$\alpha = \beta = 90°; \gamma = 120°$
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symmetry

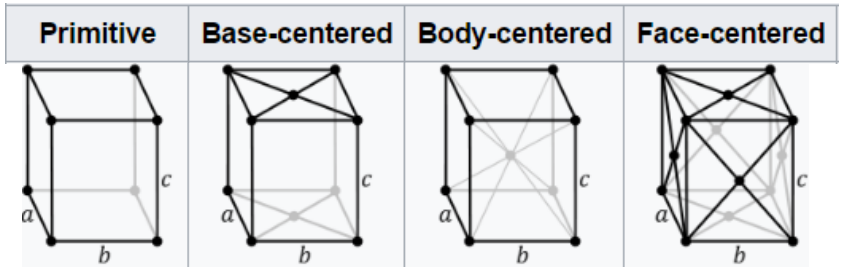
hexagonal crystal *family*

Bravais lattices

crystal systems

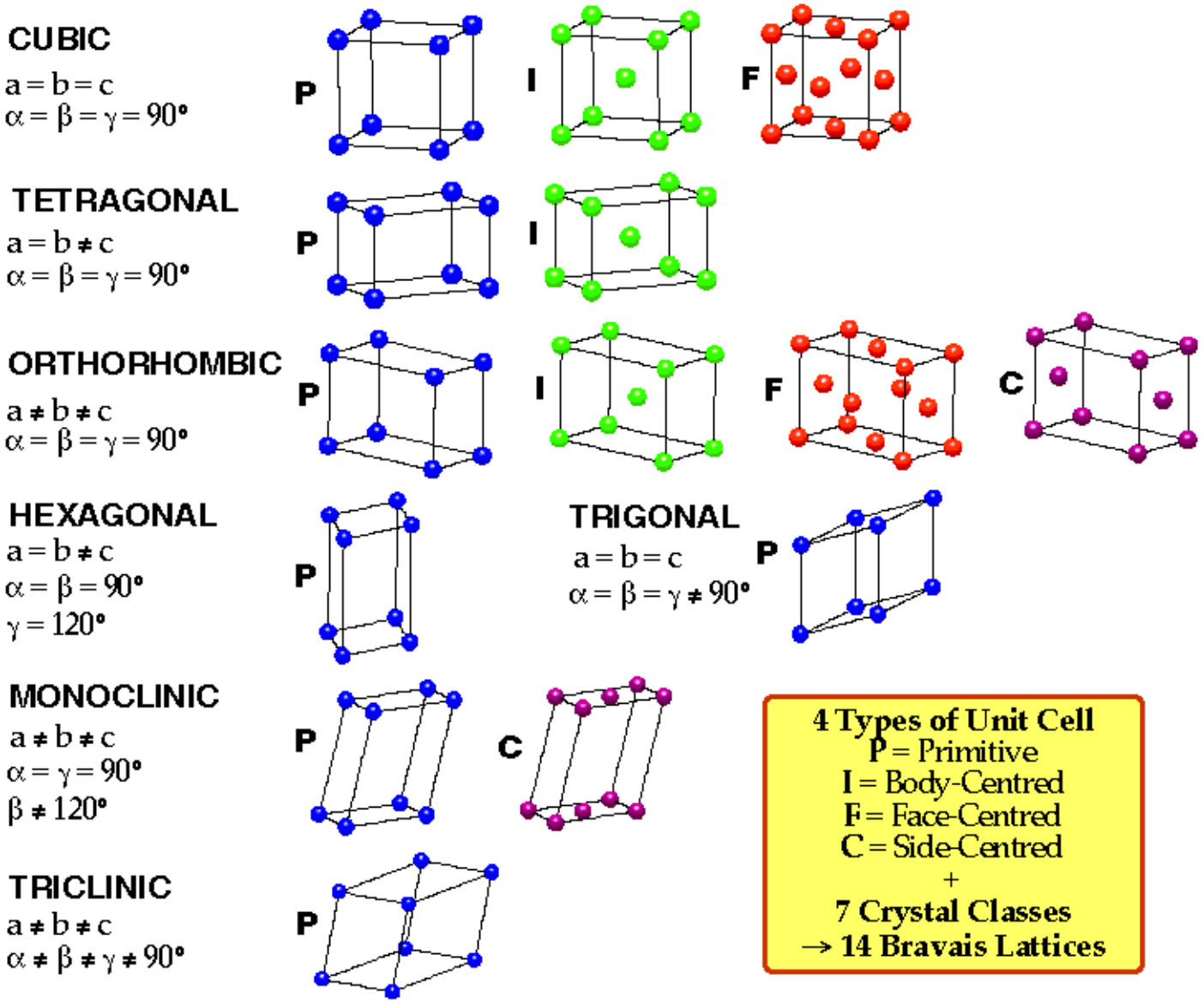
$7 \times 4 = 14$ (?)

kind of centerings



- Some of the 28 conceivable lattice types are redundant
- Some of them are not possible due to symmetry reasons

The 14 Bravais lattices

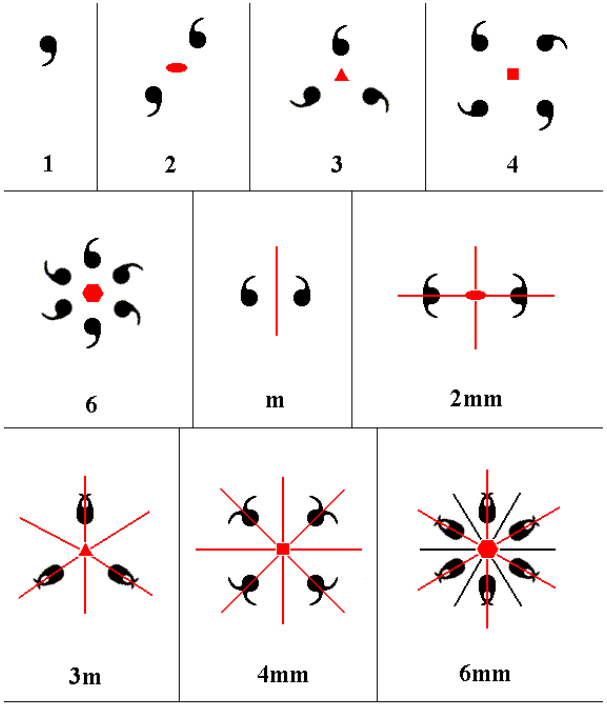


Point groups

- The 7 crystal systems consist of 32 crystal classes, corresponding to the 32 crystallographic point groups

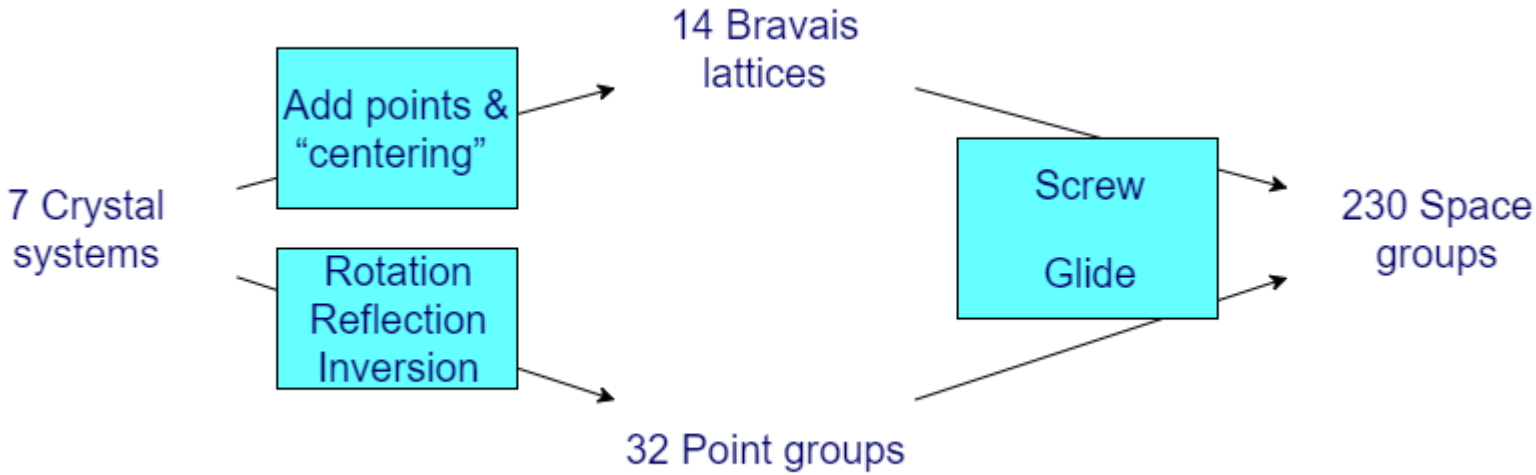
- A crystallographic point group is a set of symmetry operations

Class	Group names						
Cubic	23	$m\bar{3}$		432	$\bar{4}3m$	$m\bar{3}m$	
Hexagonal	6	$\bar{6}$	$6/m$	622	6mm	$\bar{6}2m$	$6/mmm$
Trigonal	3	$\bar{3}$		32	3m	$\bar{3}m$	
Tetragonal	4	$\bar{4}$	$4/m$	422	4mm	$\bar{4}2m$	$4/mmm$
Monoclinic Orthorhombic	2		$2/m$	222	m	mm2	mmm
Triclinic	1	$\bar{1}$					

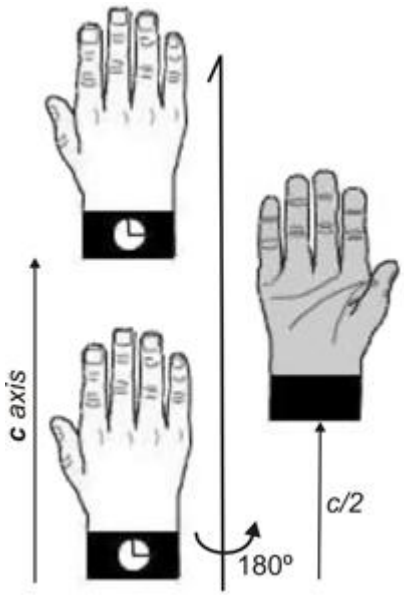


The Ten Planar Point Groups

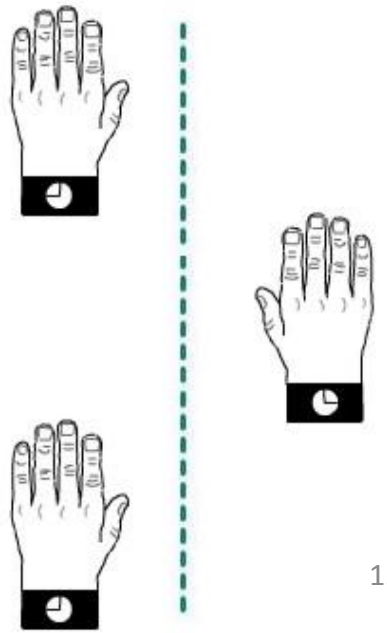
Space groups



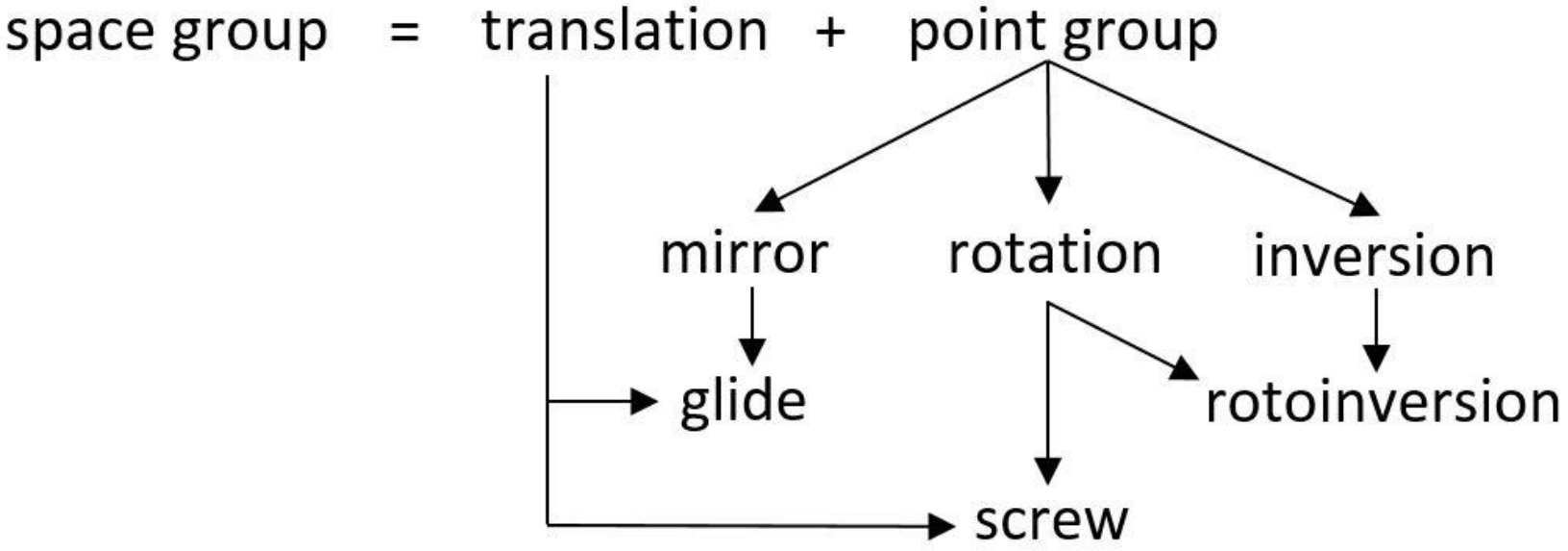
Screw axis



Glide plane



Space groups



- A space group is a combination of the translational symmetry of a unit cell including lattice centering and the point group symmetry operations

- **The symmetry of a crystal is completely described by a space group**

Symmetry operations

- The application of symmetry operations is a sequence of matrix multiplications

Translation Rotation Inversion

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\pi & 0 & -\sin\pi & 0 \\ 0 & 1 & 0 & 0 \\ \sin\pi & 0 & \cos\pi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

Application of inversion, followed by a 2-fold rotation about the b-axis and followed by a translation of [123]

- We use Miller indices because it is straightforward to derive the orientations of other faces of the same kind for different degrees of symmetry (n-fold rotations)

Miller indices

Miller indices

- Miller indices are used to denominate lattice planes and form a notation system for a family of planes
- Expressed by three integers: {h k l} such as {100}, which contains (100), (010), (001) and the negative of any of those directions

How to find a Miller plane:

1) Take the reciprocals. If the reciprocal is ∞, the plane is parallel to that direction

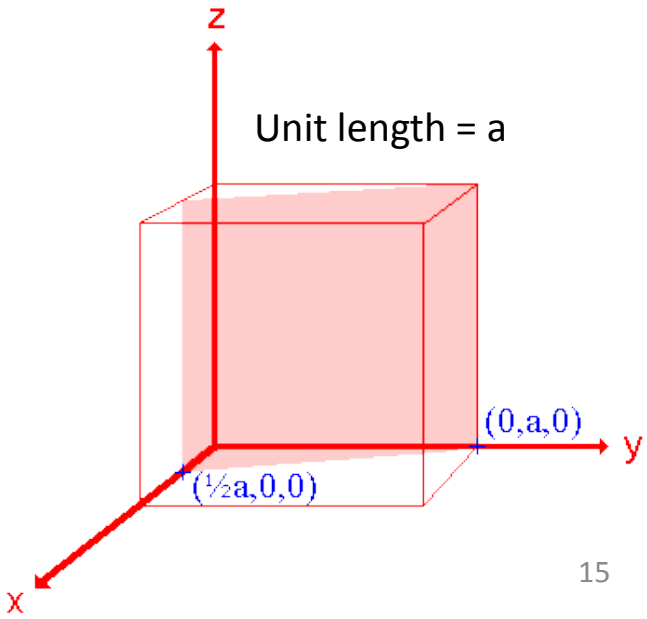
2) Multiply the reciprocals with each of the unit lengths, a, b and c

3) Mark the intercepts and draw the plane

Example:

How to find the plane with Miller indices: (210)

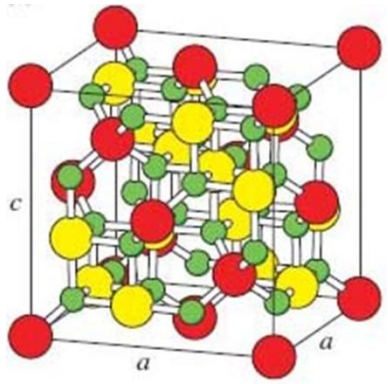
- Reciprocals (fractional intercepts): ½ , 1 , ∞
- Intercepts: ½ a , a , ∞
- Cartesian coordinates: (½ a,0,0), (0,a,0),
  parallel to z direction



Crystal shape construction

- Miller indices indicate individual planes
- Crystal shape: A polyhedron that is created as the intersection of multiple individual planes based on the unique crystal habit
- In order to construct the crystal shape we have to find the crystal faces from the symmetric Miller indices

Magnetite (Fe3O4) unit cell



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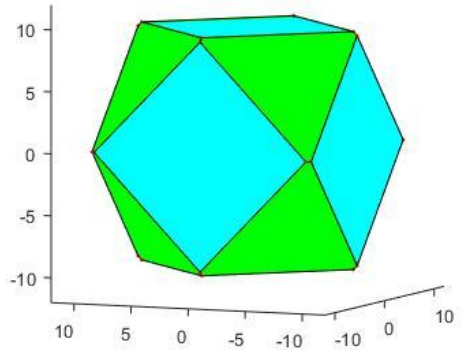
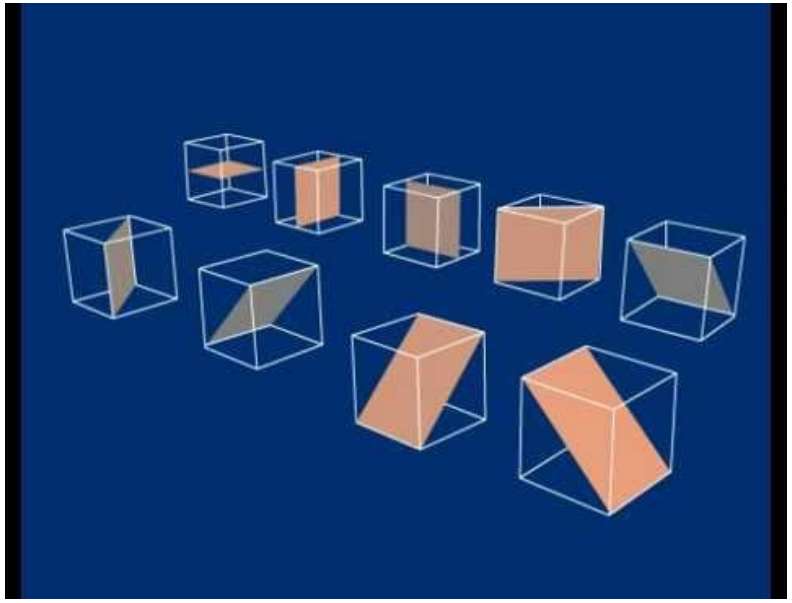
Magnetite (Fe3O4) crystal shape



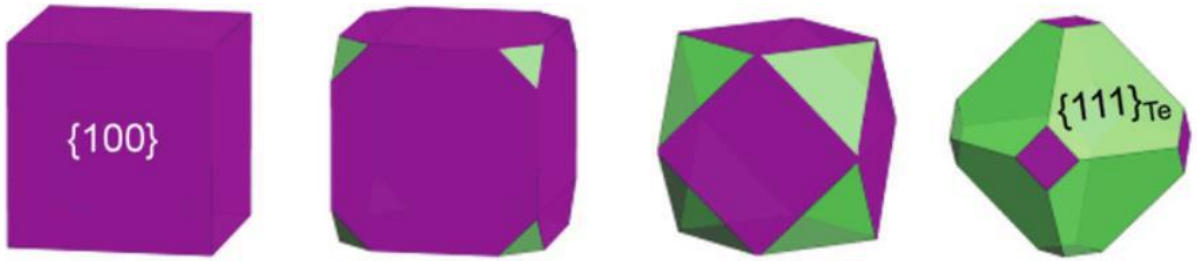
Symmetric Miller indices

- Calculate symmetric Miller indices by applying the point group symmetry operations on the initial Miller indices
- Generate Miller planes for all symmetric indices as before
- Symmetric Miller planes with respect to the point group form polyhedrons when they intersect



Nanoparticle growing planes & morphology - crystal habit

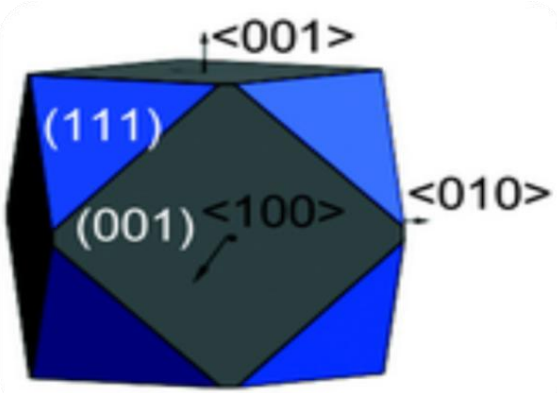
- A crystal will arrange itself such that its surface energy (Gibbs free energy) is minimized by assuming a shape of low surface energy
- The equilibrium shape of the crystal will then be that which minimizes the value of this energy (crystal habit)



$d_{hkl} = \lambda * \gamma_{hkl}$, λ=constant

Wulff morphology (crystal habit) expresses a particle produced in conditions of perfect thermodynamic equilibrium.

Magnetite: (001) plane dominates the morphology, followed by the (111) surface truncating the corners of the cube.

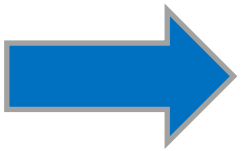


magnetite

Creating the Wulff morphology (crystal habit)

Input:

- Cif file
- Planes dominating the morphology (minimum energy surfaces) expressed in Miller indices
- Minimum surface energies of the planes
- Maximum radius from the origin



Wulff morphology

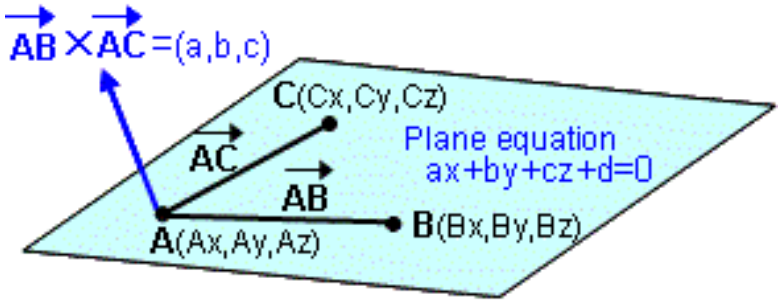
1. Based on input, calculate Miller planes

Define the Miller plane for each hkl triplet and the desired distance d:

- Calculate x,y,z coordinates.
- Calculate the coefficients A,B,C of the plane equation

$$Ax+By+Cz+D=0$$

- Apply the distance d and calculate the coefficient D
- Place the origin on the negative side: D<0



Plane equation $ax+by+cz+d=0$

(1) $\overrightarrow{AB}=(B_x-A_x,By-Ay,B_z-A_z)$

$\overrightarrow{AC}=(C_x-A_x,Cy-Ay,C_z-A_z)$

(2) $\overrightarrow{AB}\times\overrightarrow{AC}=(a,b,c)$

$a=(By-Ay)(C_z-A_z)-(Cy-Ay)(B_z-A_z)$

$b=(B_z-A_z)(C_x-A_x)-(C_z-A_z)(B_x-A_x)$

$c=(B_x-A_x)(Cy-Ay)-(C_x-A_x)(By-Ay)$

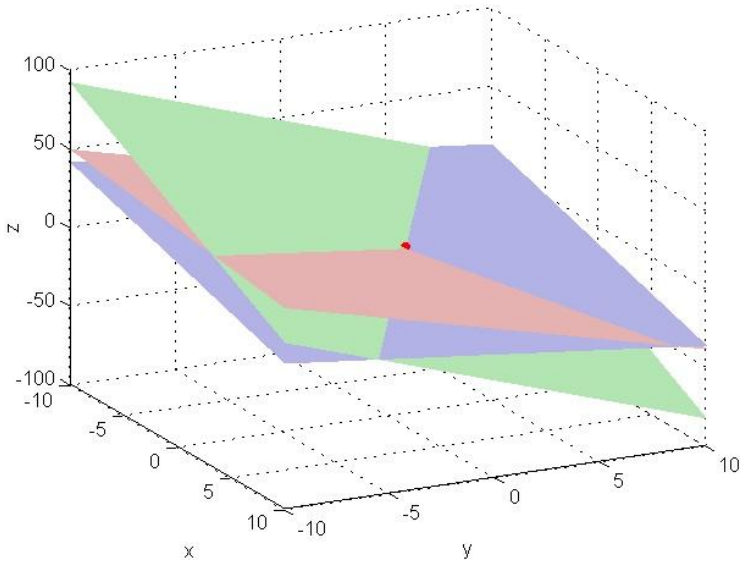
$d=-(aA_x+bAy+cA_z)$

2. Find all intersection points of three planes

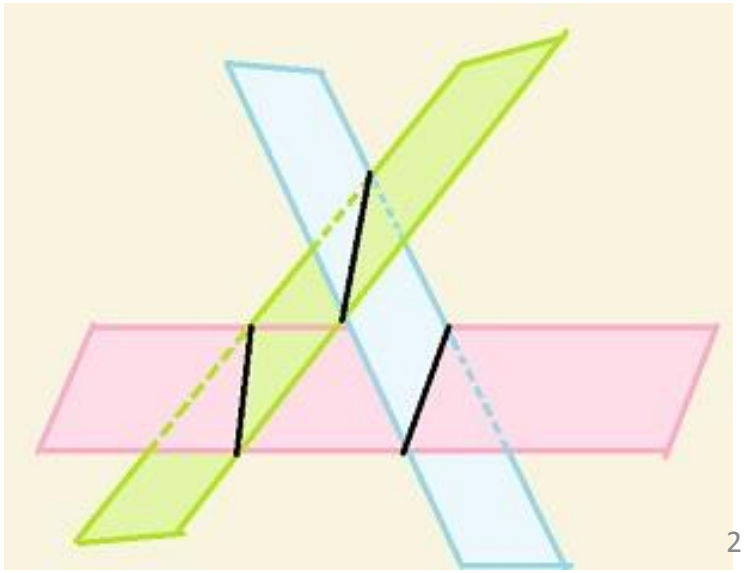
Approach: Exhaustive search for all possible intersection points -> potential vertex

- 2 non parallel planes intersection: line
- 3 planes intersection (each 2 non parallel): point

Single intersection point

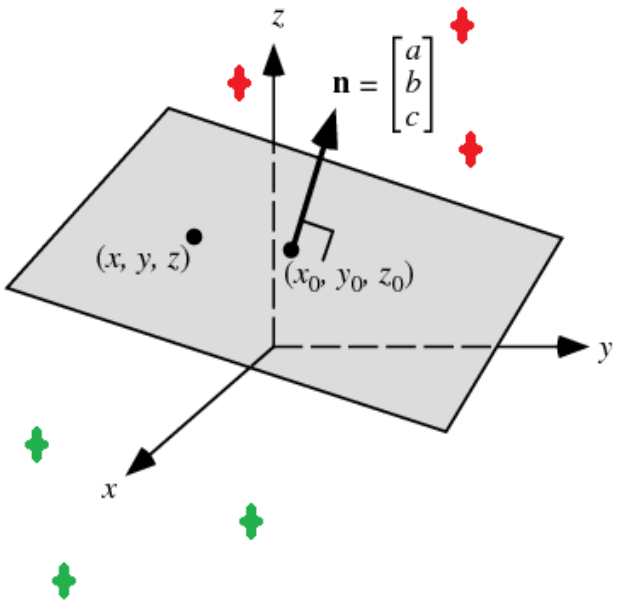


No intersection point



3. Keep points inside the polyhedron

- Discard points that fall outside the polyhedron (on the positive side of at least one of the planes)



Rejected points

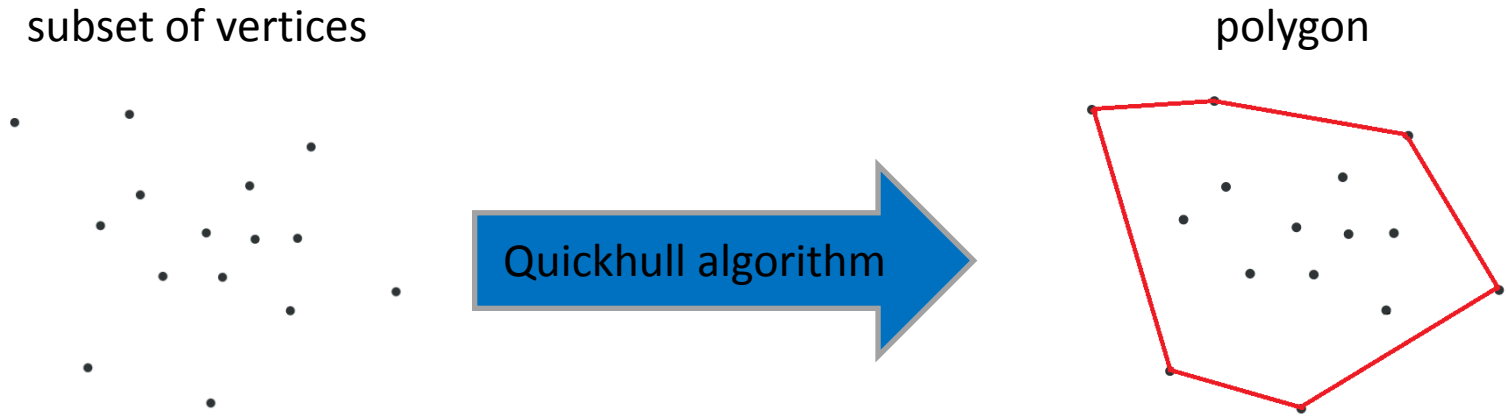
Accepted points

4. Create all faces of the polyhedron

- Each face corresponds to one of the planes
- Each face is defined by a subset of vertices

- For each plane, find all vertices that lie on it (satisfy the plane equation)
- Create a polygon of these vertices using the Quickhull algorithm

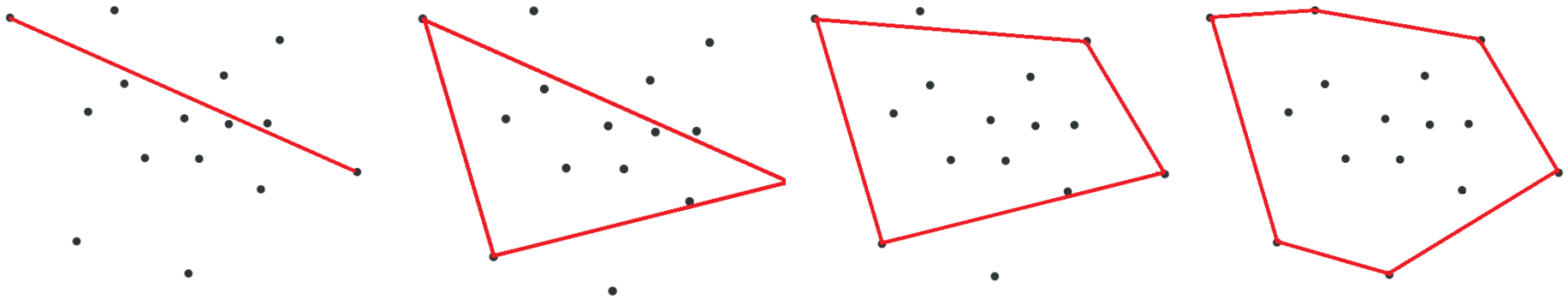
- Result: obtain a list of all faces of the polyhedron



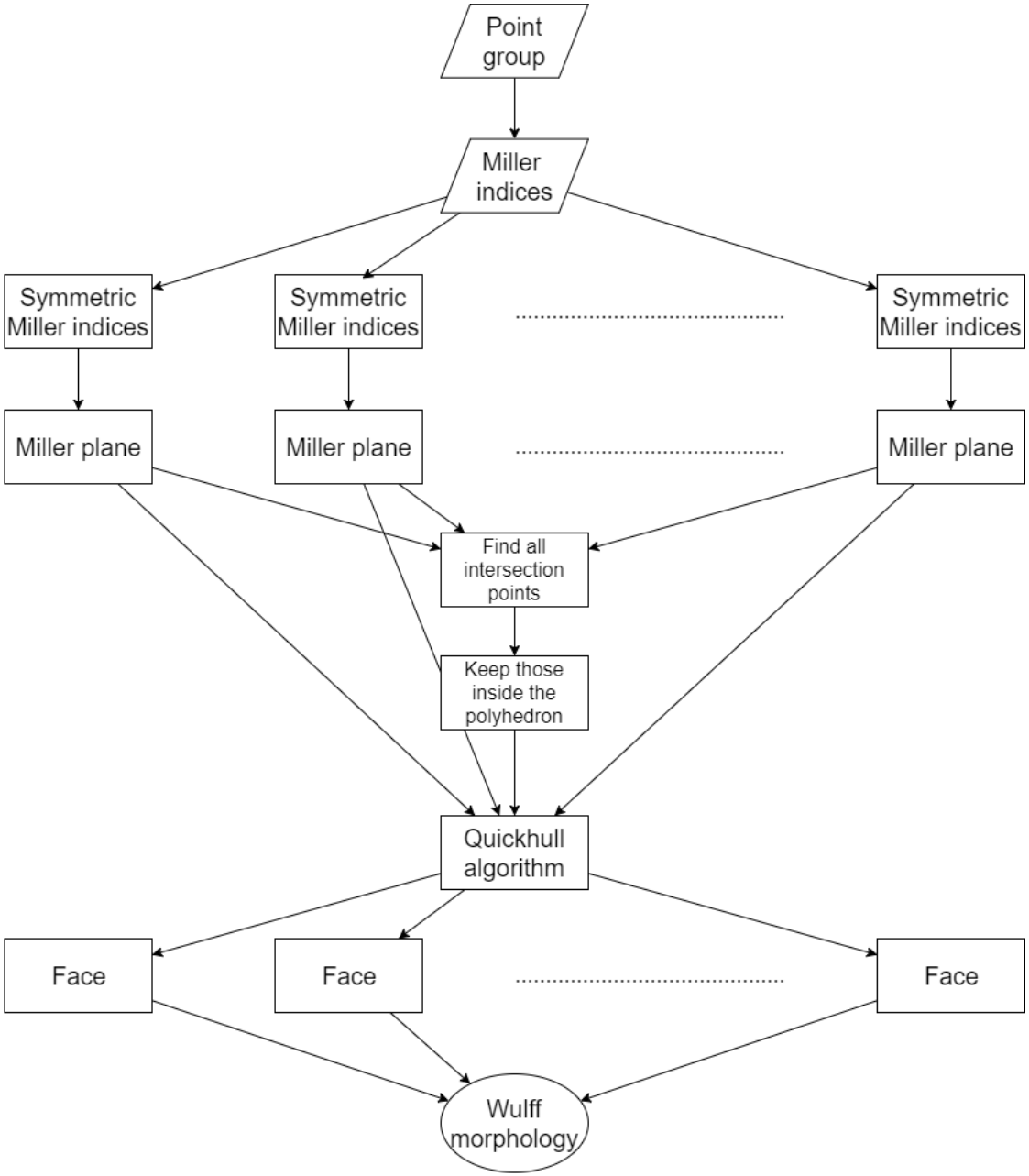
4.a Use Quickhull algorithm to define the convex hull of a set of points

Quickhull algorithm

1. Connect the most distant points with a (double) line segment
2. Find the most distant point from the line segment
3. Replace the line segment with two new ones, connecting the most distant point
4. Repeat steps 2,3 until all points are included in the convex hull

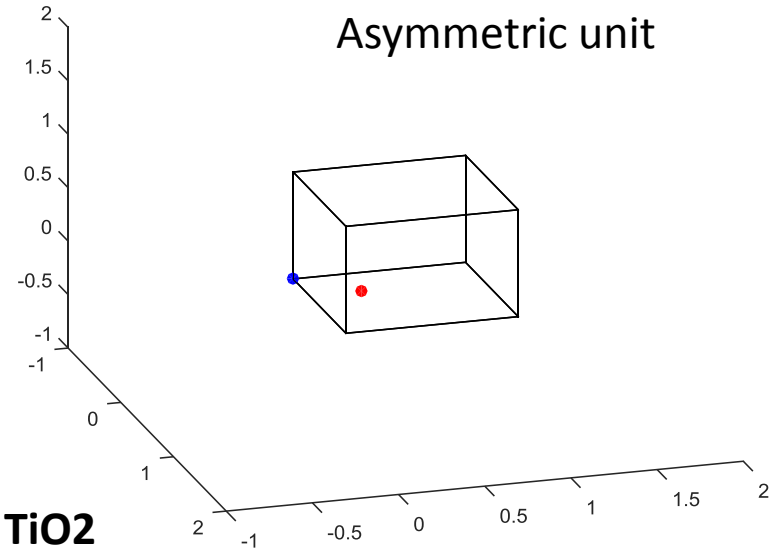


Workflow for creating the Wulff morphology



5. Create the symmetric unit from CIF file

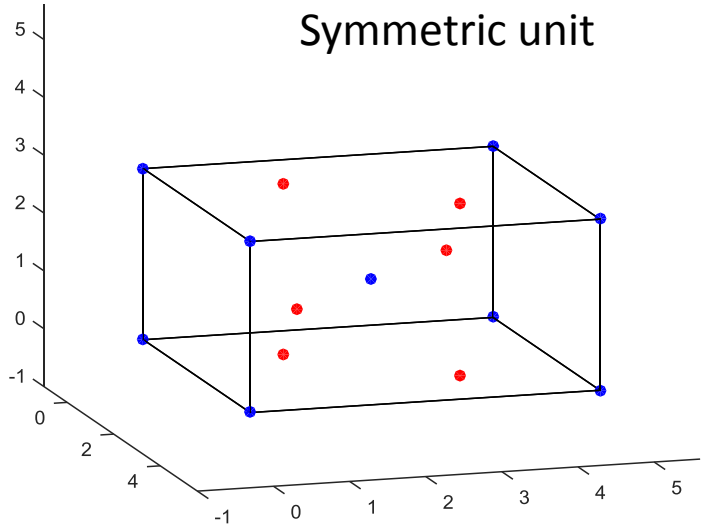
- Download from http://crystallography.net
- Cell parameters a, b, c, α, β, γ, volume, etc.
- Space group symmetry operations
- Cartesian coordinates of the atoms in the asymmetric unit



TiO2

Blue ---> Ti

Red ---> O

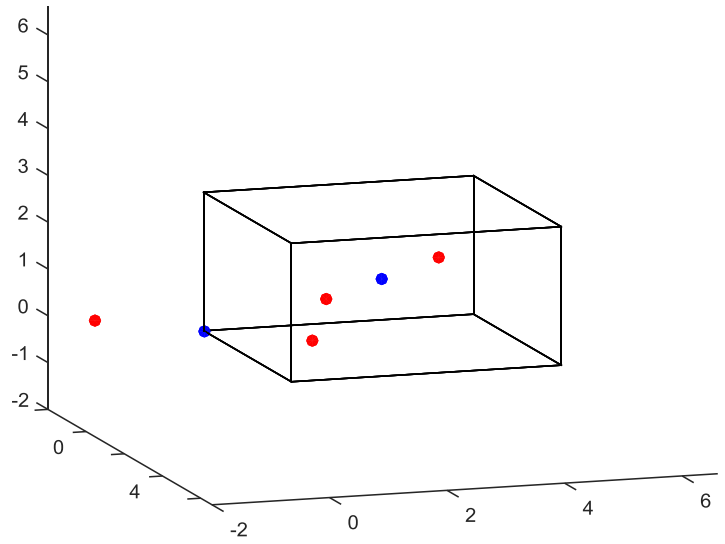


a=b=4.59373 Å, c=2.95812 Å

α=β=γ=90°

5.a Symmetric unit cell

- Apply the given symmetry operations to the atoms of the asymmetric unit with respect to the molecules lattice parameters.
- Atoms that are outside the unit cell should be moved inside.
- Atoms that are on the unit cell's faces should be copied to all parallel faces.
- Atoms that are on an edge should be copied to all edges.



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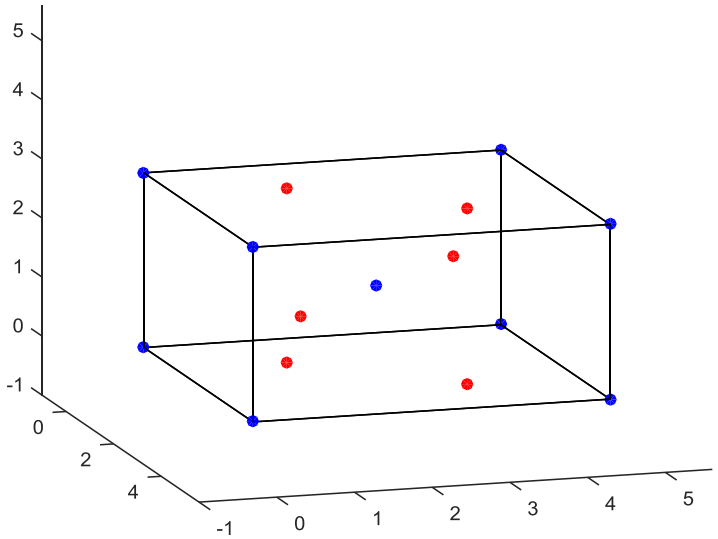
Red ---> O

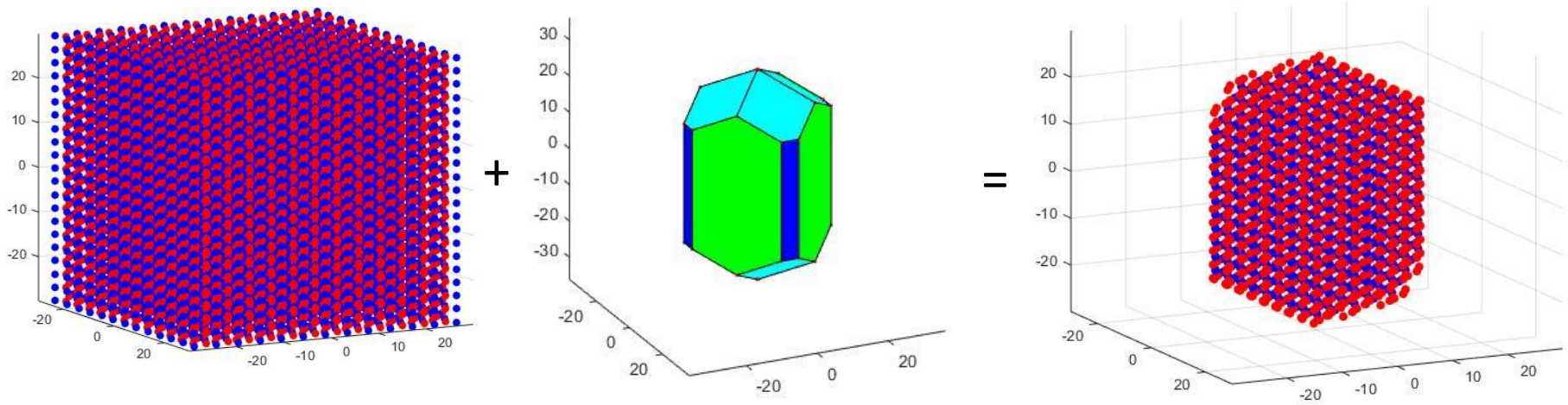


a=b=4.59373 Å, c=2.95812 Å

α=β=γ=90°

6. Replicate unit cell and overlay the Wulff construction

- Replicate unit cell across all directions until it reaches the maximum length x, y and z of its crystal shape
- Remove duplicates
- Keep the atoms that are inside the crystal shape or on it, like we did with the intersection points



Validation: TiO2 crystal shape

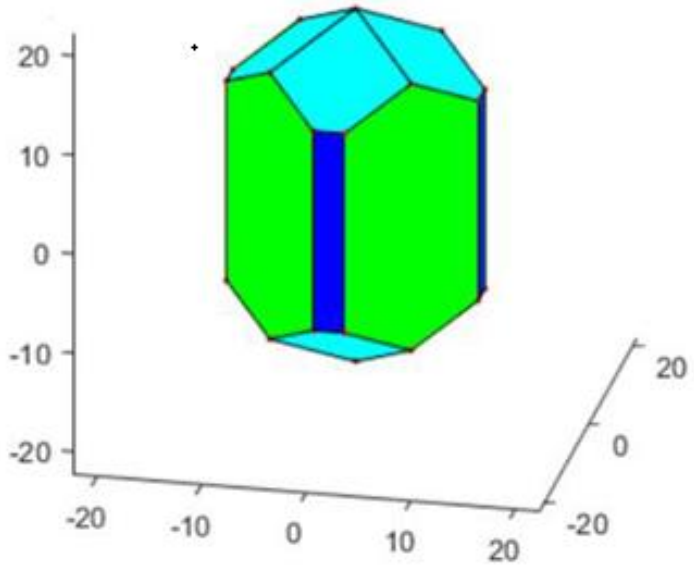
Ramamoorthy, et al., "First-principles calculations of the energetics of stoichiometric TiO 2 surfaces." *Physical Review B* 49.23 (1994): 16721.

a=b=4.59373 Å
c=2.95812 Å
α=β=γ=90°

TABLE VI. Surface atomic coordination and surface energy for several 1×1 surfaces of different orientations. The surface energies are in units of meV/(a.u.^{2}).

Surface	Surface Ti coordination	Surface O coordination	Surface energy (unrelaxed)	Surface energy (relaxed)
(110)	5,6	2,3	30.7	15.6
(100)	5	2	33.8	19.6
(011)	5	2,3	36.9	24.4
(001)	4	2	51.4	28.9

MatLab



Vesta

Validation: TiO2 nanoparticle creation

Ramamoorthy, et al., "First-principles calculations of the energetics of stoichiometric TiO 2 surfaces." *Physical Review B* 49.23 (1994): 16721.

a=b=4.59373 Å,
c=2.95812 Å
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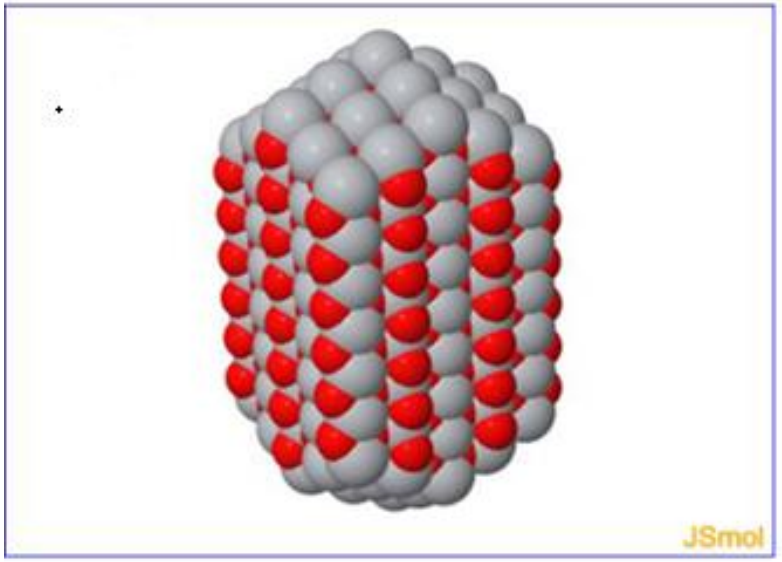
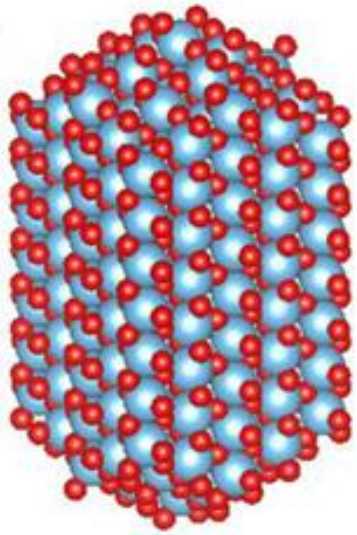
JSmol



Vesta



TiO2

Blue ---> Ti

Red ---> O

Example in Matlab

Ramamoorthy, et al., "First-principles calculations of the energetics of stoichiometric TiO 2 surfaces." *Physical Review B* 49.23 (1994): 16721.

TABLE VI. Surface atomic coordination and surface energy for several 1×1 surfaces of different orientations. The surface energies are in units of meV/(a.u.^{2}).

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(001)	4	2	51.4	28.9

- Calculated from quantum chemistry

http://nanocrystal.vi-seem.eu/CrystalTool

TiO2

Blue ---> Ti

Red ---> O

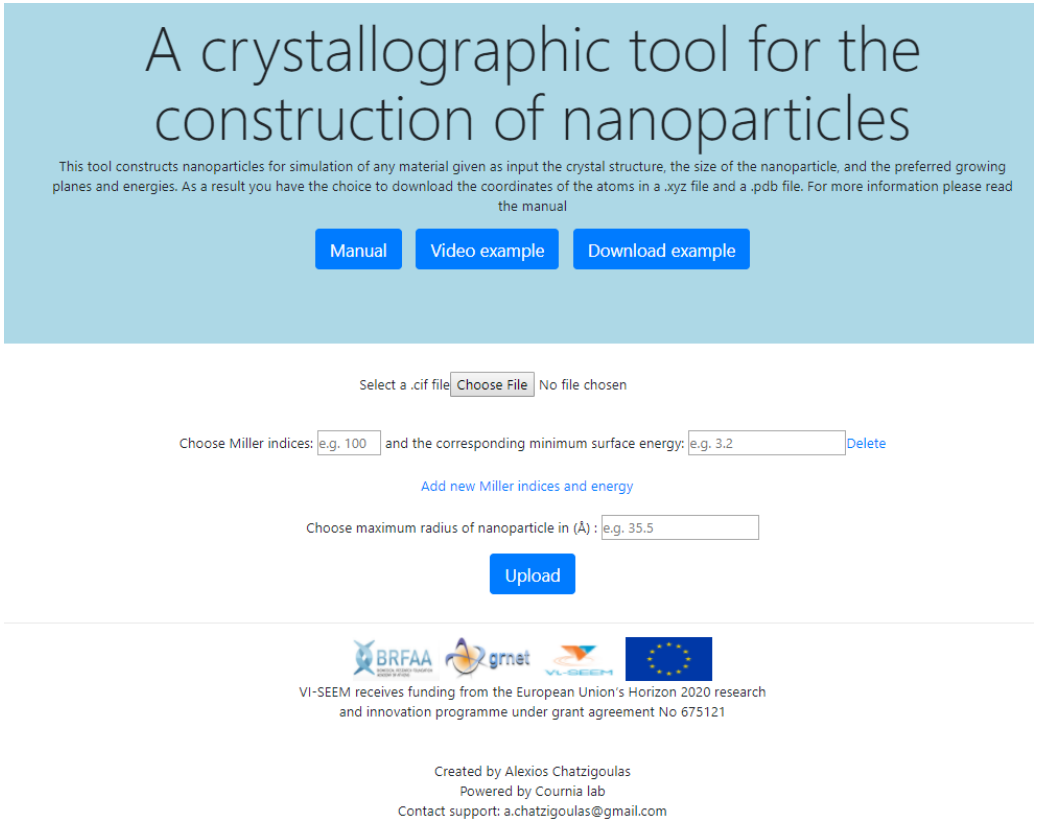
a=b=4.59373 Å, c=2.95812 Å

α=β=γ=90°

Algorithm & web-server implementation

- The algorithm was first programmed in Matlab for visualization purposes and then in C++ for speed and connectability to the web service
- The web service was programmed in PHP

http://nanocrystal.vi-seem.eu/CrystalTool



Conclusions

1. A generalized algorithm was implemented for creating crystal shapes for any kind of symmetry operations, Miller indices and distances based on the crystal preferred growing planes

2. Production and replication of the symmetric unit cell across all directions until it reaches the found crystal shape

3. Programming in MatLab, C++

4. Creation of a web service using PHP giving users a way to use the tool without installation or accounts

http://nanocrystal.vi-seem.eu/CrystalTool

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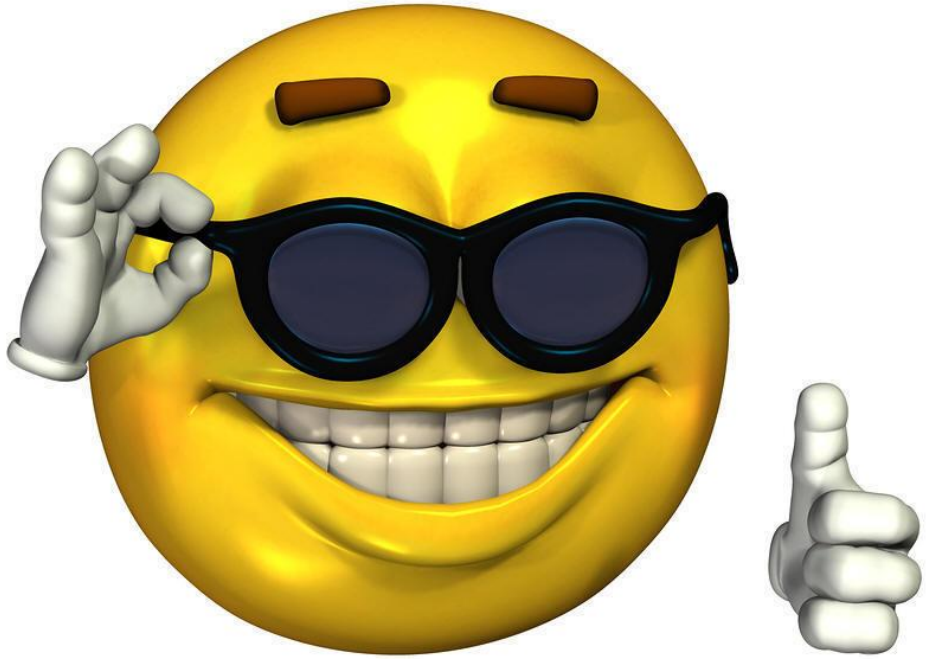
Alexandros Tsegenes, Christina Athanasiou,
Lefteris Mainas, Michalis Lazaratos`

Thank you all!!!



Surface energy

- A crystal will arrange itself such that its surface energy (Gibbs free energy) is minimized by assuming a shape of low surface energy. He defined the quantity:

$$\Delta G_i = \sum_j \gamma_j O_j$$

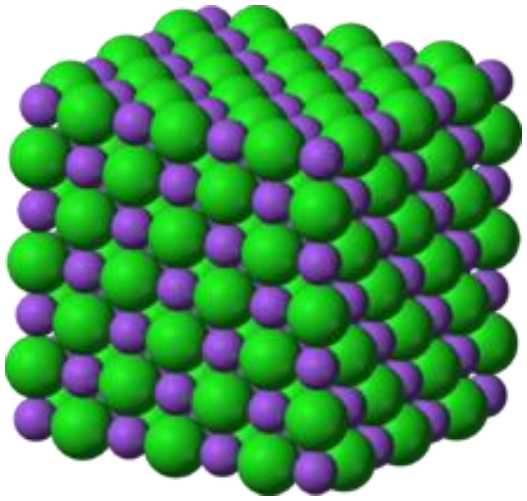
- Here γ_j represents the surface (Gibbs free) energy per unit area of the *j*th crystal face and O_j is the area of said face. ΔG_i represents the difference in energy between a real crystal composed of *i* molecules with a surface and a similar configuration of i molecules located inside an infinitely large crystal. This quantity is therefore the energy associated with the surface. The equilibrium shape of the crystal will then be that which minimizes the value of ΔG_i.

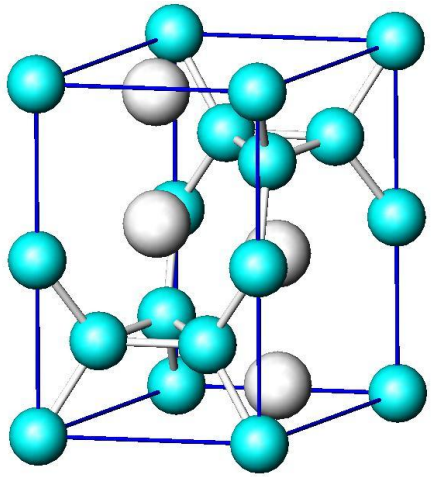
Crystallography

- Crystallography is the experimental science of determining the arrangement of atoms in the crystalline solids.

- A crystal or crystalline solid is a solid material whose constituents (such as atoms, molecules, or ions) are arranged in a highly ordered microscopic structure, forming a crystal lattice that extends in all directions.

- The description of the ordered arrangement of atoms, ions or molecules in a crystalline material is called, crystal structure.



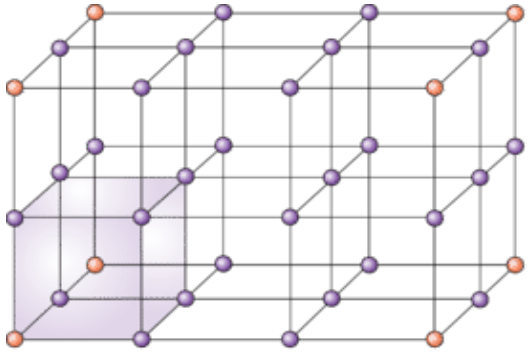


Unit Cell

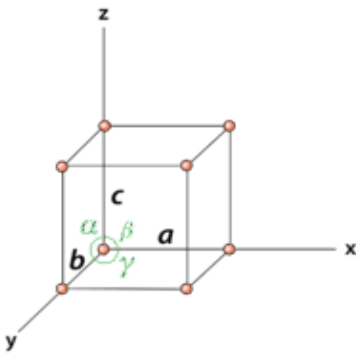
- The smallest group of particles in the material that constitutes the repeating pattern is the **unit cell** of the structure.

- The unit cell completely defines the symmetry and structure of the entire crystal lattice, which is built up by repetitive translation of the unit cell along its principal axes.

- The lengths of the principal axes, or edges, of the unit cell and the angles between them are the lattice constants, also called lattice parameters.



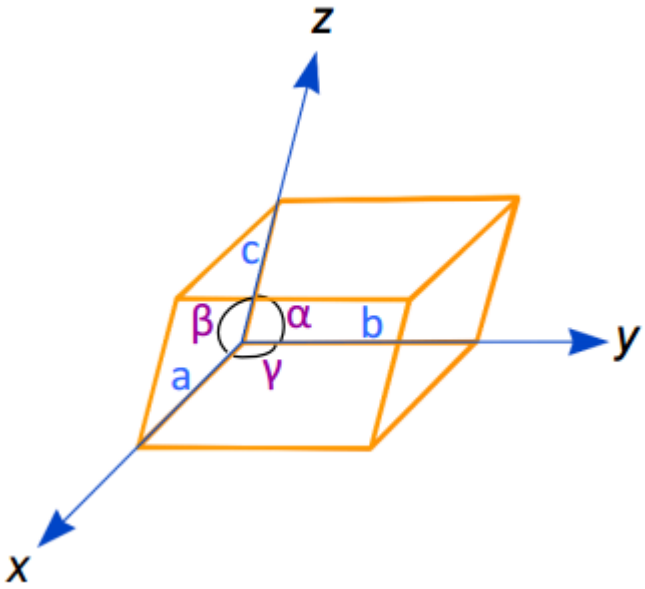
Crystal Lattice

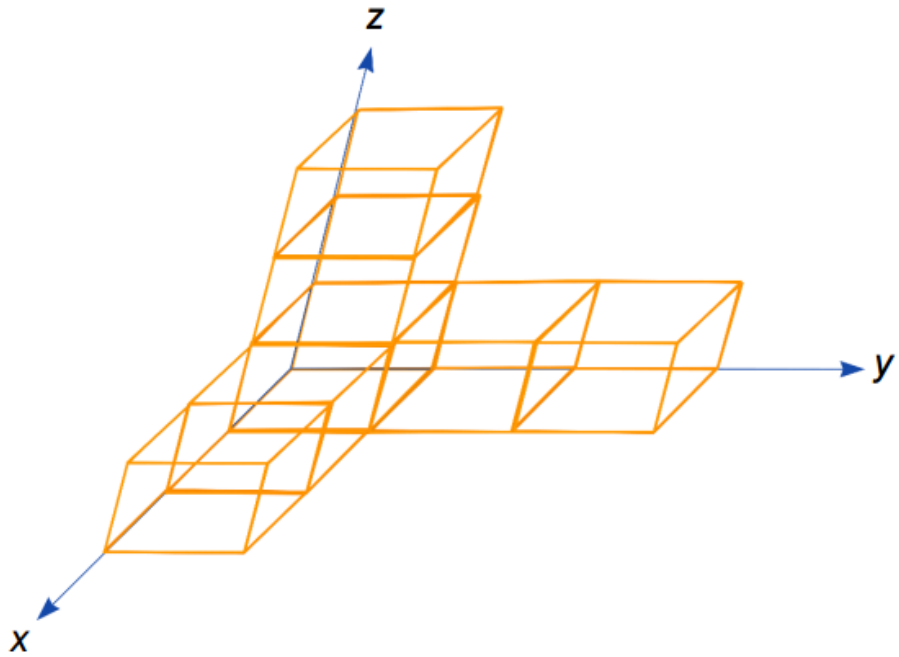


Unit Cell

Unit Cell

- The unit cell is the unit, which builds up the whole crystal structure by repeated translations along all three spatial directions.

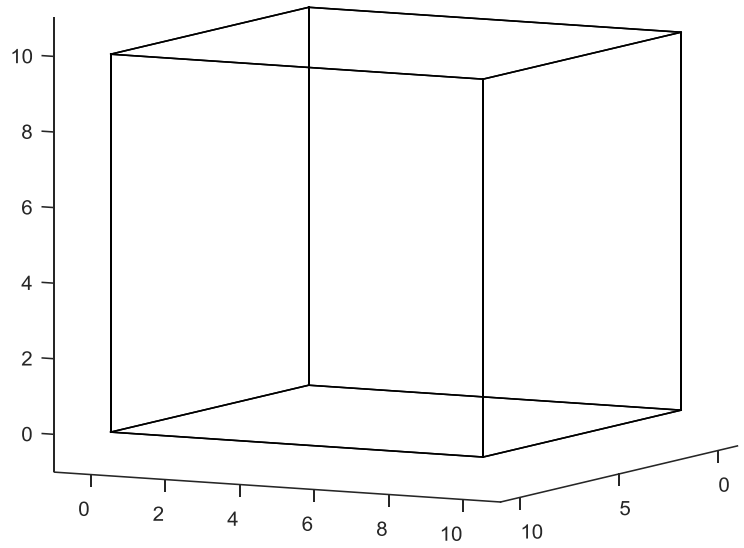




Unit Cell examples

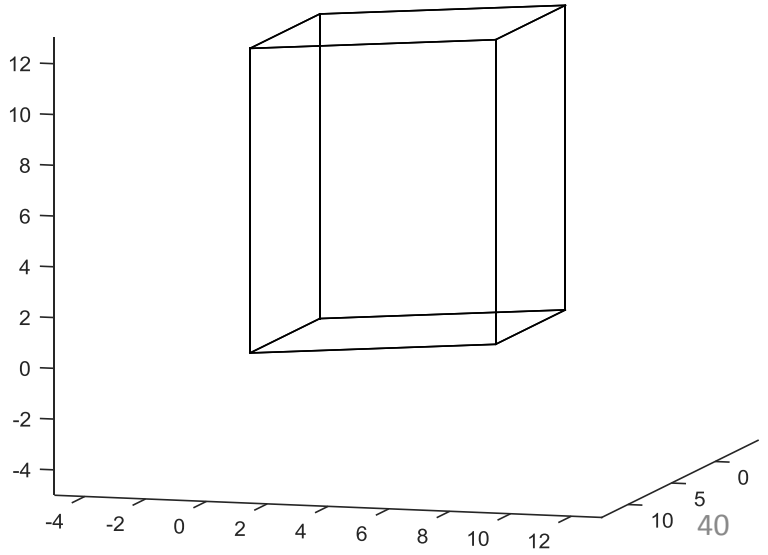
Cubic unit cell

a=b=c=10 Å.
α=β=γ=90°.



Hexagonal unit cell

a=b=8 Å, c=12 Å.
α=β=90°, γ=120°.



Crystal systems

- Every imaginable crystal of the world belongs to one of altogether 7 possible crystal systems.

restrictions for	*cell constants*	*cell angles*
triclinic	none	none
monoclinic	none	$\alpha = \gamma = 90°$
orthorhombic	none	$\alpha = \beta = \gamma = 90°$
tetragonal	a = b	$\alpha = \beta = \gamma = 90°$
trigonal	a = b	$\alpha = \beta = 90°; \gamma = 120°$
hexagonal	a = b	$\alpha = \beta = 90°; \gamma = 120°$
cubic	a = b = c	$\alpha = \beta = \gamma = 90°$

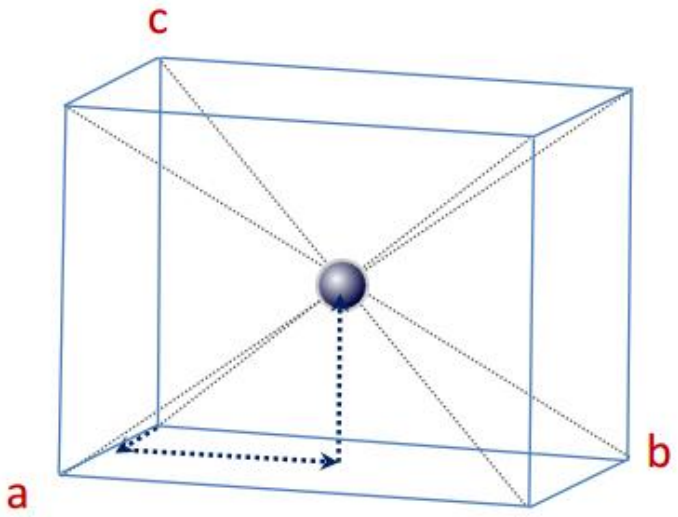
symmetry

hexagonal crystal *family*

Fractional coordinates

- Usage of the crystallographic system of coordinates.
- The lattice constants are used as units.
- The atomic site parameters are given as a coordination triple (x, y, z) and are fractional amounts of the lattice constants (a, b, c) .

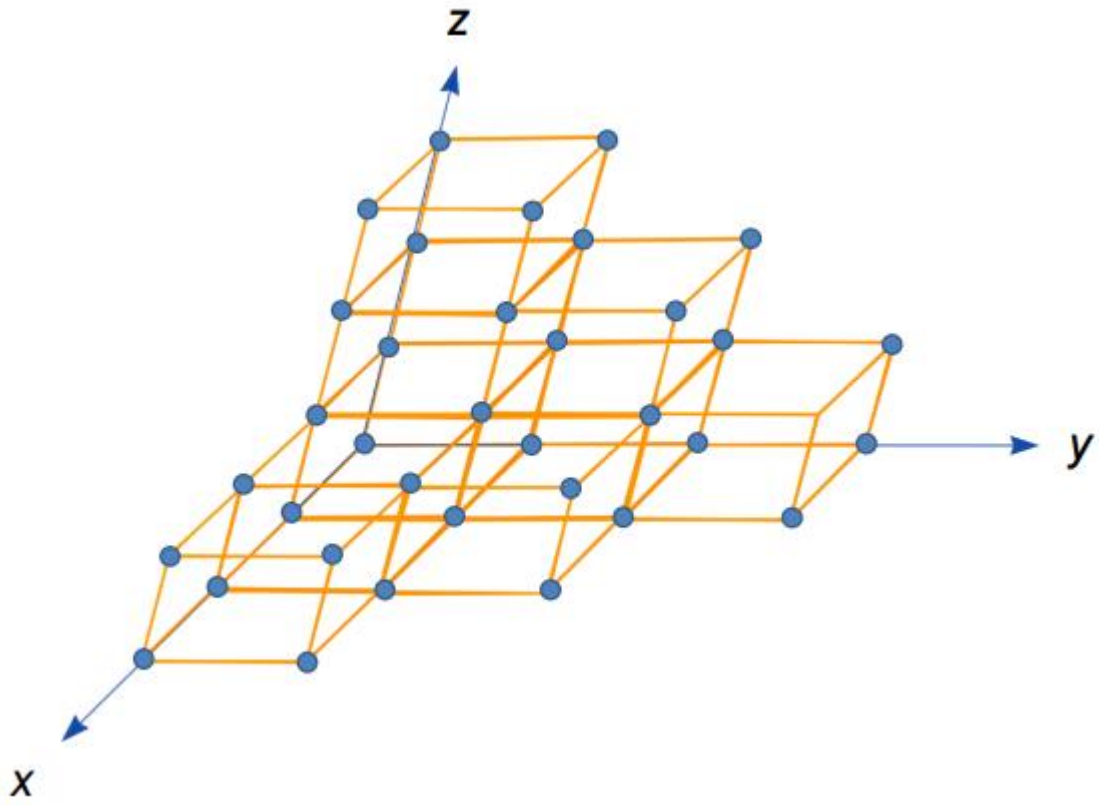
- Example:
- a = 5 Å, b = 20 Å, c = 15 Å
- $\alpha = \beta = \gamma = 90°$
- Atom's fractional coordinates: 0.5, 0.5, 0.5



- Atom's cartesian coordinates: x = 2.5 Å, y = 10 Å, z = 7.5 Å

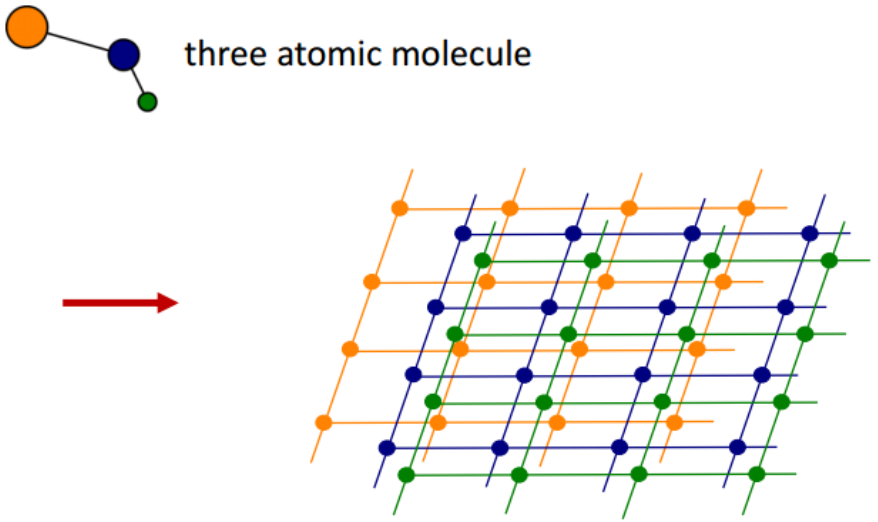
Crystal lattice

- The lattice points are the connection points between the unit cells



Base/Motif

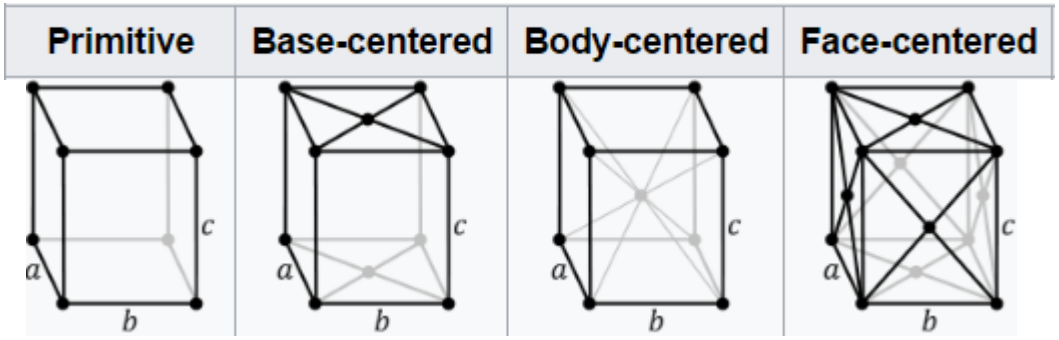
- The motif consists of the arrangement of the building blocks (atoms, molecules) of a unit cell.
- The motif is represented by a lattice point.
- All building blocks of a crystal structure are subject to the same translation principle!



Crystal Structure = Lattice + Base/Motif

Centering types

- Primitive (P): lattice points on the cell corners only.
- Base-centered (A, B, or C): lattice points on the cell corners with one additional point at the center of each face of one pair of parallel faces of the cell.
- Body-centered (I): lattice points on the cell corners with one additional point at the center of the cell.
- Face-centered (F): lattice points on the cell corners with one additional point at the center of each of the faces of the cell.
- Rhombohedrally-centered (R): lattice points on the cell corners with two additional points along the longest body diagonal (only applies for the hexagonal crystal family).



Space groups

Table 1-1

Symbols for the 230 space groups. Notation is described in the text

Triclinic

1. C_1^1 $(P1)$
2. C_i^1 $(P\bar{1})$

Monoclinic

3. C_2^1 $(P2)$
4. C_2^2 $(P2_1)$
5. C_2^3 $(B2)$
6. C_s^1 (Pm)
7. C_s^2 (Pb)
8. C_s^3 (Bm)
9. C_s^4 (Bb)
10. C_{2h}^1 $(P2/m)$
11. C_{2h}^2 $(P2_1/m)$
12. C_{2h}^3 $(B2/m)$
13. C_{2h}^4 $(P2/b)$
14. C_{2h}^5 $(P2_1/b)$
15. C_{2h}^6 $(B2/b)$

Orthorhombic

16. D_2^1 $(P222)$
17. D_2^2 $(P222_1)$
18. D_2^3 $(P2_12_12)$
19. D_2^4 $(P2_12_12_1)$
20. D_2^5 $(C222_1)$
21. D_2^6 $(C222)$
22. D_2^7 $(F222)$
23. D_2^8 $(I222)$
24. D_2^9 $(I2_12_12_1)$
25. C_{2v}^1 $(Pmm2)$
26. C_{2v}^2 $(Pmc2_1)$
27. C_{2v}^3 $(Pcc2)$
28. C_{2v}^4 $(Pma2)$
29. C_{2v}^5 $(Pca2_1)$
30. C_{2v}^6 $(Pnc2)$
31. C_{2v}^7 $(Pmn2_1)$
32. C_{2v}^8 $(Pba2)$
33. C_{2v}^9 $(Pna2_1)$
34. C_{2v}^{10} $(Pnn2)$
35. C_{2v}^{11} $(Cmm2)$
36. C_{2v}^{12} $(Cmc2_1)$
37. C_{2v}^{13} $(Ccc2)$
38. C_{2v}^{14} $(Amm2)$
39. C_{2v}^{15} $(Abm2)$
40. C_{2v}^{16} $(Ama2)$
41. C_{2v}^{17} $(Aba2)$
42. C_{2v}^{18} $(Fmm2)$
43. C_{2v}^{19} $(Fdd2)$
44. C_{2v}^{20} $(Imm2)$
45. C_{2v}^{21} $(Iba2)$
46. C_{2v}^{22} $(Ima2)$
47. D_{2h}^1 $(Pmmm)$
48. D_{2h}^2 $(Pnnn)$
49. D_{2h}^3 $(Pccm)$
50. D_{2h}^4 $(Pban)$
51. D_{2h}^5 $(Pmma)$
52. D_{2h}^6 $(Pnna)$
53. D_{2h}^7 $(Pmna)$
54. D_{2h}^8 $(Pcca)$
55. D_{2h}^9 $(Pbam)$
56. D_{2h}^{10} $(Pccn)$
57. D_{2h}^{11} $(Pbcm)$
58. D_{2h}^{12} $(Pnnm)$
59. D_{2h}^{13} $(Pmmn)$
60. D_{2h}^{14} $(Pbcn)$
61. D_{2h}^{15} $(Pbca)$
62. D_{2h}^{16} $(Pnma)$
63. D_{2h}^{17} $(Cmcm)$
64. D_{2h}^{18} $(Cmca)$
65. D_{2h}^{19} $(Cmmm)$
66. D_{2h}^{20} $(Cccm)$
67. D_{2h}^{21} $(Cmma)$
68. D_{2h}^{22} $(Ccca)$
69. D_{2h}^{23} $(Fmmm)$
70. D_{2h}^{24} $(Fddd)$
71. D_{2h}^{25} $(Immm)$
72. D_{2h}^{26} $(Ibam)$
73. D_{2h}^{27} $(Ibca)$
74. D_{2h}^{28} $(Imma)$

Tetragonal

75. C_4^1 $(P4)$
76. C_4^2 $(P4_1)$
77. C_4^3 $(P4_2)$
78. C_4^4 $(P4_3)$
79. C_4^5 $(I4)$
80. C_4^6 $(I4_1)$
81. S_4^1 $(P\bar{4})$
82. S_4^2 $(I\bar{4})$
83. C_{4h}^1 $(P4/m)$
84. C_{4h}^2 $(P4_2/m)$
85. C_{4h}^3 $(P4/n)$
86. C_{4h}^4 $(P4_2/n)$
87. C_{4h}^5 $(I4/m)$
88. C_{4h}^6 $(I4_1/a)$
89. D_4^1 $(P422)$
90. D_4^2 $(P42_12)$
91. D_4^3 $(P4_122)$
92. D_4^4 $(P4_12_12)$
93. D_4^5 $(P4_222)$
94. D_4^6 $(P4_22_12)$
95. D_4^7 $(P4_322)$
96. D_4^8 $(P4_32_12)$
97. D_4^9 $(I422)$
98. D_4^{10} $(I4_122)$
99. C_{4v}^1 $(P4mm)$
100. C_{4v}^2 $(P4bm)$
101. C_{4v}^3 $(P4_2cm)$
102. C_{4v}^4 $(P4_2nm)$
103. C_{4v}^5 $(P4cc)$
104. C_{4v}^6 $(P4nc)$
105. C_{4v}^7 $(P4_2mc)$
106. C_{4v}^8 $(P4_2bc)$
107. C_{4v}^9 $(I4mm)$
108. C_{4v}^{10} $(I4cm)$
109. C_{4v}^{11} $(I4_1md)$
110. C_{4v}^{12} $(I4_1cd)$
111. D_{2d}^1 $(P\bar{4}2m)$
112. D_{2d}^2 $(P\bar{4}2c)$
113. D_{2d}^3 $(P\bar{4}2_1m)$
114. D_{2d}^4 $(P\bar{4}2_1c)$
115. D_{2d}^5 $(P\bar{4}m2)$
116. D_{2d}^6 $(P\bar{4}c2)$
117. D_{2d}^7 $(P\bar{4}b2)$
118. D_{2d}^8 $(P\bar{4}n2)$
119. D_{2d}^9 $(I\bar{4}m2)$
120. D_{2d}^{10} $(I\bar{4}c2)$
121. D_{2d}^{11} $(I\bar{4}2m)$
122. D_{2d}^{12} $(I\bar{4}2d)$
123. D_{4h}^1 $(P4/mmm)$
124. D_{4h}^2 $(P4/mcc)$
125. D_{4h}^3 $(P4/nbm)$
126. D_{4h}^4 $(P4/nnc)$
127. D_{4h}^5 $(P4/mbm)$
128. D_{4h}^6 $(P4/mnc)$
129. D_{4h}^7 $(P4/nmm)$
130. D_{4h}^8 $(P4/ncc)$
131. D_{4h}^9 $(P4_2/mmc)$
132. D_{4h}^{10} $(P4_2/mcm)$
133. D_{4h}^{11} $(P4_2/nbc)$
134. D_{4h}^{12} $(P4_2/nnm)$
135. D_{4h}^{13} $(P4_2/mbc)$
136. D_{4h}^{14} $(P4_2/mnm)$
137. D_{4h}^{15} $(P4_2/nmc)$
138. D_{4h}^{16} $(P4_2/ncm)$
139. D_{4h}^{17} $(I4/mmm)$
140. D_{4h}^{18} $(I4/mcm)$
141. D_{4h}^{19} $(I4_1/amd)$
142. D_{4h}^{20} $(I4_1/acd)$

Trigonal

143. C_3^1 $(P3)$
144. C_3^2 $(P3_1)$
145. C_3^3 $(P3_2)$
146. C_3^4 $(R3)$
147. C_{3i}^1 $(P\bar{3})$
148. C_{3i}^2 $(R\bar{3})$
149. D_3^1 $(P312)$
150. D_3^2 $(P321)$
151. D_3^3 $(P3_112)$
152. D_3^4 $(P3_121)$
153. D_3^5 $(P3_212)$
154. D_3^6 $(P3_221)$
155. D_3^7 $(R32)$
156. C_{3v}^1 $(P3m1)$
157. C_{3v}^2 $(P31m)$
158. C_{3v}^3 $(P3c1)$
159. C_{3v}^4 $(P31c)$
160. C_{3v}^5 $(R3m)$
161. C_{3v}^6 $(R3c)$
162. D_{3d}^1 $(P\bar{3}1m)$
163. D_{3d}^2 $(P\bar{3}1c)$
164. D_{3d}^3 $(P\bar{3}m1)$
165. D_{3d}^4 $(P\bar{3}c1)$
166. D_{3d}^5 $(R\bar{3}m)$
167. D_{3d}^6 $(R\bar{3}c)$

Hexagonal

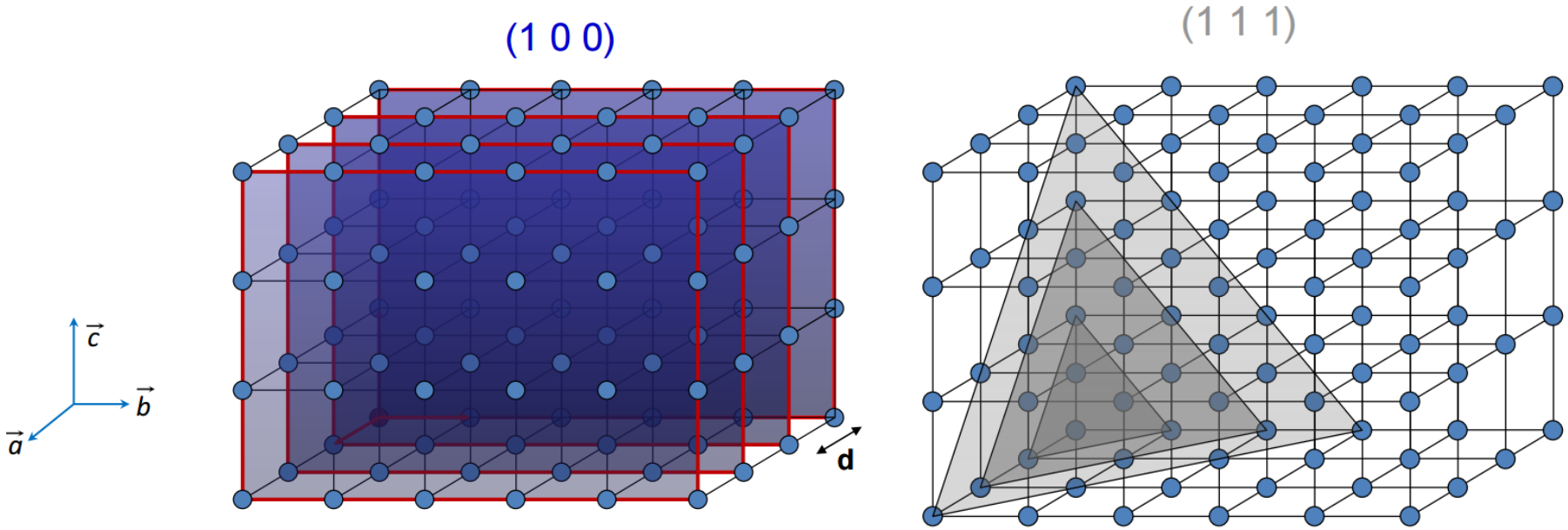
168. C_6^1 $(P6)$
169. C_6^2 $(P6_1)$
170. C_6^3 $(P6_5)$
171. C_6^4 $(P6_2)$
172. C_6^5 $(P6_4)$
173. C_6^6 $(P6_3)$
174. C_{3h}^1 $(P\bar{6})$
175. C_{6h}^1 $(P6/m)$
176. C_{6h}^2 $(P6_3/m)$
177. D_6^1 $(P622)$
178. D_6^2 $(P6_122)$
179. D_6^3 $(P6_522)$
180. D_6^4 $(P6_222)$
181. D_6^5 $(P6_422)$
182. D_6^6 $(P6_322)$
183. C_{6v}^1 $(P6mm)$
184. C_{6v}^2 $(P6cc)$
185. C_{6v}^3 $(P6_3cm)$
186. C_{6v}^4 $(P6_3mc)$
187. D_{3h}^1 $(P\bar{6}m2)$
188. D_{3h}^2 $(P\bar{6}c2)$
189. D_{3h}^3 $(P\bar{6}2m)$
190. D_{3h}^4 $(P\bar{6}2c)$
191. D_{6h}^1 $(P6/mmm)$
192. D_{6h}^2 $(P6/mcc)$
193. D_{6h}^3 $(P6_3/mcm)$
194. D_{6h}^4 $(P6_3/mmc)$

Cubic

195. T^1 $(P23)$
196. T^2 $(F23)$
197. T^3 $(I23)$
198. T^4 $(P2_13)$
199. T^5 $(I2_13)$
200. T_h^1 $(Pm3)$
201. T_h^2 $(Pn3)$
202. T_h^3 $(Fm3)$
203. T_h^4 $(Fd3)$
204. T_h^5 $(Im3)$
205. T_h^6 $(Pa3)$
206. T_h^7 $(Ia3)$
207. O^1 $(P432)$
208. O^2 $(P4_232)$
209. O^3 $(F432)$
210. O^4 $(F4_132)$
211. O^5 $(I432)$
212. O^6 $(P4_332)$
213. O^7 $(P4_132)$
214. O^8 $(I4_132)$
215. T_d^1 $(P\bar{4}3m)$
216. T_d^2 $(F\bar{4}3m)$
217. T_d^3 $(I\bar{4}3m)$
218. T_d^4 $(P\bar{4}3n)$
219. T_d^5 $(F\bar{4}3c)$
220. T_d^6 $(I\bar{4}3d)$
221. O_h^1 $(Pm3m)$
222. O_h^2 $(Pn3n)$
223. O_h^3 $(Pm3n)$
224. O_h^4 $(Pn3m)$
225. O_h^5 $(Fm3m)$
226. O_h^6 $(Fm3c)$
227. O_h^7 $(Fd3m)$
228. O_h^8 $(Fd3c)$
229. O_h^9 $(Im3m)$
230. O_h^{10} $(Ia3d)$

Miller indices

- Miller indices are used to name the crystal faces in a systematic manner, and are also used to denominate lattice planes.
- Miller indices form a notation system for a family of planes and are expressed by three integers: {h k l} such as {100} which contains (100), (010), (001) and the negative of any of those directions.



Cif files

- Contain all the required information of a molecule :
- 1)It's cell's parameters a, b, c, α, β, γ,volume etc.
- 2)It's space group symmetry in fractional coordinates.
- 3)The cartesian coordinates of the asymmetric unit.

```
_journal_page_last                 444
_journal_volume                    1
_journal_year                      1963
_chemical_formula_sum              'O2 Ti'
_chemical_name_mineral             Rutile
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_symmetry_space_group_name_Hall    '-P 4n 2n'
_symmetry_space_group_name_H-M     'P 42/m n m'
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_cell_angle_beta                   90
_cell_angle_gamma                  90
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_cell_length_b                     4.59373
_cell_length_c                     2.95812
_cell_volume                       62.423
_exptl_crystal_density_diffrn      4.250
_[local]_cod_chemical_formula_sum_orig 'Ti O2'
_cod_database_code                 9009083
_amcsd_database_code               AMCSD#0011415
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_symmetry_equiv_pos_as_xyz
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y,x,-z
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1/2-y,1/2+x,1/2+z
1/2+x,1/2-y,1/2+z
1/2-x,1/2+y,1/2-z
x,y,-z
-x,-y,z
y,x,z
-y,-x,-z
1/2-y,1/2+x,1/2-z
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-x,-y,-z
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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Ti 0.00000 0.00000 0.00000
O 0.30530 0.30530 0.00000
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