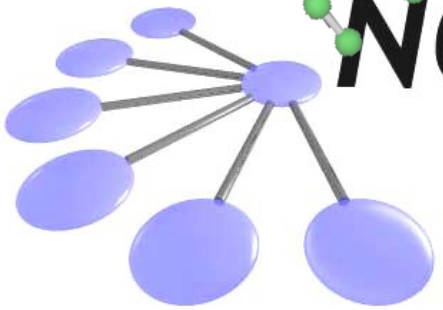
First Time User Guide to

Crystal Viewer Tool

on

nanoHUB.org

NCN



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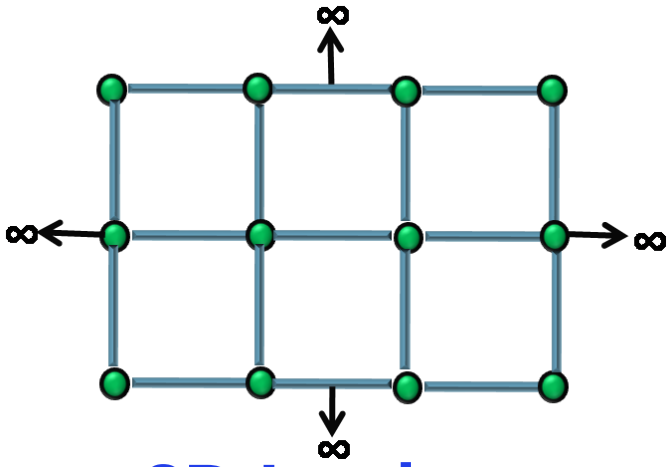
Topics discussed

- What are crystals ?
  - How are they represented ?
- Basics of crystallography :
  - Lattice vectors, primitive cells, unit cell
  - Bravais lattices, Miller indices and planes
- What is Crystal Viewer tool ?
  - Features .
- Capabilities in the tool.
- Types of Inputs.
- What happens when you just hit SIMULATE?
- Example run for a complete simulation.
- Limitations of the tool.
- Few Words About the tool.
- References .
- Appendix

What are crystals ?

- *Crystals are*
  - » Periodic arrangement of atoms in space (**called Lattice**).
- Simplest periodic block can be a single atom
  - » Eg: Copper, Gold, Silver, Iron, etc.

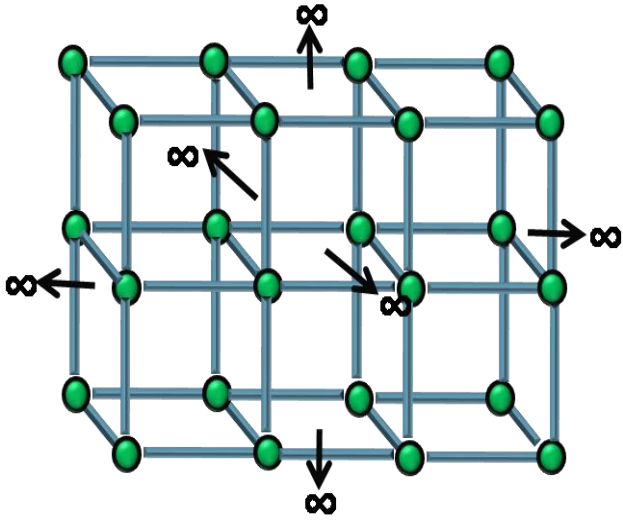
1D Lattice



2D Lattice

Atoms can be arranged periodically in 1, 2 and 3 D to produce

CRYSTALs

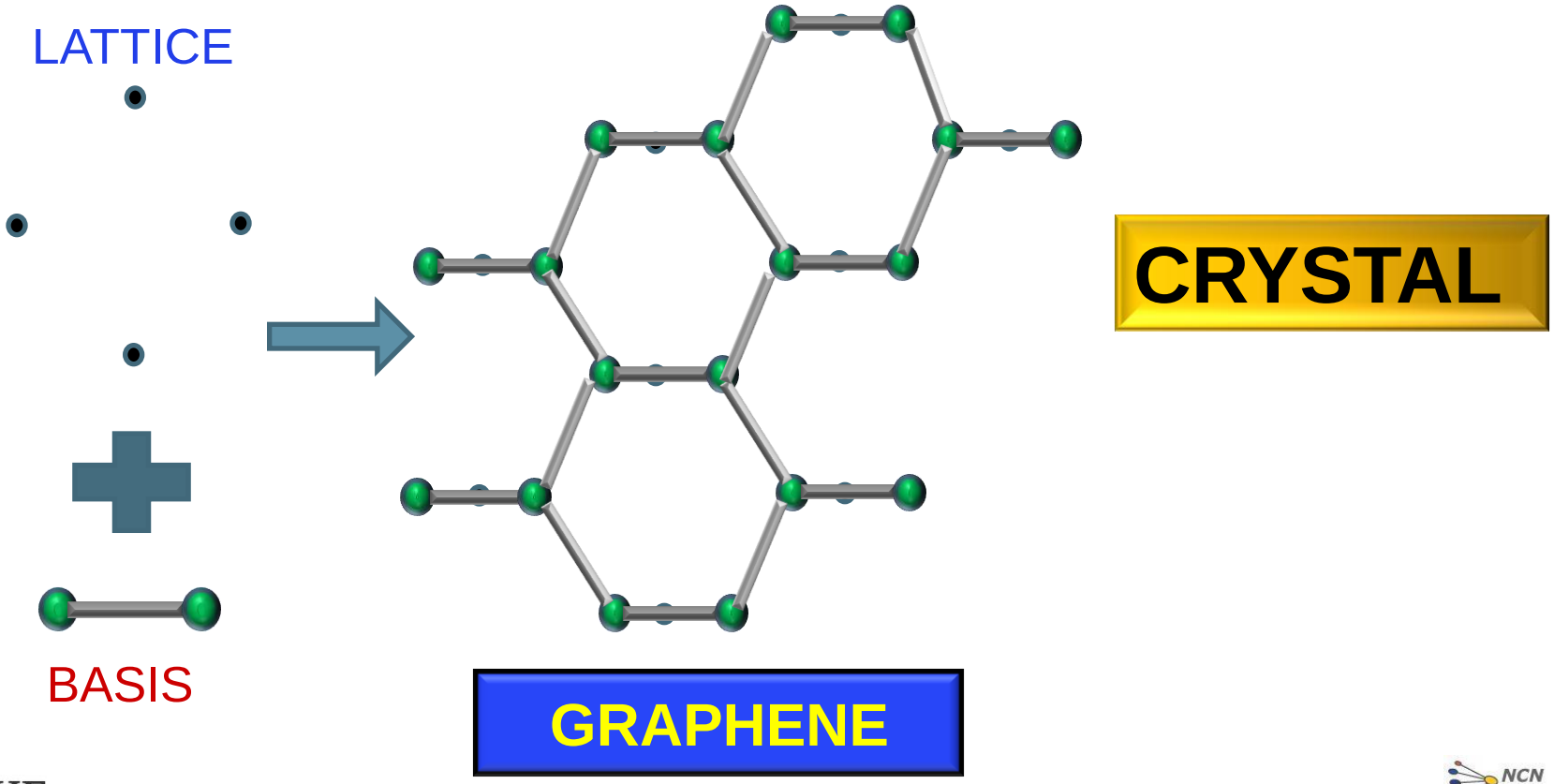


3D Lattice

Images obtained from Crystal Viewer tool on nanoHUB.org

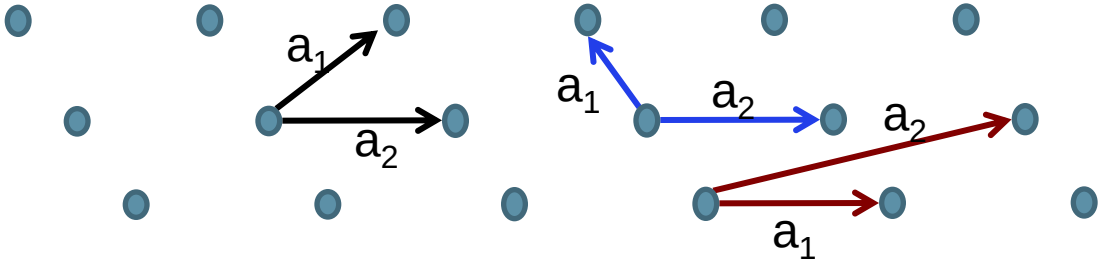
Representation of Crystals

- Crystal is represented by
  - » **Lattice :** Points in space repeated periodically
  - » **Basis :** Group of atoms repeated each lattice point.



Steps to construct a crystal

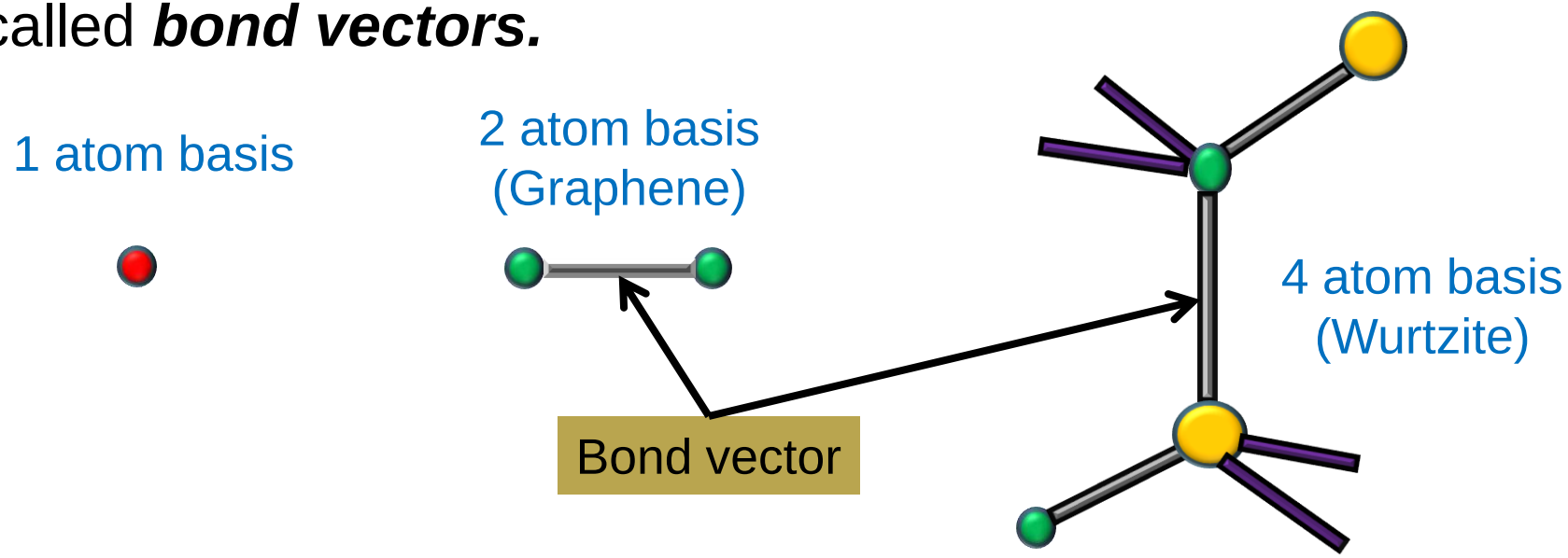
- Basis & Lattice together form the crystal.
- A basis can have one or more than one atom
  - » In the last slide basis had 2 atoms.
- Translate the basis in the space (at lattice points) to obtain the crystal structure.
  - » $T = La_1 + Ma_2 + Na_3$ T = Translational vector. L,M,N => integers
- a_1, a_2 & a_3 are called Lattice vectors.
- Lattice Vectors are not necessarily ***unique.***



Three different lattice vectors produce the same lattice structure.

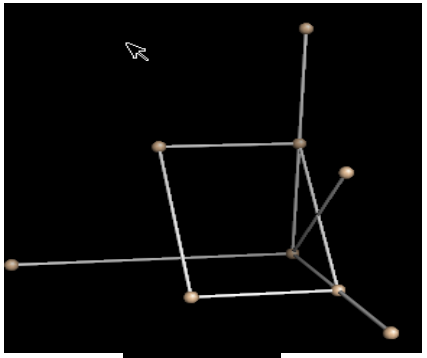
Crystallography : About the Basis…

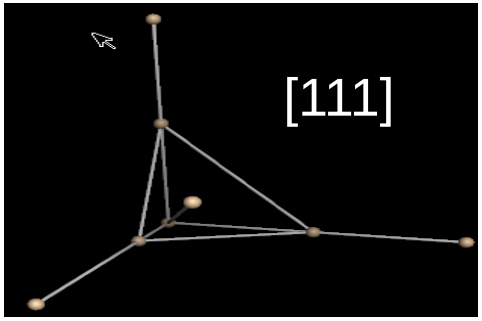
- Basis : Can be as simple as one atom, or a complex many atom system.
- Basis is also called a ***unit cell*** or simply a ***cell.***
- Unit cell with minimum volume is a ***Primitive cell.***
- In complex cells atoms are linked together using vectors called ***bond vectors.***



Miller Planes and Indices

- Miller indices are method to describe :
  - » planes and directions in crystals.
- Indices are denoted using l, m, n along x,y,z respectively.
  - » These are inverse of intercepts on the x,y,z axis.
  - » Convert these into full integers.
  - » **Eg: intercept (3,2,6) => l,m,n = 6X(1/3,1/2,1/6) = (2,3,1).**
- (lmn) represents a miller plane along direction l,m,n.
- [lmn], denotes a direction in the basis of direct lattice.
- <lmn> denotes direction that are eqv. to [lmn].
- {lmn} denotes the family of planes eqv. to (lmn).
- Negative integers are represented by with a bar on the number.



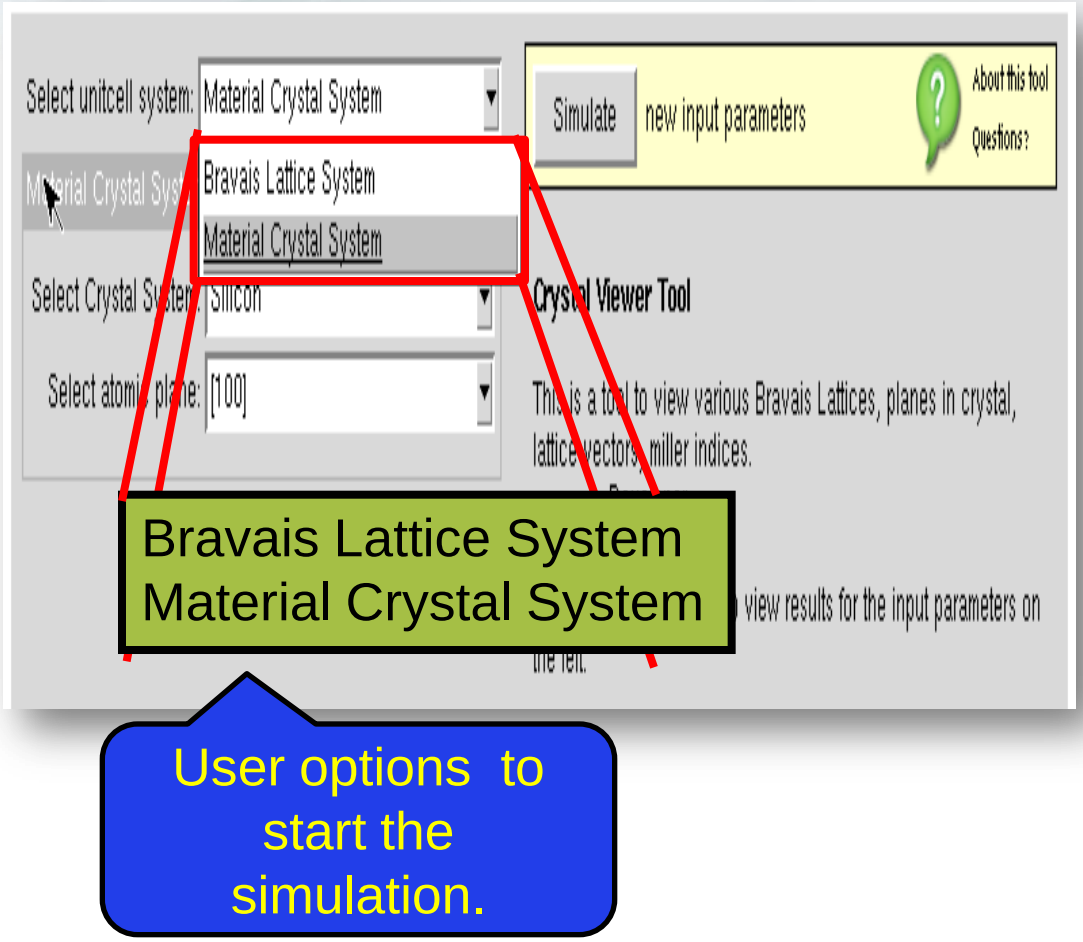


Images obtained from Crystal Viewer tool on nanoHUB.org

What is Crystal Viewer Tool ?

- Crystal Viewer Tool :
  - »A MATLAB® based.
  - »Used for visualization of :
    - ✓ Different material crystals.
    - ✓ Different Bravais Lattices.
  - »Provides information about miller indices and planes.
  - »Provides information about crystals.
  - »Tool has been developed at Purdue University.
    - ✓ Part of the teaching tools on nanoHUB.org.
- Developers : (version 1.23)
  - »Abhijeet Paul / Purdue University.
  - »Gerhard Klimeck / Purdue University.

Crystal Viewer Tool : First look

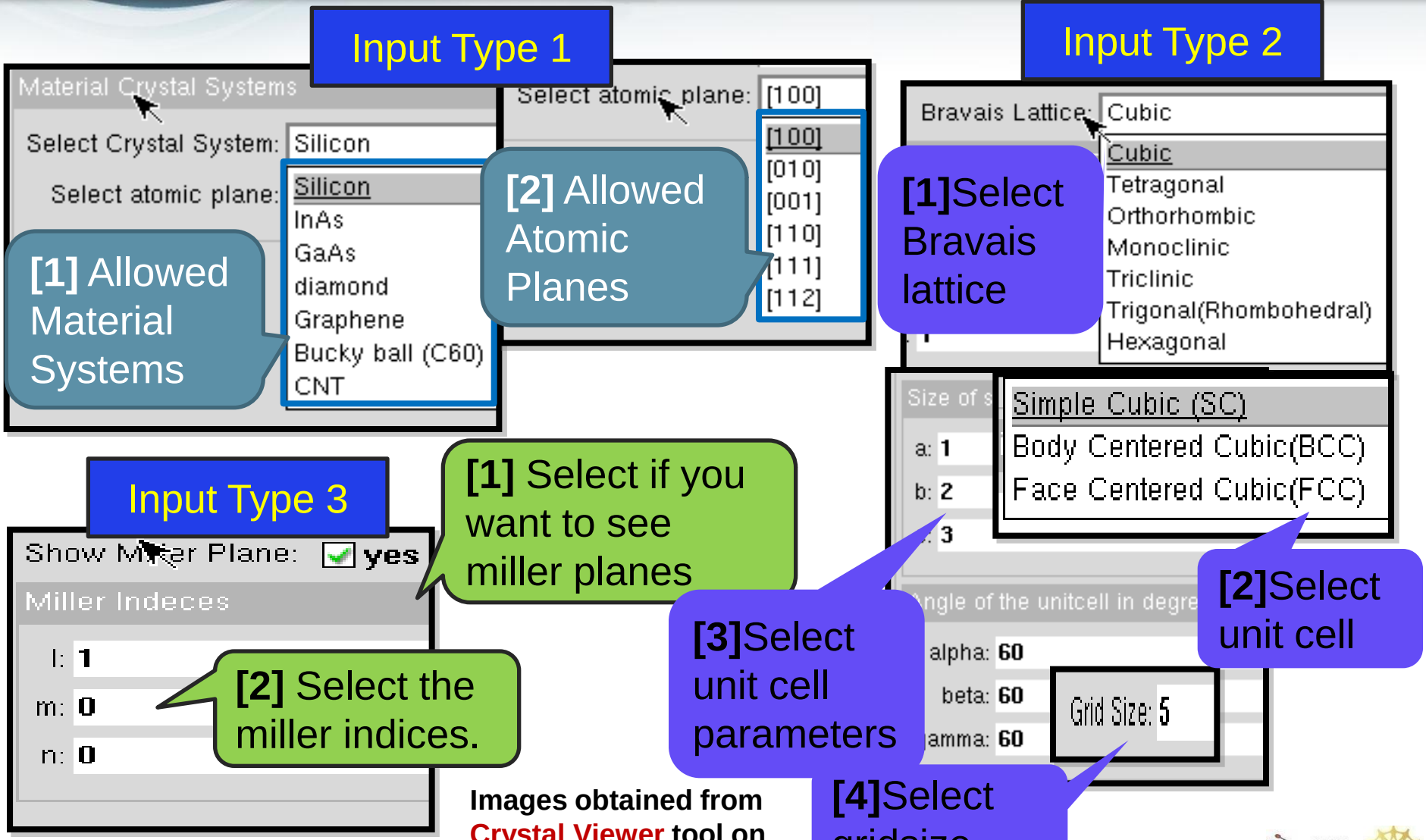


Capabilities of the tool :

- ✓ Visualize Bravais lattices.
- ✓ Visualize larger grids.
- ✓ Visualize miller planes.
- ✓ Visualize material crystals.
- ✓ Visualize atomic planes.
- ✓ Obtain crystal information.

Check out the tool webpage for latest updates, features and bug fixes at : : http://nanohub.org/resources/crystal_viewer

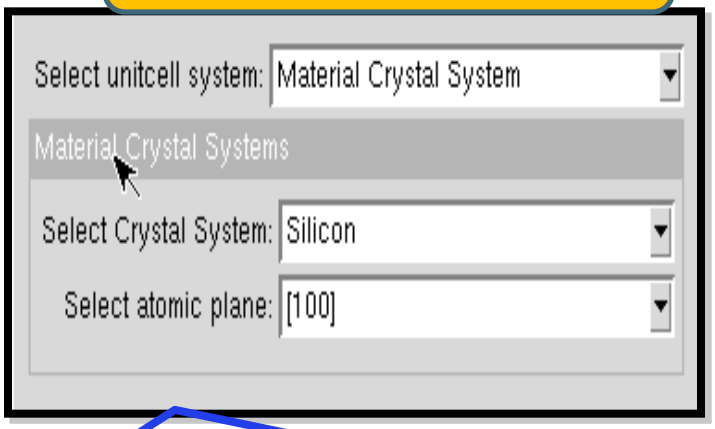
Types of Inputs



Images obtained from Crystal Viewer tool on nanoHUB.org

What happens when you just hit SIMULATE?

Default Inputs



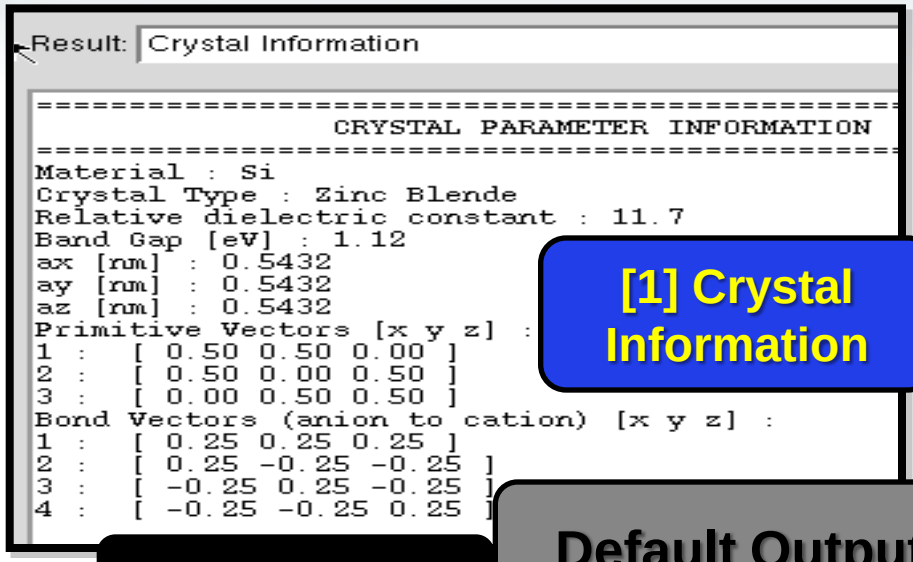
Runs with the following default inputs:

[Select unitcell system]: Material Crystal System.

[Select Crystal Material]: Silicon

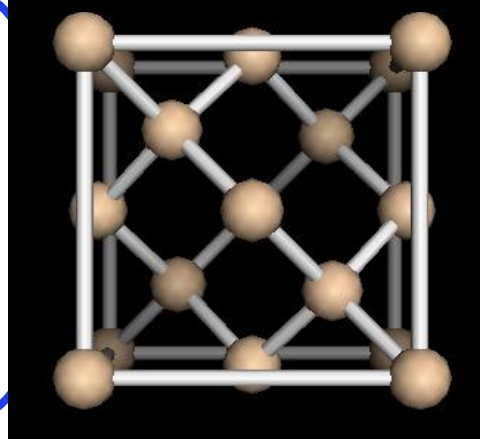
[Select atomic plane]: [100]

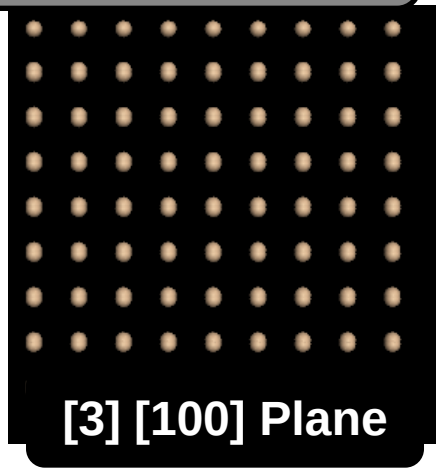
Default Outputs



[1] Crystal Information

[2] Unitcell





[3] [100] Plane

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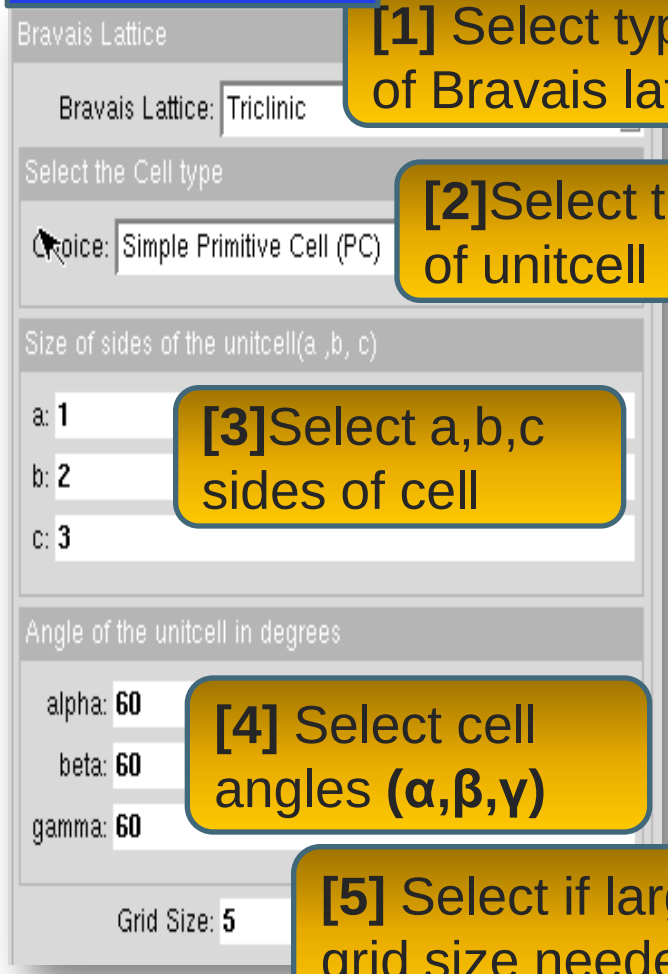
Images obtained from Crystal Viewer tool on nanoHUB.org

Bravais lattice simulation : Input to Output

INPUTs



[1] Select type of Bravais lattice

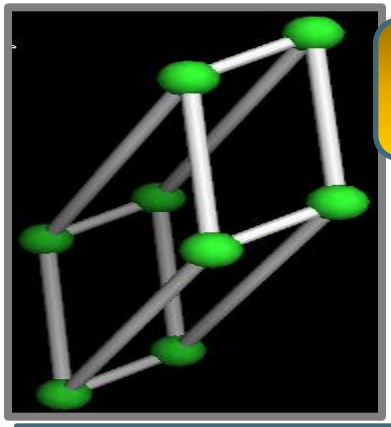
[2]Select the type of unitcell

[3]Select a,b,c sides of cell

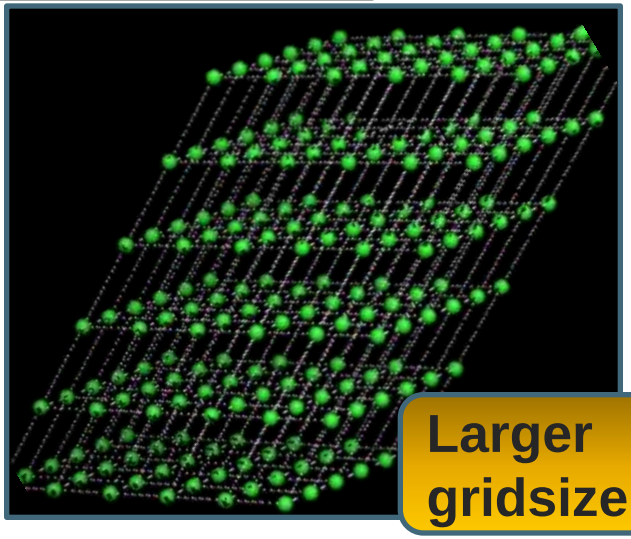
[4] Select cell angles **(α,β,γ)**

[5] Select if larger (>1) grid size needed.

OUTPUTs



Triclinic unitcell



Larger gridsize

Images obtained from Crystal Viewer tool on nanoHUB.org

Limitations of the tool

- Visualization of miller planes is not very good
  - »normal vector and plane are not very helpful.
    - ✓ work is underway to improve this.
- Cannot take cut planes in the larger crystal systems.
- Improvement in atomic plane visualization needed.

Always keep checking the tool web-page for latest features, releases and bug-fixes at : http://nanohub.org/tools/crystal_viewer

Few words regarding the tool

- Use this tool to learn about crystals.
- Feel free to post about
  - »the bugs
  - »new features you want.
- Contact the developers in case you want to collaborate for some work using this tool.

Always keep checking the tool web-page for latest features, releases and bug-fixes at : http://nanohub.org/tools/crystal_viewer

References

- URLs on crystal information, miller index & Bravais lattice
  - »http://cst-www.nrl.navy.mil/lattice/
  - »http://en.wikipedia.org/wiki/Bravais_lattice
  - »http://serc.carleton.edu/research_education/crystallography/xldatabases.html
  - »http://webmineral.com/
  - »http://en.wikipedia.org/wiki/Miller_index
- Books to read about crystals
  - » Kittel, Charles (1996) [1953].Introduction to Solid State Physics (Seventh Edition ed.). New York: John Wiley & Sons. pp. 10. ISBN 0-471-11181-3. http://www.wiley.com/

References

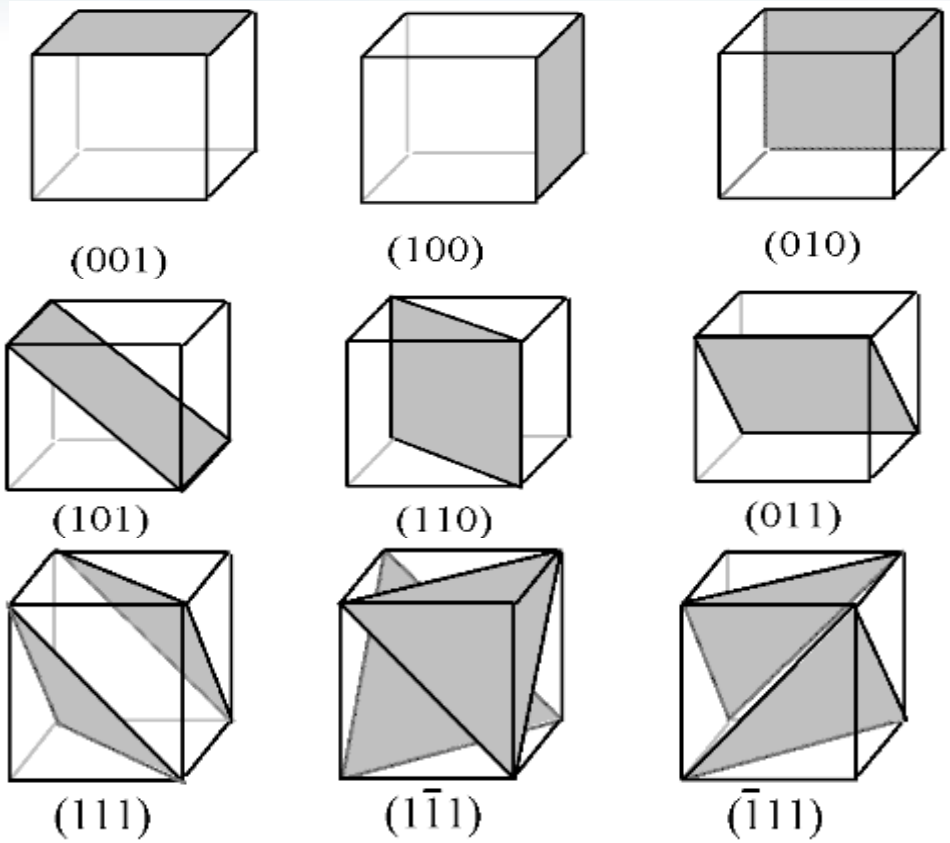
- Homework assignment using the tool.
  - » https://nanohub.org/resources/4200
- Link for the tool :
  - » http://nanohub.org/resources/crystal_viewer

Appendix A : Bravais lattices

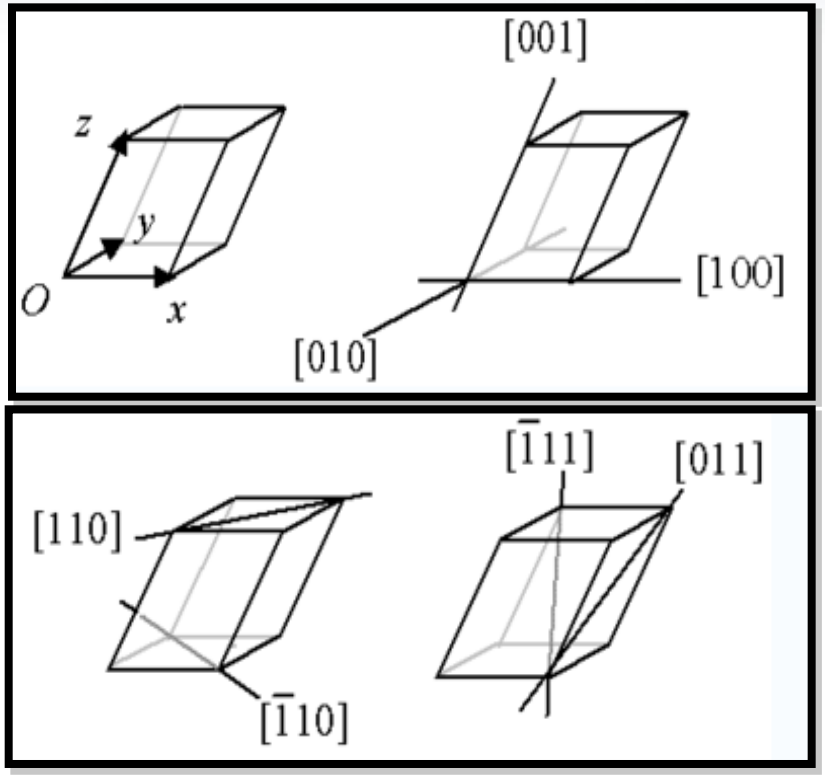
Distance Parameters (a, b, c)	Angle Parameters (α,β,γ)	Name	No. of Lattices / Types	Example
a = b = c	$\alpha = \beta = \gamma = 90^0$	Cubic	**3** S,B,F	CsCl, NaCl
a = b ≠ c	$\alpha = \beta = \gamma = 90^0$	Tetragonal	**2** S,B	TiO_2 (Rutile), SnO_2 (Cassiterite)
a ≠ b ≠ c	$\alpha = \beta = \gamma = 90^0$	Orthorhombic	4 S,B,E,F	KNO_3, $BaSO_4$ (Baryte)
a = b = c	$\alpha = \beta = \gamma < 120^0 \neq 90^0$	Rhombohedral (Trigonal)	1 S	Ice, Al_2O_3
a = b ≠ c	$\alpha = \beta = 90^0$; $\gamma = 120^0$	Hexagonal	1 S	Mg, Zn, PbI_2
a ≠ b ≠ c	$\alpha = \gamma = 90^0$; $\beta \neq 90^0$	Monoclinic	2 S,E	Monoclinic Sulphur, $Na_2SO_4.10H_2O$
a ≠ b ≠ c	$\alpha \neq \beta \neq \gamma \neq 90^0$	Triclinic	1 S	$CuSO_4.5H_2O$

S: simple B: body centered F: face centered E: end face centered

Appendix B: Miller Planes & Directions



Some Important Miller planes



Some Important Miller directions

Images from **http://en.wikipedia.org/wiki/Miller_index** Author: **Christophe Dang Ngoc Chan**