First Time User Guide to Crystal Viewer Tool on nanoHUB.org

Abhijeet Paul, Gerhard Klimeck & Ben Haley
NCN @Purdue University
West Lafayette, IN 47906, USA
• 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
• **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**

**3D Lattice**

Images obtained from Crystal Viewer tool on [nanoHUB.org](http://nanoHUB.org)
• 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.
  
  » \( T = L \mathbf{a}_1 + M \mathbf{a}_2 + N \mathbf{a}_3 \)  
  
  \( T \) = Translational vector. \( L,M,N \Rightarrow \) integers

• \( \mathbf{a}_1, \mathbf{a}_2 \) & \( \mathbf{a}_3 \) are called **Lattice vectors**.

• Lattice Vectors are not necessarily **unique**.

Three different lattice vectors produce the same lattice structure.

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• 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**.

1 atom basis

2 atom basis (Graphene)

4 atom basis (Wurtzite)

Bond vector
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 $(3, 2, 6) \Rightarrow l, m, n = 6 \times (1/3, 1/2, 1/6) = (2, 3, 1)$.

$(l,m,n)$ represents a miller plane along direction $l,m,n$.

$[l,m,n]$, denotes a direction in the basis of direct lattice.

$\langle l,m,n \rangle$ denotes direction that are eqv. to $[l,m,n]$.

$\{l,m,n\}$ denotes the family of planes eqv. to $(l,m,n)$.

Negative integers are represented by with a bar on the number.
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.
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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

Images obtained from Crystal Viewer tool on nanoHUB.org
Types of Inputs

Input Type 1

- Silicon
- InAs
- GaAs
- diamond
- Graphene
- Bucky ball (C60)
- CNT

- [100]
- [010]
- [001]
- [110]
- [111]
- [112]

Input Type 2

[1] Select Bravais lattice
- Cubic
- Tetragonal
- Orthorhombic
- Monoclinic
- Triclinic
- Trigonal (Rhombohedral)
- Hexagonal

[2] Select unit cell
- Simple Cubic (SC)
- Body Centered Cubic (BCC)
- Face Centered Cubic (FCC)

Input Type 3

[1] Select if you want to see miller planes
[2] Select the miller indices
- I: 1
- m: 0
- n: 0

[3] Select unit cell parameters
- alpha: 60
- beta: 60
- gamma: 60

[4] Select gridsize
- Grid Size: 5

Images obtained from Crystal Viewer tool on nanoHUB.org

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nanoHUB online simulation and more
What happens when you just hit SIMULATE?

**Default Inputs**

- Select unitcell system: Material Crystal System
- Select Crystal System: Silicon
- Select atomic plane: [100]

**Default Outputs**

1. **Crystal Information**
   - Material: Si
   - Crystal Type: Zinc Blende
   - Relative dielectric constant: 11.7
   - Band Gap [eV]: 1.12
   - \( a_x \) [nm]: 0.5432
   - \( a_y \) [nm]: 0.5432
   - \( a_z \) [nm]: 0.5432
   - Primitive Vectors \([x \ y \ z]\):
     - 1: [0.50 0.50 0.00]
     - 2: [0.50 0.00 0.50]
     - 3: [0.00 0.50 0.50]
   - Bond Vectors (anion to cation) \([x \ y \ z]\):
     - 1: [0.25 0.25 0.25]
     - 2: [0.25 -0.25 -0.25]
     - 3: [-0.25 0.25 -0.25]
     - 4: [-0.25 -0.25 0.25]

**Runs with the following default inputs:**
- [Select unitcell system]: Material Crystal System.
- [Select Crystal Material]: Silicon
- [Select atomic plane]: [100]

Images obtained from Crystal Viewer tool on [nanoHUB.org](http://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
• URLs on crystal information, miller index & Bravais 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
• Homework assignment using the tool.
  » https://nanohub.org/resources/4200

• Link for the tool:
  » http://nanohub.org/resources/crystal_viewer
# Appendix A: Bravais lattices

<table>
<thead>
<tr>
<th>Distance Parameters ((a, b, c))</th>
<th>Angle Parameters ((\alpha, \beta, \gamma))</th>
<th>Name</th>
<th>No. of Lattices / Types</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a = b = c)</td>
<td>(\alpha = \beta = \gamma = 90^0)</td>
<td>Cubic</td>
<td>3 S,B,F</td>
<td>CsCl, NaCl</td>
</tr>
<tr>
<td>(a = b \neq c)</td>
<td>(\alpha = \beta = \gamma = 90^0)</td>
<td>Tetragonal</td>
<td>2 S,B</td>
<td>TiO\textsubscript{2} (Rutile), SnO\textsubscript{2} (Cassiterite)</td>
</tr>
<tr>
<td>(a \neq b \neq c)</td>
<td>(\alpha = \beta = \gamma = 90^0)</td>
<td>Orthorhombic</td>
<td>4 S,B,E,F</td>
<td>KNO\textsubscript{3}, BaSO\textsubscript{4} (Baryte)</td>
</tr>
<tr>
<td>(a = b = c)</td>
<td>(\alpha = \beta = \gamma &lt;120^0\neq 90^0)</td>
<td>Rhombohedral (Trigonal)</td>
<td>1 S</td>
<td>Ice, Al\textsubscript{2}O\textsubscript{3}</td>
</tr>
<tr>
<td>(a = b \neq c)</td>
<td>(\alpha = \beta = 90^0;\gamma = 120^0)</td>
<td>Hexagonal</td>
<td>1 S</td>
<td>Mg, Zn, PbI\textsubscript{2}</td>
</tr>
<tr>
<td>(a \neq b \neq c)</td>
<td>(\alpha = \gamma = 90^0;\beta \neq 90^0)</td>
<td>Monoclinic</td>
<td>2 S,E</td>
<td>Monoclinic Sulphur, Na\textsubscript{2}SO\textsubscript{4}.10H\textsubscript{2}O</td>
</tr>
<tr>
<td>(a \neq b \neq c)</td>
<td>(\alpha \neq \beta \neq \gamma \neq 90^0)</td>
<td>Triclinic</td>
<td>1 S</td>
<td>CuSO\textsubscript{4}.5H\textsubscript{2}O</td>
</tr>
</tbody>
</table>

S: simple    B: body centered    F: face centered    E: end face centered
Some Important Miller planes

Images from [http://en.wikipedia.org/wiki/Miller_index](http://en.wikipedia.org/wiki/Miller_index) Author: Christophe Dang Ngoc Chan