

Crystal Viewer Lab Exercise

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Exercise Background

A central problem in the investigation of material properties involves the examination of the underlying blocks that aggregate to form macroscopic bodies. These underlying blocks own a definite arrangement that is repeated in three dimensions to give the crystal structure. We will try to explore the geometry of some well known class of materials (e.g., diamond, zinc-blende, wurtzite etc,) and learn techniques of identifying planes (Miller indices) and directions in these crystal structures. Finally, we will see that the crystals are provided with a certain symmetry which is reflected in their physical properties.

Exercise Objectives

We will use these arguments when we learn more about the electronic structure of materials in a separate assignment.

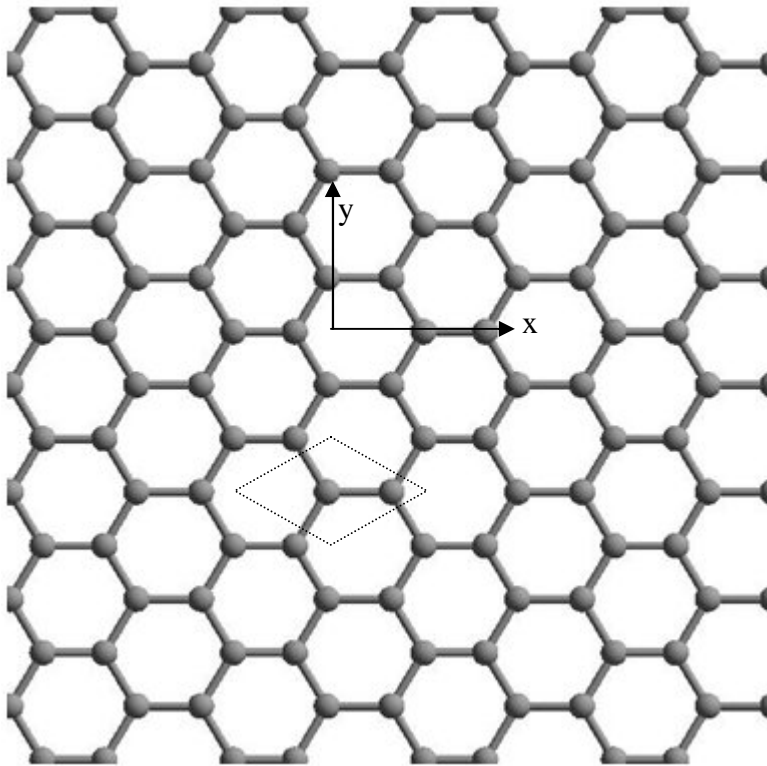
Relevant Literature

A few useful books to learn more about crystals are given below:

1. Martin. T. Dove, *Structure and Dynamics: An Atomic View of Materials*, Oxford University Press, (2003).
2. N. Ashcroft, D. Mermin, *Solid State Physics*, Brooks/Cole (1976), Chapter 7.

Exercise:

1. Graphene is a 2D crystal with carbon atoms arranged in a honeycomb structure as shown below.



- a) Assuming that the unit cell is a hexagon of carbon atoms, determine how many carbon atoms are there per unit cell. What is the basis vectors needed to reproduce the whole 2D crystal? If a_{CC} is the carbon-carbon spacing. Verify that the basis vectors are of the same length in this case.
- b) The dashed area in the figure above is often given as the primitive unit cell for graphene. a) determine the basis vectors for this unit cell, and b) determine the area of this unit cell and compare it to that of the hexagon in part 1a) and comment.

2. Directions in a crystal

- a) Prove that the $[h\ k\ l]$ *direction* is normal to the $(h\ k\ l)$ *plane* in a cubic system.
- b) Show that the angle between two planes (or two directions) is

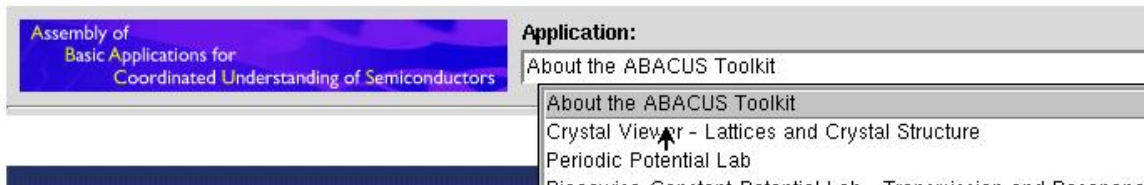
$$\cos(\theta) = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

- c) Visualize a zinc-blende crystal system from three different directions $[100]$, $[110]$, $[111]$ taken from three different crystal cuts..

Utilize the Crystal Viewer Tool in ABACUS on nanoHUB The tool can be found at:

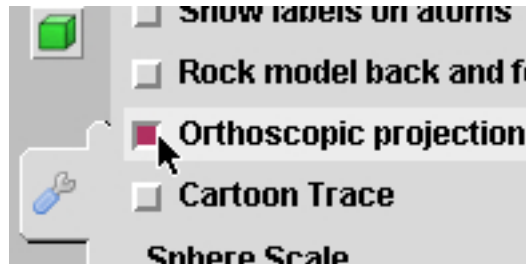
<https://nanohub.org/tools/abacus> (you will need a free nanoHUB login)

ABACUS contains many useful tools – for this exercise choose the crystal viewer



In Crystal viewer chose zinc-blende as a “Material Lattice Type” and pick GaAs as a material.

A) Rotate the crystal computed with (100) Miller plane into three different directions [100], [110], and [111]. You may find it useful to turn off the “Orthoscopic Projection” to see the depth of the crystal better



Download the three different plots by clicking on the right green arrow.



- B) repeat A) but start from a (110) Miller plane.
 - C) repeat A) but start from a (112) Miller plane.
3. For silicon (Fig. 1.5a in ASF), answer the following questions.
- a) How many Si atoms per sq. cm are there on a (100) plane?
 - b) How many on a (110) plane?
 - c) How many on a (111) plane?
 - d) Utilize the Crystal Viewer Tool in ABACUS on nanoHUB to prove your results in a, b and c.
 - e) In Crystal viewer use the Silicon material system. Choose the Miller indices of the plane you are interested in for Si, rotate the plane so you can observe the surface well and download the results by clicking on the right green arrow.