EE669: Simulation Exercise

Crystal Growth

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To study the Zinc Blend lattice using VESTA

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Credits: First version of this exercise, Ms. Bazila Parvez

Credits: K. Momma and F. Izumi: An integrated three-dimensional visualization system VESTA using wxWidgets, Commission on Crystallogr. Comput., IUCr Newslett., 7, 106-119 (2006).

Introduction

All electronic properties and many of the chemical and mechanical properties that are important from a processing perspective are related to the crystal structure of the semiconductor.

In this exercise, you would be introduced to the VESTA crystal viewer program that allows you to see the crystal lattice in 3D. Please see the exercises at the end to familiarize with some of the specific aspects of crystals that we would frequently refer to in this course.

Installing VESTA

- Open https://jp-minerals.org/vesta/en/
- Click on "Software => Download" on the left panel of the page. The download page starting with "License agreement" would open.
- Scroll down to "Latest versions". Download the version suitable for your computer's operating system.
- Install the software on your computer.

Setting up the view of GaAs crystal

- Download the file "GaAs-ZnS.vesta" supplied with this document into your computer.
- Open the VESTA program on your computer.
- To open the "GaAs-ZnS.vesta", click "File => Open".
- On the top panel with "a b c ……", click on the "football" symbol to view the crystal in the "standard orientation of crystal shape".

Playing around with the software

- You are encouraged to explore the software. More crystal structures can be downloaded from the website mentioned above. Some of the settings that are useful for the exercises of interest to us are given below.
- Under "View", make sure that "parallel" (and NOT "perspective") is turn on.
- On the left panel different symbols can be seen. These represent different tools available for analysis. For example, the arrow tool can be turned on to "rotate" the crystal.

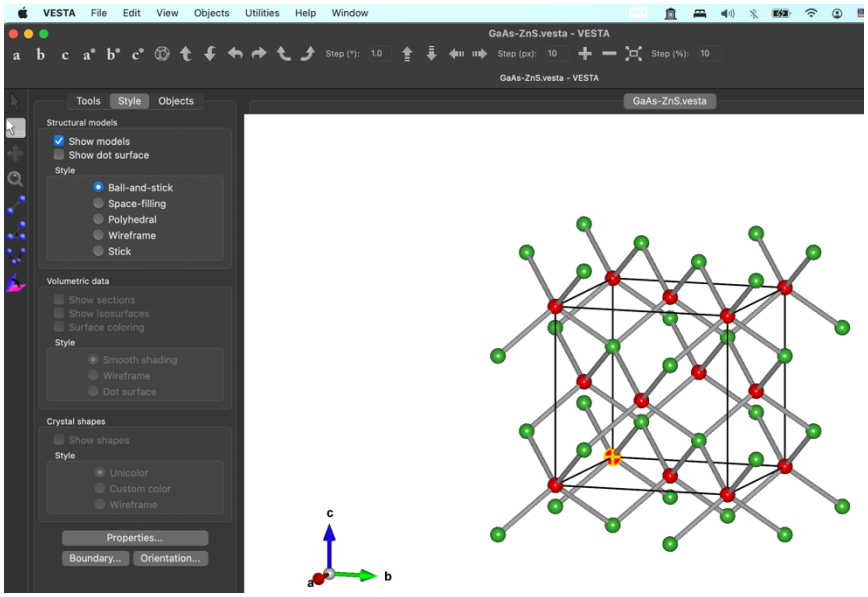
- You also see “Tools Style Objects” panel. You may explore these. The recommended settings under “Style” are “Show models” and “Ball-and-stick”.
- Now to the crystal displayed. The cube is the unit cell of GaAs, drawn to scale. The edge of the cube has a length equal to 0.56537 nm, the lattice constant of GaAs. Green balls represent the Arsenic atoms and the red balls represent Gallium atoms.
- The definition of the coordinate system is shown on the left bottom. The unit vectors in the 3 orthogonal axes directions are represented as **a, b, c**.
- You may rotate the crystal and see the reference coordinate system also rotate in tandem. Identify the corner of the cube that is the origin of the coordinate system. This can be marked using the “Select” tool on the left most panel, that is the arrow with a small rectangle next to it.
- You can also view planes in the crystal.
    - In “Edit” pull down menu, select lattice planes. To add a plane, click on “New”. Enter the hkl values for the plane. For example, h = 1, k = 0, and l = 0 for plane (100). “d” is the distance of the plane from the origin of the coordinate system.
    - The value of “d” may be specified to make the plane cut specific points on different axes. As an exercise, set the plane to (110). By default the distance of the plane from the origin is set to the lattice constant. This would result in a plane that is parallel to the usual definition of the (110), but would not cut both the a and b axes at 1 as per standard notation. To make the plane pass through (a, b) = (1, 1), the “Distance from origin” can be set to 3.99 A.
    - To view the plane (111) that passes through (a, b, c) = (1, 1, 1), set the “Distance from origin” to 3.3 A, after setting the values of h,k,l to 1,1,1.

Exercise

Through these exercises, we would try to develop and understanding of the origin of anisotropic properties of crystals.

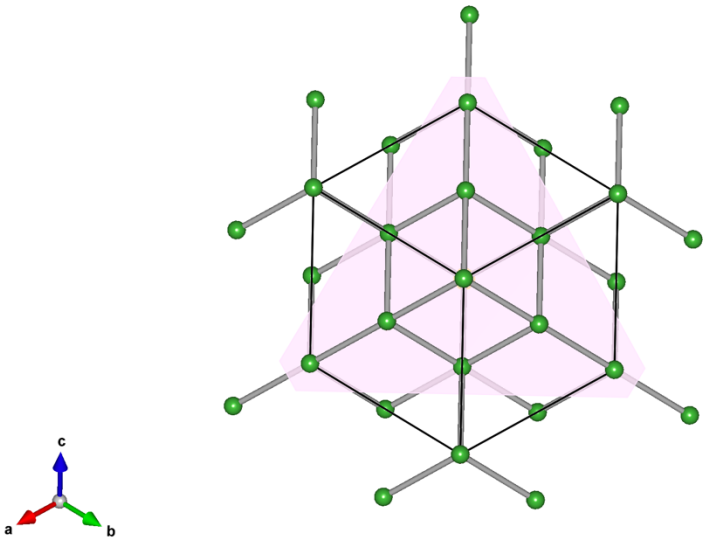
1. Define the plan (100) as described above. Rotate the crystal in such a way that you are viewing it along or opposite the [100] direction. This can be ensured by observing the colour of the plane. You may note that the colour turns darker or lighter as you rotate the crystal. The plane turns lightest when the plane is parallel to the screen of the computer (the direction of view is along or opposite to the direction perpendicular to the plane). You may note the arrangement of the atoms as projected on to the (100) plane. Take a screen shot of this for comparisons. Do the same exercise for the (110) plane and [110] direction. Take a screen shot. Repeat for (111) and [111]. Place the three screen shots side by side in a powerpoint presentation. What do you observe?
2. Determine the arial density of atoms (number of atoms per cm^2) on the three planes (100), (110) and (111). For doing this, please note the boundaries of the plane that confines the plane within the cube, and determine that area. You may also note that the atoms at the edges of this area are only partially within this area, and that should be carefully accounted for. Are the arial densities the same in different ?

Appendix



Screen shot of the VESTA GUI with GaAs-ZnS.vesta loaded.

The yellow cross shows the origin of the coordinate system.



View of the crystal along the (111) direction.