NanoLab (Phys4790) Name ___________________

Crystal Model Lab (150pts)

In this lab activity you will familiarize yourself with some basic concepts of the structure of crystals and crystal surfaces. A basic understanding is necessary in nanoscience for two reasons: the properties of nanoparticles can be dominated by the properties of their surfaces because a significant fraction of their constituent atoms reside there; and nanostructures that we wish to create will be supported on surfaces, thus an understanding of the structure and properties of those surfaces is critical.

BASIC CONCEPTS THAT SHOULD BE FAMILIAR TO YOU:

Common crystal structures: simple cubic (sc), face centered cubic (fcc), body centered cubic (bcc), hexagonal close packed (hcp), cubic close packed (ccp).

Miller indices and the nomenclature to describe crystal planes and directions: The following nomenclature should make sense to you. You should be able to describe what they mean and give examples.

(hkl)	a specific plane
{hkl}	family of planes
[hkl]	a specific direction
<hkl>	a family of directions

Surface Sites: 3-fold hollow, 4-fold hollow, bridge, atop.

Ad-Atoms.

Coordination Number: (for atoms in the bulk crystal and for ad-atoms on the surface.)

The bar: Sometimes one or more of the numbers in the Miller index have a bar over them. What does the bar signify?

SAFETY

In this lab you will use 1” diameter polypropylene spheres.

- They can be harmful if swallowed or inhaled.
- Escaped spheres are a hazardous and may cause injury from slipping and falling.

Please be considerate of others. Keep your spheres under control. Track down escaped spheres.

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General Questions (You may find it useful to use your models for some questions.)
In questions 1-6, consider only the cubic lattice, e.g. fcc.)

1. 2pts) Name every possible crystal plane in the {100} family.

2. 2pts) Name every possible crystal plane in the {110} family.

3. 2pts) Name every possible crystal plane in the {111} family.

4. 2pts) Name every possible crystal plane tin the {211} family.

5. 2pts) What crystal direction is normal to the $(1\bar{2}3)$ surface and points *away from* the origin? (Be careful of signs!)

6. 2pts) The $[2\bar{1}1]$ direction points *into* what crystal surface plane?

7. 4pts) What is the coordination number of the balls in:

the FCC lattice?

the HCP lattice?

8. 6pts) Consider crystals with an **FCC** lattice. What is the shape of the crystal with a surface composed of all possible planes of: (The surface is exclusively one family of planes.) If you cannot name the solid, state the number and shape of the resulting faces.

{111} planes?

{110} planes?

{100} planes?

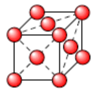
9. 2pts) The cubic-close-packed structure is also known as ___________________.

10. 10pts) Surface sites. Starting with each of the FCC surfaces below, state how many different types of sites are present and the coordination number for each. (Not every surface has all types of sites.)

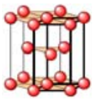
	3-fold hollow		4-fold hollow		bridge		atop	
surface	# sites	coord #	# sites	coord #	# sites	coord #	# sites	coord #
{111}								
{110}								
{100}								

Working with the frame supported models. You will construct and experiment with crystal models built from 1” balls. Your crystals will be built from surfaces defined by frames. We will focus on the low index FCC crystal face families {100}, {110}, and {111}. We will also compare FCC and HCP crystal structures.

Orienting the Cartesian coordinate system.



- FCC: Use the FCC cell (based on the 4-ball basis) to help you find the Cartesian coordinate directions. This is best done by embedding the cell into the crystal.



- HCP: Use the HCP cell (based on the 6-ball basis) to help you find the Cartesian coordinate directions. This is best done by embedding the cell into the crystal.

hexagonal frame. use frame __________________.

triangular frame. use frame __________________.

square frame. use frame __________________.

rectangular frame. use frame __________________.

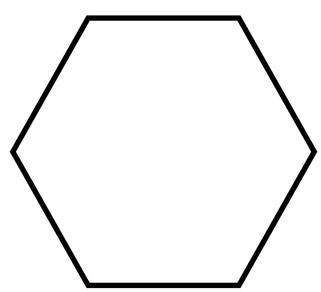
HEXAGONAL FRAME

Building crystals from close-packed layers. Place the frame on the table in the pen. Add balls to create the first layer. When balls are packed on a flat surface they naturally tend to form a close-packed layer. Notice that the balls form the familiar hexagonal/triangular pattern.* Add a second layer of balls to the model. The second layer is also close packed. The balls naturally rest in the 3-fold hollow sites of the layer below. Observe that the second layer only covers half of the 3-fold hollow sites. Look down on the second layer and observe that the second layer has two types of 3-fold hollow sites, those with balls in the layer below and those without balls in the layer below. It follows that there are two different ways to build the third layer of balls, both sit in 3-fold hollow sites, but differ in their relationship to the underlying layer.

ABC stacking (CCP) of the close-packed layers places the new layer (C) over the 3-fold hollow sites in the previous layer (B) that have no balls in the layer below (A). The new layer will be directly over the balls 3 layers below (another C layer). You cannot see more than 3 layers into a crystal that is built using ABC stacking when looking in the 3-fold hollow sites of the close-packed layers. Continue the ABC stacking as high as it will go.

11. 2pts) What surface family is in the plane of the table?

12. 10pts) What family of surfaces are exposed on the sides of the stack? Make a sketch showing a top-down view of your stack. Show the frame and the stack edges. Then label the exposed faces on this sketch.



13. 4pts) Two types of surfaces are exposed on the sides of the stack. The two surfaces alternate around the sides of the stack (three occurrences of each surface). What determines the orientation theses surfaces? After all, you start with a hexagonal frame, so should not all six sides of the stack be identical? What would you need to do to your crystal to switch the two surfaces? (Rotate the model is not the answer.) Hint: What did you do that determined the orientation of the surfaces?

14. 4pts) How many sets of close-packed planes exist in this crystal? Use the clear plastic sheet to slice into the crystal.

15. 2pts) Continue the crystal stack as high as it will go. How many balls are in the top most layer?

AB stacking (HCP) of the close-packed layers places the new layer (A) over the 3-fold hollow sites in the previous layer (B) that have balls in the layer below (A). Thus the new layer will be directly over the balls 2 layers below (another A layer). You can see through a crystal that is built using AB stacking when looking in the 3-fold hollow sites of the close-packed layers. One set of 3-fold hollow sites is never occupied.

16. 2pts) What surface family is in the plane of the table?

17. 4pts) How many sets of close-packed planes exist in this crystal? Use the clear plastic sheet to slice into the crystal.

18. 2pts) Continue the crystal stack as high as it will go. How many balls are in the top most layer?

TRIANGULAR FRAME

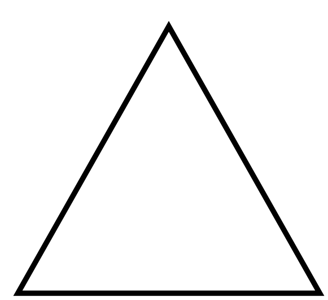
Place the frame on the table in the pen. Repeat the activity you did for the hexagonal frame.

ABC stacking (CCP)

19. 2pts) What surface family is in the plane of the table?

20. 10pts) What surfaces are exposed on the sides of the stack? Make a sketch showing a top-down view of your stack. Show the frame and the stack edges. Then label the exposed faces on this sketch.

21. 4pts) How many sets of close-packed planes exist in this crystal? Use the clear plastic sheet to slice into the crystal.



22. 2pts) Continue the crystal stack as high as it will go. How many balls are in the top most layer?

23. 4pts) When you slice off the edges running from the point of the triangular frame to the apex of the stack, what surface is exposed?

AB stacking (HCP)

24. 2pts) What surface family is in the plane of the table?

25. 4pts) How many sets of close-packed planes exist in this crystal? Use the clear plastic sheet to slice into the crystal.

26. 2pts) Continue the crystal stack as high as it will go. How many balls are in the top most layer?

SQUARE FRAME

Building crystals from square-array layers. Place the frame on the table in the pen. Insert the plastic square, which helps start the square array. The correct size plastic square will position all of the balls in the first layer.** Add balls to create the first layer. This will take a little work to get the balls to form the correct structure. It is not automatic. Flooding the frame with balls at this point will make the task of forming the first layer more difficult. When first layer is finished, add more balls to from the second layer. Note that the second layer rests in the 4-fold hollow sites and that *every* 4-fold hollow site is filled by the second layer. Hence there is only one possible way for the balls to stack.

27. 2pts) What surface family is in the plane of the table?

28. 10pts) What surface is exposed on the side of the stack? Make a sketch showing a top-down view of your stack. Show the frame and the stack edges. Then label the exposed faces on this sketch.

29. 4pts) Define the +z axis upward and perpendicular to the table, mark arrows on your sketch above to show the Cartesian coordinate axes.

30. 4pts) Find the {100} planes in this crystal. Use the clear plastic sheet to slice into the crystal. Mark them on your above sketch with dashed lines. In a new sketch, show the arrangement of the balls in this plane when looking parallel to the table. The plane of the table should be obvious in your sketch.

31. 4pts) If the square frame had vertical sides, what surface would be exposed there? Use the clear plastic sheet to extend one side of the frame and build the crystal against it. In a new sketch, show the arrangement of the balls in this plane when looking parallel to the table. The plane of the table should be obvious in your sketch.

32. 2pts) Continue the crystal stack as high as it will go. How many balls are in the top most layer?

RECTANGULAR FRAME

Building crystals from layers of spaced rows. Place the frame on the table in the pen. Place the rods in the frame, which separate the rows. Add balls to create the first layer, which consists of close-packed rows of balls separated by the rods. (The rows should rest against the frame on two sides, thus the number of rods should be one less than the number of rows.) When the first layer is finished, add more balls to from the second layer. Note that the second layer rests in the 4-fold hollow sites and that *every* 4-fold hollow site is filled by the second layer. Hence there is only one possible way for the balls to stack. Unlike the 4-fold hollow sites in the square frame, the 4-fold hollow sites on this surface are rectangular, AND the ball also contacts the ball two layers directly below it.

33. 2pts) What surface family is in the plane of the table?

34. 10pts) What surface is exposed on the side of the stack? Make a sketch showing a top-down view of your stack. Show the frame and the stack edges. Then label the exposed faces on this sketch.

35. 4pts) Find the {100} planes in this crystal. Use the clear plastic sheet to slice into the crystal. Mark them on your above sketch with dashed lines. In a new sketch, show the arrangement of the balls in this plane when looking parallel to the table. The plane of the table should be obvious in your sketch.

36. 4pts) If the rectangular frame had straight sides, what surfaces would be exposed? Use the clear plastic sheet to extend the long side and the short side of the frame and build the crystal against it. In two new sketches, show the arrangement of the balls in this plane when looking parallel to the table. The plane of the table should be obvious in your sketch.

37. 2pts) Continue the crystal stack as high as it will go. How many balls are in the top most layer?

38. 8pts) Did you find this lab activity helpful to understand crystal structures?

What would you do differently to improve it (be specific)?

What would you did you like about it (be specific)?

FOOTNOTES

*Often the adjective *hexagonal* is applied to describe this 2D layer. It is also sometimes called a *triangular* lattice because the smallest polygon is a triangle, which distinguishes it from the non-close-packed lattice of a honeycomb. We will not get tied up in the semantics, it is sufficient to note that different terminologies are applied to this close-packed 2D layer.

**The square array is not a stable packing a 2D array of balls compared to the close packed layer.