Goodie bag #6: Crystallography

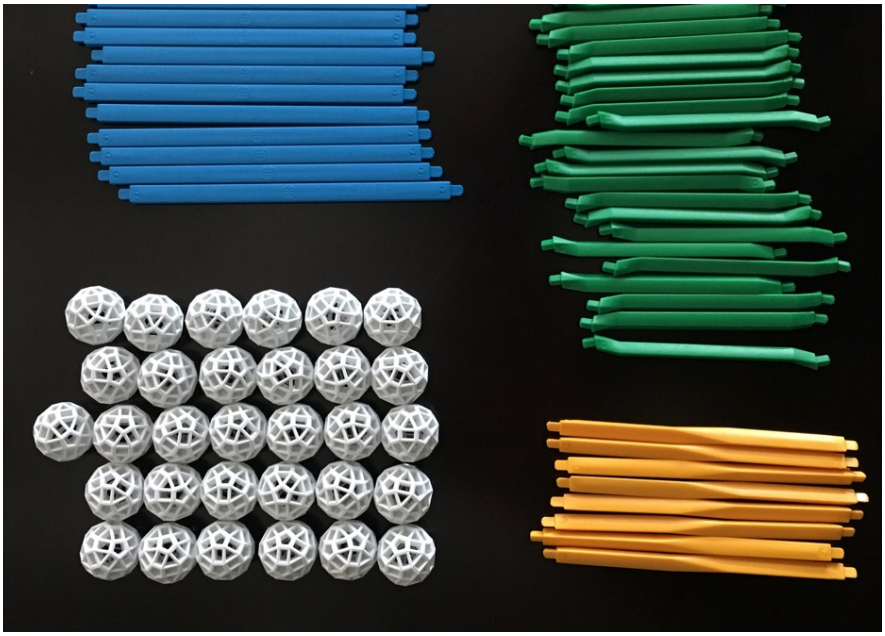
Handed out on 10.22.18 | Quiz #6 on 10.25.18

3.091

Do yourself a solid.

This bag contains:

- **31 white balls**
- **12 blue struts (for SC)**
- **24 green struts (for FCC)**
- **8 yellow struts (for BCC)**



What to bring to the quiz: a pre-built FCC structure

Introduction

This goodie bag will explore the different structures of crystalline materials. Core knowledge and practice: crystal lattice, plane and direction, packing density.

Instructions & Questions

Question 1: Basic unit cells

Use the pieces to build 3D models of Simple Cubic, Body Centered Cubic, and Face Centered Cubic unit cells. Remember that since they are cubic the length of each edge of the cube should be the same.

Let's now focus on the SC structure.

Question 2a: Crystallographic direction

Your SC model has 8 unique atoms in it. If you look down the [100] direction, how many atoms do you see that are not hidden behind other atoms?

Question 2b: Crystallographic plane
How many of these atoms (from Question 2a) are completely bisected by the (100) plane (i.e. their center lies exactly on the (100) plane)? What are the coordinates of these atoms? Use proper crystallographic notation.

Question 2c: Angles
Identify and calculate the angles between

(i) the [100] and [110] directions
(ii) the [100] and [111] directions

Let's now focus on the BCC structure.

Question 3a: Crystallographic direction
If you arrange your model so that you are looking down the [110] direction, how many atoms do you see that are not hidden behind other atoms?

Question 3b: Crystallographic plane
How many of these atoms (from Question 3a) are completely bisected by the (110) plane (i.e. their center lies exactly on the (110) plane)? What are the coordinates of these atoms? Use proper crystallographic notation.

Question 4: Linear packing density
Look down each of the [010], [101] and [111] directions.

- Intuitively, which direction would you say has the higher atom density?

  Let us now confirm (or refute) this intuition.

- How many atoms lie along each direction?

- Are they touching (yes or no for each direction)?

- Deduce the radius *r* of an atom as a function of the lattice parameter *a*.

- For each direction, determine the linear packing fraction (% of the distance occupied by atoms) and the linear packing density (# of atoms per nm) in the case of an atom of Lithium.

Question 5: Planar packing density
Consider the (101) plane.

- How many atoms lie on this plane?

- Sketch this plane. Represent the atoms by circles. Indicate the significant lengths used as a function of *r* and *a* (exact values for atomic radius or lattice parameter are not necessary, but relative atom positions are important).

- Calculate the planar packing fraction and planar packing density of the (101) BCC plane in the case of an atom of Barium.

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