Crystal structure

1. **crystals.** Grains in a polycrystalline material are typically 50um across. Metal ions have a diameter of approximately 0.30nm. In the following, we estimate the fraction of ions near a grain boundary.

   (a) Calculate the volume of the grain, assuming that it's a cube with side length of 50um.
   (b) Calculate the volume of one ion.
   (c) Estimate the number of ions in the grain: $N = V_{grain}/V_{ion}$.
   (d) Calculate the surface area of same the cube.
   (e) Calculate the cross sectional area of one ion.
   (f) Estimate the number of ions at/near the cube's surface.
   (g) From (c) and (f), estimate the fraction of ions at/near the grain boundary.

   adapted from 2.example1 Turton.

2. **structure**. Determine the volume occupied by the spheres in the fcc structure as a percentage of the total volume. *(Turton 2.2.)*

3. **structure.** Another property to describe the crystal structure is its *coordination number.*

   (a) Determine (or look up) the coordination numbers for the following: simple cubic, bcc, fcc, hcp.
   (b) How are coordination numbers determined?
   (c) Diagram this for the simple cubic and the bcc structures.

   This isn't covered in Turton. Hofmann devotes 1 sentence to it. I suggest looking it up somewhere on the www.

4. **the lattice.** A given lattice can be described by *any* set of lattice vectors which, when repeated, creates the lattice. Each set of lattice vectors creates a unit cell. Find definitions for the following:

   (a) unit cell
   (b) primitive unit cell
   (c) non-primitive unit cell
   (d) conventional unit cell
   (e) Wigner-Seitz cell

   Use text and a diagram in your answer.

5. **the lattice.** 2.4 in Turton

6. **the lattice.** In 2D, there are only 5 lattices types. There are 14 in 3D. Each lattice is characterized by its symmetry. These are called Bravais lattices.

   (a) Name and briefly sketch the 5 Bravais lattices in 2D.
   (b) Describe the relationship between the lattice vectors, $\vec{a}_1$ and $\vec{a}_2$. Sketch these on the lattices, and use words or equations.

   You'll have to look this up on the www. It's not in your text. Choose a reputable source.

7. **Review.** In the following, refer to your intro physics text's section on wave optics.

   (a) Describe in 1-3 sentences and a diagram, the results of the double slit experiment and the physical reasons behind it.
   (b) The angular position of the maxima is given by $d\sin\theta = m\lambda$. What do d and θ refer to? Indicate these on the diagram.
   (c) $d\sin\theta$ is a distance. Indicate this distance on the diagram.
   (c) Why would the waves interfere destructively? Why would the waves interfere constructively?

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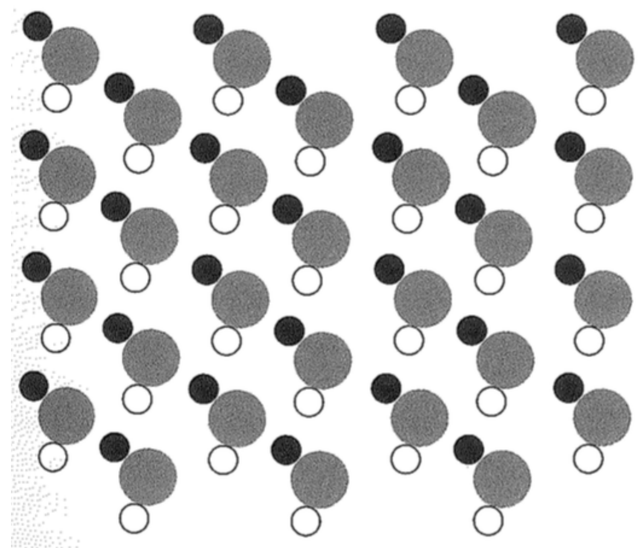
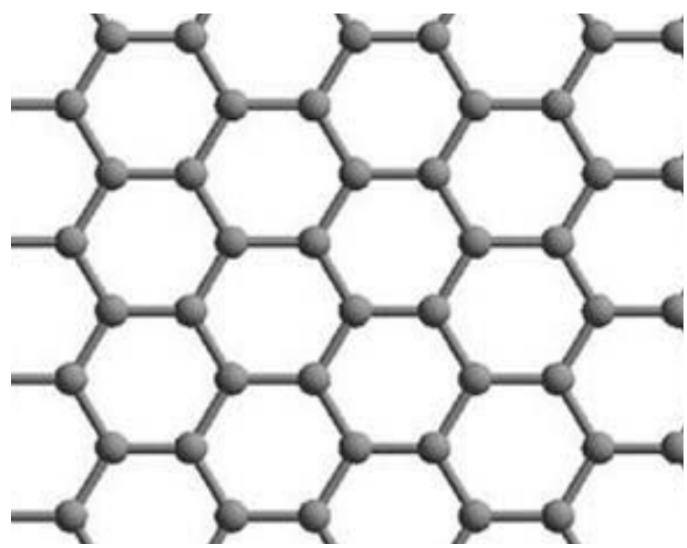
8. In the 2D crystal below, identify



   (a) a primitive unit cell and its lattice vectors
   (b) a non-primitive rectangular unit cell and its vectors
   (c) the bases associated with each of the above
   Adapted from Hofmann 1.1

9. The honeycomb lattice is the structure graphene[1].



   (a) Identify sets of atoms that are identical to each other. To determine if two atoms are "the same",

[1] Graphene is a 2 dimensional form of carbon. It's effectively the layers that make up graphite. Geim and Novoselov were awarded the Nobel Prize in 2010 for their experimental studies of graphene.

consider the positions of their nearest neighbors.
(b) Determine a pair of lattice vectors, the associated unit cell, and the basis that can be used describe graphene.

Adapted from Hofmann 1.3

10. Sketch a few cubic unit cells and draw the following lattice planes

    (1 0 1), (0 1 1), (0 2 1), (2 1 0), (2 1 1)

    Adapted from Hook and Hall 1.2

11. The Miller indices $(h\ k\ \ell)$ define a lattice plane. Show that the following vector

    $$[h\ k\ \ell] = h\vec{a} + k\vec{b} + \ell\vec{c}$$

    is perpendicular to the $(h\ k\ \ell)$ plane. Here, $\vec{a}, \vec{b}$, and $\vec{c}$ are the lattice vectors.

    If you're not sure what to do, try the following:
    (a) Sketch a cubic unit cell and draw the lattice plane $(h\ k\ \ell)$, where $h, k, \ell > 1$.
    (b) The $(h\ k\ \ell)$ plane intersects the ab plane. This line can be described by the vector $\vec{P} = \frac{1}{h}\hat{a} + \frac{1}{k}\hat{b}$. The $(h\ k\ \ell)$ plane also intersects the bc plane. Determine a vector $\vec{Q}$ that describes this line.
    (c) Use what you know about vector products to determine a vector perpendicular to both $\vec{P}$ and $\vec{Q}$.

12. 2.9 in Turton

13. 2.10 in Turton

14. (a) Determine the maximum wavelength for which constructive interference can be observed in the Bragg model for a simple cubic crystal with a lattice constant of 0.36 nm.

    (b) What is the energy of the x-rays in electron volts?

    (c) If you were to perform neutron diffraction, what would the energy of the neutrons have to be in order to obtain the same deBroglie wavelength?

    Adapted from Hofmann 1.5. If you're not sure what to do for (b) and (c), refer to your Modern Physics text.

15. (a) An electron has kinetic energy E. Derive the following expression for the electron's wavelength

    $$\lambda = \frac{h}{\sqrt{2mE}}$$

    (b) Calculate the wavelength of an electron with a kinetic energy of 100keV.

    Adapted from Turton 2.11. If you're not sure what to do, refer to your Modern text. Also, it's helpful to write E in terms of momentum.