Protein Structure Determination. Xray Homework 1:

Due Thursday Oct 29, 2020. PDF format.
http://www.bioinfo.rpi.edu/bystrc/courses/bcbp4870/homework.html

(1) Short answers.

(a) Define *crystal lattice* using a vector equation.

(b) Define *morphology* using crystal contact strength.

(c) Define *nucleation point* using kinetics of crystal growth and dissolution.

(2) Space group symmetry. (**See pp 3-4**)

(a) Draw all of the **symmetry operators** that you can find. Place symbols at axes of symmetry for rotations in the xy plane. For rotations out of the xy plane, place the sym op symbol in the margin and draw a line indicating the axis. Indicate the height in Z.

Each foot or hand represents one molecule. The black foot or hand is facing **down** and centered at z=½, the grey foot or hand is facing **up,** centered at z=0. In-plane 2-folds are 1/2 way between the equivalent positions (feet or hands).

(b) Outline the **unit cell**. Outline the **asymmetric unit (*asu*)**.
Use the point of highest symmetry as the **origin** of the unit cell.
(To check your work, make sure the *asu* can fill all space when repeated by symmetry.)

(3) Wave addition.

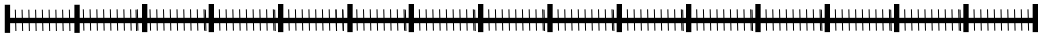
Add the following waves in Argand space. Draw each wave as a vector and use a protractor and ruler to measure the total **amplitude** and **phase** of the summed waves. Use graph paper. Each wave below is a (amplitude, phase) pair. Phases are in degrees.

(1.5, 120.)
(2.0, -60.)
(3.0, 180.)
(1., 0.)
(2., 90.0)

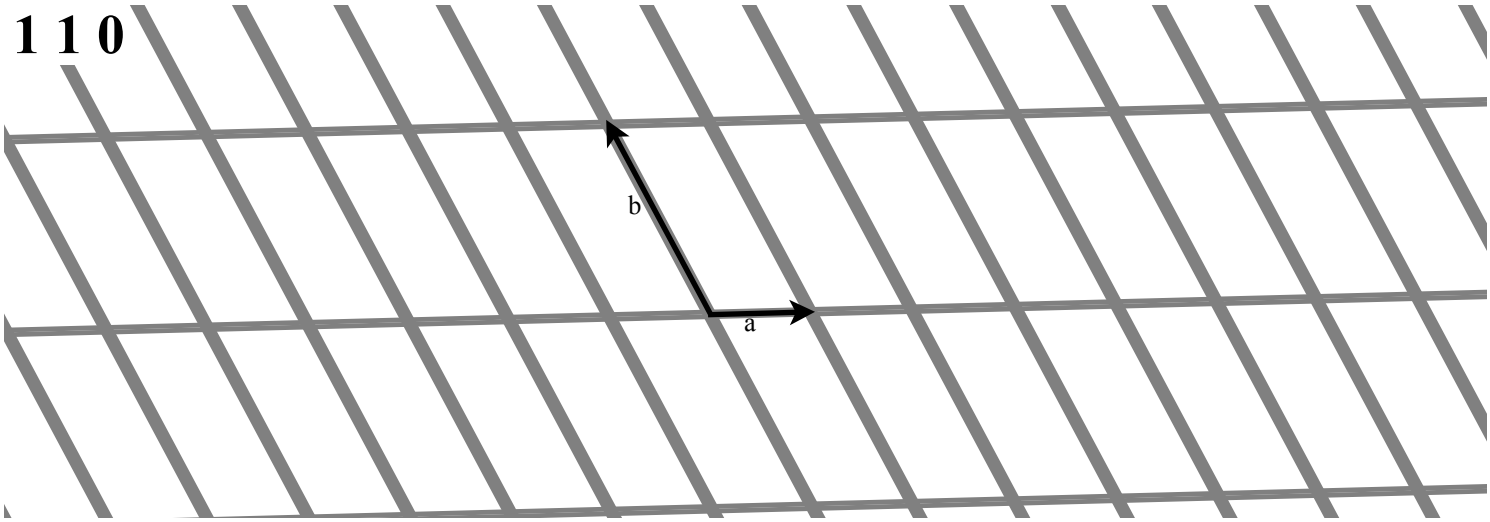
(4) Using the crystal lattice paper (**see p. 2**) **a** and **b** axes are specified.

(a) Draw the sets of crystal planes as defined by the given Miller indeces *hkl*.

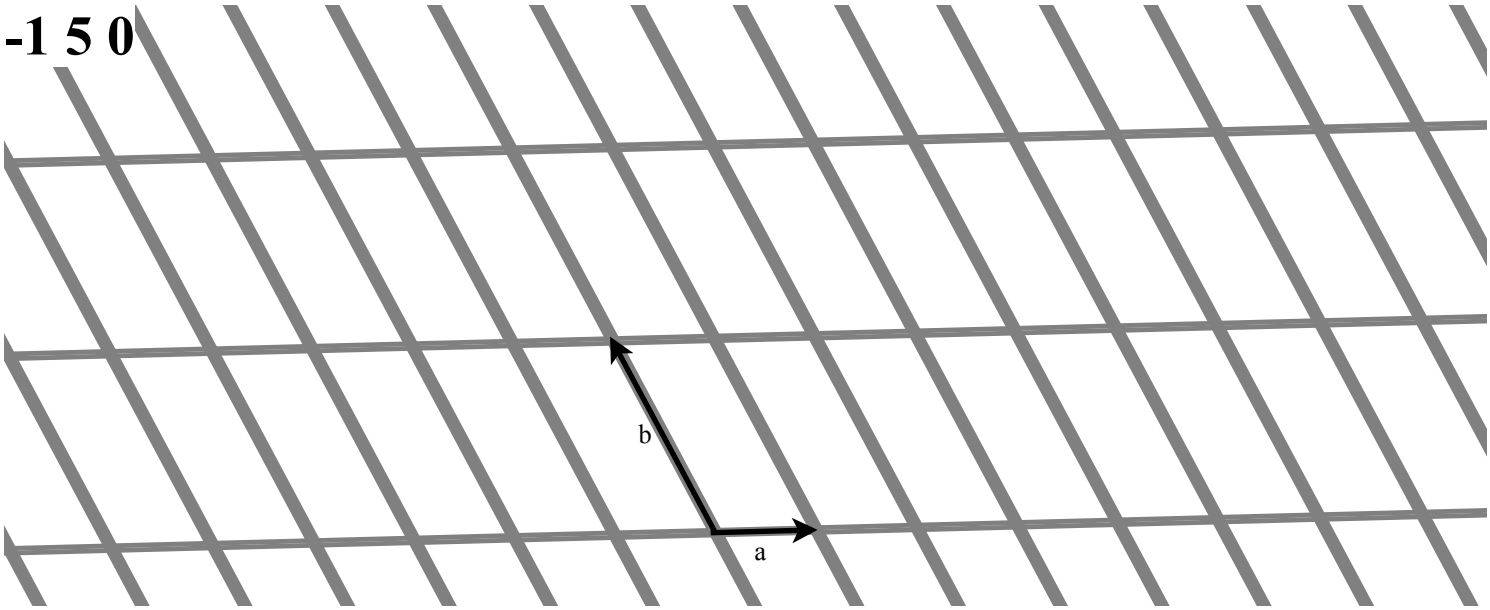
(b) Use the ruler provided to measure the Bragg distance. Calculate the Bragg angle. Draw the direction of the *beam* and the *reflection*. Use λ=1.54Å.



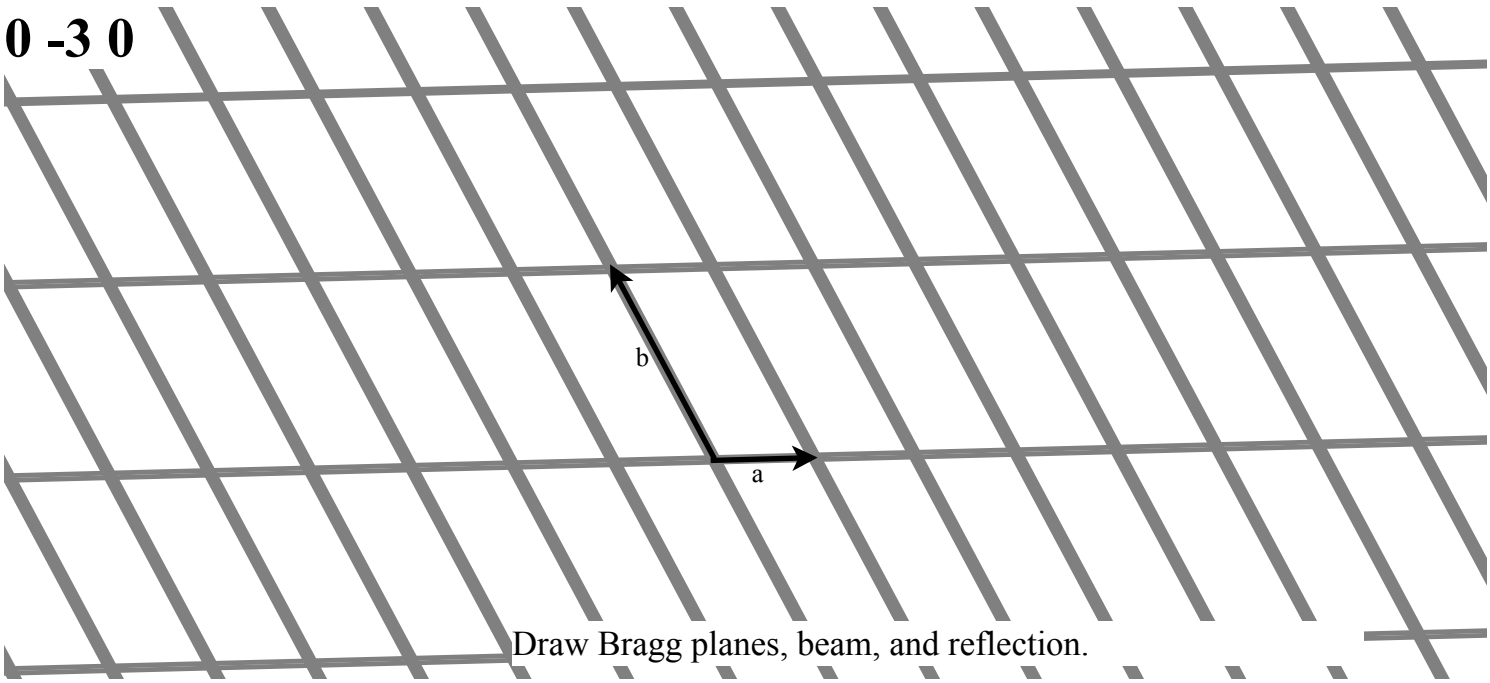
1 1 0



-1 5 0

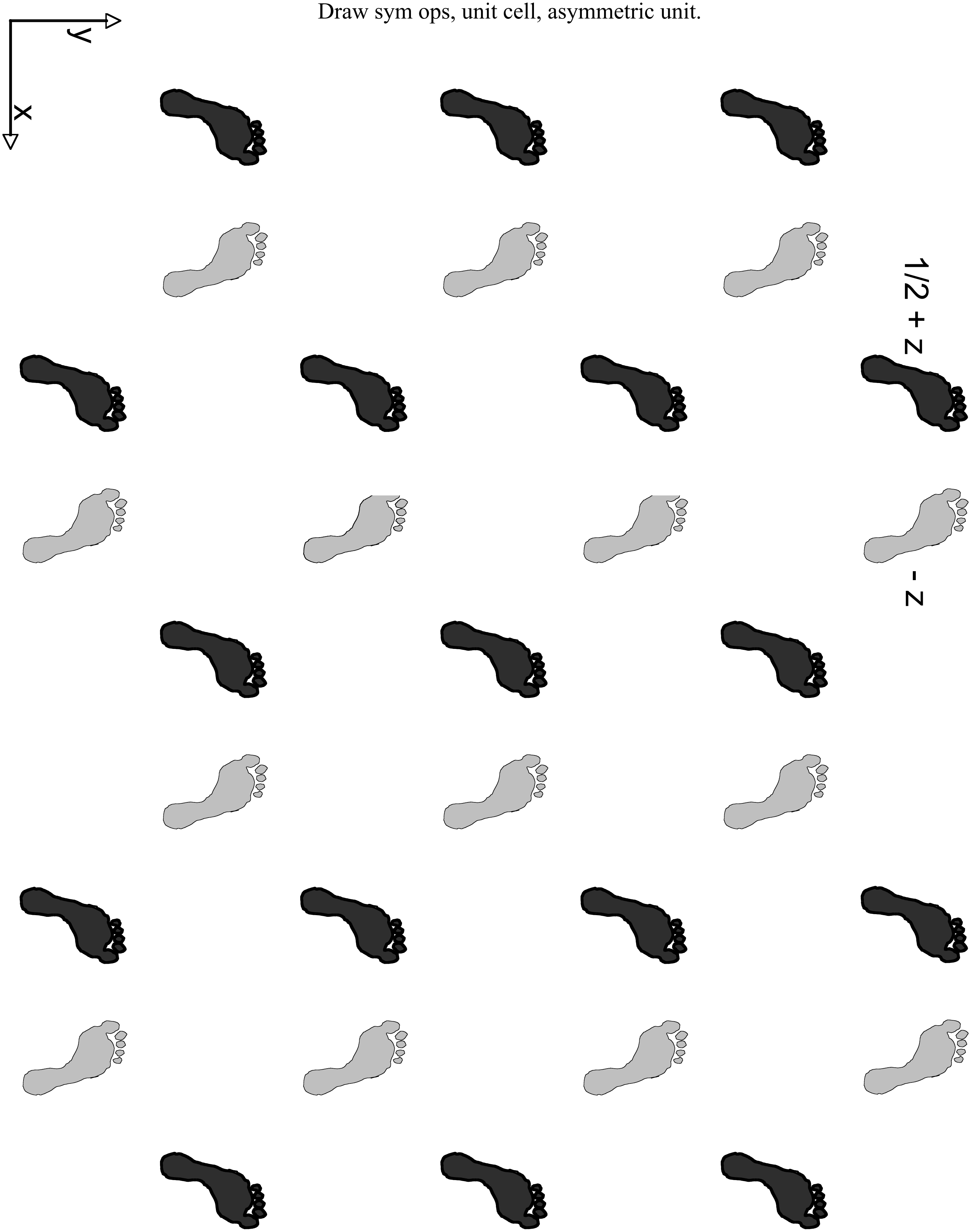


0 -3 0



Draw Bragg planes, beam, and reflection.

Draw sym ops, unit cell, asymmetric unit.



Draw sym ops, unit cell, asymmetric unit.