Bravais simulation report

Name:

PRESET 1 shows the honeycomb structure where each atom has three nearest neighbors. The associated lattice of points (the Bravais lattice) can be seen by clicking on the LATTICE button above the left hand display. The position of the two atoms in each of the cells, the basis, is specified by their coordinates with respect to a corner of the unit cell, in units of the cell edges.

Ex.1. Move either atom around by dragging the handle of one of its coordinate sliders. Does the Bravais lattice change?

Ex. 2. Remove the second atom by clicking on the ATOM B toggle. Is the associated Bravais lattice the same or different? Why?

The smallest unit cell which can be used to define a crystal structure is called a primitive unit cell, and is determined by the primitive axes.

PRESET 2 gives a structure with a rectangular unit cell and a two-atom basis.
Ex. 3. Show that this unit cell is not a primitive cell. What is a possible pair of axes and the angle between them which give a primitive cell for this structure? Draw the lattice and indicate your choice of axes.

Ex. 4. Select PRESET 1 again. Can you find a smaller unit cell, with only a single atom in the cell, which can be used to define this structure? Explain your answer.

Ex. 5. Select PRESET 3. Give a more convenient but non-primitive choice of lattice plus basis that gives the same structure and orientation. Draw the axes and give the basis in units of $\mathbf{a_1}$ and $\mathbf{a_2}$. What is the most obvious primitive cell to use (not available to "bravais" because the $\mathbf{a_1}$ axis is not horizontal)?

In PRESET 4 you see two atomic planes drawn in the real-space (left hand) picture. Sets of planes are conventionally defined in terms of Miller indices (read the description on page 12 of the SSS book). "bravais" gives the Miller indices below the right hand window. Typing in the Miller indices defines the selected planes.

Ex. 6. Check out a number of (h k) values. Draw one example. Explain the meaning of the (0 1) planes.

Ex. 7. Return to PRESET 1 and click on SHOW PLANES, and on the real-space LATTICE, to show two of the set of (1 1) planes. There are no atoms on the planes drawn here. Change the basis to ATOM A at [0 0] and ATOM B at [1/3 1/3]. What fraction of the atoms lie on the planes? Enter (1 -1) for the Miller indices. What has happened to the positions of the atoms relative to the planes?

The reciprocal lattice is defined by a unit cell with axes b_1 and b_2 such that

$$\boldsymbol{b}_i \cdot \boldsymbol{a}_j = 2\pi\delta_{ij}$$

Ex. 8. PRESET 5 shows a rectangular real-space lattice and its reciprocal, with no atoms. Vary the magnitude of the axes a_1 and a_2 and verify that the reciprocal lattice vectors are appropriate to maintain the above relation. Draw one example and write down $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{b_1}$ and $\mathbf{b_2}$.

Now vary the angle between $\mathbf{a_2}$ and $\mathbf{a_1}$. Verify that the orthogonality condition is maintained. Draw one example and write down $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{b_1}$ and $\mathbf{b_2}$. Then look carefully at the magnitudes b_1 and b_2. Explain why they both increase as the angle departs from 90º, though a_1 and a_2 remain fixed.

Ex. 9. Return to PRESET 1 and click on LATTICE above the right hand frame to display the lattice reciprocal to the honeycomb structure. Remove one of the atoms in the unit cell by clicking on ATOM B. Does the reciprocal lattice change?

The reciprocal lattice vectors and lattice planes are strongly related (read the description on page 15 of SSS).

Ex. 10. Use PRESET 1 with both the reciprocal LATTICE and SHOW PLANES activated. Double click on one of the reciprocal lattice points; the corresponding (h k) values are displayed below and a pair of the (h k) planes appear in real space. Repeat a couple of times, write down your observations. Verify that (i) the vector from the origin of the reciprocal lattice to the (h k) reciprocal lattice point is perpendicular to the lattice planes shown at the left; (ii) the higher the (h k) values the more closely spaced are the planes.

Ex. 11. In PRESET 6 “bravais” simulates a two-dimensional diffraction experiment. On the right of the screen is the diffraction pattern for the honeycomb structure on the left. Switch on the display of the reciprocal LATTICE as a reminder that the positions of the diffraction peaks give a scaled map of the reciprocal lattice. Move the atoms around or remove and replace one of the atoms in the basis. Do the diffraction spots’ positions change? Do the intensities of the spots change?

Ex. 12. Choose PRESET 7 to recover a monatomic rectangular crystal structure. Notice that the intensities of the x-ray peaks fall off with increasing magnitude of $\mathbf{\Delta k}$. This is a

consequence of the destructive interference of components of the wave scattered from different parts of the atom (read the description on page 20 of SSS). Change the SIZE of the atom A by a factor of 2 (both larger and smaller) and verify that the envelope of the intensities of the diffraction peaks varies at it should.

Ex. 13. PRESET 8 demonstrates the effect of the interference between the waves scattered from the two atoms in the cell. Include the reciprocal LATTICE display. Remove and add ATOM B while watching the diffraction pattern. Does the pattern change? Does the reciprocal lattice change? Explain. What if you delete ATOM A instead of ATOM B?

Ex. 14. With both atoms present, click on the SHOW PLANES button and then double click on the (1 0) reciprocal lattice point. In the crystal structure display note that there are as many atoms midway between the lattice planes as there are on them. Check out several low index planes and compare the number of atoms in the lattice planes with the numbers midway between the planes. How do these comparisons relate to the presence or absence of peaks at the corresponding reciprocal lattice points? Write down a few examples.

Ex. 15. Vary the ATOMIC NUMBER of one of the atoms and watch the behavior of the diffraction pattern. Be aware that “bravais” normalizes the diffracted intensities to keep the central spot at a fixed brightness. What happens to the extinctions you noted in the previous exercise?