Step-by-Step Guide to Crystallographic Points, Directions, and Planes

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Naming points, directions, and planes in a unit cell can seem overwhelming at first, but will become easy as you practice and follow the following procedures. Indices of crystallographic points, directions, and planes are given in terms of the lattice constants of the unit cell. For points and directions, you can consider the indices to be coefficients of the lattice constants. Remember that **you only need to invert the indices for planes.** It is essential to label axes, lattice constants, and identifying information for directions (vector arrow head) and planes (axes intercepts) in order to receive full credit.

For extra practice with indexing directions, visit the University of Liverpool's interactive site for crystallographic directions. For extra practice with planes, visit the University of Liverpool's interactive site for crystallographic planes. This website from Cambridge has an excellent website about crystallographic planes along with plug-ins that will draw a plane given its indices and will let you match indices to a range of planes.

Points

Labeling points in a unit cell follows the same procedure for listing points in any Cartesian coordinate system. The indices used to refer to points are q, r, and s. They are listed without commas, parentheses, or brackets. Consider point P in Figure 1a. If you were standing at the origin of the unit cell, you could travel $q \cdot a$ in the x-direction, $r \cdot v$ in the y-direction, and $s \cdot c$ in the z-direction to get to point P. Thus we would say that point P corresponds to the qrs point coordinates.
To find q, r, and s when you are shown a drawing with a point:

1. Start with your pencil at the origin.

2. Count the number lattice constants you must move in the x-, y-, and z-directions to reach the point.

3. Write the point as qrs without commas, parentheses, or brackets. Do not convert the coordinates to reduced integers. The $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ point in the BCC structure is not the same as the 111 point.

To draw a point given qrs:

1. Start with your pencil at the origin.

2. Count $q \cdot a$ in the x-direction, $r \cdot v$ in the y-direction, and $s \cdot c$ in the z-direction.

3. Draw and label the point.

In the BCC system shown in Figure 1b, the path to point 9 would be $0 \cdot a$ in the x-direction, $1 \cdot a$ in the y-direction, and $1 \cdot a$ in the z-direction. Thus the point coordinates of point 9 are 011. The point coordinates for point 5 are $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

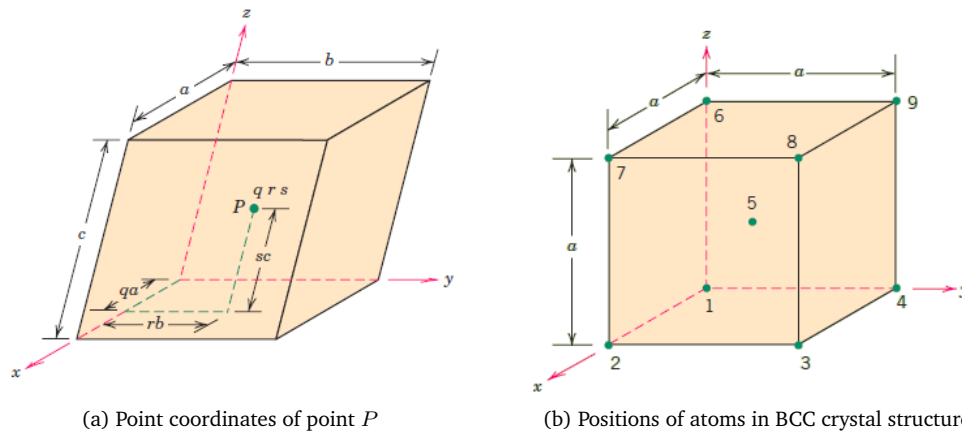(a) Point coordinates of point P (b) Positions of atoms in BCC crystal structure

Figure 1: Crystallographic point coordinates

Directions

To draw a direction given the $[uvw]$ indices:

1. Choose a point for the origin of your vector. Simple directions, such as those shown in Figure 2a, are easy to draw using the 000 crystallographic point as the origin. For more complicated directions (see Figure 2b), it is more convenient to translate (add or subtract) or scale (multiply or divide) the indices of the direction. If you translate your origin to the point 001 for example, the tail of your direction vector will be at this point.

2. Start with your pencil on your chosen origin. Move your pencil $u \cdot a$ in the x-direction, $v \cdot b$ in the y-direction, and $w \cdot c$ in the z-direction. If u, v, or w are negative, move in the negative direction on that axis.

3. Draw and label a point.

4. Draw a line from your chosen origin to the point you just drew. Add an arrow head at the point.

It is extremely important when drawing directions that you **label the point that lies at the end of your direction vector**. If the TAs cannot tell where your direction is ending, you will not receive full credit. Is it also highly preferred that you shift the origin and scale of the direction vector so that it is contained inside the unit cell.

If you shifted the origin, a way to check that you drew your direction properly is to subtract the point coordinates of the arrow head from those of its tail. The resulting indices should be $[uvw]$.

To write the $[uvw]$ indices given a drawing of a direction:

1. Place your pencil at the tail of the given vector.

2. Count how many lattice constants you must move in the x-, y-, and z-directions to reach the head of the vector. Write them down. Be mindful of negatives.

3. If necessary, multiply by a common number to make the indices integers.

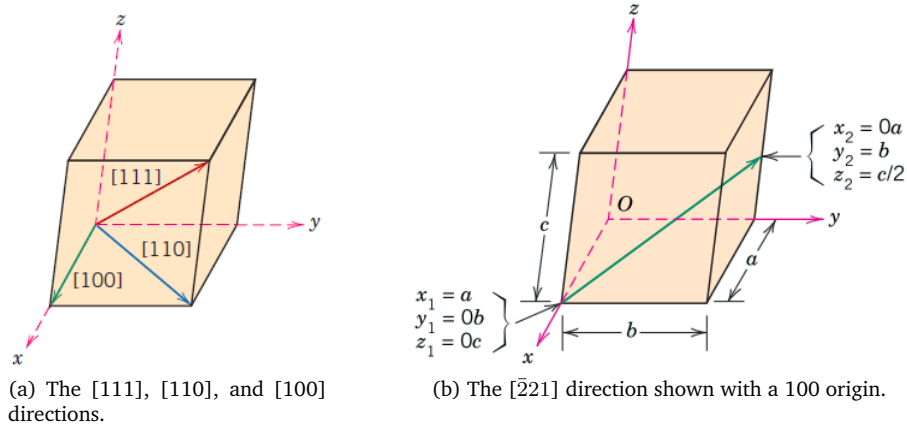4. Rewrite the indices and enclose them in square brackets $[uvw]$.

(a) The [111], [110], and [100] directions.

(b) The [$\bar{2}$21] direction shown with a 100 origin.

Figure 2: Crystallographic directions

Planes

To draw a plane given the (hkl) indices:

1. Find the reciprocal of (hkl). If one or more of the indices is zero, consider the reciprocal to be infinity. The values $\frac{1}{h}$, $\frac{1}{k}$, and $\frac{1}{l}$ are the intercepts of the x-, y-, and z-axes, respectively. If one or more intercept is infinity, this means that the plane will never intercept that axis (it is parallel to that axis). For the (221) plane shown in Figure 3a, the reciprocals would be $^1/_2$, $^1/_2$, and 1.

2. For all non-zero indices, draw a point on the x-axis at $^a/_h$, a point on the y-axis at $^b/_k$, and a point on the z-axis at $^c/_l$.

3. Connect the dots.

4. If you had a zero index - for example, the (001) plane in Figure 3b - draw two points at 111 and 011, and 110, then connect the dots.
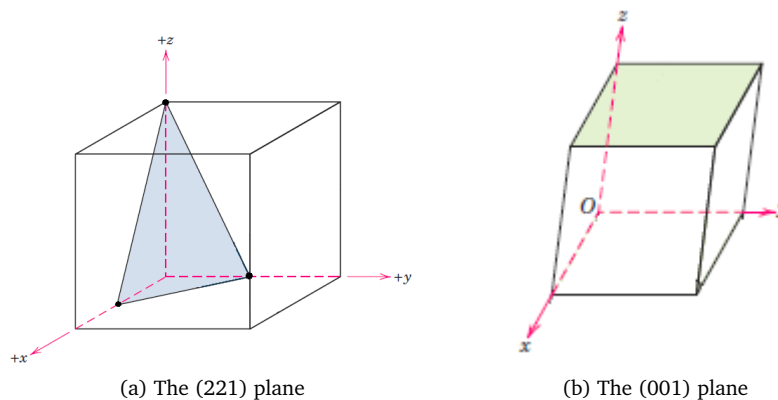

(a) The (221) plane

(b) The (001) plane

Figure 3: Crystallographic planes

To list the (hkl) indices given a drawing of a plane:

1. Check to see if the plane goes through the origin, as in Figure 4a. If not, proceed to step 2. If it does, shift the plane 1 lattice constant in an axis such that it no longer passes through the origin (see Figure 4b). This new plane is equivalent to the first.

2. Find the coefficients by which you would multiply the lattice constants to identify where the plane intercepts the x-, y-, and z-axes. Be mindful of negative intercepts. If the plane doesn't intercept an axis (it is parallel to that axis), call the intercept infinity. Write down these values.

3. Take the reciprocal of these intercepts. The value of $\frac{1}{\infty}$ is zero.

4. If necessary, multiply or divide by a common number to put the indices in the most reduced integer form. Sometimes you will be asked to leave the indices unreduced - for example, (220) instead of (110) - for use in x-ray diffraction questions.

5. Enclose the indices in parentheses without commas (hkl).

(a) Plane that passes through the origin

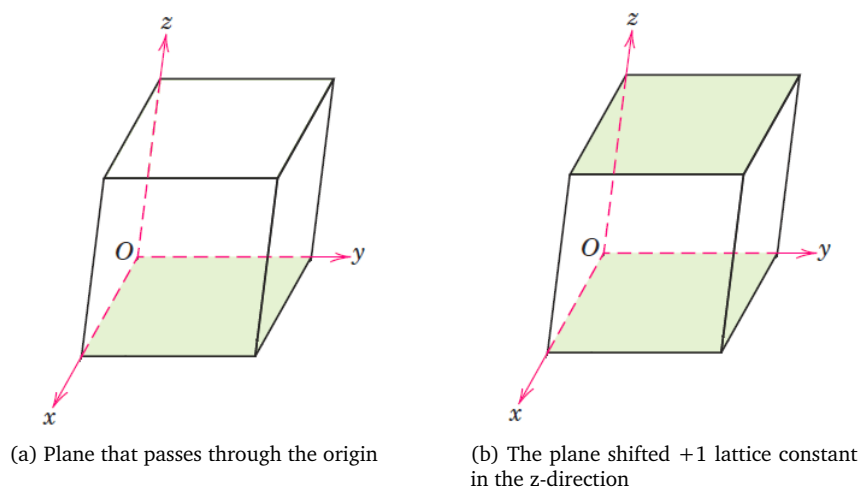(b) The plane shifted +1 lattice constant in the z-direction

Figure 4: The method used to determine the indices of a plane that passes through the origin

It is extremely important when drawing planes that you **label where the plane intersects the axes**. If the TAs cannot tell where your plane intersects the axis, you will not receive full credit.

Note: The hkl indices define a vector that starts at the origin and it perpendicular to the plane. Recall from your multi-variable or vector calculus class that the equation of a plane can be written as $a\overrightarrow{x} + b\overrightarrow{y} + c\overrightarrow{z} = d$, where the vector $[abc]$ is perpendicular to the plane. In our case, a crystallographic plane can be written as $h\overrightarrow{a} + k\overrightarrow{b} + l\overrightarrow{c} = d$.