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ENEE416: Group Activity 1

Miller Indices

Background / Overview

Miller index is the method of describing the crystalline lattes structures in space. This method is first developed by a professor named William Hallowes Miller. W. H. Miller was a professor of mineralogy at St John's College, Cambridge University, England with extended work on crystallography.

In the study of crystalline solid structures, some solid atoms are oriented in a way that the molecules or atoms are periodically arranged. This means that similar crystals appear the same way as their neighboring crystals in the entire structure. In order to represent the lattice structure in space, a set of integer values are used. These integer values represent the position and direction vector of a given lattice. Indexing a lattice helps to further know about the properties of different materials in the study of material science. Such investigations include the determination of the shape of a single crystal, and mechanical properties of the material.

The main purpose in the use of Miller indices is that in finding the orientation of a crystalline structure, the planes formed by the repeated properties may have an infinite intercept. Having an infinite intercept will further complicate our desire to locating the lattice. In addition to encountering an infinite intercept, Miller indices also have a resemblance to the conventional x, y, and z coordinate system. These similarities help us to determine the orientation without having to deal with infinite planes. Furthermore, representing unit cells by integers helps us to replicate the lattice into several lattices.

How to determine Miller indices of crystal planes

The first step of finding Miller indices is to identify the intercepts of the crystal planes. The intercepts are the points where the planes intersect the coordinate planes (the x, y, and z plane for a 3D cubic lattice). Planes that do not intersect the coordinate plane are considered infinite planes, and have an infinite intercept.

After finding the intercepts of the crystal planes, we take the inverse of each intercept to avoid having an infinite intercept. Then the numbers are reduced to the lowest integer number by multiplying each value by another number that will give us the lowest number. The final sets of numbers are the Miller indices representing crystal planes. In the case where we have a negative intercept, the Miller indices are denoted by an over bar on the specific index.

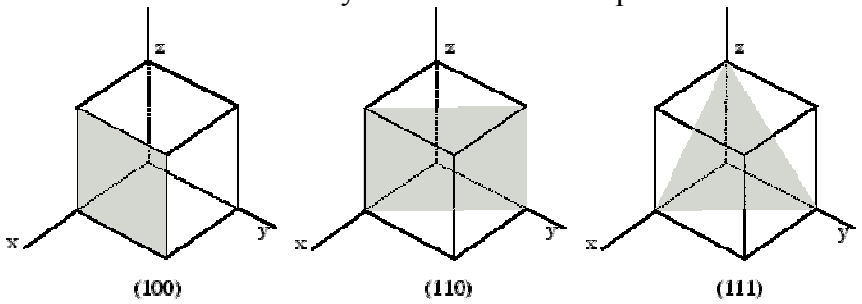

Figure 1: Different cubic lattice structures with their Miller Indices

Miller Indices can also be used represent directions as well. This process is similar to finding a miller index for a plane, but simpler. First project the vector of interest onto the all three of the coordinate axes. After this, determine the corresponding x, y, and z coordinates. Once you have these three numbers, reduce or enlarge them in order to have the smallest possible whole numbers.

Unique Aspects of Miller Indices

Now that we've defined the procedure in finding miller indices, we must explain some of the specifics or instances where the miller indices are easy to find. Those instances regard differentiating planes and directions, ambiguity with results, negative regions of the coordinate system, and having the plane of interest parallel to a coordinate axes.

Miller indices, as shown above, can be used for both direction and planes. With that said, we need to be able to differentiate between the two. Plane miller indices will be designated with ( ) brackets while directional miller indices will be designated with [ ] brackets.

Due to the symmetry of the unit cells of elements such as silicon, some Miller Indices are indistinguishable. These certain miller indices look equivalent. An example of such are: (100), (001), and (010). Instead of trying to differentiate all three, we call this a set and use {} for brackets. Using this system, the miller indices used in the previous example would be referred to as the {100} planes, rather than just (100), (001), (010).

With the procedure we listed above in determining miller indices, there is another instance that we must consider. If the plane falls into the negative region and has a miller index of (121), we cannot tell the difference with a plane that falls in the positive region with the same miller index. In order to distinguish these two apart, a bar is placed over the relevant index. For example, the negative region (121) would look something like (**1**21), (1**2**1), or (12**1**). Keep in mind that these bars are suppose to be above the number, Microsoft word does not allow us to do that. Figure 2 is a good example of how we distinguish negative miller indices.

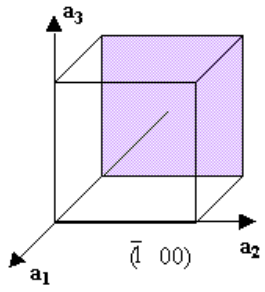

Figure 2

The last instance to understand is miller indices when the plane of interest is parallel to one of the coordinate axis. This means that the plane will not intersect either one or two, which does not give us a discrete intercept point. However, this is easily solved when you follow the procedure in finding miller indices. Since there is no intercept point, we set it as infinity. When you take the inverse of it, it becomes 0 and then looks like a normal miller index.

References

University of Cambridge: http://www.doitpoms.ac.uk/tlplib/miller_indices/index.php
Wikipedia: http://en.wikipedia.org/wiki/Miller_index