

Miller Indices and Slip Symmetries: A Brief Primer

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1 Introduction

In the previous primer, we talked about how to describe cells, and the atoms in those cells - however we lacked the ability to talk about one important property: **orientation**. Orientation in crystal structure is kind of arbitrary, insofar as for any given orientation, repeating the cell in all directions forms a crystal. The difficulty comes when you wish to form a film, for example, which requires repeating the cell in only 2 directions. This again is not necessarily a problem for cubic lattices, which have a high degree of symmetry, but for the other cells, specifying which ‘side’ to repeat is tricky (saying the ‘top’ of the cell does not really have any meaning). Luckily, we have a method of describing sides of a cell, which we refer to as **Miller Indices**.

2 Miller Indices

2.1 Real-Space Lattice

The Miller indices (often denoted (h, k, ℓ)) are simply the coefficients of the **reciprocal space**, as described in the following equation:

$$\mathbf{G}_m = h\mathbf{b}_1 + k\mathbf{b}_2 + \ell\mathbf{b}_3 \quad (1)$$

In order to understand where this comes from, we must first take a more rigorous look at the lattice vectors described in the previous primer. As we last left it, we described each point individually, a_1, a_2, \dots, a_n . However, we can describe all of these points generally (and thus the entire lattice) with the following:

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \mid (n_1, n_2, n_3) \in \mathbb{Z} \quad (2)$$

Let’s break this equation down. \mathbf{R} denotes the entire lattice, \mathbf{a}_i denotes a primitive vector (essentially describes the location of a point, a direction with a fixed length ¹.) and n_i is some integer (which is what the second half of the equation means mathematically). The purpose of describing it this way is that by combining these vectors in various proportions, we can systematically build the entire crystal. Let’s use a primitive cubic cell as an example:

¹The point of using vectors here is that it allows us to relate our principle axes (i.e. $\{x, y, z\}$) to the axes of the crystal itself, so regardless of the angles inside the unit cell, and regardless of if the crystal is rotated relative to the principle axes, we can still simply describe the crystal. We are also only looking at 3D systems, hence the three primitive vectors and coefficients.

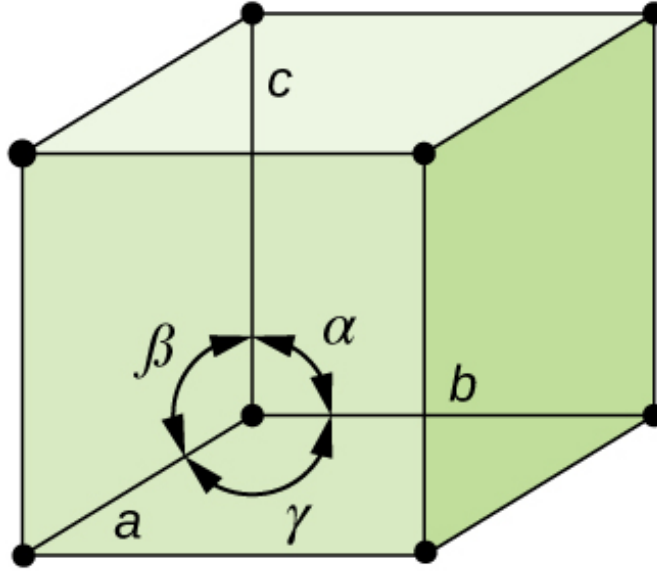


Figure 1: An example primitive cubic cell.

In this figure, the cell lengths are labelled $\{a, b, c\}$, and if we move in only one cardinal direction at a time, we find a point at a , b and c distance from the origin, in each of their respective directions. Mathematically, we write this as:

$$\mathbf{a}_1 = a \hat{\mathbf{e}}_1 \quad (3)$$

$$\mathbf{a}_2 = b \hat{\mathbf{e}}_2 \quad (4)$$

$$\mathbf{a}_3 = c \hat{\mathbf{e}}_3 \quad (5)$$

$\hat{\mathbf{e}}_1$ denotes a unit vector, which is a direction with a length of 1. Now we can see if we substitute this into equation 2, and start incrementing n_i (i.e. $(0,0,0)$, $(1,0,0)$, $(0,1,0)$, $(0,0,1)$, $(1,1,0)$, etc.), we slowly generate the whole crystal. For now, we won't derive this for all crystal structures, but it is important to know this, as the **reciprocal lattice** comes from this description.

2.2 Reciprocal Lattice

Hopefully you will have come across Fourier transforms, which convert lengths into frequencies. Frequencies have dimensions of 1 divided by a length (i.e. in a cubic cell, there is one atom per length a in the x direction). Thus, when we apply a Fourier transform to a lattice, the lattice spacings between the two lattices become inversely proportional. If we increase the spacing in the real lattice, the frequency decreases, meaning the points in the reciprocal lattice become closer together. Now this ends up being useful to describe planes in a lattice, as any vector can be attributed to a plane (normal from it). Say we have a set of planes spaced x apart, normal to some reciprocal space vector. If we decrease the spacing between the planes, the vector gets longer. If we mark the points of the end of the reciprocal vector where the planes cut through the unit cell an integer number of times, we form a crystal structure, which is the reciprocal lattice. As such, **any point in the reciprocal lattice corresponds to a plane in real space**. The **Miller indices** $\{h, k, \ell\}$ describe that point, just as $\{n_1, n_2, n_3\}$ describes a real point (i.e. an atom).

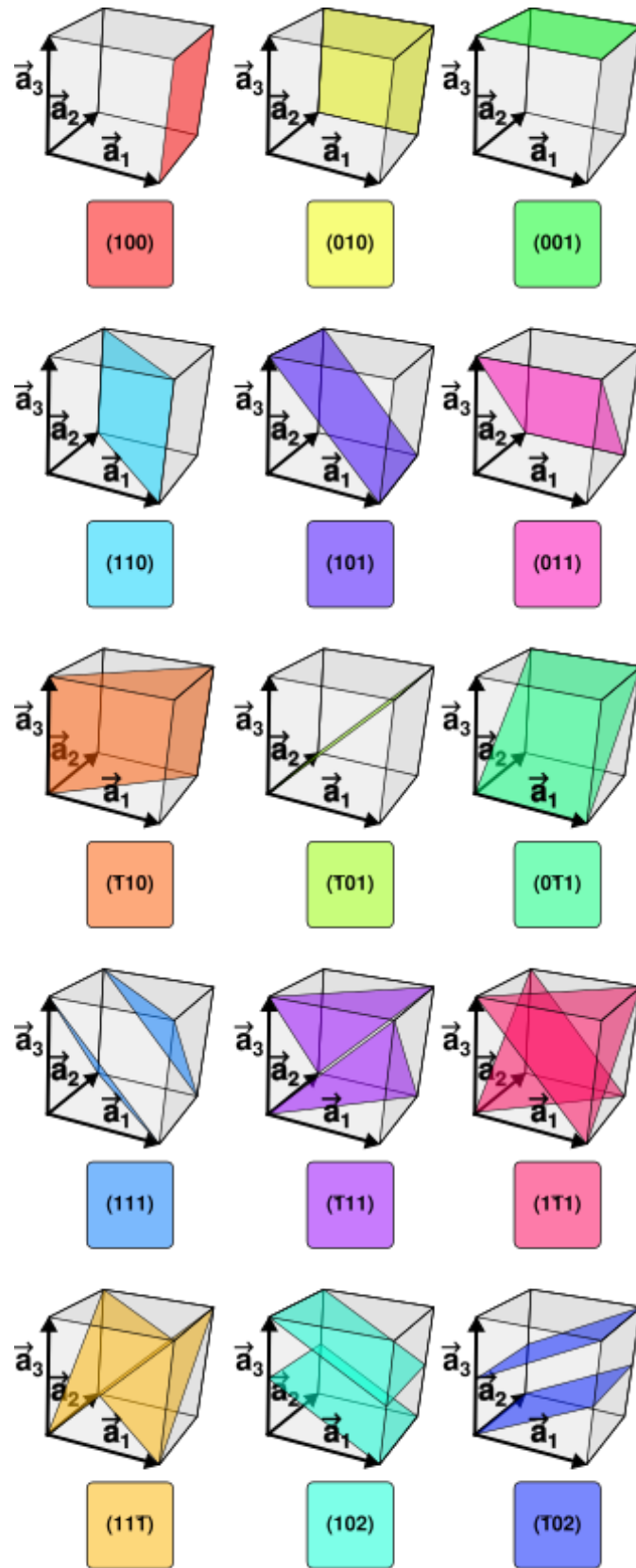


Figure 2: A diagram showing a collection of planes, with the corresponding Miller indices. The bar on top of certain indices represents a negative, meaning it acts opposite in that specific direction.

3 Slip Symmetries

Now the purpose of being able to actually describe planes in a crystal structure is that certain crystal structure will ‘slip’ or displace along specific ‘weaker’ planes. For example, FCC crystals can slip along the $\{1, 1, 1\}$ plane. As you are now accustomed to how Miller indices work, you should now hopefully be able to understand the directions involved when discussing slip symmetries.