Lecture Notes - Mineralogy - Miller Indices

- All directions and planes in a mineral are referenced to a crystallographic coordinate system. This is always a right-handed coordinate system based on the unit cell of the mineral.

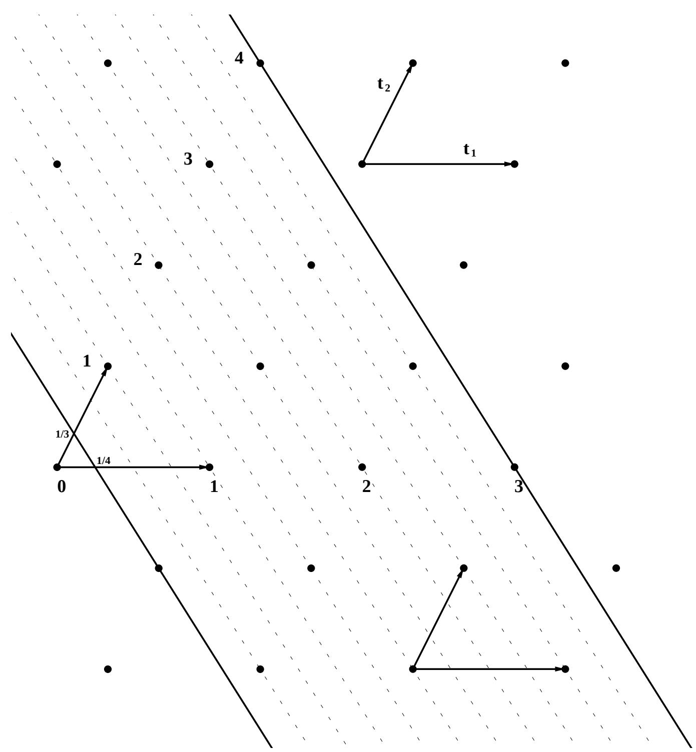
- **Rational directions** in a mineral may be located by extending a vector from the lattice point that is the origin of the unit cell to any other lattice point. The direction is labeled with the coordinates of the lattice point placed in **square brackets** without commas. For example, the direction parallel to the **b**-axis of a crystal would be **[010]**. This is the same direction as **[020]** and **[030]**. By convention, **[010]** is used instead of **[020]**, **[030]**, etc.

- **Rational planes** in crystals are identified by **Miller indices**, which may be determined for any plane (or any line in two dimensions) from the intersections of the plane (or line) with the crystallographic axes. The recipe for Miller indices is:

> (a) Determine the intecepts of the plane of interest with the crystallographic axes;
> (b) Invert each intercept (so that x becomes 1/x);
> (c) Multiply all terms by the lowest common denominator.

The indices determined by this recipe are placed in **parentheses** without commas. For example, a plane that intersects the **a**-axis at **2**, the **c**-axis at **1**, and that is parallel to the **b**-axis, would have a Miller index of **(102)**. $(2,\infty,1) \rightarrow (1/2,1/\infty,1/1) \rightarrow (2/2,2/\infty,2/1) \rightarrow (102)$. Note that planes parallel to a crystallographic axis will have a zero in the Miller index for that axis. If the intecepts are negative, a bar is placed over the appropriate index. When saying out loud a Miller index that contains a negative number, one says **bar** before the number. For example, $(1\bar{2}1)$ is pronounced "one, bar two, one."

- Miller indices are convenient because **all parallel planes in a crystal have the same Miller index**. Consider the set of parallel lines shown on page 2 of these notes. Choosing an arbitrary origin as indicated on the figure, one of the lines has rational intercepts at $3\mathbf{t}_1$ and $4\mathbf{t}_2$, giving a Miller index of (4 3). The line with intercepts $(1/4)\mathbf{t}_1$ and $(1/3)\mathbf{t}_2$ also has a Miller index of (4 3). Similarly, the line with intercepts $(3/4)\mathbf{t}_1$ and $(3/3)\mathbf{t}_2$ also has a Miller index of (4 3). Note that in this example there are 11 planes with at least one non-rational intercept for each plane with rational intercepts, making a total of 12 planes. 12 is the lowest common denominator used to obtain (4 3)! Because all parallel planes have the same Miller index, the Miller index you determine from observations of the faces of a crystal will be same as the index one might determine for a parallel plane from a model of the crystal structure.



- Miller indices also conveniently give the **equation** for the plane of interest. In two-dimensions, if **A** and **B** are the itercepts of a line on the **x** and **y** axes, the equation of this line would be:

$$\frac{x}{A} + \frac{y}{B} = 1$$

If **A**=1/4 and **B**=1/3, then the equation becomes 4x + 3y = 1. If **A**=3 and B=**4**, the equation becomes:

$$\frac{x}{3} + \frac{y}{4} = 1 \text{ or } 4x + 3y = 12$$

Thus, the Miller indices **(hkl)** are the rational (whole number) coefficients for the equations for any of a set of planes with

$$h\mathbf{x} + k\mathbf{y} + l\mathbf{z} = \text{constant.}$$

- By convention, when one refers to a set of planes for which one or more axis intercept is unspecified, the letters **h**, **k**, and **l** may be used for the unspecified **a**, **b**, and **c** indices, respectively. Thus, a general Miller index would be **(hkl)**, which would refer to any or all rational planes. All the planes parallel to a given line in a crystal are said to belong to a single **zone**. For example, all **(h0l)** planes are parallel to the **b**-axis, which would be the zone axis for all **(h0l)** planes.

- If one can **index** the faces of a crystal, the relative orientation of the faces may be used to determine the ratios of the lengths of the crystallographic axes. For example, the crystal pictured below has a **(110)** face as well as **(100)** and **(010)** faces. Measurement of the interfacial angles **(100)^(110)** and **(010)^(110)** will yield φ and θ with some rearangement. **(010)^(110)** is **90-**θ (or **90+**θ if the obtuse angle is used). To find **a/b** solve the expression

$$\tan\theta = \mathbf{a}/\mathbf{b}.$$

If the plane **(110)** were actually **(210)**, then the equation would be

$$\tan\theta = \mathbf{a}/(2\mathbf{b}).$$