PLANES, FORMS, AND RECIPROCAL LATTICE:

Reading Assignment: Zoltai and Stout, pp. 40-63, Appendix 4.

Planes and forms:

Planes are natural features associated with the crystalline state. When the macroscopic shape of a crystal is considered the bounding surfaces are disturbances in the bonding of the atoms.

They have an associated Gibbs free energy associated with the disturbance caused by having the lattice end.

The specific free surface energy is defined as

$$\gamma \triangleq \frac{d\Delta G}{dA} \simeq \lim_{dA \to 0.0} \frac{dW}{dA}$$

For each mineral, γ is, in general, a function of the orientation of the surface normal with respect to the crystal, of temperature, of pressure, and of the chemistry of any pore fluid, gas, or absorbate that is present. The total energy of the finite crystal depends on the sum of the product of γ_I x total area of the surface i. Values of $\gamma \approx 1\text{-}10$ J/m^2(0.4- 4.0ev or 1-10 x10^3 ergs/cm^2).

Free energy is minimized when certain special surfaces occur, for example, when a crystal is cleaved. In addition, as crystals grow from a solution, the growth rate of each face is affected by the orientation of its normal, so, special planes also tend to occur during crystal growth, although they may be different than the cleavage planes. The observation of these special surfaces led to the hypothesis of elementary building blocks (unit cells) by such early crystallographers as Huygens, Haüy, Hessell, and Bravais (see following page).

In addition to the bounding surfaces formed by cleavage or crystal growth, one may consider internal surfaces within the crystal. Such surfaces may be important when considering mechanical strength, twin structures, grain boundaries, antiphase domains, magnetic properties, or x-ray patterns.

Nomenclature and Definitions

Planes can be described by

1. the symmetry of the shape of the face, as in cleavage *rhombs* in calcite.
2. the pole symmetry, e.g., *4mm* or *4*.
3. a classical name, pedion, pinacoid, etc.
4. a letter, e.g., *m, r, f, c, e,* …
5. a set of three indices called Miller indices.

*Planes that intersect along a line common to all are **co-zonal**. The line along which they intersect is called a zone axis or more simply, a **zone**.*

Crystal Forms

*The assemblage of two or more faces/sufaces/planes that are related by symmetry are called **forms.***
Forms may be open or closed depending on whether or not the surfaces completely enclose a volume. Forms that are parallel to some symmetry axis (that is, the normal is parallel) are called special forms.

Of course, γ, like every other crystal property is governed by the symmetry of the crystal, thus, planes in the same form have the same specific free energy.

There are 150 different names for the forms in thirty two different space groups. For an exhaustive (and exhausting) look at all the forms see [Bloss, 1994, Chapter 5] and the next two pages .

Some classical names:

Name	Description	Sym. Op.
Pedion	No relationship	1
Pinacoid	Any two parallel (‖)faces	$\bar{1}$
Scalenohedron	2 scalene triangles connected on a side	
Domes	2 non-‖ faces related by a mirror	M
Sphenoids	2 non-‖ faces related by a 2-fold	2
Disphenoids	2 sphenoids rel. by another element (e.g. m)	2m 2/m
Prisms	3 or more faces that meet in a zone	3, 4, 6
Pyramids:	3 or more faces that intersect at a point	3, 4, 6
Rhombs	6 rhombs related by a three fold	3
Dipyramid	Two pyramid forms	3/m, 4/m
Dodecahedron	12 rhomb faces	Isometric
Octahedral	8 trianular faces	Isometric
Cubic	6 square faces	isometric

(a) 001

(b) hh0

(c) hh$\bar{1}$

(d) hk0

(e) hk$\bar{1}$

(f) 4 a₂ m • 1 $\frac{1}{4}$ $\frac{m}{4}$ a₁
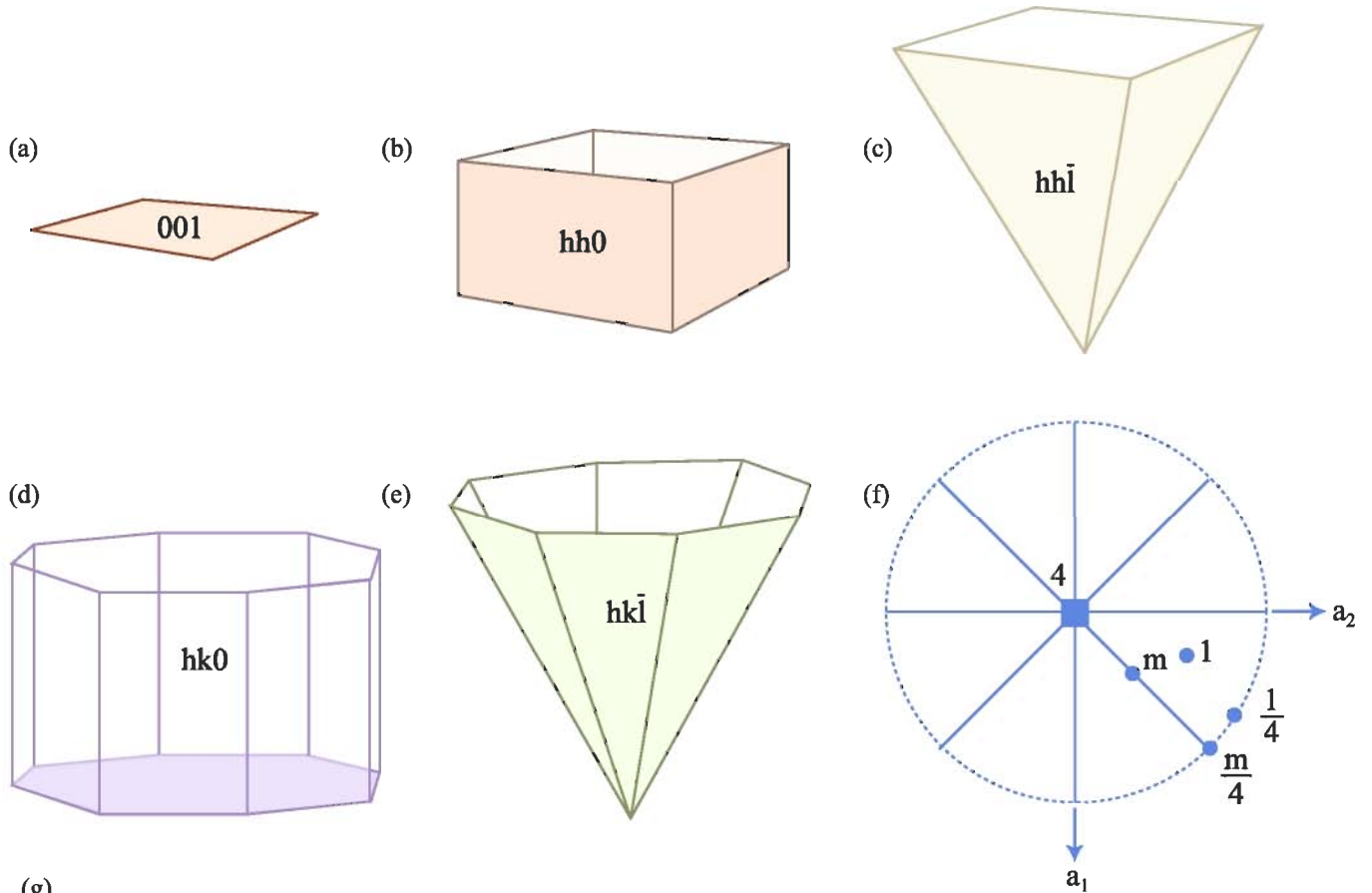
(g)

Classical name of crystal form	Symmetry of faces	Short symbol of form	No. of faces	Indices of a face
Ditetragonal pyramid	1	1	8	hkl
Ditetragonal prism	1	1/4	8	hk0
Tetragonal pyramid	m	m	4	hhl
Tetragonal prism	m	m/4	4	110
Pedion	4mm	4	1	001

(f) Stereographic projection of 4mm point group showing representative face normals of the general position, 1, semispecial position, 1/4, special positions, m, m/4, and 4. The resulting three-dimensional forms are (a) pedion, 4, (b) tetragonal prism, m/4, (c) tetragonal pyramid, m, (d) ditetragonal prism, 1/4 and (e) ditetragonal pyramid, 1.

Information is summarized in (g), a section of the crystal form tables.

MATHEMATICAL DESCRIPTION: MILLER INDICES

Although the classical names, letter symbols, and structural symmetry of the face are often used to describe the external features of the crystal, the most common method to describe both external and internal plane orientations is one that assigns a set of three indices similar to the method used to describe rational lattice vectors. These three indices are called the Miller indices.

*Planes that contain more that one lattice point are called **rational planes***

***Miller indices,** (h k l), are used to indicate lattice planes. The Miller indices are derived from the inverse of the intercept distance of the plane on the crystal axes. The Miller indices are also the coefficients of the equation specifying the position of a general point on the plane.*

A recipe for determining the Miller[1] indices is

> 1. Find the intercepts of the plane with the crystallographic axes.
>
> 2. Take the reciprocal of each intercept, express the indices as a row or column vector.
>
> 3. Multiply the reciprocals by the lowest common denominator to get a set of three integral indices

Parentheses are used to indicate that the indices represent a plane (rather than a lattice vector). Braces are used to indicate a form. Thus, in the isometric system, (100) and $(\bar{1}00)$ are planes within the form $\{100\}$.

The fact that step 2 can be done for all planes of interest is the law of rational intercepts, as surmised by Haüy. If just the intercepts are used, then the indices are called the Weiss intercepts, a method that is in disfavor.

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[1] The use of the reciprocal construction and the resulting indices was actually first suggested by William Whewell at Cambridge. William Miller succeeded him and popularized their use in a crystallography textbook published in 1839. Zoltai, T., and J.H. Stout, *Mineralogy: Concepts and Principles*, 505 pp., Macmillan Publishing Company, New York, 1984.

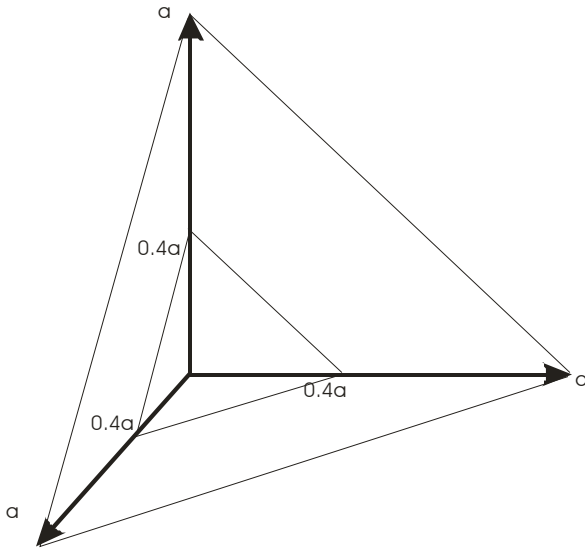Determine the Miller indices for the following planes:
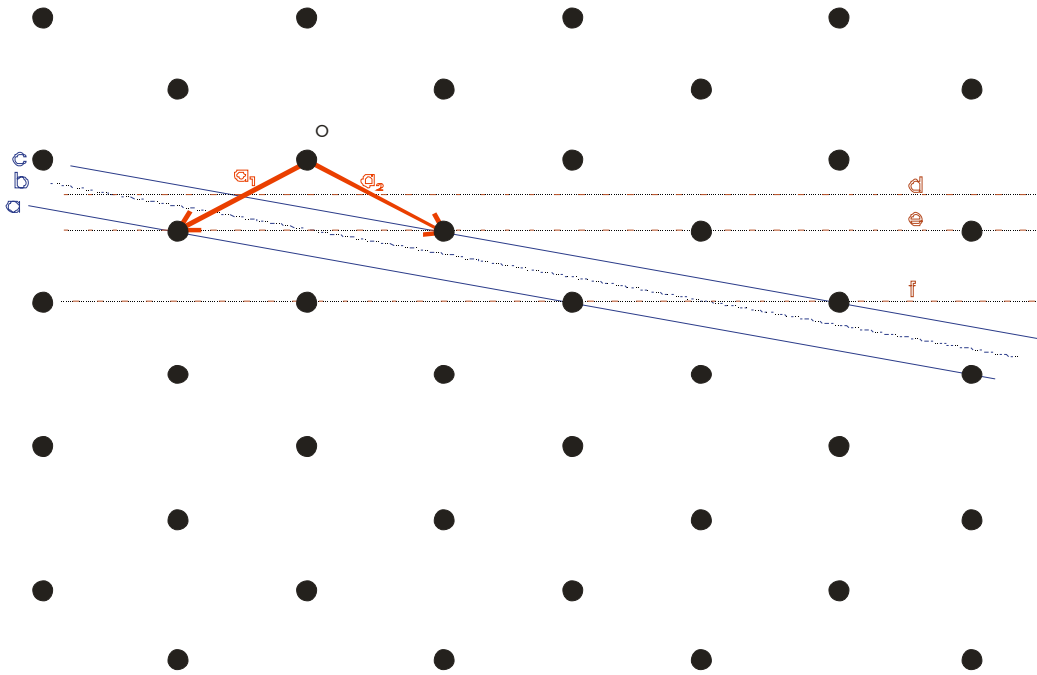
Try the planes below:
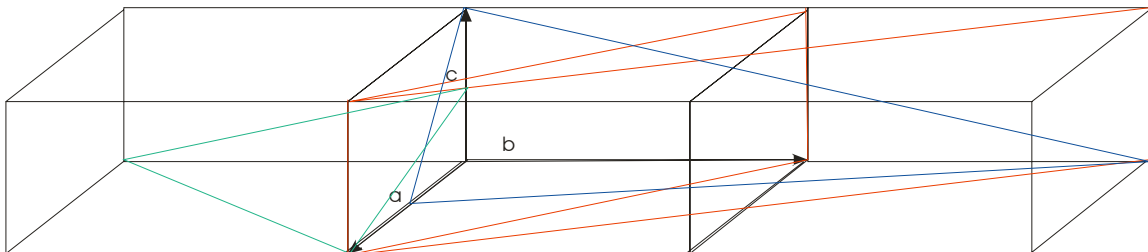
Miller indices are useful because all parallel planes have the same Miller indices when reduced.

Rational planes have integral values of Miller indices.

In a three-dimensional space with orthonormal axes, the equation of a line is

$\dfrac{x}{A} + \dfrac{y}{B} + \dfrac{z}{C} = 1$ where A, B, and C are the intercepts with the x, y, z axes.

So at least for orthonormal coordinates, the Miller indices are the coefficients for the equation of a set of planes.
So, (h k l) can be thought of as standing for the components of the equation:
$hx + ky + lz = \text{constant}$ *where the constant gives an indication of the spacing between planes.*

But, what about non-orthonormal axes?

Reciprocal Lattice:

Reciprocal vectors are defined to be perpendicular to two of the three lattice vectors and with length equal to 1/length of the third vector.

$$\mathbf{a}^* = \frac{\mathbf{b} \times \mathbf{c}}{|\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})|}$$

$$\mathbf{b}^* = \frac{\mathbf{c} \times \mathbf{a}}{|\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})|}$$

$$\mathbf{c}^* = \frac{\mathbf{a} \times \mathbf{b}}{|\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})|}$$

Notice that this definition insures that
**a×a* = b×b* = c×c*** $= 1$ *and*   **b×a* = c×b* = a×c*** $= 0$

Or $a_i \cdot a^{*j} = \delta_i^j$ where the sub and super script denote the three different real and reciprocal vectors, respectively.

Notice that $|\mathbf{a}^*| = \dfrac{1}{|\mathbf{a}| \sin \gamma}$ where γ is the angle between **a** and **b**.

Exercise: Below is a plan view of two lattice vectors; assume that the third axis extends perpendicular to the paper; draw the reciprocal vectors:
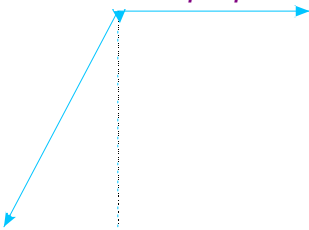
A general real lattice is given below in the left hand picture. Draw the reciprocal lattice vectors in the right hand picture. For comparison, the real vectors are dotted in the right hand picture:
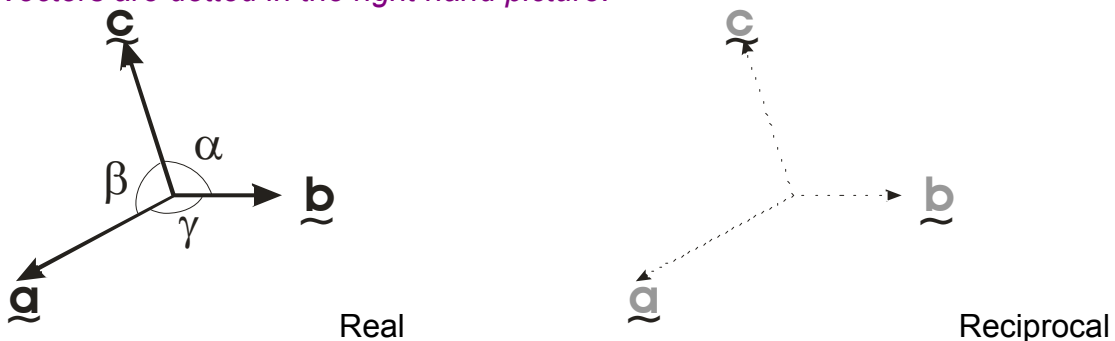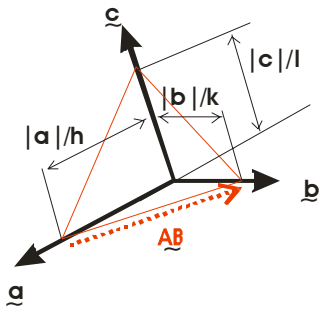
Real   Reciprocal

Relation between Miller indices and reciprocal lattice:

The reciprocal vector formed by using the Miller indices of a plane as its components forms a vector in space that is normal to the plane. The length of the reciprocal vector for the plane is the distance between two similar planes.

Proof:

If the normal to the plane is given by $\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ Then the dot product of the normal with any vector lying in the plane will be zero.

Consider vector AB which lies in the plane:

By vector addition, $\dfrac{\mathbf{a}}{h} + \mathbf{AB} = \dfrac{\mathbf{b}}{h}$.

The dot product, $\mathbf{AB} \cdot \mathbf{r}^* = \left(\dfrac{\mathbf{b}}{h} - \dfrac{\mathbf{a}}{h} \right) \bullet \left(h\mathbf{a}^* = k\mathbf{b}^* + l\mathbf{c}^* \right)$

$$= -1 + 1 + 0 = 0$$

because of the properties of the reciprocal vectors.

The spacing between planes (h k l) is $1/\left| \mathbf{g}^*_{hkl} \right|$.

Proof: In the figure above the spacing between the planes is the projection of $\dfrac{\mathbf{a}}{h}$ on $\dfrac{\mathbf{r}^*}{|\mathbf{r}^*|}$

$$d_{hkl} = \dfrac{\mathbf{a}}{h} \bullet \dfrac{\mathbf{r}^*}{|\mathbf{r}^*|} = \dfrac{h}{h} \cdot \dfrac{1}{|\mathbf{r}^*|} = \dfrac{1}{|\mathbf{r}^*|}$$

SUMMARY: LATTICES PLANES, CRYSTAL FORMS, AND RECIPROCAL LATTICE

1.   Miller Indices arise from finding the plane intercepts, inverting, forming a vector and clearing fractions or common factors

2.   The Miller indices are the components of the equation for the plane.

3.   Each set of Miller indices represents a set of parallel planes. Indices that are integral multiples of another set are parallel planes with a smaller interplanar spacing e.g. (4 4 2) and (2 2 1).

4.   In general a given direction is not parallel to the pole of a plane with the same Miller indices.

5.   Equivalent planes may be discovered by examining a stereogram and considering the symmetry elements.

6.   Some planes in the crystal (crystal forms) are common enough or important enough to be given special names. The naming can be by Miller indices, classical terminology, by pole symmetry, or be lower case letters.

7.   Reciprocal vectors are formed by choosing a vector perpendicular to two lattice vectors and of length reciprocal to the third lattice vector.

8.   Linear combinations formed from these reciprocal vectors and the Miller indices are vectors that are in the same direction as the poles to the corresponding planes. The vector length of this vector is the reciprocal of the plane spacing.

BIBLIOGRAPHY

Bloss, F.D., *Crystallography and Crystal Chemistry: An Introduction*, 543 pp., Mineralogical Society of America, Washington, DC, 1994.

Zoltai, T., and J.H. Stout, *Mineralogy: Concepts and Principles*, 505 pp., Macmillan Publishing Company, New York, 1984.