| EENS 2110 | Mineralogy |
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Crystallographic Calculations

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Crystallographic Calculations

Crystallographic calculations involve the following:

1. Miller Indices (hkl)

2. Axial ratios - . a: 1: c

3. ρ and ϕ angles corresponding to a Miller Index (hkl)

4. angles between crystallographic axes if in monoclinic, or triclinic systems.

Most of what you will do in lab or on exams will involve crystallographic calculations in the orthorhombic, tetragonal, hexagonal, or isometric systems, where the axes angles are fixed. Note that you will always be given enough information to solve the problem. Some of the problems you might be expected to solve involve determination of Miller Indices from the ρ and ϕ angles, to determine the ρ and ϕ angles for faces of mineral with known axial ratios, or to determine axial ratios of minerals that have faces of known ρ and ϕ angles.

First let's review some of the things we know about Miller indices and ρ and ϕ angles. In the orthorhombic, tetragonal, or isometric systems.

- If h is 0, i.e. (0kl) is the Miller Index, then the face is parallel to the **a** crystallographic axis.

    So, $\phi = 0^o$ or $\phi = 180^o$

- If k is 0 i.e. (h0l) is the Miller Index, then the face is parallel to the **b** crystallographic axis.

    So, $\phi = 90^o$ or $\phi = 270^o$

- If l is 0, i.e. (hk0) is the Miller Index, then the face is parallel to the **c** crystallographic axis.

    So, $\rho = 90^o$

- If h & k are 0, i.e. (00l) is the Miller Index, then the face is perpendicular to the **c** axis

    So, $\rho = 0^o$ or $\rho = 180^o$, and ϕ is undefined.

- If h & l are 0, i.e. (0k0) is the Miller Index, then the face is perpendicular to the **b** axis.

    So, $\rho = 90^o$ and $\phi = 0^o$ or $\phi = 180^o$.

- If l and k are 0, i.e. (h00) is the Miller Index, then the face is perpendicular to the **a** axis.

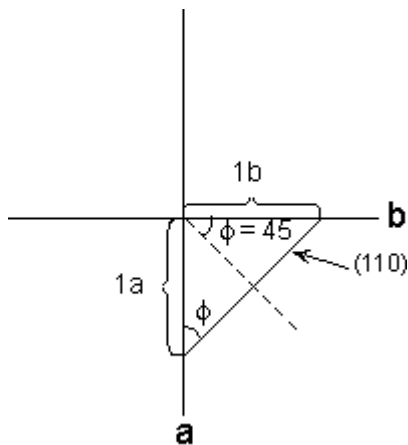   So, $\rho = 90^o$ and $\phi = 90^o$ or $\phi = 270^o$.

Now let's do some examples

1. Given Miller indices and ρ and ϕ angles for crystal faces that, in combination, intersect all crystallographic axes, calculate the axial ratios of the mineral.

    a.
Faces	ρ	ϕ
(110)	90°	45°
(011)	70°	0°

    For the (110) we note that it does not intersect the c axis, so we can look at it in the two dimensional plane containing the a and b axes, as shown in the drawing below. From this face we should be able to determine the a/b axial ratio. Since the ϕ angle is the angle between the normal to the face and the b axis, by similar triangles we know that the ϕ angle also occurs between the a axis and the face.
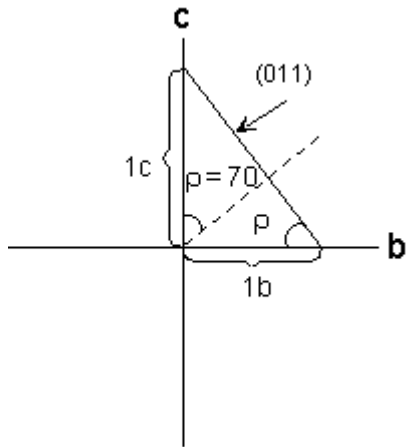

    Thus, we can write:

    $$\tan 45^o = 1b/1a$$

    then

    $$1a/1b = 1/\tan 45^o = 1$$

    So, a/b: b/b = 1: 1

    We next note that the (011) intersects the b and c axes only, so we can examine this face in the plane containing only b and c, as shown below. From this drawing we can obtain the c/b axial ratio. Since the ρ angle is the angle between the pole to the face and the c axis, again by similar triangles we know that the ρ angle also occurs between the b axis and the (011) face.

c

(011)

1c ρ=70

ρ
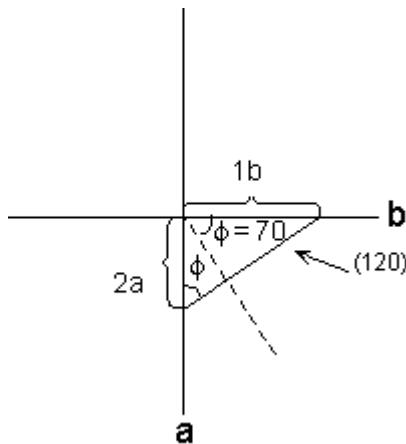
b

1b

Thus, we can write:

$$\tan 70^o = 1c/1b$$

then

$$c/b = \text{arctan } 70^o$$

$$\text{So, } c/b = 2.7475$$

so, a : b : c = 1 : 1 : 2.7475 and the mineral must be tetragonal, since a/b =1.

b. Faces   ρ   φ
   (120)   90° 70°
   (011)   32° 0°

The face (120) does not intersect the c axis, so we can look at this face in the plane containing only the a and b axes. We must also remember that Miller Indices represent the inverse of the intercepts, so the face (120) intersects the a axis at twice the number of unit lengths that it intersects the b axis. Since the φ angle is the angle between the normal to the face and the b axis, by similar triangles we know that the φ angle also occurs between the a axis and the (120) face.
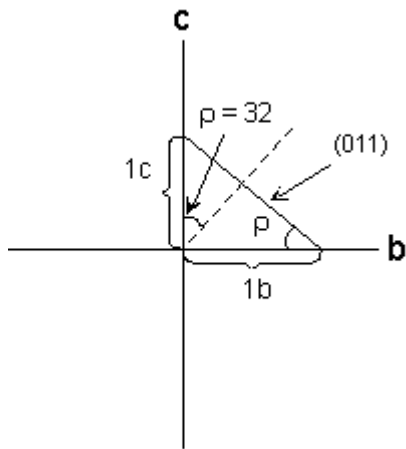
1b

φ=70   b

φ

2a

(120)

a

Then we can write:

$$\tan 70^o = 1b/2a$$

$$a/b = 1/2\tan 70^o$$

$$1a/1b = 0.18199$$

We next note that the (011) intersects the b and c axes only, so we can examine this face in the plane containing only b and c, as shown below. From this drawing we can obtain the c/b axial ratio. Since the ρ angle is the angle between the face and the c axis, again by similar triangles we know that the ρ angle also occurs between the b axis and the (011) face.

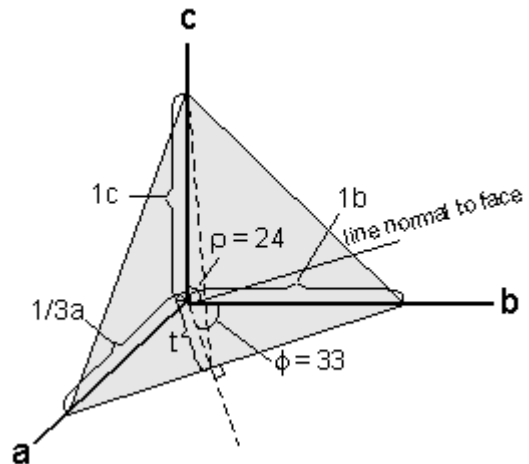For this face we can determine that

$$\tan 32^o = 1c/1b$$

$$1c/1b = 0.6248$$

so, a : b : c = 0.18199 : 1 : 0.6248, and the mineral is orthorhombic
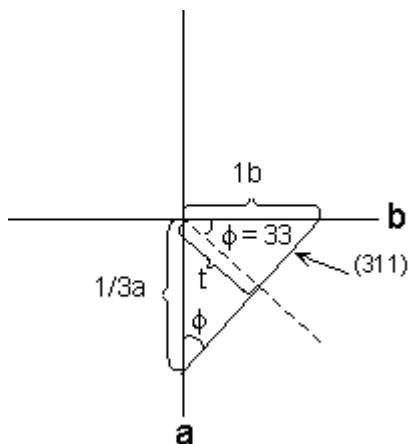
c. Faces   ρ   φ
    (311)   24° 33°

This face is more complicated because it intersects all three axes.

We first attempt to draw a 3-dimensional view of this face. Notice that the φ angle is measured in the horizontal plane that includes the a and b axes. The ρ angle is measured in a vertical plane that includes the **c** axis and the line normal to the face in the a - b horizontal plane, and is measured between the c axis and a line normal to the face.

Note also, that for the (311) face, the intercept on the a axis is 1/3 what it is on the b and c axes, because the Miller Index is the inverse of the intercepts..

We can determine the a/b part of the axial ratio by looking at the projection of this face in the a - b plane.

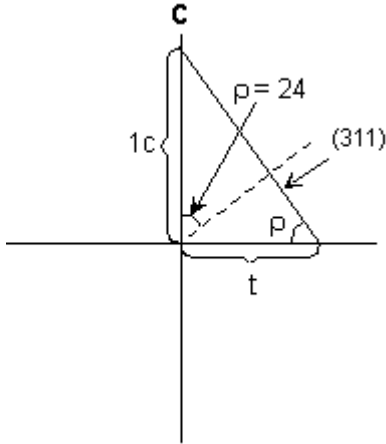$$1b/(1/3)a = \tan 33^o$$

$$1a/3b = 1/\tan 33$$

$$1a/1b = 3/\tan 33$$

$$1a/1b = 4.6196$$

In order to determine the length of the **c** axis, we need to know the length of the line labeled t, because this line forms the base of the triangle in which the ρ angle is measured. The length of the line t is:

$$t/b = \cos 33^o$$

$$t/b = 0.8397$$

$$t = 0.8397\ b$$

We can now use this to determine the c/b axial ratio.

$$1c/t = \tan 24^o$$

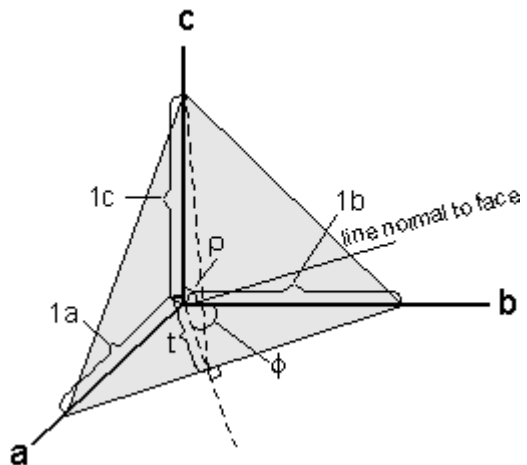$$1c = 0.8387\ b \tan 24^o$$

$$c/b = 0.3747$$

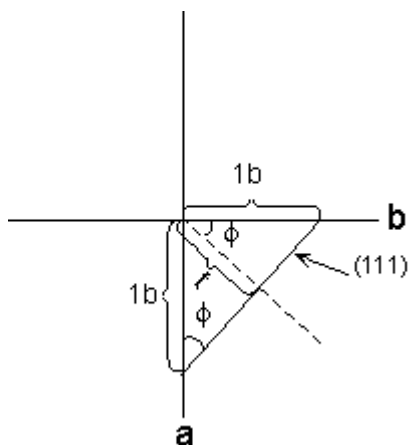Thus, the axial ratio for this mineral is 4.6196 : 1 : 0.3747

Now we'll look at an example where we are given the axial ratio of the mineral and asked to calculate the ρ and ɸ angles for the faces.

1. Given the axial ratio for a mineral is 1 : 1 : 5.0, what are ρ and ɸ for the face (111).

We first attempt to draw a 3-dimensional view of this face. Notice that again the ɸ angle is measured in the horizontal plane that includes the a and b axes. The ρ angle is measured in a vertical plane that includes the c axis and the line normal to the face in the a - b horizontal plane, and is measured between the c axis and a line normal to the face.

In this case the intercept on the all three axes is 1.

Since the ϕ angle for this face is measured in the horizontal a - b plane, we can draw the plane containing only the a and b axes to determine the angle.

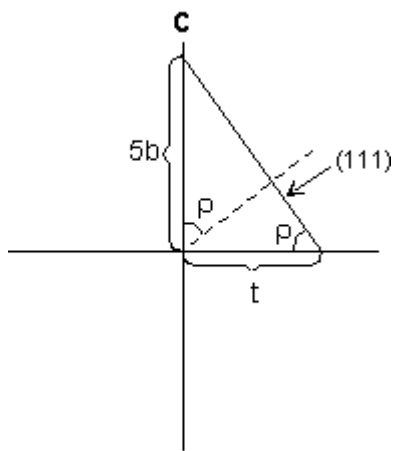Since the axial ratio tells us that the relative lengths of the a and b axes are equal

$$\tan \phi = 1b/1b = 1$$

$$\phi = 45^o$$

In order to determine the ρ angle, we need to know the length of the line labeled t, because this line forms the base of the triangle in which the ρ angle is measured. The length of the line t is:

$$t/b = \cos 45^o$$

$$t = 0.7071 \ b$$

Now we can determine the angle by drawing the plane that includes the c axis and the line t. In this plane we can let the length of the c = 5b, from the axial ratio. Then:

$$\tan \rho = 5b/t$$

$$\tan \rho = 5b/0.7071b$$

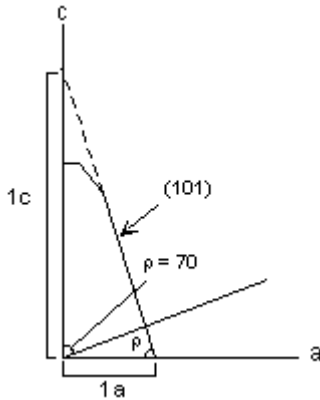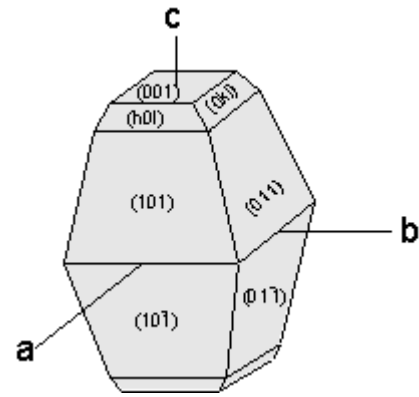$$\tan \rho = 5/0.7071$$

$$\tan \rho = 7.071$$

$$\rho = \arctan (7.071) = 81.95^o$$

So for the (111) face in this crystal $\rho = 81.95^o$ and $\phi = 45^o$.

2. Given the tetragonal crystal shown below and the following information:

For the face (101) $\rho = 70^o$ $\phi = 90^o$
  a. What is the axial ratio for this crystal?
  b. What are the Miller Indices for the faces labeled (0kl) and (h0l), given that both of these faces have $\rho = 53.9478^o$?

a. To find the axial ratio we note that we can use the face (101) and draw this in plane of the a and **c** axes (since the face doesn't intersect the b axis. Then, we can determine that

$$\tan \rho = 1c/1a$$

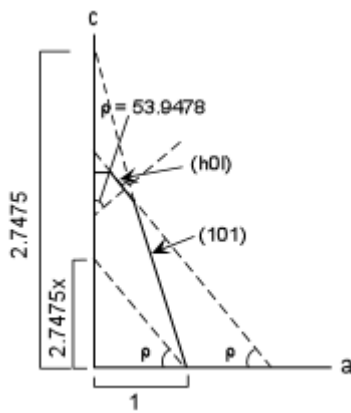so, $\tan 70^o = c/a = 2.7475$

and the axial ratio is: 1 :1 : 2.7475

b. To find the Miller indices of the face (h0l) we proceed as follows:

Since all we need is the relative lengths of intersection to calculate the parameters, we can assume one of the lengths = 1, i.e. 1a. This is the same as moving the face parallel to itself so that it intersects the a axis at a unit length of 1. The face intersects the c axis at 2.7475x, where the 2.7475 value is the length of the c axis relative to the unit length of the a axis. Then

$$\tan (53.9478) = 2.7475x/1, \text{ and thus, } x = 0.5$$

The parameters for this face are then:

1, ∞, 1/2, which can be inverted to give the Miller Index - (102).

Since the mineral is tetragonal, the face labeled (0hl) would have the Miller Index (012).

Problems such as these could be asked on any laboratory exam.

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