Novel Digital Goniometry (A midnight goniometric folly)

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January 27, 2014

It has been known, since the 17th century, that fixed relationships exist between the planar faces of mineral crystals. However, it took nearly a hundred years more before a simple method of measuring the angle between adjacent crystal faces was implemented in the form of the contact goniometer. This simple, but fairly accurate tool, could measure angles on macro crystals with an accuracy of about a quarter of a degree. Soon after, the optical goniometer was invented and evolved in many forms, incrementally improving on the accuracy and ease of use, as well as being less limited by the size of the crystals being measured. At the dawn of the 20th century, with the invention and development of x-ray diffraction spectrometers, the goniometers that were once the mainstay of crystallographers found less and less use and eventually were discarded as useful tools. At the present time, goniometers are mostly of interest only to amateurs and to historical museums, and are of little use to professional crystallographers and mineralogists.

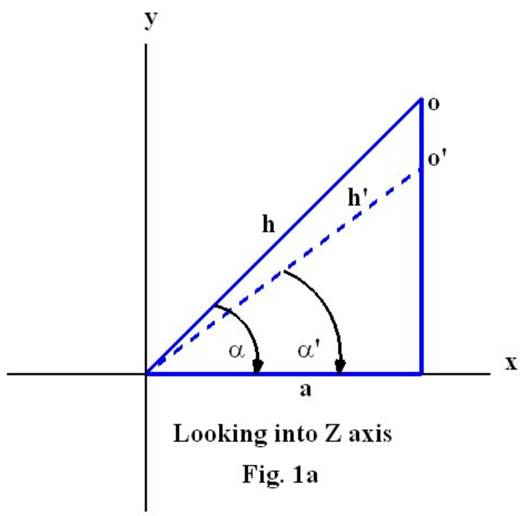
Having an interest in learning crystallography, at an amateur level, led me to investigate the construction of a simple optical goniometer. While I have experience at instrument building, what originally seemed like a fairly simple project turned out to be quite complicated and time consuming and soon my patience wore thin. As a result, the miniature precision measuring heads and optical parts that I acquired are still packed away in a drawer waiting for another day when I will find the time and fortitude to revive the project. Irrationally, I also gave up the idea of studying crystallography, as I can usually only remain absorbed in something when I have a hands on involvement.

Some years later, while using a digital microscope with measurement capabilities, it occurred to me that perhaps this would be a useful tool for measuring crystals. For many obvious reasons, I realized that this tool could not replace an optical/mechanical goniometer, but perhaps it could be used for learning and experimentation. The thought persisted, but I took no action on it until a friend posed a mineral identification problem that I thought could be solved by goniometry. I then set out to see if I could make any sort of meaningful determinations using "digital goniometry", a fancy term that I coined for angular measurements made using a simple digital protractor program. For existing images, this method can be used under some circumstances that I will eventually address. My first attempts were made with images of crystals that were pre-existing and that I had no control over the orientation. It was apparent that the faces that I wished to measure were not perfectly orthogonal to the optical axis of the camera, or planar with the sensor, when the digital images were taken. That set me to thinking about how much error in off-plane orientation could be tolerated. In my mind's eye I could picture the result, but couldn't quantify it without calculations. When I finally mentioned the idea to some associates, it wasn't well received for reasons based upon their own intuitions. That gave me the renewed interest to pursue this idea (or folly) and so I set out to do the analysis which, to my surprise, actually turned out to be a trivial exercise. We consider a digital image of a hypothetical crystal face bounded by sides h, o and a on the x, y plane (Fig.1a). We wish to measure the angle α on the computer monitor by digital means and it seems obvious that, if the image of the crystal face was not imaged with the optical axis of the camera orthogonal to it, a measurement of the angle α would result in an error. This is certainly true, but to what extent, and how much error is tolerable? At first glance, it may seem that any non-parallelism of the face to the x, y plane would be intolerable when trying to achieve fractional degree accuracy. Surprisingly, the measurement accuracy is not affected as much as it would seem.

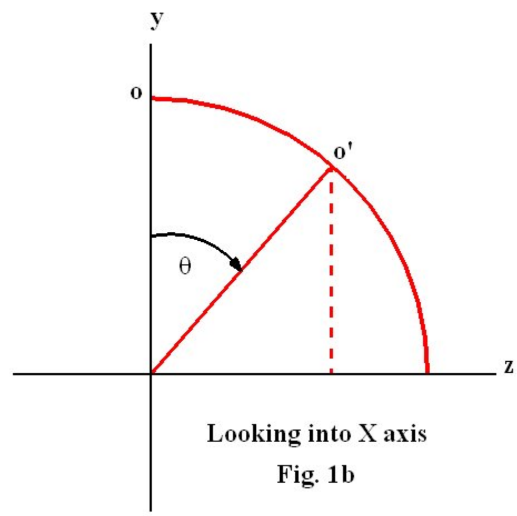
The assumptions and calculations:

To see how an error is introduced into our measurement, imagine a crystal face bounded by line segments h,o,a that is planar to the x,y plane and then rotate the crystal about the x axis so as to reduce angle α to α', from a view into the z axis (figure 1a). As we do so, we note that the height of the face at point o appears to shrink to point o' and angle α is now reduced to the apparent angle α' and the error introduced is $\alpha - \alpha'$. Calculation of the error is straightforward. Though not rigorous, the names of the sides will also denote the lengths of the sides for simplicity. Effects due to foreshortening are small and therefore ignored in the following simplified analysis.

Rotation about X axis



Looking into Z axis
Fig. 1a



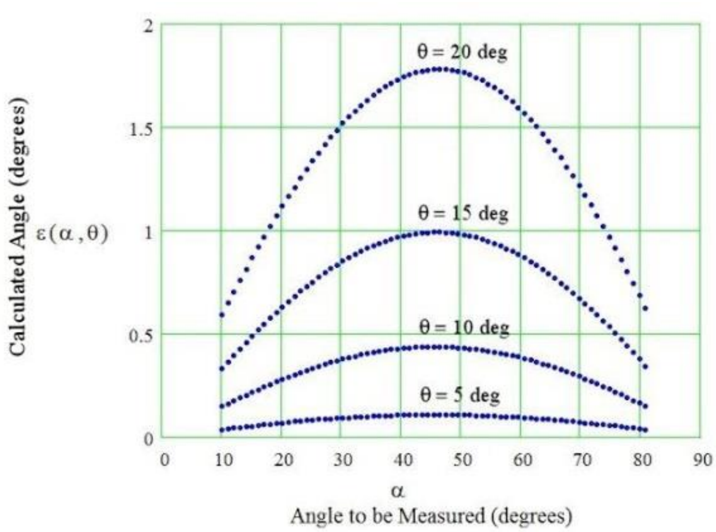
Looking into X axis
Fig. 1b

α = actual angle to be measured of face bounded by h,o,a
α' = apparent angle of rotated face bounded by h',o',a
o = height of side o
o' = apparent height of rotated side o
θ = angle of rotation about the x axis

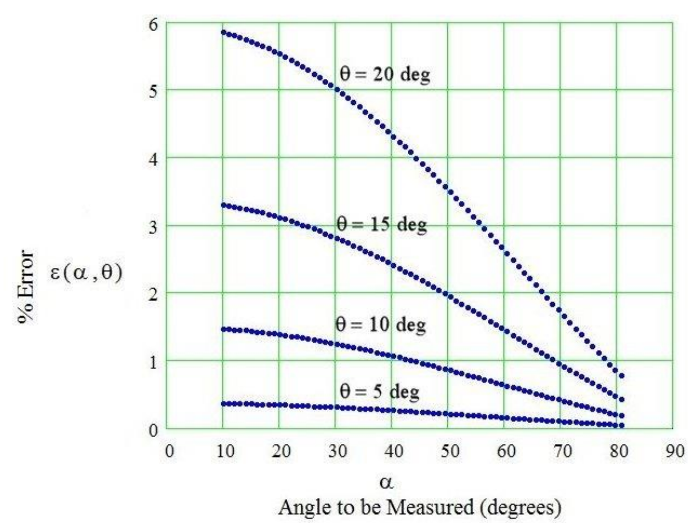
$\alpha = \dfrac{o}{tan\alpha}$ and $o' = \sin(90 - \theta)$ therefore, it follows that

$\alpha' = \arctan[\sin(90 - \theta)\, tan\alpha]$ and the error ε is: $\varepsilon = \alpha - \arctan[\sin(90 - \theta)\, tan\alpha]$

As an example, the case where the angle to be measured (α) is 45^0 and the angle of rotation (α') is 10^0, the calculated error is $\varepsilon = 0.44^0$. Graph 1 and Graph 2 below provide a broader view of how the measured angle is affected by its rotation about the x axis in figures 1a and 1b above.



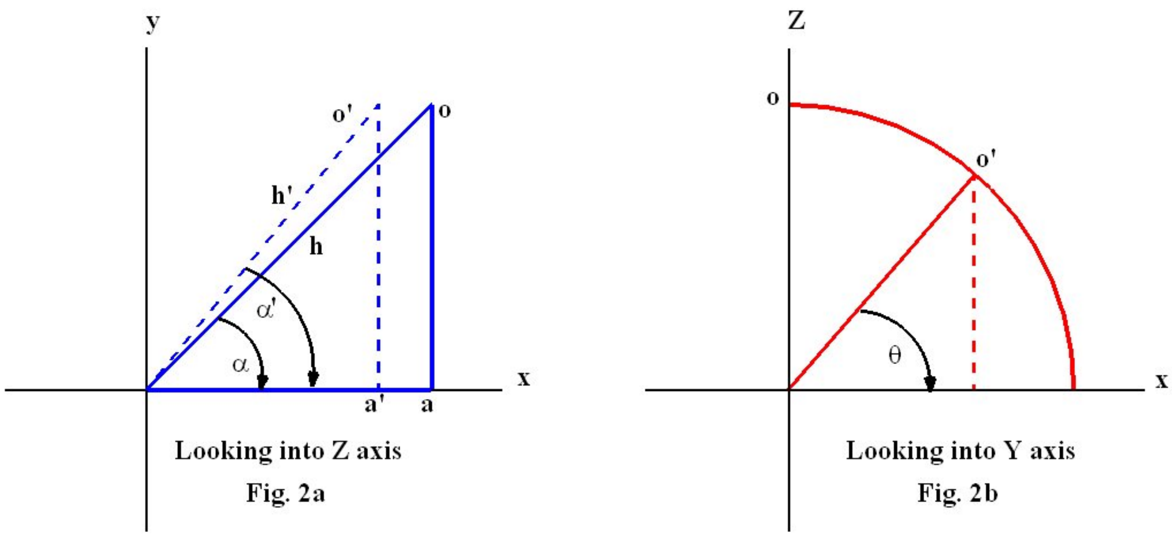
Graph 1.



Graph 2.

Now imagine the crystal face bounded by line segments h,o,a that is planar to the x,y plane and then rotate the crystal about the y axis so as to increase α to α' from a view into the y axis (figure 2a). As we do so, we note that the side of the face a appears to shrink to point a' and angle α is increased to the apparent angle α' and the error introduced is α-α'. The calculation of the error is again straightforward, as follows.

Rotation about Y axis



Looking into Z axis
Fig. 2a

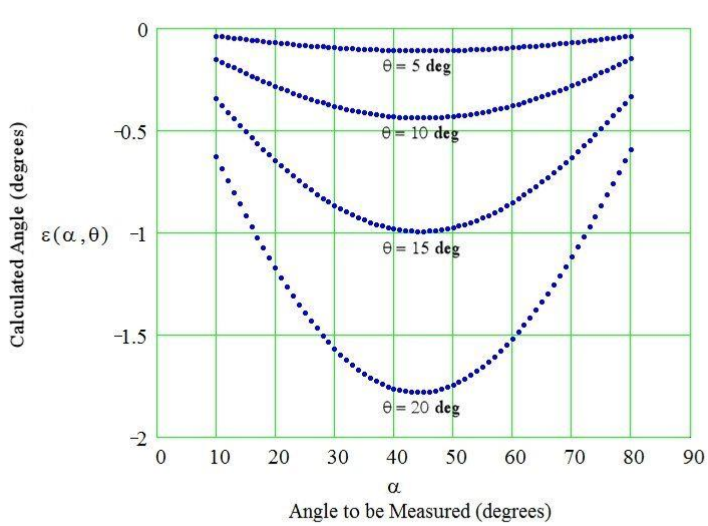
Looking into Y axis
Fig. 2b

α = actual angle to be measured of face bounded by h,o,a
α' = apparent angle of rotated face bounded by h',o',a
a = length of side a
a' = apparent length of rotated side a
θ = angle of rotation about the y axis

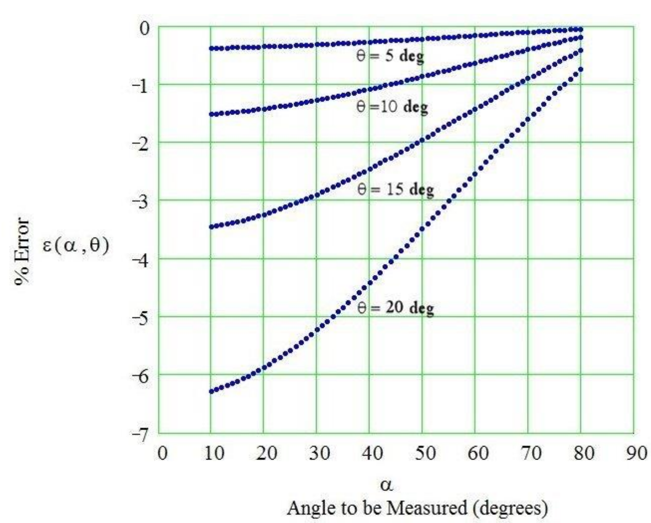
$a\tan\alpha = a'\tan\alpha'$ and $a' = a\cos\theta$ therefore it follows that:

$\alpha' = \arctan\left[\frac{\tan\alpha}{\cos\theta}\right]$ and the error ε is: $\varepsilon = \alpha - \arctan\left[\frac{\tan\alpha}{\cos\theta}\right]$

For example, the case where the angle to be measured (α) is 45^0 and the angle of rotation (θ) is 10^0, the calculated error is again $\varepsilon = 0.44^0$. Notice that the introduced error ε has increased the measured α rather than decreasing it, as in the previous example of rotation about the x axis. Graph 3 and Graph 4 below provide a broader view of how the measured angle is affected by rotation about the y axis in figures 2a and 2b above.



Graph 3.



Graph 4.

It can be seen from the above that significantly large rotations on either axis do not introduce errors that would render this method of measurement useless. The accuracy of an angular measurement could be greatly improved by having a prior knowledge of, or guessing, the amount of rotation of the face to be measured, and compensating for that using the calculations and/or the graphs above. Also, note from Graph 2 and Graph 4 that larger angles to be measured are not as affected by out-of-plane rotation as smaller angles. Note that there are situations whereby the additive angular errors, due to rotation about two planes, compensate for the error in the angle of interest. I will eventually do a more complete analysis, but this serves as a start towards that end. With this in mind, it is always better to adjust the position of a crystal face such that it is reasonably orthogonal to the optical axis of the imaging device. To that end, it is very easy to do this with images made at magnification, i.e. photomicrographs. Contrary to the bane of microphotography, lack of depth of field actually helps in this case. The specimen can be adjusted very easily by making sure that the crystal face of interest is uniformly in focus at each corner, or across its plane.

Having quantified the magnitude of the errors introduced by rotating a crystal face from being planar to the x,y axis, I could proceed to revisit my earlier trials on my friend's crystal and others with a better confidence in the accuracy of the measurements. The original crystal in question was a Boleite that had an epitaxial growth on its faces, as many do. The object of the exercise was to determine whether the epitaxial growth was Psuedoboleite or Cumengeite. When I originally took the photo, I had no idea that I would ever be trying to measure angles on it, so I had oriented it for aesthetics rather than measuring. As luck would have it, the angle that I wanted to measure was actually rotated forward to make the face of interest nearly orthogonal to the optical axis. The measurement turned out to be very close to the expected angle for Psuedoboleite. As a further check, I measured a Cumengeite crystal for comparison. The results are shown in Photo 1, and Photo 2.

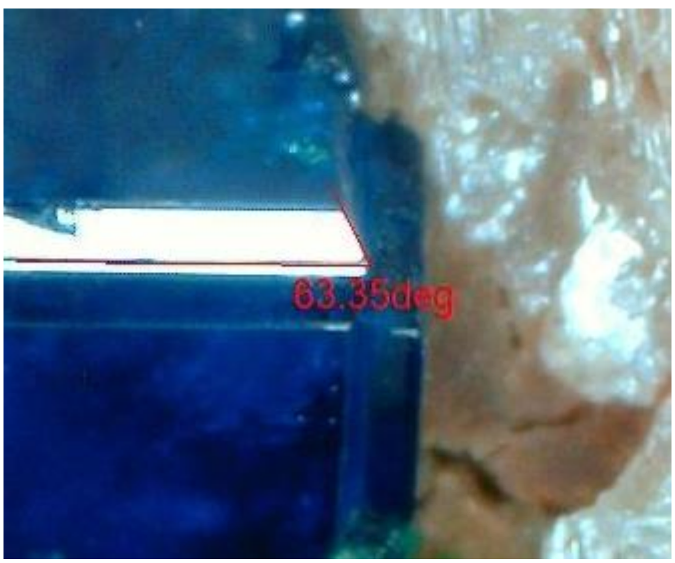


Photo 1.
Pseudoboleite
Expected = 63.63^0
Measured = 63.35^0
Error = 0.28^0

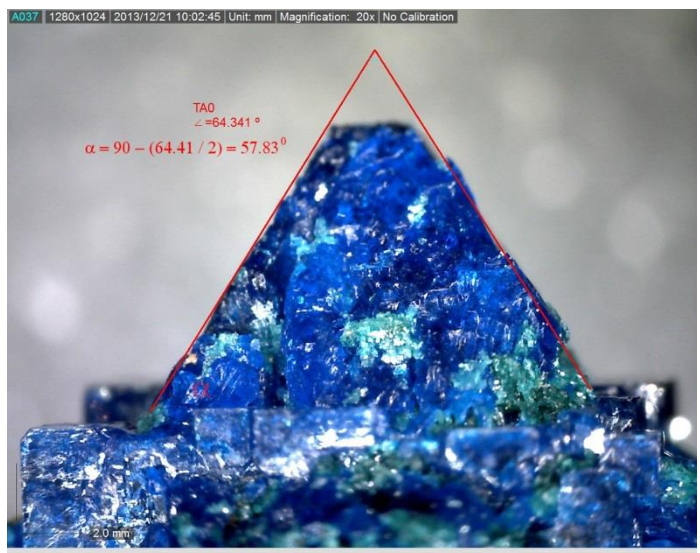


Photo 2.
Cumengeite
Expected = 58.35^0
Measured = 57.85^0
Error = 0.5^0

This result is optimistically in favor of Pseudoboleite, but not conclusive, so I will confirm it later when I again have access to the specimen and can better align it for measurement. In making these measurements, I noted how well the eye can interpolate a best line fit to rough, or otherwise not well defined edges.

Many other possibilities exist for the use of this simple method, though it cannot compete with a professional reflection goniometer. However many useful determinations can be made, though with less accuracy. The verification of Quartz Japan Twins is easily performed by this method. Here are a few examples.

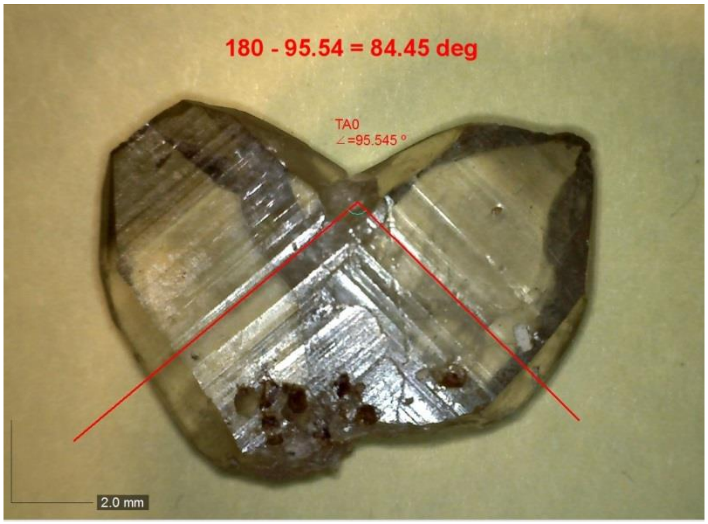


Photo 3.

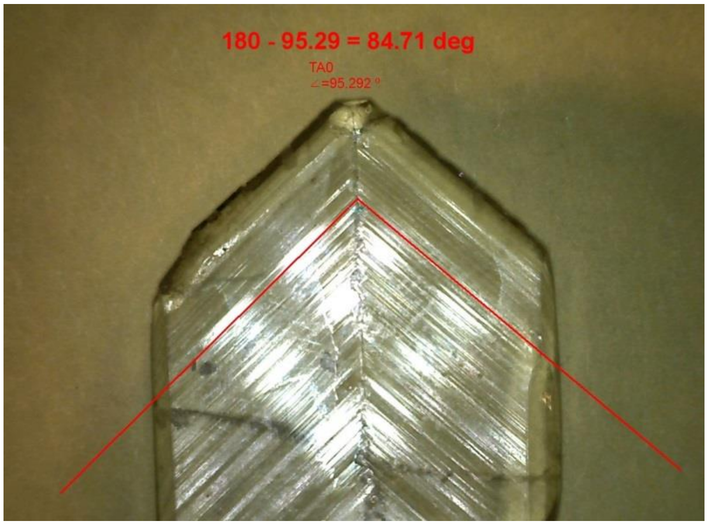


Photo 4.

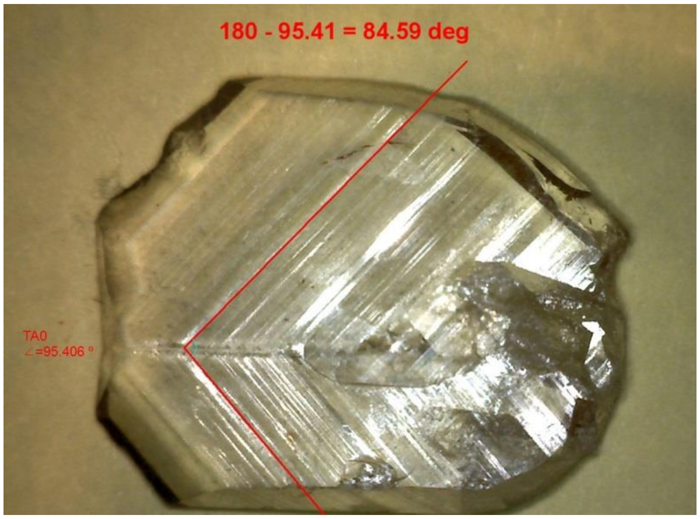


Photo 5.

Note that the accuracy of the measurements is very close to the Japan law twin angle of 84.55^0 . The worst case error, for these measurements, is ~0.16^0. In this case, the striations and the alignment of the crystals make this measurement fairly easy. None of the three crystals are larger than ~12mm and it would be very difficult to measure them with a regular protractor.

In conclusion, a digital protractor can be useful in determining the angles included in crystal faces with reasonable accuracy. Some digital microscopes, such as the Dino-Lite, have angular measurement capability built into the DinoCapture software. There are also digital protractor freeware programs, such as MB-Ruler, that can be used to make angular measurements on most digital images.

The mathematical treatment developed is useful in assessing the accuracy of the angular measurement of adjacent crystal faces. If an estimate of the non-planar angle of the face to be measured can be made, then the introduced angular error can be calculated and used to correct the final result. From this exercise is also apparent that the eye is very good at interpolating the best line fit to a rough edge as in Photo 2. However, further improvement in accuracy can be achieved by averaging several measurements. Having gone through this exercise, I am now satisfied that this method can be useful for some work where an accuracy of perhaps 0.5^0 still allows for a meaningful determination. This simple and inexpensive method can provide the student of crystallography a tool with which to experiment, and to make determinations where high accuracy is not required.