Rowland Circle Geometry based X-ray Spectrometer Alignment Guide XRS TECH LLC.

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Figure 1, Rowland circle geometry based x-ray spectrometer, Rowland circle diameter equal to the radius of bent crystal analyzer

The alignment task is to allow the crystal analyzer, detector, and single x-ray energy (monochromator) to be linked together. Only after the spectrometer is aligned, can it be used to do all necessary measurements. Fig.1 shows the principle of Rowland circle geometry based x-ray spectrometer.

One is suggested to use the elastic line to align the spectrometer. It can take at least half a day to get the alignment done. Fig. 2 describes why it is a demanding job. In fig. 2, it shows $\Theta - \chi$ plane, where Θ is the analyzer Bragg angle, and χ is the analyzer tilt angle. In fig.2 (a), after initial laser alignment, due to crystal miss-cuts and limited goniometer accuracy, detector (rectangle), analyzer (circle) and single x-ray elastic energy (vertical line) are not always aligned at the same point. One can imagine how difficult it is to align these three devices from fig.2.(a) to fig.2.(b). The reason is one needs move two out of these three devices to make them align in a two dimensional plane in **BLINK**.



Figure 2, spectrometer alignment with single energy x-ray from elastic scattering

Fortunately, we have a simpler way to do this job. The key is to use band energy x-ray in place of single energy x-ray. Fig. 3 shows this principle. Band energy x-ray can be from knowable emission lines which need to cover or can be close to our spectrometer measuring point. From

fig. 3(a), we see the detector and analyzer both are in the band energy x-ray field (presented as the rectangle filled with gray color). The alignment requires just moving one of two devices (between the analyzer and detector, usually the analyzer) in Θ - χ plane to align, since the detector can always can get signal if they are aligned in the same band energy x-ray field. Fig. 3(b) shows the aligned picture. With this method, one can make complete the job in only 30 minutes.



Figure 3, spectrometer alignment with band energy x-ray from knowable emission lines

In the following, we will list all steps for alignment with band energy x-ray:

- 1) Laser initial alignment (necessary for rough alignment before x-ray):
 - (a) Based on the energy range for the measurement, calculate the scattering spot and analyzer and detector position on the Rowland circle. Then put these three objects on the Rowland circle;
 - (b) Using a tiny point laser, point on the scattering spot, watch the reflecting point focus from the analyzer, and then rotate the analyzer to let the reflecting point back to the scattering spot. Here the Bragg angle is defined as 90 degrees;
 - (c) Rotate the analyzer to the desired Bragg angle, and set the detector at its laser reflecting-focusing point position. Record both of their position parameters as position A;
 - (d) rotate the analyzer to another Bragg angle in the energy range, and move detector to its new laser reflecting-focusing point position. Record both of their position parameters as position B;
 - (e) Use position A and B parameters to calculate and set analyzer and detector motion parameters to be linked together (on a presumed linear relationship);
- 2) Band energy x-ray alignment:
 - (a) set up a sample at a scattering spot. The sample's emission lines need to cover or be close to the spectrometer measuring energy range. For example, if one wants to set the spectrometer to measure energy around 6500eV, one can use Mn K_{β} lines (band center at 6490eV) for alignment;
 - (b) Move the analyzer and detector to the Bragg angle of the sample emission energy(not necessarily on the peaks);
 - (c) Open the detector slit widely to maximize its active entry area;
 - (d) Put on a vacuum path or helium path to reduce air absorption if necessary;
 - (e) Turn on the x-ray and set the monochromator energy above the sample emission edge to create expected emission lines;
 - (f) If there is signal in the detector, fine tune the analyzer to maximum. If there is no signal, tune the analyzer Θ or χ to get signal and maximization (after laser alignment, real x-ray alignment position should not be far away);

- (g) Narrow the detector slit to reduce background and tune the analyzer to maximum signal again;
- (h) Scan spectrometer energy to find the peak of the emission lines and calibrate spectrometer energy. One can also scan the monochromator to calibrate if possible.

For the system with multiple crystals, alignment is similar to above. All crystals first need to be aligned in laser simulation. In x-ray alignment, you need to align one at a time by shielding all others. First align the center crystal following the above steps. After the center crystal is aligned in 2)-(f), don't move the whole crystal set Θ . Only adjust each remaining crystal by its own tilting and rotating angles. After all crystals are aligned, you can show all crystals in x-ray before step 2)-(g).

Note, for XAFS mini-spectrometer alignment (such as R=182mm case), if one is only interested in one energy position measurement without scanning spectrometer, then one can reduce some steps above, such as item 1)-(d) and 1)-(e).