Spec orientation matrix notes (sixc)
Ian Robinson 8/10/2020

1. Starting from scratch, you need to use a dummy matrix to overwrite what the previous user was doing.

Commands:
"or0 H K L" uses the current angles to define the primary reflection to be HKL
"or1 H K L" uses the current angles to define the secondary reflection to be HKL
"setor0 del th chi phi mu gam H K L" uses the given angles to define the primary reflection to be HKL
"setor1 del th chi phi mu gam H K L" uses the given angles to define the secondary reflection to be HKL
"or_swap" interchanges primary and secondary
"setlat a b c al be ga" enters the lattice parameters
"LAMBDA = number" sets the wavelength

For samples on a flat substrate lying along the theta axis, we usually want 00L to be the surface normal and H00 to be in-plane, near th=0. The lengths of the vectors are unimportant, just the directions, so we set this with:
"setor0 0 0 90 -10 0 20 0 0 1"
- at th=0, phi=-10 tilts the sample towards the beam and gam=20 sets symmetric diffraction
"setor1 20 10 90 0 0 0 1 0 0"
- del=20 th=10 sets symmetric diffraction in plane

We would then use "br H 0 L" to go to a reflection with both in-plane and out-of-plane Q components, with both H and L non-zero. Pure 00L can't be calculated by sixc and pure H00 would be exactly grazing across the surface.

2. Substrate optical surface alignment, sigtau
Completely separate from the crystal is the optical alignment of its surface. This is set by grazing the beam exactly parallel to the surface and watching for the reflection in the Tischler camera. Reduce the reflected beam height to merge with the direct beam on the horizon. Do this at th=0 (adjust phi) and th=90 (adjust chi) until the sample is flat to the beam. Then type "sigtau" and accept the current phi, chi readings to define the flat optical surface.

This is the time to accurately focus the Confocal (CF) microscope and note its lens distance. The beam will always be at the position where the CF image is bright

Choose the desired incidence angle with "freeze value", which sets the value to the angle Alpha appearing in the reciprocal lattice position, seen using "wh" or "ca HKL".

3. Here is an example of a valid final orientation matrix (August 2020)
The sigtau feature was not used, because the CF microscope at Alpha = 5 was used to set the sample height for all the settings

Primary Reflection (at lambda 1.37756):
del th chi phi mu gam = 21.9288 12.868 91.1218 -4.87285 0 18.44
HKL=103

Secondary Reflection (at lambda 1.37756):
del th chi phi mu gam = 21.9902 -76.898 85.1283 -1.12696 0 18.5047
HKL=013

Lattice Constants (lengths / angles):
real space = 3.754 3.754 12.65 / 90 90 90
reciprocal space = 1.674 1.674 0.4967 / 90 90 90

Azimuthal Reference:
sigma tau = -90 0
H K L = -0.00010391 -0.00012683 1

Lambda = 1.37756