

SMART-1k.exe

Mouse

- Left mouse button: rotate the goniometer
- Right mouse button: zoom in and out

Controls tab

- Use slider to change the angles 2-theta, omega and phi (alternatively, point to the yellow box with the number and then drag the mouse to change the angle).
- You can animate omega and phi using the up/down arrows under their values. The small slider on the left regulates the speed.
- Shutter button – self-explanatory, but the R.L. won't be visible if the beam is off
- Antialias – turn it on for a slight improvement of graphic quality (not too useful)
- 2Theta/Omega Scales – if you have the file scale.jpg in the same folder as the program, the scale will be shown on these two axes
- X-ray Source – makes the tube housing vanish and reappear
- Detector – as for the source, and the slider changes the distance
- Realistic beam – the model has been constructed to scale, but this makes the beam a bit small to see if you are trying to show something to the students. This option allows you to unrealistically scale up the beam and crystal to make them more visible.
- Elongated Crystal – turns the crystal into a needle with one dimension larger than the beam diameter. This is useful to show students that sometimes the crystal can be completely in the beam, but you can rotate the goniometer axes such that the crystal protrudes
- Persistent RL points – when turned off, only the RL points outside the Ewald sphere are visible
- Show Reflections – will show thin red beams for the spots touching the sphere
- Ewald Sphere – turns the sphere on and off. The two sliders control its scale and transparency. When scaled up and down, the RL will scale accordingly. This nicely highlights the fact that the reciprocal space can be scaled arbitrarily because scaling up and down doesn't affect the magnitude of an angle.
- Background Color and Mouse Rotation Sensitivity – self-explanatory (actually, the latter doesn't work as I have disabled it)

R.L. Tab

The purpose here is to create a reciprocal lattice based on a real unit cell. Obviously we don't want to create an infinite reciprocal lattice because your video card's memory won't handle so many objects - therefore you can create a finite sphere of reflections that is limited by the real unit cell and the value of $2\theta_{\max}$.

- Direct Unit Cell – enter the cell parameters in real space
- The yellow text boxes are not editable – just informative
- $2\theta_{\max}$ – use this to limit the size of the reciprocal lattice (i.e. the lattice of reflections) to a manageable sphere of reflections. The default works well for Mo.
- λ - here you can select the radiation wavelength (choices of anode targets include Ag, Mo, Cu, Co, Fe, Cr). You can make this choice even after the R.L. has been created, but the Miller indices are limited according to the choice at the time that you press the "Update R.L." button. However, after updating the wavelength, you can press the "Update R.L." button again to create a reciprocal lattice using the cell and the new wavelength. This feature is nice when

you have the Ewald Sphere and R.L. visible because it will immediately demonstrate what happens to the RL if the wavelength is changed (i.e. the scale of the Ewald sphere will change and this will have consequences for the RL points that are in diffracting positions).

- When you create the RL, intensities are randomly generated, but they do drop off in intensity with 2θ - and the RL has inversion symmetry only.

Strategy Tab

- Here you can set the starting values of the goniometer angles and detector distance. Although it seems like you can choose between omega and phi scans, I have not yet implemented phi scans. Therefore checking the Phi box has no effect. The No. of Frames and Step Size will determine the overall omega angle for the sweep.
- Press "GO!" to simulate the data collection.
- Note – you can enter a value for the frame time, but this is not in real time. The collection is speeded up.
- When you press "GO!", the data collection will be simulated – the reflections will start as grey spheres, and will turn red when they get into diffracting positions. Once a reflection has been in a diffracting position, it will stay red. Of course, any reflections that have been in diffracting positions will be red, and not just the ones that hit the detector. This is something that may be attended to in the future if there is ever an update.

X.exe

Much the same as SMART1k.exe, but will less functionality. Reflections that get into diffraction positions go yellow only while they touch the Ewald sphere. There is no simulation of a data collection strategy and you can't see the reflections. Sometimes it is nicer to just use this simpler version precisely because there are fewer options.