# EwaldSphere Manual

Len Barbour, Department of Chemistry and Polymer Science, University of Stellenbosch, Stellenbosch 7600, South Africa. Email: ljb@sun.ac.za

**EwaldSphere** is a teaching aid. It superimposes the Ewald sphere construction on a simulation of a Bruker SMART 1000 single-crystal X-ray diffractometer. The software is distributed as Freeware. Updates can be downloaded from the author's group web site: http://academic.sun.ac.za/barbour/Software.html.

## Mouse

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

## Control tab (Left)

- This tab shows the view from the camera and allows you to center the crystal
- Centering
  - Allows novice users to practice and understand the crystal centering process. By default, when a unit cell is defined (see below), the crystal is placed in a random orientation, and it is randomly off centre (as would be the case in a "real" experiment).
  - There are checkboxes to show/hide the camera (also hides the camera view) and to illuminate the crystal
  - The Zoom slider zooms the image in and out
  - The Intensity slider changes the intensity of illumination
  - Preset buttons: the **A**, **B**, **C** and **D** buttons control preset goniometer angles for centering the crystal:
    **A** – set Omega to -30° and toggle Phi between 0° and 180°
    **B** – set Omega to -30° and toggle Phi between 90° and -90°
    **C** – set Omega to 150° and toggle Phi between 0° and 180°
    **D** – set Omega to 150° and toggle Phi between 90° and -90°
  - Gonio-X, Gonio-Y and Gonio-Z are used to control the X, Y and height adjustment of the goniometer head, respectively. The X and Y pins on the goniometer head are color coded so that you can see which is which.
  - Cheat! – if you don't want to practice centering the crystal (you will be informed by how far the crystal was off centre).
  - Bump Crystal – randomly changes the orientation of the crystal (but not its position).

## Control tab (bottom)

- Goniometer
  - Use slider to change the angles 2-theta, omega and phi (alternatively, point to the yellow box with the number and then left-drag the mouse left or right to change the angle).
  - You can animate omega and phi using the up/down arrows.
  - Zero any of the three axes using their "Zero" buttons.

- Detector (Active area of chip = 62 × 62 mm)
  - The checkbox will show or hide the detector
  - Use the slider to change the distance from the crystal
  - The "Show Frames" checkbox allows you to display a small window that simulates the frames
  - Use the slider to scale the frame window
  - You can change the background color of the frames
  - You can clear the current frame using the "Clear Frame" button
- X-Ray Source
  - The checkbox will show/hide the tube housing
  - "SHUTTER" button – self-explanatory, but the R.L. won't be visible if the shutter is closed
  - $\lambda$ - the dropbox allows you to choose the wavelengths for Ag, Mo, Cu, Co, Fe or Cr sources
  - The first slider allows you change the wavelength continuously between 0.1 and 4.0 Å
  - The Intensity slider controls the intensity of the beams – this will affect the intensity of the spots on the frames
  - You can choose to keep the shutter open between movements of the goniometer axes. By default, the frames are cleared each time an axis is moved, or the detector distance is changed.
- Ewald Sphere
  - Use the checkbox to show or hide the Ewald Sphere
  - 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 does not affect the magnitude of an angle.
  - You can customize the color of the sphere

**Menu – File**

Not implemented yet. Possible future enhancements would be to read an experimental data file containing the orientation matrix and reflection data.

**Menu – Tools**

- Options
  - Realistic beam – the model has been constructed to scale, but this makes the 0.5 mm beam difficult to see. This option allows one 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 that you can rotate the goniometer axes such that the crystal protrudes from the beam.
  - Only Detected Reflections – only the reflections that strike the detector chip will be shown.
  - Mouse Rotation Sensitivity and Background Color – these options should be self-explanatory
  - Reset Reflection Colors – turns all of the R.L. points grey (by default, R.L. points that have been detected become red). The colors are reset (i) when a new crystal is defined, (ii) a data collection strategy is initiated or (iii) this button is pressed.
- Define Crystal

- The purpose here is to create a reciprocal lattice based on a real-space unit cell. Obviously we don't want to create an infinite reciprocal lattice because your video card's memory won't handle that 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
- Reciprocal Unit Cell – The yellow text boxes are not editable but are intended to be informative.
- Resolution Limit – limits the resolution of the reciprocal lattice (i.e. the lattice of reflections) to a manageable sphere of reflections.
- Always Visible – when this is checked, the R.L. will be visible even if the beam is not turned on
- Update R.L. - creates a RL with only -1 Laue symmetry and no systematic absences. Intensities are randomly generated, but they do drop off in intensity with resolution.
- **NOTE:** The first time you run the program the default unit cell parameters define a cubic unit cell with *a* = 5 Å. The default resolution of the R.L. is 1.20 Å. You can edit these values, and when you exit the program the last-used values will be saved in the Windows registry.

- Automate Sweep
  - You can set the starting values of the goniometer angles, and the detector distance. The No. of Frames and Step Size will determine the overall omega angle for the sweep.
  - Press "GO!" to simulate a single sweep through the reciprocal lattice.
  - Note – exposure time is given in ms (otherwise the simulation will take a long time to complete).
  - "GO!" – the sweep will begin. The colors of all the reflections will be reset to grey, and those that are detected during the sweep will become red.

When the beam is turned on and a R.L. is defined, the R.L. points that are in contact with the surface of the Ewald sphere give rise to diffracted rays. The thickness of each diffracted ray is proportional to (1) the beam intensity, (2) the size of the R.L. point and (3) the amount of overlap between the R.L. point and the surface of the Ewald sphere. Diffracted rays are shown as red lines, unless they strike the detector chip, in which case they are green.