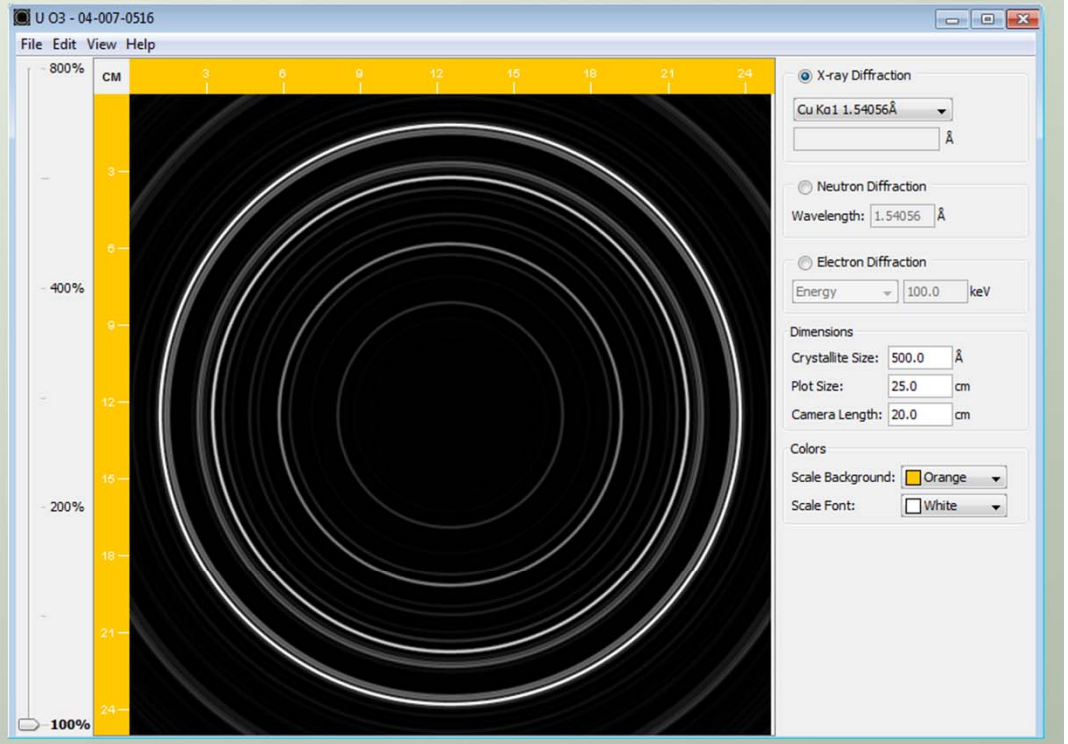
Use 2D Patterns

Use 2D Patterns

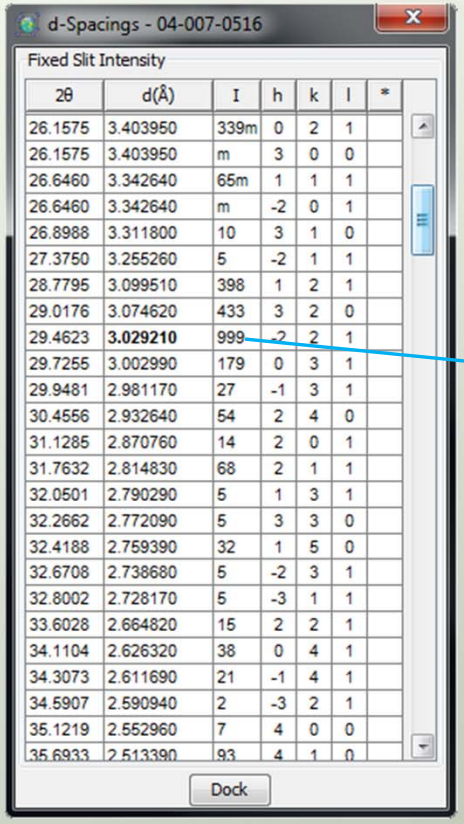
- A graphical 2D diffraction pattern, or *Ring Pattern*, can be produced for every entry in the ICDD PDF-4+ database.
- A Ring Pattern provides a 2-dimensional simulation of the X-ray pattern for a given phase as it would appear on a flat 2-dimensional detector such as:
  - Photographic film
  - Phosphor image plates
  - Solid state arrays



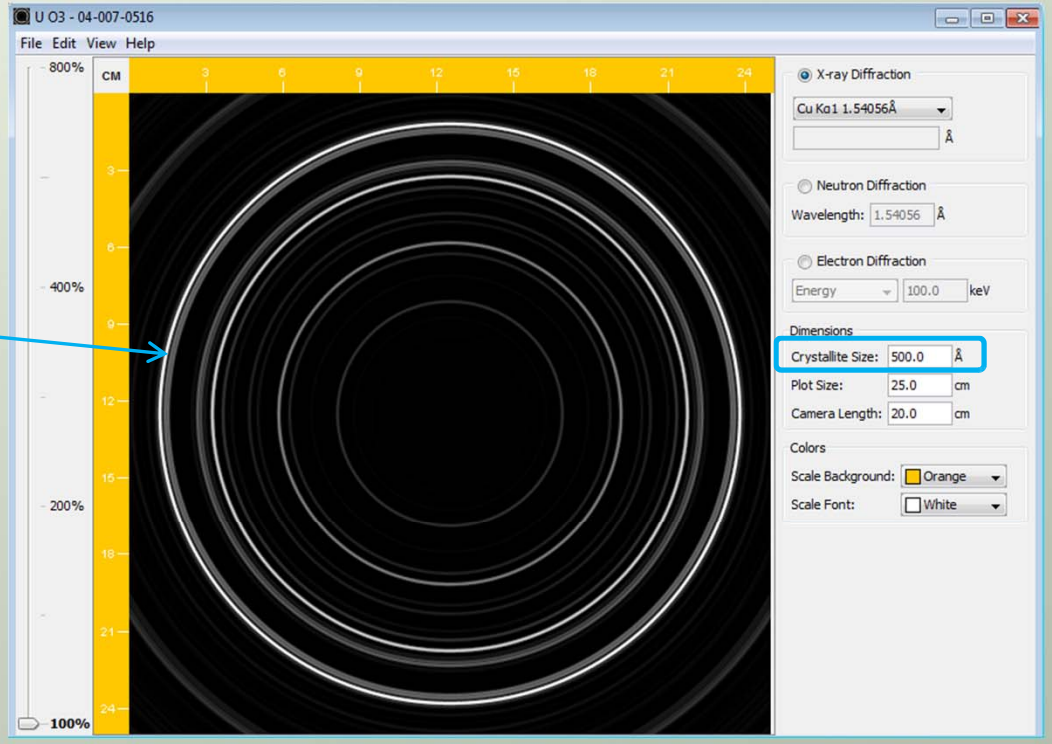
Ring Pattern for Uranium Oxide (500Å crystallite size)

Use 2D Patterns

- Each ring corresponds to a peak (d-spacing and intensity) calculated using the ***Crystallite Size*** parameter specified in the 'Ring Pattern'.
- The higher the intensity, the brighter the ring.



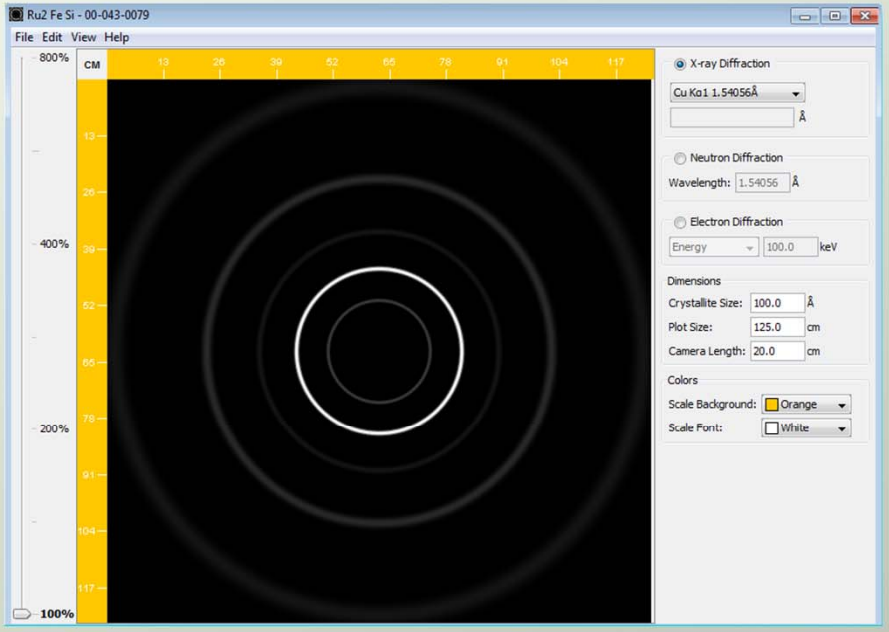
2θ	d(Å)	I	h	k	l	*
26.1575	3.403950	339m	0	2	1	
26.1575	3.403950	m	3	0	0	
26.6460	3.342640	65m	1	1	1	
26.6460	3.342640	m	-2	0	1	
26.8988	3.311800	10	3	1	0	
27.3750	3.255260	5	-2	1	1	
28.7795	3.099510	398	1	2	1	
29.0176	3.074620	433	3	2	0	
29.4623	**3.029210**	999	-2	2	1	
29.7255	3.002990	179	0	3	1	
29.9481	2.981170	27	-1	3	1	
30.4556	2.932640	54	2	4	0	
31.1285	2.870760	14	2	0	1	
31.7632	2.814830	68	2	1	1	
32.0501	2.790290	5	1	3	1	
32.2662	2.772090	5	3	3	0	
32.4188	2.759390	32	1	5	0	
32.6708	2.738680	5	-2	3	1	
32.8002	2.728170	5	-3	1	1	
33.6028	2.664820	15	2	2	1	
34.1104	2.626320	38	0	4	1	
34.3073	2.611690	21	-1	4	1	
34.5907	2.590940	2	-3	2	1	
35.1219	2.552960	7	4	0	0	
35.6933	2.513390	93	4	1	0	



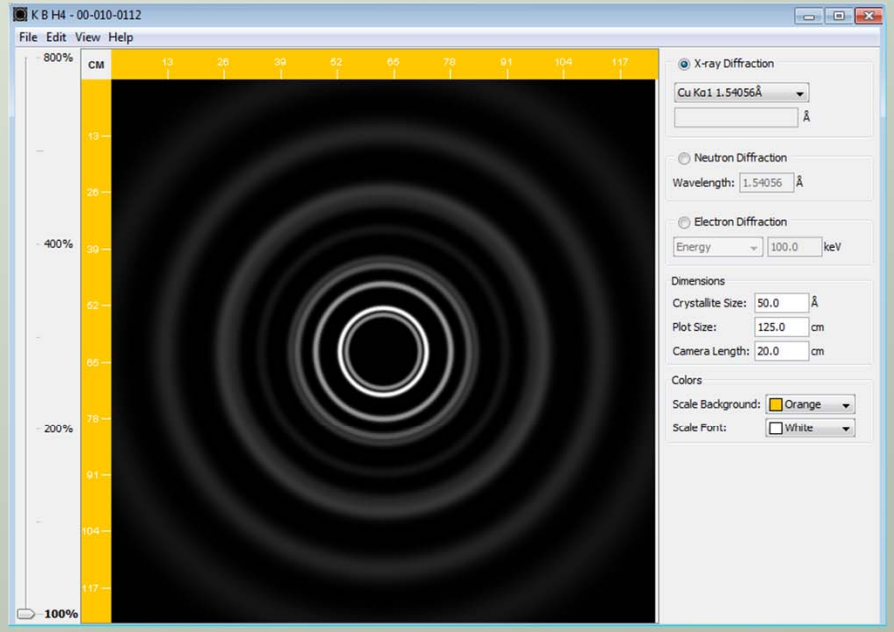
Ring Pattern for Uranium Oxide (500Å crystallite size)

Use 2D Patterns

- The simulation assumes:
  - No preferred orientation in the specimen
  - Uniaxial positioning of the detector (transmission geometry with incident beam centered)
  - An infinite number of randomly oriented crystallites



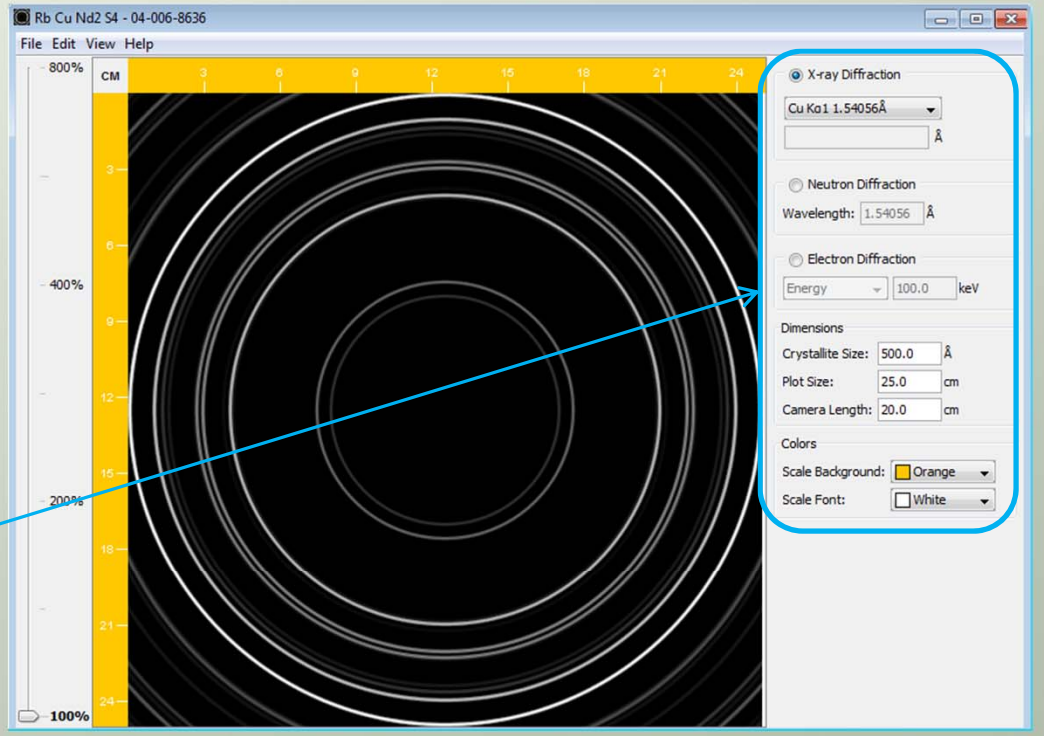
Ring Pattern for Iron Ruthenium Silicon (100Å crystallite size)



Ring Pattern for Potassium Boron Hydride (50Å crystallite size)

Ring Pattern Preferences

- There are various preferences used to control how the Ring Pattern is simulated and displayed.
  - X-ray, Neutron (new), and Electron (new) Diffraction
  - Wavelength, energy (new)
  - Crystallite Size
  - Plot Size
  - Camera Length
  - Colors
- You can dynamically change the preferences on the form for that individual Ring Pattern.

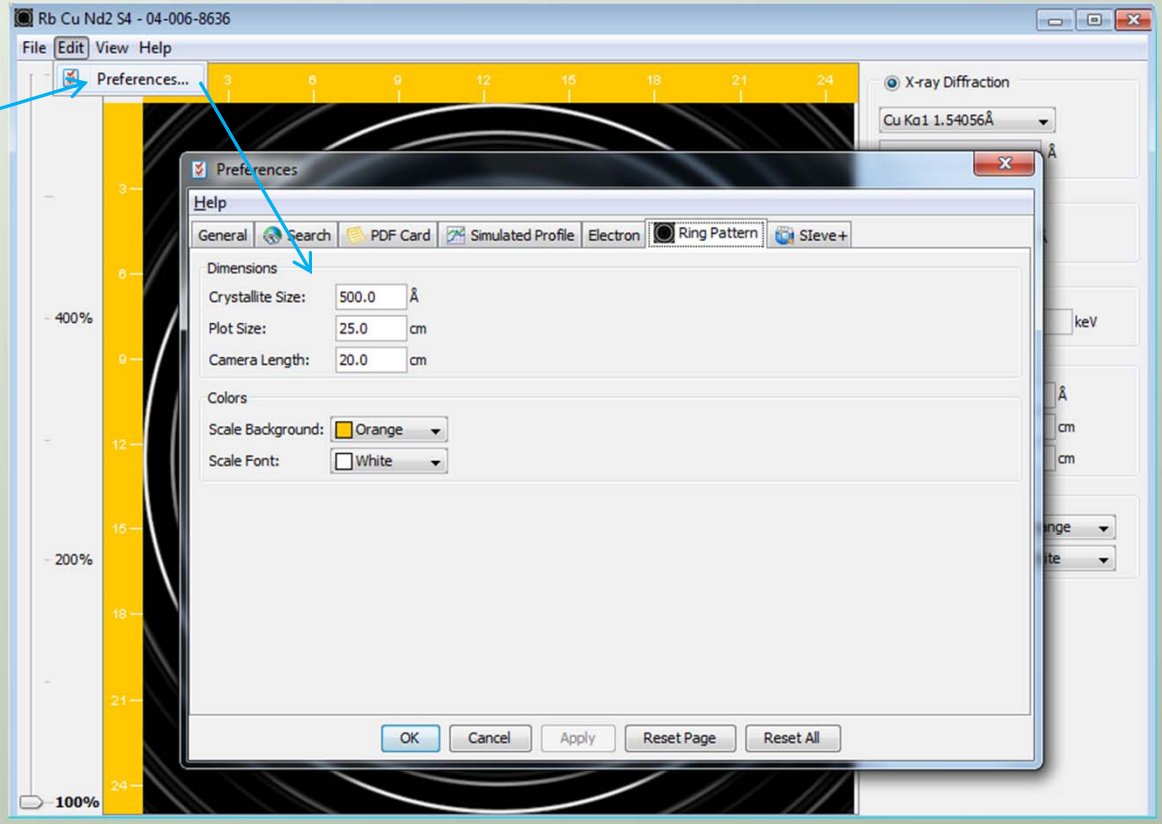


Ring Pattern for Rubidium Copper Neodymium Sulfide (500Å crystallite size)

Ring Pattern Preferences

- Alternatively, you can change the preferences for all Ring Patterns by using the Ring Pattern Preferences form.

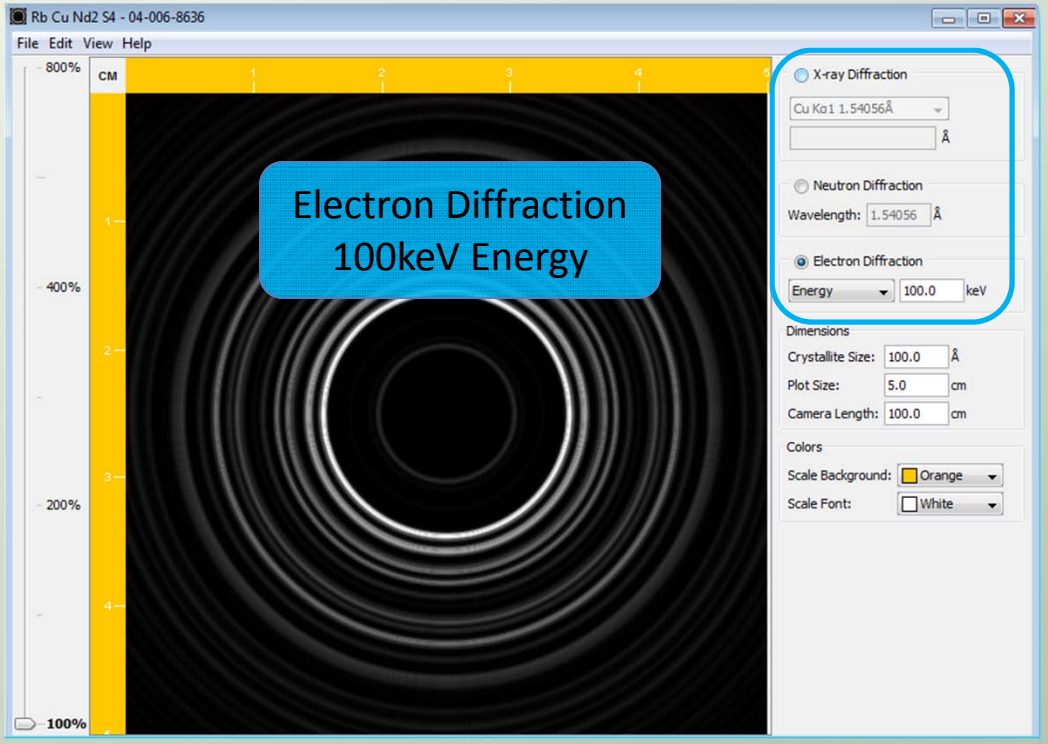
Click *Preferences* in the *Edit* menu



Ring Pattern Preferences

Ring Pattern Preferences

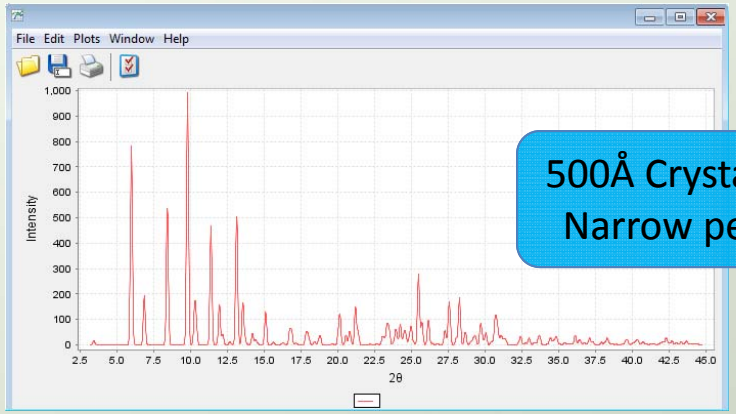
- The diffraction type of the Ring Pattern can be set to:
  - **X-ray diffraction** using a wavelength
  - **Neutron diffraction** using a wavelength (new)
  - **Electron diffraction** using a wavelength or energy (new)
- To change the diffraction type and wavelength/energy for all Ring Patterns, use the Simulated Profile Preferences.



Ring Pattern for Rubidium Copper Neodymium Sulfide (100Å crystallite size)

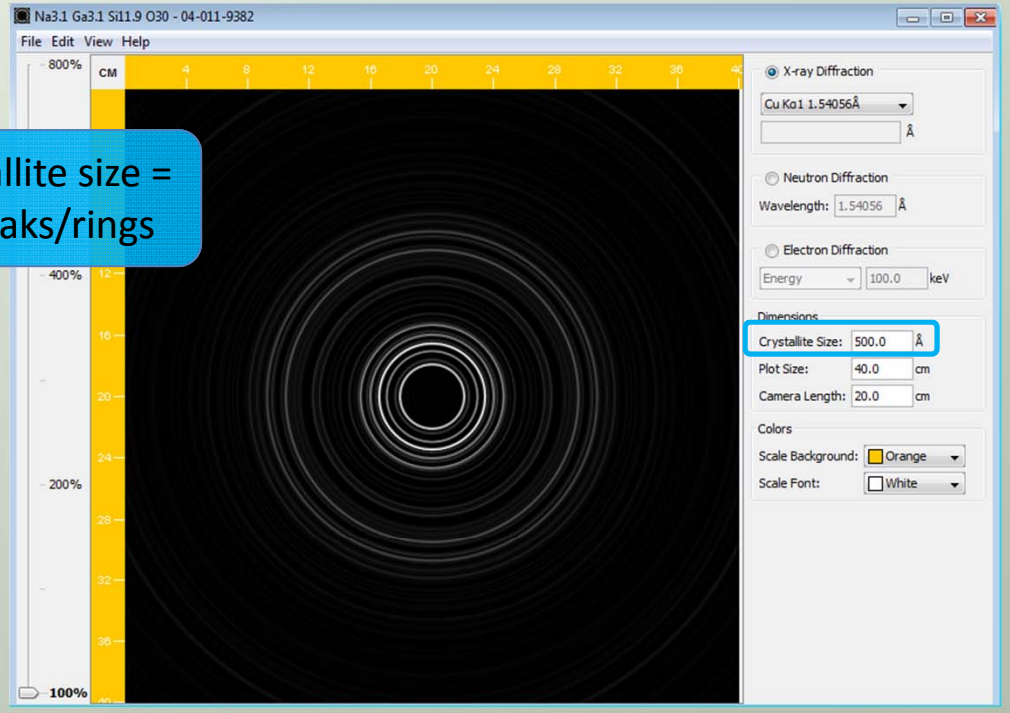
Ring Pattern Preferences

- The ***Crystallite Size*** parameter (in Å) affects the broadness of the rings.
- Narrow rings correspond to larger ***Crystallite Sizes***.



Diffraction Pattern for Sodium Gallium Silicon Oxide

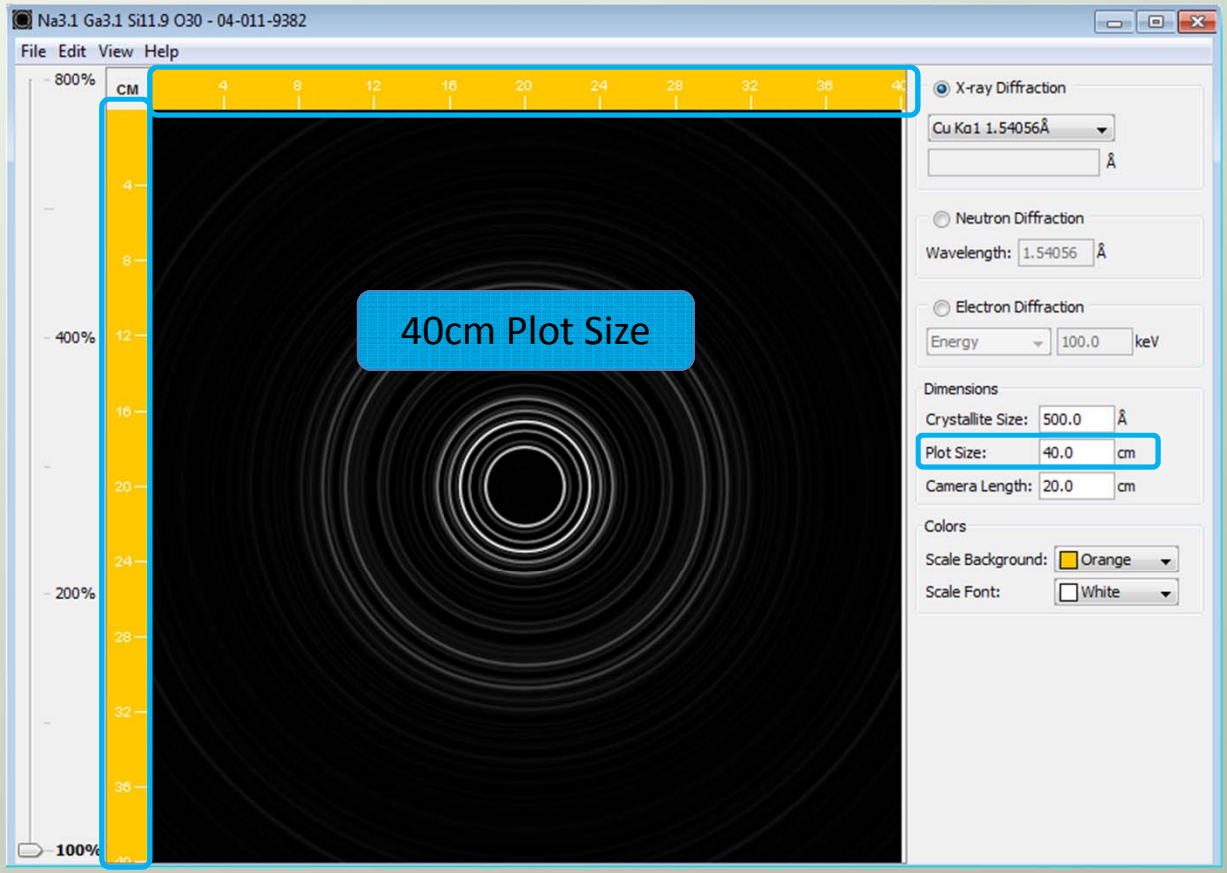
500Å Crystallite size =
Narrow peaks/rings



Ring Pattern for Sodium Gallium Silicon Oxide (500Å crystallite size)

Ring Pattern Preferences

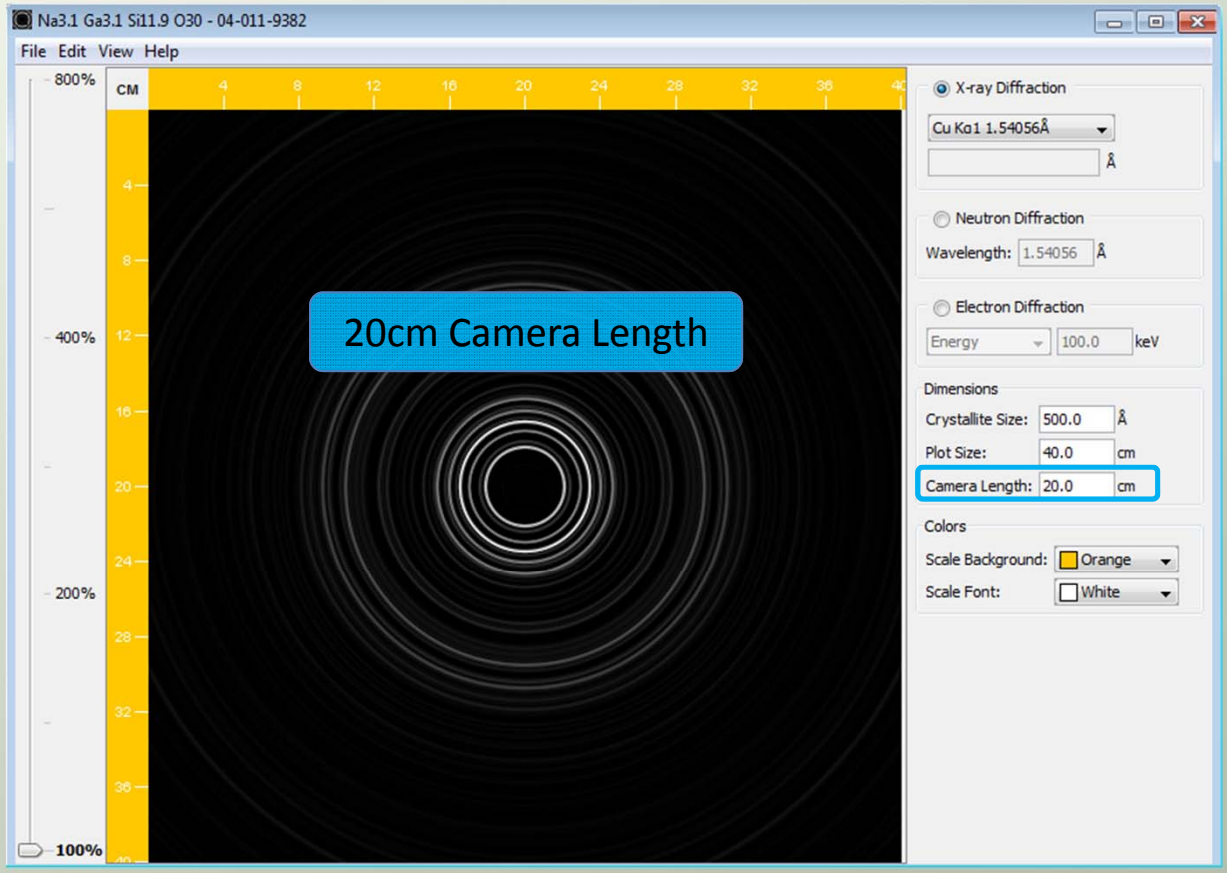
- The ***Plot Size*** controls the detector dimensions (width and height in cm).
- If the Ring Pattern is not visible on the form, try increasing the ***Plot Size***.



Ring Pattern for Sodium Gallium Silicon Oxide (500Å crystallite size)

Ring Pattern Preferences

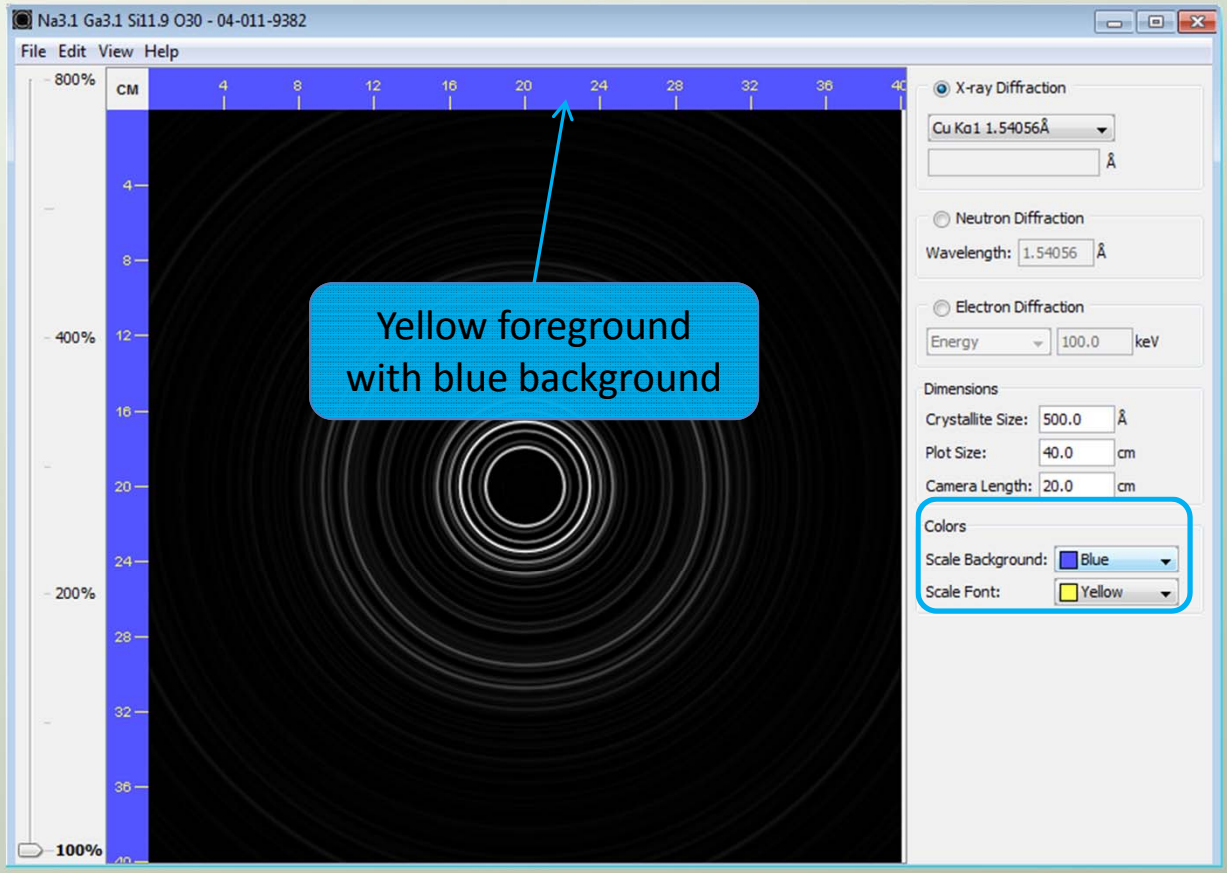
- The ***Camera Length*** controls the sample-to-detector distance (in cm).



Ring Pattern for Sodium Gallium Silicon Oxide (500Å crystallite size)

Ring Pattern Preferences

- The ***Scale Background*** and ***Scale Font*** colors control the appearance of the Ring Pattern.



Ring Pattern for Sodium Gallium Silicon Oxide (500Å crystallite size)

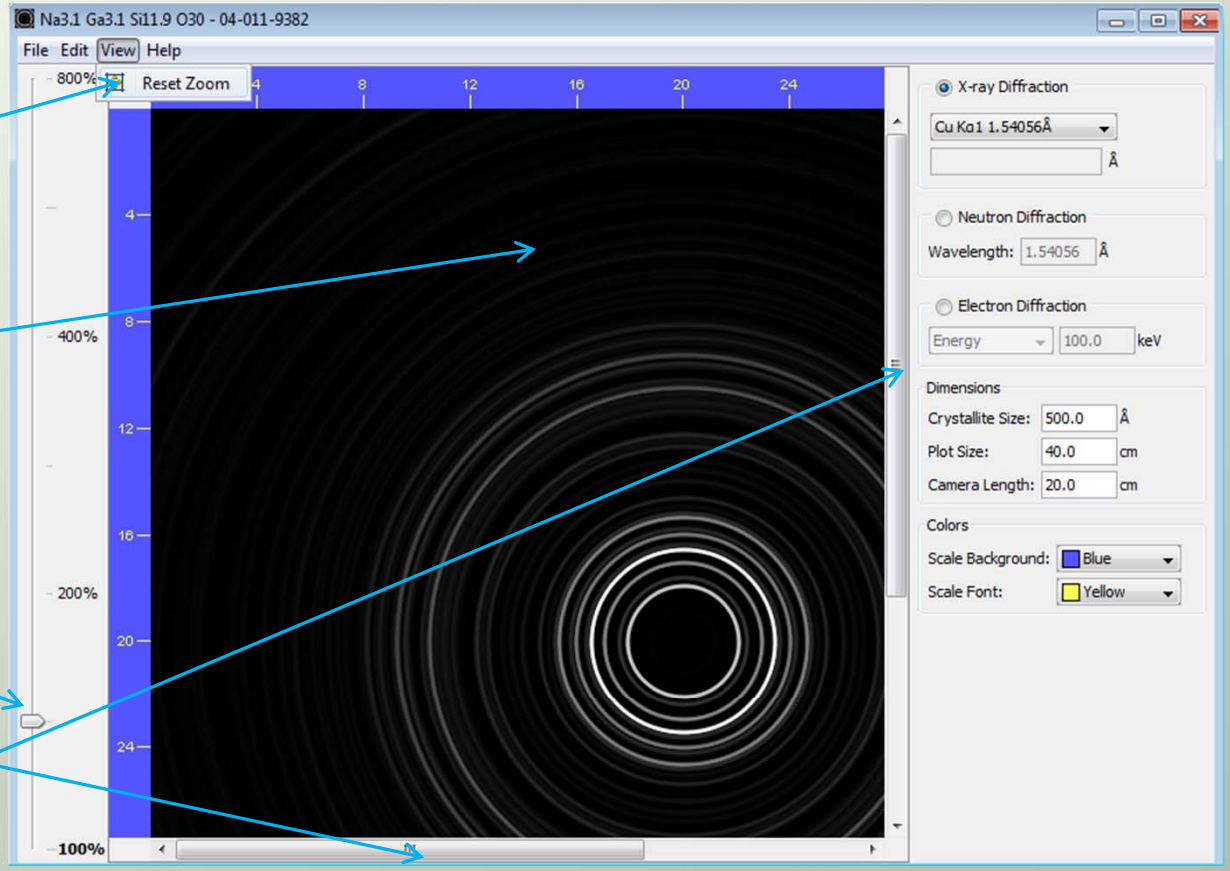
Ring Pattern Manipulation

Click to reset zoom

Double-click anywhere to reset zoom

Drag the slider to zoom

Drag the scrollbars to pan



Ring Pattern for Sodium Gallium Silicon Oxide (500Å crystallite size)

Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website.
www.icdd.com

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