



New Features for Release 2021

New Features for Data Mining

- New searches
 - Refined Formula – A formula derived from the occupancies and site multiplicities of the elements in the atomic coordinates.
 - Wyckoff Sequence
 - Topology* – The topological descriptors as per RCSR database (<http://rcsr.anu.edu.au/>).
- Automatically resize search results window to fit the data.
- Sort on multiple columns in the search results.

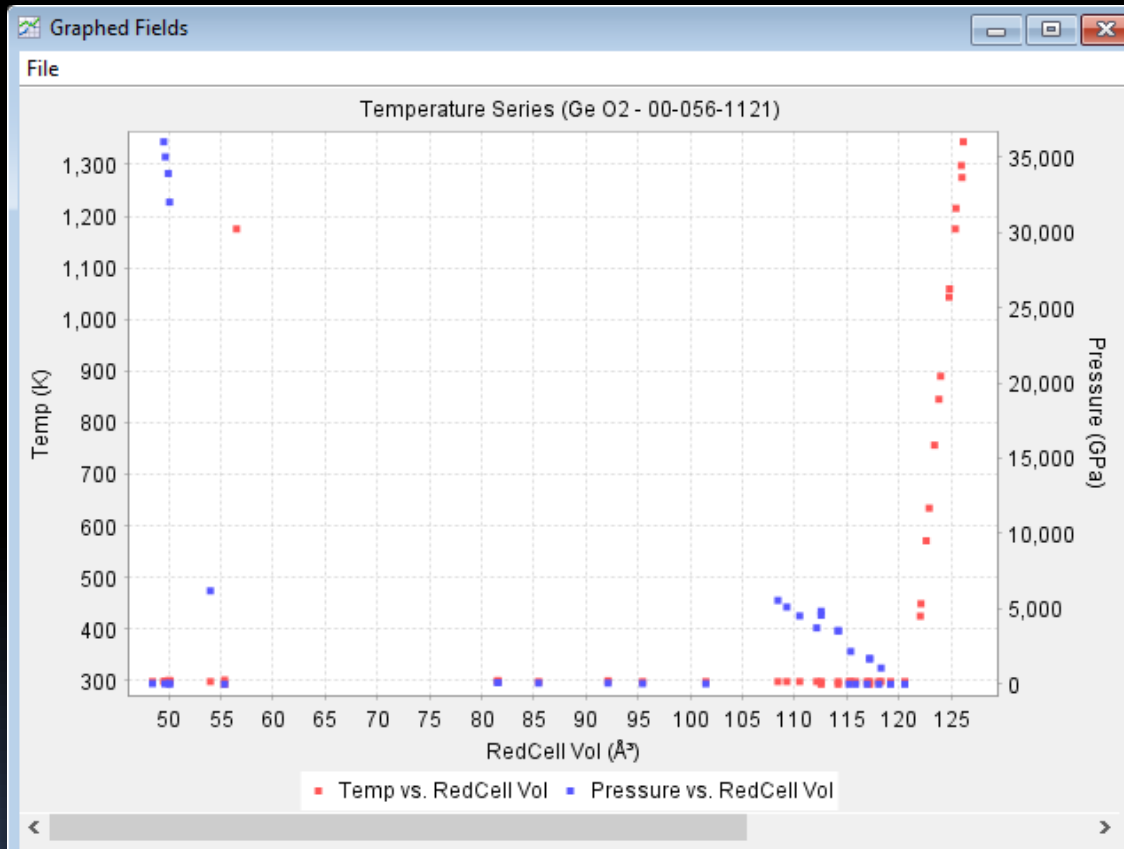
The screenshot displays the RCSR database search interface. The search criteria include 'Subfile' (Custom PDF Set), 'Environment' (Ambient, Non-ambient), 'Status' (Primary, Alternate), 'Quality Mark' (Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision), and 'Database' (ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05)). The search results are displayed in a table with columns: PDF #, QM, Chemical Formula, Compound Name, SYS, and Wyckoff Sequence. The results are filtered by the Wyckoff sequence 'd2 c14'.

PDF #	QM	Chemical Formula	Compound Name	SYS	Wyckoff Sequence
04-013-9441	B	$\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2$	Zinc Azide Ammonia	O	d2 c14
04-013-9623	S	$(\text{CN}_4\text{H}_7)_2\text{ZrF}_5$	Aminoguanidinium Zirconium Fluoride	O	d2 c14
04-013-9624	S	$(\text{CN}_4\text{H}_7)_2\text{ZrF}_5$	Aminoguanidinium Zirconium Fluoride	O	d2 c14
04-013-9625	S	$(\text{CN}_4\text{H}_7)_2\text{ZrF}_5$	Aminoguanidinium Zirconium Fluoride	O	d2 c14

The search results window is titled 'Results - 4 of 444,133'. The search criteria are: [Wyckoff Sequence Exactly 'd2 c14'] And [Status (Primary, Alternate)].

Data mining search results for the Wyckoff sequence "d2 c14".

New Features for Data Mining

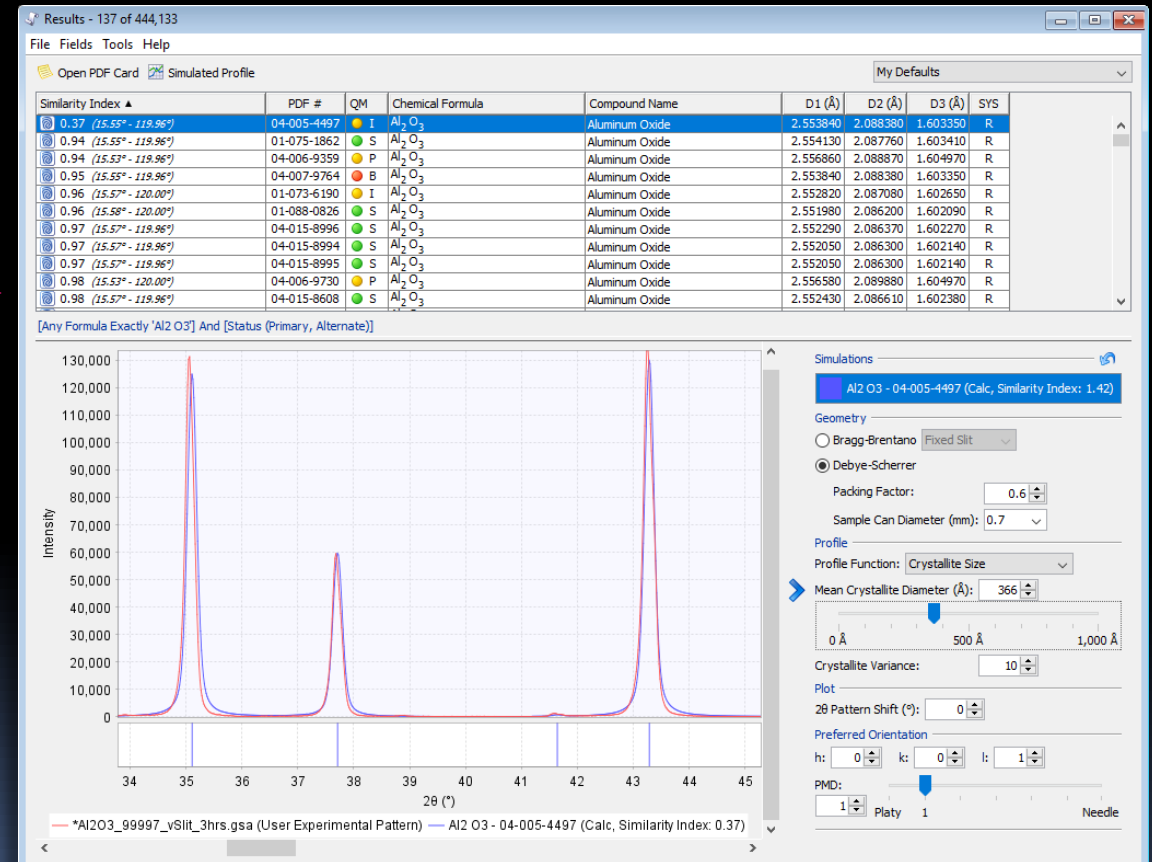


- Plot left and right y-axes of data mining searches
- Applies to any numeric field

Temperature series graph for Ge O2 displaying both temperature (left y-axis) and pressure (right y-axis) as a function of reduced cell volume.*

New Features for Simulations

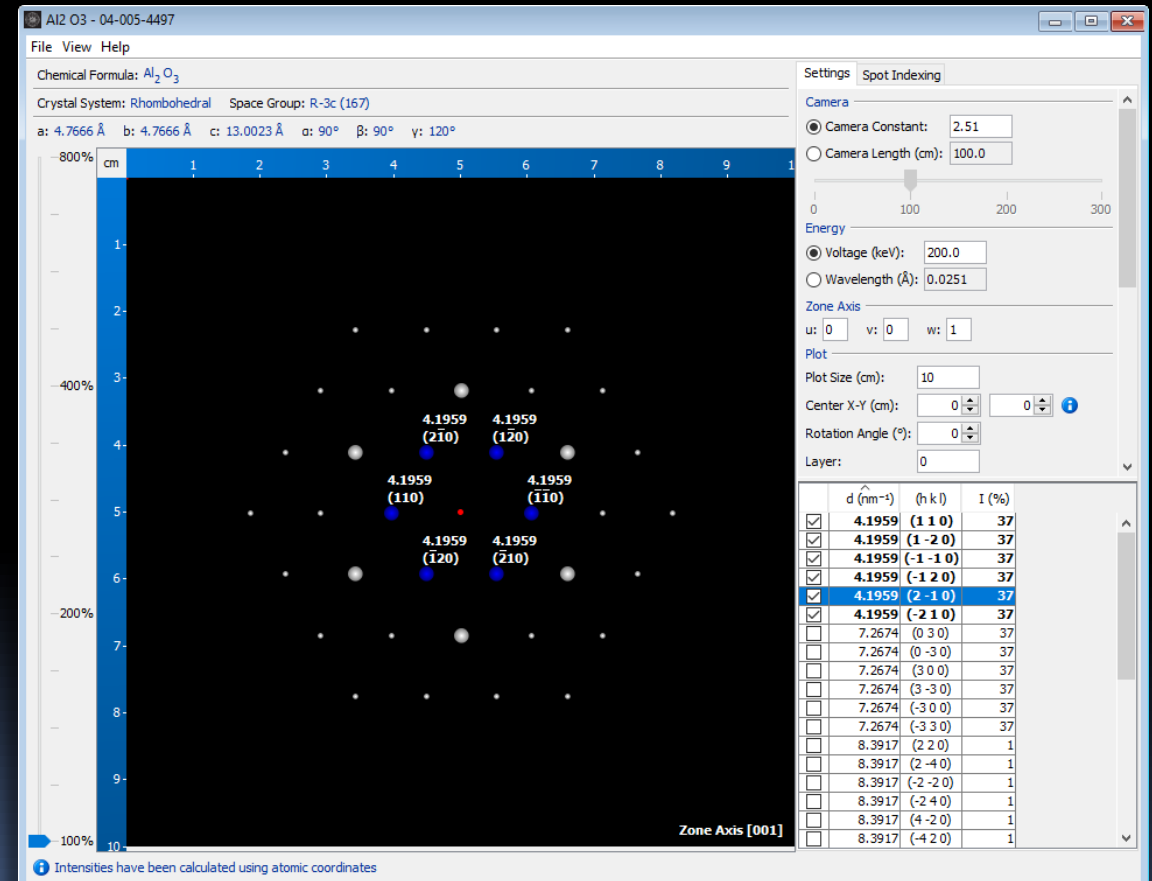
- Quick settings panel for pattern simulations*
- Mouse wheel pans the graph left and right
 - Holding SHIFT will autoscale the y-axis (intensity).



Quick settings panel allows the user to dynamically change various simulation settings directly on the graph.

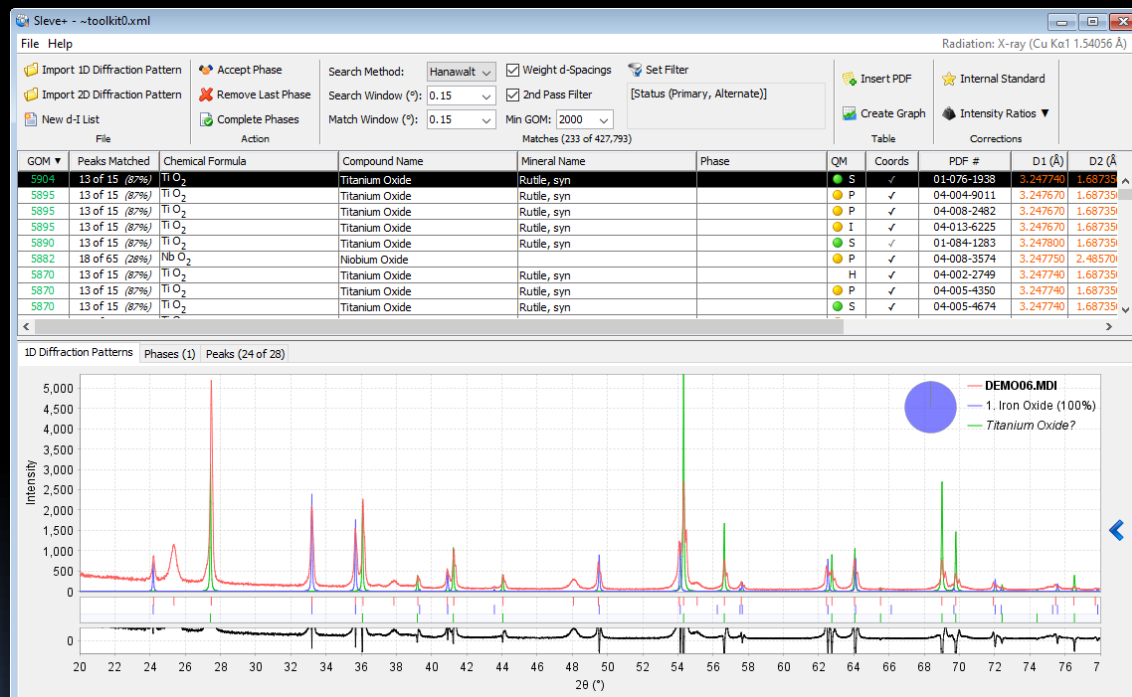
New Features for Simulations

- New SAED features*
 - Interactive d-spacings table
 - User-defined background color
 - Transparency setting for visual overlay of imported images
 - Customize position of zone axis label



New table displays the d-spacings, HKL's, and intensities for all spots in the SAED pattern simulation window. Spots can be highlighted by clicking on them in the table or directly in the simulation.

New Features for Phase ID (Sieve/Sieve+)

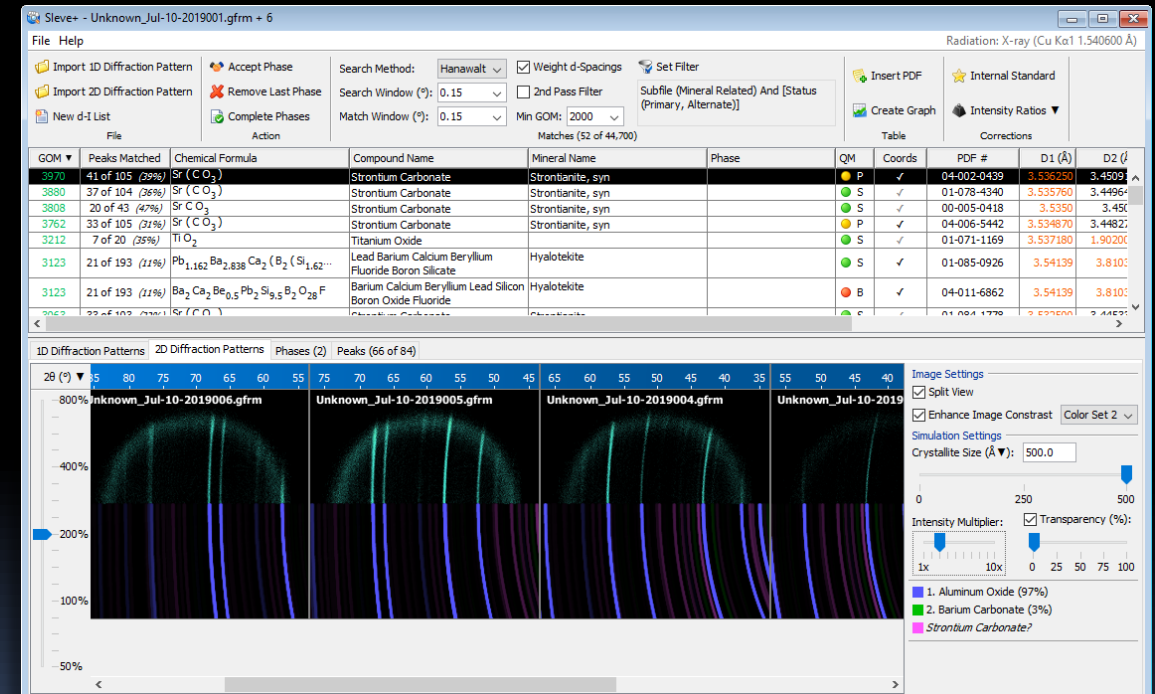


- Import JADE projects directly into Sieve/Sieve+ for phase identification
- Export the Sieve/Sieve+ d-I list to a file as 2θ-intensity values

Experimental data that was imported and processed in JADE, can now be imported into Sieve+ for complimentary phase identification.

New Features for Phase ID (Sieve+)

- Intensity scaling for 2D multiphase analysis
- New color sets for enhancing the image contrast of imported 2D patterns.



Intensities are now scaled for ring pattern simulations when doing 2D multiphase analysis.