CrystalMaker® SOFTWARE

Technical Specifications

Program features and operating requirements.

Mac

Operating Systems

- macOS 14 "Sonoma"
- macOS 13 "Ventura"
- macOS 12 "Monterey"
- macOS 11 "Big Sur"
- macOS 10.15 "Catalina"
- macOS 10.14 "Mojave"

Hardware

- Apple Silicon or Intel Mac running macOS 10.14 or later
- 1 GB free disc space
- 8 GB RAM

Notes

- CrystalMaker 11 for Mac is a **Universal Binary** which runs natively on Apple Silicon (M-series processors) as well as older, Intel-based Macs.
- As a bundled application all program resources, documentation and example files are saved inside a single application icon, making for easy drag-and-drop installation.

Windows

Operating Systems

- Windows 11 *(recommended)*
- Windows 10
- Windows 8
- Windows 7

.NET Framework 4.8 or later required

Hardware

- 64-bit PC running Windows 7 or later.
- Graphics card with OpenGL 3.2 (or later) capability.
- 1 GB free disc space.
- 4 GB RAM.

Notes

- CrystalMaker 11 for Windows is distributed as a compressed Microsoft-Installer package, ready for auto-run.

Usability

Elegant, user-friendly & interactive

- 64-bit native Mac & Windows applications.
- Optimized for Apple Silicon and Intel.
- Supports macOS Sonoma & Windows 11.
- Elegant user interface: power without clutter.
- Supports drag-and-drop for fast data import.
- Multiple undo/redo levels.
- Multi-document synchronization.
- Haptic feedback (Mac): feel atoms & bonds.

Visualization

Pixel-perfect 3D graphics

- Gorgeous high-DPI "Retina" graphics.
- Depth fading and depth zoom/profiling.
- Stereo-pair plots.
- Out-of-the-screen red/blue stereo (colour).
- Auto perspective.

Molecule Builder

Point-and-click with optimization

- Duplicate, detach, move, edit atoms.
- Automatically add H atoms.
- Optimize geometry (minimize energy).
- Calculate energy.
- Simulate vibration modes & IR spectra.

Crystal Building

Easy to build complex structures

- Crystal editor with symmetry browser.
- Supports mixed/disordered site occupancies.
- Atomic displacement parameters (Uiso, Uij).
- Dynamic plot range control: arbitrary range in fractional coordinates along each axis with real-time update.
- Automatic range optimization to repair cation coordination at cell edges.

Crystal Engineering

Design new structures

- Slab and surface generation.
- Insert block of space into crystal lattice.
- Place one structure inside another.
- Visualize interfaces/domain boundaries.
- Insert atoms; change element types.
- Move/rotate selected atoms in crystal.
- Spherical nanocrystals.

Crystal Energy Modelling

No supercomputers required!

- Relax any crystal structure on your desktop.
- Relax arbitrary surfaces or structural blocks.
- Fast Monte Carlo relaxation with subsequent least-squares refinement.
- Integrated potentials library.
- Smart potential selection.
- Monte-Carlo pressure/temperature simulations (constant NPT or NVT).
- Simulate temperature option.

Lattice Dynamics

Visualize phonons interactively

- Full phonon calculations.
- Density of states.
- Dispersion curves between arbitrary points.
- Visualize, rotate, scale vibrational modes.

Thermodynamic Properties

Calculated from energy modelling

- Entropy.
- Heat capacity.
- Helmholtz free energy.
- Zero-point energy.
- Vibrational energy.

Physical Properties

Calculated from energy modelling

- Elastic constants.
- Bulk modulus, shear modulus.
- Young's Modulus.
- Poisson's Ratio.
- Acoustic velocities.
- Dielectric constants.

Calculations

Explore structural properties

- Porosity calculation.
- 3D porosity map.
- Distance map.
- Molecular volume.
- Surface area/volume calculations.
- Electron density map.
- Centre-of-gravity.
- Molecular centroids.
- Cavity Finder (add translucent centroids).
- Rings through selected atom.
- Interatomic distances.
- Atom density/distance histograms.
- Pair distribution functions: X-ray, neutrons.
- Polyhedral distortion indices.
- Planar packing factors.
- Inter-planar/vector angles.
- D-spacing calculator.
- Best-fit line/plane through selected atoms.
- Distance from selected atom(s) to plane.
- Unit cell volume, density, chemical formula.
- Framework automation: stylized display.

Animation

Structural behaviour & dynamics

- Synchronize multi-structure sequences.
- Visualize structural behaviour.
- Visualize large-scale simulation trajectories.
- Rotate and zoom whilst animating.
- Scrubber control: fast-forward/reverse.

Direct Measurement

Measure atoms, distances, angles

- Selected atoms show coordination summary.
- Interatomic distances (with error propagation).
- Projected distances (in plane of screen).
- Arbitrary angles in plane-of-screen.
- Angle between any 3 atoms (with rollover).
- Torsion angle between any 4 atoms.

Bonding

Fast custom bond search & display

- Bonds Inspector with interactive editing.
- Distance histograms for element pairs.
- Primary and secondary bonds.
- Double, triple, dashed, dotted, striped styles.
- Thick or thin cylinder option.
- Customizable bond radius.
- Optional bond distance labels.

Polyhedra

Simplify complex structures

- Generated automatically, with bond search.
- Visualize massive zeolite cages, MOFs, etc.
- Solid, translucent, hybrid, blank styles.
- Show ellipsoids or spheres at vertices.
- Visualize concave polyhedra (curved faces).

Lattice Planes

Explore symmetry, surfaces & slabs

- Show multiple planes/sets of parallel planes.
- Generate symmetry-related planes.
- Move through structure; snap to intercepts.
- Slice structures; define slabs.

Surface Overlay

Molecular shapes & cavities

- Space-fill, van-der-Waals, solvent-excluded.
- Real-time probe sphere radius control.
- User-defined colour and opacity.

Volumetric Data

Visualize structure + properties

- Import and visualize multiple 3D datasets.
- Add/subtract datasets.
- Iso-surfaces/volumes, point clouds, slices.
- Real-time range slider control (with presets).

Overlays

Label with text, lines and arrows

- Add lines, arrows and rich-text boxes.
- Display customizable axial vectors.
- Legend, ruler/scale bar.

File Formats

Comprehensive import and export

Format	Import	Export
1. 3ED	•	
2. ATOMS	•	
3. CASTEP Cell	•	•
4. CASTEP Output	•	
5. CASTEP Volumetric	•	
6. CCL	•	
7. Chem3D Cartesian	•	•
8. CIF[a]	•	•
9. CMDF	•	
10. CMDX	•	•
11. CMMF	•	
12. CMTX	•	•
13. CSSR	•	
14. Gaussian CUBE	•	
15. DEN (Volumetric)	•	
16. DL_POLY Config	•	
17. DL_POLY Revcon	•	
18. DL_POLY History	•	
19. DMol3 ".car"	•	•
20. DMol3 ".arc"	•	
21. FDAT (CSD)	•	
22. GRD (Volumetric)	•	•
23. GROMACS	•	
24. GSAS	•	
25. GULP	•	
26. ICSD	•	
27. LAMMPS	•	
28. Molfile	•	
29. PDB	•	•
30. Prismatic	•	
31. RMCProfile	•	•
32. SDfile	•	
33. SHELX[b]	•	
34. STRUPLO	•	
35. SYSTRE[c]	•	
36. TOPAS	•	
37. VASP Structure	•	
38. VASP Trajectory	•	
39. VASP Volumetric	•	
40. VESTA	•	
41. Voxel	•	•
42. WIEN2k	•	•
43. XCrySDen Structure	•	
44. XCrySDen Animation	•	
45. XYZ	•	•

Import Notes.

a. CIF: Imports multiple structures from a single CIF file, including thermal and error parameters (where available).

b. SHELX: Supports multi-part SHELX files, with the option to display a composite structure or individual states of the disordered model.

c. SYSTRE: Automatic colour-coordinated display of symmetry-related bonding.

Other Data Formats

Format	Import	Export
1. Elements	•	•
2. Coordinates		•
3. Visible Coordination		•
4. Crystal Coordination		•
5. HTML Structure		•
6. Distances & Angles		•
7. Vibrations List		•

Output

Export graphics, video and data

- High-resolution graphics with transparency.
- Rotation, animation & vibration videos.
- 3D printing (via STL) + COLLADA 3D.
- Structures, coordinates, bonds, distances.
- Works with CrystalDiffract® and SingleCrystal™ (sold separately) to provide live structure/diffraction rotation and recalculation: edit a structure in real time at the atomistic level, and see its diffraction pattern update.

Structures Library

(CrystalViewer)

- 1400 reference structures, for instant display.
- Major rock-forming minerals (400+)
- Zeolite frameworks (230).
- Structural architecture (animations).
- Basic structure types.
- Thematic libraries.

Support

Welcome to the family!

- 30-year track record of service and support.
- Full user's guide (400 page PDF).
- Quick-start tutorial (PDF).
- Video tutorials + YouTube™ channel.
- Free technical support.
- Regular updates.

For Further Details & Queries, Contact:

SCUBE Scientific Software Solutions (P) Ltd.

An ISO 9001:2008 Certified Company

1217, 12th Floor, Hemkunt Chambers, 89 Nehru Place, N.Delhi-19

Phone : 91-11-41618828, 41618829 | Fax : 91-11-41618828

E-mail : info@scubeindia.com | Website: www.scubeindia.com

Corporate Identity No. : U72200DL2004PTC126289

CrystalDiffract 7

File Input
Live diffraction – or just drag-n-drop!

- **CIF** – including multi-structure files (each structure generates a separate diffraction pattern, within the same window).
- **STRUPLO**
- **CMTX** (CrystalMaker text file: an easy, human-readable format: much safer than CIF!).
- **CMDF** (CrystalMaker 7–9 Document).
- **CMDX** (CrystalMaker 10–11 Document).
- **Direct Simulation Link** via CrystalMaker's `Transform > Powder Diffraction` submenu, including "Live Powder Diffraction" mode.
- **XY** (space-delimited) text file for observed data.
- **CSV** text file.
- **Rigaku-Scintag ASC** diffractometer file.

Diffraction Simulations
X-rays, Neutrons or Electrons

- **Constant-wavelength X-ray Diffraction** (traditional laboratory source). Intensity as a function of 2θ, d-spacing, 1/d or Q-space (2π/d).
- **Constant-Wavelength Neutron Diffraction** (e.g., reactor source). Intensity as a function of 2θ, d-spacing, 1/d or Q-space (2π/d).
- **Constant-Wavelength Electron Diffraction** (e.g., powder rings in a transmission electron microscope). Intensity as a function of 2θ, d-spacing, 1/d or Q-space (2π/d).
- **Energy-Dispersive X-ray Diffraction**, (synchrotron source). Intensity as a function of energy, d-spacing, 1/d or Q-space (2π/d).
- **Time-of-Flight Neutron Diffraction** (neutron spallation source). Intensity as a function of time-of-flight, d-spacing, 1/d or Q-space (2π/d).

Instrument
Your Virtual Diffractometer

- **Wavelength** (angle-dispersive diffraction)
- **Detector 2θ Angle** for energy-dispersive and time-of-flight simulations.
- **Neutron Flight Path**: total distance, in metres, for time-of-flight simulation.
- **Peak Profile**: Lorentzian, Gaussian, Pseudo-Voigt (variable eta), Delta
- **Instrumental Peak Broadening**: constant values for constant-wavelength and EDX simulations; variable broadening for time-of-flight neutron diffraction according to the specified instrument resolution (Δd/d)
- **Zero Correction** plus intensity offset and scale factor (for observed datasets).
- **Background Function.** Users can specify a background function by editing control points in an easy and intuitive manner. The background can be toggled on or off at any time.
- **Logarithmic Intensity Mode.** Intensities can be displayed on either a linear (default) or logarithmic scale. In "Film" mode, you can also simulate the photographic film response, by adjusting the film's gamma parameter in real time.

Display Options
Custom Visualization

- **Show/Hide Patterns.** Toggle pattern visibility with checkbox controls.
- **Rearrange pattern order.** Drag-and-drop patterns in the Patterns List to rearrange the plot order or use arrangement commands on the Patterns menu. Patterns can also be sorted by: Title, Colour, Visibility and Kind (i.e., Simulated, Mixture or Observed), via the Patterns List Actions menu.
- **Stack Patterns** in "Graph" mode, using the toolbar and menu controls (a Collapse command is also available)
- **Label reflexions.** Choice of label types, styles and colours. Option to suppress labelling for weaker reflexions by specifying a minimum relative-intensity threshold. Label content can include: hkl, d-spacing, x-value, phase name (or blank). Optional label rotation, arrow/tick display, and positioning: top or bottom of the screen, or "floating" above each profile.
- **Overlay Peak Profiles.** You can optionally display peak overlays for individual reflexions in a simulation: a good way to reveal overlapping influences in a complex diffraction profile.
- **Graph Plot Style.** Extensive control over profile line style (solid, dashed, dotted, hidden), line width, colour, shadow, fill-from-zero. Optional display of data markers, in a wide range of styles, with size control. (Automatic pattern colouring options, including Spectrum colouring and a reset facility, are available from the Patterns List Actions menu.)
- **Film Style.** CrystalDiffract provides a number of colour scales for depicting "film" simulations, including traditional Film Negative or Positive, plus Spectrum, Fire and Ice themes. The simulated film's gamma response can be adjusted in real time: higher gamma values help to accentuate weaker reflexions, in the presence of stronger ones (i.e., mimics the traditional, non-linear, photographic intensity response curve).

Phase ID
Comprehensive Diffraction Lookup

- Integrated diffraction database (~500,000 entries), created from the full Crystallography Online Database (COD).
- Instantly identify candidate phase(s).
- Browse publication data.
- Superimpose calculated peaks.
- Load full simulated pattern via the COD.

Rietveld Refinement
It's Quick and Easy

- Multi-phase support.
- Constant and dual-wavelength XRD.
- Constant-wavelength & time-of-flight neutrons.
- Sophisticated background shaping (Chebyshev polynomials, up to 13 terms).
- Automatically determines refinable parameters from crystal system & space-group.
- Fully-automatic refinement mode, with option of further (manual) refinement cycles.
- Unlimited cycle undos/redos.
- Change profile type and fitting range during refinement.
- Anisotropic temperature factor constraints.
- Equivalence constraints option for isotropic temperature factors.
- Optional damping parameters.
- Trajectory window with quality-of-fit metrics.
- Interactive colour-coded correlation matrix.

Sample
Your Virtual Powder Sample

- **Full Crystal Structure.** CrystalDiffract provides complete control over the crystal structure, including spacegroup symmetry, lattice parameters, fractional coordinates of sites in the asymmetric unit, site occupancies (unlimited occupants per site), isotropic and anisotropic atomic displacement parameters ("thermal ellipsoids").
- **Real-Time Lattice Parameter Control.** Adjust cell parameters and cell volume in real time, using slider and text controls in the Parameters List. Great for simulating structural distortions and the effects of displacive phase transitions.
- **Real-Time Site Occupancy Control.** Site occupancies can be adjusted in real time, using slider and tet controls in the Parameters List. Any number of elements can be assigned to an individual site, to simulate the effect of substitutional disorder: simply use the Add or Remove controls in the Parameters List. Precise site composition can be set using the Zero Occupancies commmand, and then typing in individual values in the Occupany list in the Parameters List.
- **Toggle Control for Displacement Parameters.** You can enable or disable thermal parameters for any site, using a checkbox control in the Parameters List. This is a good way of assessing the contribution made by atomic displacement parameters to the overall intensities.
- **Size Broadening.** Isotropic particle size broadening correction to the peak widths.
- **Strain Broadening.** Isotropic, percent strain broadening correction to the peak widths.
- **Preferred Orientation.** Choice of sample geometry: platy crystals or needle-like crystals in a capillary. Degree of alignment can be continuously varied, with simulation assuming a weighted (constant sample) March-type correction.

SingleCrystal 5

File Input
Live diffraction – or just drag-n-drop!

- CMDX (CrystalMaker X document)
- CMDF (CrystalMaker 7–9 document)
- CMTX (CrystalMaker text format)
- CIF
- Direct Simulation Link via CrystalMaker's `Transform > Powder Diffraction` submenu, including "Live Powder Diffraction" mode.
- Images in JPEG, GIF, TIFF, PNG, PDF (etc.) formats (for observed patterns)
- DM3, DM4 (observed patterns)
- SCDX (SingleCrystal 4–5 document)
- SCDF (SingleCrystal 3 document)

Structures Library
Crystals to Go

- Integrated library of ~1,000 curated crystal structures
- 500 mineral structures are included here.
- Indexed with metadata, annotations.
- Searchable, with scope bar.

Multi-Phase Simulation
X-rays, Neutrons or Electrons

- Reciprocal lattice sections (including upper layers)
- Weighted reciprocal lattice sections
- Zero-layer & upper-layer Precession patterns
- Laue front-plate, back-plate & cylinder patterns
- Transmission electron microscope (TEM) diffraction patterns with the option of Kikuchi Lines and Powder Rings
- 3D Weighted reciprocal lattice
- 3D Brillouin Zone
- 3D Crystal Shape

Instrument
Your Virtual TEM

- Wavelength (range for Laue patterns) and/or microscope voltage (TEM)
- Polarized radiation correction (Laue patterns)
- Crystal thickness (TEM)
- Beam convergence angle (TEM)
- Reflexion spot size
- Intensity saturation
- Volume fraction
- Kikuchi Line intensity (TEM)
- Minimum d-spacing for reflexion generation
- Maximum number of reflexions
- Gamma correction (intensity-greyscale mapping function)
- Automatic "Cleanup" (background subtraction and smoothing for observed patterns)

Display Options
Custom Visualization

- High-DPI "Retina" graphics.
- Colour-coded display of intensity, wavelength or phase angle, with opacity control.
- Show/hide systematic absences: lattice, spacegroup, other.
- Show/hide reflexion labels (hkl values), with minimum-intensity threshold.
- Reflexion, label, selection & background colours.
- Colourize observed diffraction image using fixed colour + opacity, or by applying a colour gradient.
- Control observed intensity range using minimum and maximum "threshold" limits, with the option of showing outliers as transparent or saturated regions.

Manipulation
Multi-Touch and More

- Rotation (real-time multi-touch, mouse, trackpad, Touch Bar, keyboard controls; view direction dialog)
- Scaling (real-time multi-touch, mouse, trackpad, Touch Bar, toolbar and Inspector options)
- Movement (xy offsets)
- Lattice layer control (e.g., reciprocal lattice sections)

Measurement
Interactive Screen Tools

- Miller indices, intensity, structure factor – for a clicked reflexion.
- Distances between two clicked reflexions.
- Angles between three clicked reflexions.
- Arbitrary distances, using the Ruler overlay.
- Arbitrary angles, using the Protractor overlay.
- Grid dimensions and angles, using the Grid overlay.
- Auto-indexing, for a loaded diffraction image and its simulation – via the Grid overlay.
- Profile tool for measuring cross-sections of diffraction data, with real-time updates and profile-width adjustment.
- Peak Markers to measure positions and intensities of observed reflexions.

Fourier Transforms
Optical Diffraction on Your Computer

- Generate a Fourier Transform of any displayed image or diffraction simulation.
- Interactive Fast Fourier Transform mode.
- Scale bar and ruler.
- Represent intensity as colour or gradient.
- Custom scale.

Brillouin Zones
Reciprocal Periodicity

- Visualize first Brillouin Zone for any crystal.
- Adjust colouring and opacity.
- Display adjacent reciprocal lattice points, including absences.
- Measure vertices, edges and face centres.
- Shift-click to define a trajectory in reciprocal space.

Crystal Shapes
Build Your Gems

- Dedicated Faces Inspector.
- Add symmetry-related faces.
- Adjust colouring and opacity.
- Real-time distance control (interactive "Wulff Construction").
- Measure face properties.
- Measure inter-facial angles.
- Measure vertex distances and angles.
- Combine multiple shapes for twinning/chiral relations.

Stereographic Projection
Symmetry Relationships in 2D

- Add arbitrary poles as vectors or plane normals in any colour.
- Show traces as great circles or small circles (user-specified radius).
- Add all symmetry-related directions, and/or all directions out to a maximum hkl index.
- Group poles by symmetry or N-value.
- Miller-Bravais (four-index) notation is available, as an option, for trigonal and hexagonal crystals.
- Hover the mouse over a pole to display its bearing and elevation.
- Double-click a pole to set this as your view direction.
- Measure angles between any pair of selected poles.
- Click-and-drag the stereogram to smoothly change the crystal orientation.
- Optional rotatable stereonet.
- Customize visibility and labelling of South Hemisphere projections.
- Export stereograms as pixel or vector images.

Data Output
Simulations and Observed

- Structure Factors.
- Relative intensities.
- Screen intensities.
- Raw intensities.
- Zone Axes file (for manual TEM indexing).
- Profile output (Ruler Profile).

Graphics Output
Patterns & Projections

- High-resolution pixel graphics: JPEG, GIF, TIFF, PNG, PSD (Mac), PICT (Mac), etc.
- Vector graphics: PDF (Mac) or WMF (Windows)

Support
Welcome to the Family!

- Deluxe 236-page user's guide (PDF).
- Self-Guided Tutorials (PDF).
- "What's New?" guide (PDF)
- Video tutorials (online)
- First-class technical support for registered users.