

LANDYNE

CRYSP v. 2

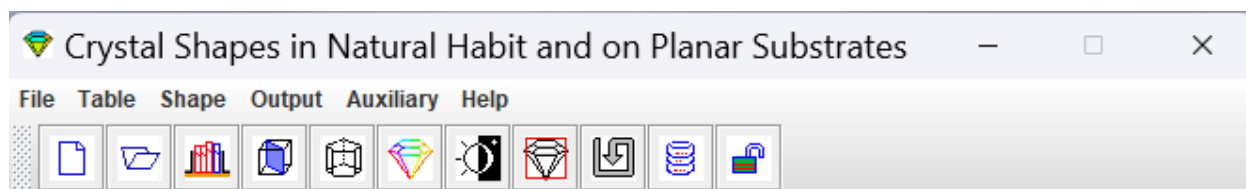
User Manual

*Construction and Visualization of Crystal Shapes and Cleavage
in Natural Habit and on Planar Substrates*

自然形态和平面基底上晶体形状和解理面的构建与显示

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1. Introduction

The shape of crystals has played a crucial role in the early development of crystallography. Faceted Wulff shapes offer illustrative examples of crystalline structures and behavior. During the late nineteenth century, crystallography was largely focused on observing the symmetrical patterns of faceted morphologies. In recent decades, interest in crystal shapes has been revitalized, driven by developments in nanostructures and heteroepitaxial islands (Medeiros-Ribeiro *et al.*, 1998; Robinson *et al.*, 2009; Longo *et al.*, 2011; Falub *et al.*, 2012). The morphology of crystallites is a fundamental factor—among others—in determining important physical properties, such as facet energy (Stekolnikov & Bechstedt, 2005), step formation energy (Giesen *et al.*, 2001; Bonzel & Nowicki, 2004), and facet growth velocity (Sun *et al.*, 2008, 2011; Romanyuk *et al.*, 2007), as well as other physical phenomena (Kim *et al.*, 2009). The crystallite shape itself can be predicted using the Wulff theorem and construction (Wulff, 1901).

A variety of software tools for visualizing crystal morphology have been developed—available as both open-source and commercial products. Notable examples include *Crystal Shape* (Dowty, 1980), *Wulffman* (Roosen *et al.*, 1998), *JShape* (Weber, 1999), *WinXMorph* (Kaminsky, 2005, 2007), *VESTA* (Momma & Izumi, 2011), *Wulffmaker* (Zucker *et al.*, 2012), *SOWOS* (Scopece, 2013), *NanoCrystal* (Chatzigoulas *et al.*, 2018), *Mercury* (Macrae *et al.*, 2019), and *Wulffpack* (Rahm & Erhart, 2020). These tools differ in functionality: some offer end-to-end solutions from generation to visualization, while others focus solely on shape generation for external rendering. The algorithms used also vary, with some tools implementing the classical Wulff method and others incorporating efficient convex hull algorithms, such as Qhull (Barber *et al.*, 1996). While certain software packages are actively maintained, others are unsupported. Moreover, many lack essential features—such as facet area calculation or user extensibility—highlighting the need for flexible, accessible, and well-supported alternatives. A recent comparative evaluation of several such tools was presented by Boukouvala, Danieland, and Ringe (2021).

Three-dimensional visualization enabled by Wulff-based modeling provides critical insights into experimentally observed crystal shapes, facilitates the construction of theoretically grounded models, and supports deeper analyses of shape-dependent crystal properties. These capabilities also enhance educational experiences by demonstrating how symmetry manifests in morphology. In this context, we developed **CRYSP**, a component of the **Landyne suite**, designed for the construction and visualization of crystal shapes in natural habit, cleavage planes, and crystals on planar substrates. CRYSP generates Wulff constructions based on user-specified crystal symmetries and energetics. It converts a crystal's space group to its corresponding point group symmetry, and requires as input the lattice parameters, a defined set of crystal facets, and their associated surface energies or growth rates.

Deriving the crystallographic point group (crystal class) from the space group

1. Leave out the Bravais lattice type.
2. Convert all symmetry elements with translational components into their respective symmetry elements without translation symmetry. (Glide planes are converted into simple mirror planes; screw axes are converted into simple axes of rotation.)

3. Axes of rotation, rotoinversion axes, and mirror planes remain unchanged.

In combination with **SVAT** (Li, 2020) and **SPICA** (Li, 2016), CRYSP has strong pedagogical potential, particularly in demonstrating how symmetry influences crystal shape. By adjusting surface energies in real time, users can reconstruct and visualize equilibrium polyhedra, gaining a deeper understanding of the thermodynamic and symmetry-based factors that govern crystal shape. This flexibility makes CRYSP a valuable tool for both research and education in the field of crystal morphology.

2. Theory background

In 1878 Josiah Willard Gibbs proposed that a droplet or crystal will arrange itself such that its surface Gibbs free energy is minimized by assuming a shape of low surface energy. He defined the quantity

$$\Delta G_i = \sum_j \gamma_j S_j \quad (1)$$

Here γ_j represents the surface (Gibbs free) energy per unit area of the j th crystal face and S_j is the area of said face. ΔG_i represents the difference in energy between a real crystal composed of i molecules with a surface and a similar configuration of i molecules located inside an infinitely large crystal. This quantity is therefore the energy associated with the surface. The equilibrium shape of the crystal will then be that which minimizes the value of ΔG_i .

2.1 Wulff construction

George Wulff (1901) made use of Gibbs theory (1928) and created a methodology to determine the equilibrium shape of a crystal based on its preferred growing planes (crystal habit). He also showed that the distance d_j of a crystal plane from its origin is proportional to its minimum surface energy γ_j :

$$d_j = \lambda \cdot \gamma_j \quad (2)$$

where λ is a constant, d_j is the distance of the Miller plane (hkl) from the origin of the lattice, and γ_j is its minimum surface energy. This is known as the Gibbs-Wulff theorem. Equation 2 denotes that lower surface energy leads to a larger plane area closer to the origin, because when the surface energy γ_j is reduced, the d_j is also reduced, and as a result, that plane truncates the other planes at a greater extent. A gamma plot, also known as a γ -plot, or Wulff plot, is a polar plot showing the surface free energy (γ) of a crystal as a function of orientation, and the Wulff construction uses this plot to determine the equilibrium shape that minimizes the total surface free energy of a fixed volume. When the surface free energy density, $\vec{\gamma}(\hat{n}) \equiv |\vec{\gamma}(\hat{n})|\hat{n} = \hat{n}\gamma(\hat{n})$, is given as a scalar function of the interfacial orientation $\hat{n}$, the resulting Wulff shape that follows from the Wulff construction is predominantly composed of those orientations that have the lowest surface energy. When $\vec{\gamma}(\hat{n})$ is very anisotropic, the Wulff shape can exhibit a faceted morphology composed only of planes, edges and corners. The Wulff constructions can also be applied to non-crystallographic crystals, e.g., based on decahedral and icosahedral symmetry, which can be viewed as consisting of five and twenty tetrahedral grains, respectively.

The Wulff construction is straightforward. Each face is represented by an equation, which is based on its Miller indices (hkl) and the central distance. The central distances may be measured (actual shape) or represent relative growth velocities (ideal growth shape) or surface energies (equilibrium shape). To build the shape, all triplets of face equations are solved to give the possible corners, then the smallest polyhedron is found by eliminating corners which are further from the center than any face. Edge line is made by connecting corners which have two faces in common. The crystal can be viewed from any angle, and both orthographic and perspective projections are supported. This method is considered as the traditional Wulff construction, which is adopted in CRYSP. The technique using Quickhall algorithm may also be used for fast generating Wulff shape, especially for a large number of faces involved, e.g., Wulffman (Roosen *et al.*, 1998) and Wulffpack (Rahm & Erhart, 2020).

The Wulff construction has several important properties:

- The shape of the resulting polyhedron depends only on the *ratios* between the surface energy values of the different crystal planes. This means surface energies can be given in any units, as long as the units are consistent for all inputs.
- Crystal planes with high surface energy (usually those with high Miller indices) tend to be *less likely* to appear on the equilibrium shape.
- High-index faces are often hidden behind low-index faces, even if their surface energy (γ_{hkl}) is relatively low.
- The additional energy from edges and vertices—where two crystal faces meet—is *neglected* in the Wulff construction.
- The polyhedron produced has the *same symmetry* as the underlying crystal structure.
- Regarding point (d), since the Wulff construction considers only flat facets meeting at sharp edges and corners, it does not account for the energy cost of these edges. If edge energies were included, the crystal faces would become *rounded* rather than sharp. This rounding effect typically appears at temperatures above absolute zero (0 K) and can be observed in simulations of nanoparticles when temperature is increased.

Furthermore, the Wulff construction assumes an equilibrium shape that minimizes the surface Gibbs free energy in a vacuum. In real systems, factors like solution environment, pH, temperature, and other conditions can influence surface growth, leading to changes in crystal shape away from the ideal Wulff form.

2.2 Winterbottom construction

The Wulff construction only applies to isolated crystals (particles) in homogeneous environments. However, in many contexts of practical importance (e.g., solid-state dewetting, catalysts, micropatterned surfaces, pores in a sintered body) a crystal (particle) can be attached to one or more interfaces. The equilibrium shape must minimize the sum of each total interfacial energy while maintaining other constraints, such as crystal (particle) volume and connectivity of the interfaces. The simplest example is a deformable crystal (particle) with a fixed volume that abuts a non-deformable (rigid) planar interface (e.g., a liquid drop on an inert-solid planar surface). In addition to the interfacial energy between the crystal (particle) and its environment in the absence of the substrate (γ_{pV} , where V refers to the environment, which is often a vapor phase), there are

two additional interfacial energies: the interface where the substrate abuts the crystal (γ_{SP}) and where the substrate is not in contact with the crystal (γ_{SV}). The isotropic crystal (particle) case is familiar: minimization produces a spherical cap that intersects the substrate with a uniform wetting angle, θ , for the crystal (particle) on the substrate, with

$$\theta = \cos^{-1} \frac{\gamma_{SV} - \gamma_{SP}}{\gamma_{PV}} \quad (3)$$

Equation 3 is known as the Young equation and can be interpreted as a force balance or as a boundary condition that derives from global energy minimization—these interpretations are not independent. The Young Equation is independent of particle size (in the absence of other defect energies), but the curvature of the spherical cap is determined by the particle volume. If ($\gamma_{SV} - \gamma_{SP}$) is positive, then most of the sphere is discarded, and only a small cap remains. This is the Winterbottom construction for an isotropic particle (Winterbottom, 1967). The Young equation is helpful in determining the equilibrium shape of an isotropic particle, but it is not obvious how it pertains to a general anisotropic particle. Winterbottom showed that the $\gamma = 0$ point will be a distance ($\gamma_{SV} - \gamma_{SP}$) below the substrate not only for isotropic particles, but for a particle with a general Wulff shape (Winterbottom, 1967).

The crystal (particle) shape on a planar substrate is characterized by the aspect ratio (AR), defined as $\beta_1 \equiv h_{\max}/S_{\text{base}}^{\frac{1}{2}}$, the height of the island divided by the square root of its base (Zhang *et al.*, 2010). Other parameters widely employed in multiscale modelling of heteroepitaxy are the facet area divided by the volume of the entire crystal to the power of 2/3: $\beta_2 \equiv S_{\text{base}}/V_{\text{tot}}^{\frac{2}{3}}$. (Chen *et al.*, 2012; Scopece *et al.*, 2012; Scopece & Beck, 2013). If we define the average height as $h_{\text{avg}} = V_{\text{tot}}/S_{\text{base}}$, then $\beta_2 \equiv S_{\text{base}}/V_{\text{tot}}^{\frac{2}{3}} = S_{\text{base}}/(h_{\text{avg}}S_{\text{base}})^{\frac{2}{3}} = S_{\text{base}}^{\frac{1}{3}}/h_{\text{avg}}^{\frac{2}{3}}$. Since $\beta_1^2 \equiv h_{\max}^2/S_{\text{base}}$, $\beta_2^3 \equiv S_{\text{base}}/h_{\text{avg}}^2$, thus, $\beta_2^3 \approx 1/\beta_1^2$. These values are pure numbers and are independent of the volume of the solid. Comparison of the β values give a direct comparison of the relative abundance of the facets in the crystal and this parameter may turn out to be useful in crystallography as well. Because of the properties of the Wulff construction, facets with larger distance will have a lower β_2 , vanishing for a larger enough value of distance. For this consideration, the definition as β_2 is recommended.

2.3 Bravais–Friedel–Donnay–Harker (BFDH) model

In addition to its application in studying surface free energies, the Wulff construction can also be adapted to predict steady-state growth shapes of crystals. In this context, the method is used when the growth velocity depends only on the interfacial orientation $\hat{n}$. To obtain the growth shape, the velocity as a function of orientation $\vec{v}(\hat{n})$ replaces $\vec{\gamma}(\hat{n})$ in the Wulff construction. The slowest growing interfaces are the largest on the steady-state shape and the faster orientations grow out of existence at the corners. Thus, the Wulff shape can be used for studies of growth shapes as well.

Bravais–Friedel–Donnay–Harker (BFDH) law (Donnay & Harker, 1937; Hartman, 1978) is a classical theory of crystal growth. It states that a crystal in a polyhedral shape is achieved by different growth rates along different crystal orientations and the relative growth rate R_{hkl} of a face

(hkl) is inversely proportional to the distance d_{hkl} . The surfaces with the lowest growth rate will be maintained as the final crystal facets. The morphological importance (MI) of a face (hkl) is defined as the relative statistical frequency of occurrence of the face (hkl) or the relative size of the face (hkl) occurring on a set of crystals of a certain compound, the interplanetary spacing and the morphological importance (MI) has the following relationship, $d(h_1k_1l_1) > d(h_2k_2l_2) \rightarrow MI(h_1k_1l_1) > MI(h_2k_2l_2)$.

According to Bravais and Friedel, the value of d_{hkl} ought to be corrected for non-primitive cells if these cells are used to calculate d_{hkl} (Friedel, 1911). These corrections may lead to integers h, k and l that are mutually non-prime. According to Donnay & Harker (1937), d_{hkl} need to be corrected for screw axes and glide planes of the space group of the crystal structure because exactly the same crystal surfaces are separated by d_{nhnknl} . An intuitive extension of the Donnay-Harker law was given by Donnay & Donnay (1961) for the case that surfaces separated by d_{nhnknl} are almost exactly the same. For a treatment of the BFDH law Hartman (1978), the modified formulation of the BFDH law is that the growth rate R_{hkl} is proportional to $1/d_{hkl}^m$, where m is between 1 and 2.

The BFDH "theory" provides a useful model, however, limited by the fact that it is based only on geometrical properties of crystals. This means that physical and chemical-physical properties are not considered to interpret the results of growth. For a rough estimate based on crystal structure: the BFDH model provides a quick and reasonable first approximation. In general, d_{hkl} has, at least, to be corrected by the crystallographic selection rules as given in International Tables for X-ray Crystallography (2005). If the space group and elementary cell of a given structure are known, all d_{hkl} values can be calculated and then the crystal forms can be constructed.

The BFDH model and the Wulff construction are related approaches to predicting crystal morphologies, but they differ in their underlying principles and do not typically yield the same morphology. The BFDH model focuses on the relative growth rates of crystal faces based on their interplanar spacing, and predicts that faces with larger d-spacings will be more prominent in the crystal morphology (i.e., grow slower and therefore become larger) while the Wulff construction considers the equilibrium shape of a crystal by minimizing its total surface energy, and predicts the equilibrium shape of a crystal by constructing a polyhedron where the distance from the center to each face is proportional to the face's surface energy. For predicting equilibrium shapes with surface energy considerations: the Wulff construction is generally more accurate and realistic. For situations where non-equilibrium growth or other factors are dominant: neither method may be entirely accurate, and more advanced models incorporating growth kinetics and other environmental factors might be needed.

2.4 Atom cluster

Particle shapes of crystal nanoparticles can affect their properties, functionality, and applications. Furthermore, the surface-level atomic arrangements of compound are even important for application. With CRYSP, the atomic arrangement can be obtained by filling the crystal structure within the facets. The atom cluster can be used in the following cases:

- Relating structure to reactivity: different crystal faces (like {100}, {110}, or {111}) expose different densities of atoms and dangling bonds. An atomic model helps researchers link specific surface structures directly to catalytic or electrochemical performance.
- Controlling nanoparticle stability: at the nanoscale, shape dictates stability. Atomic models reveal how atoms move, diffuse, or hop along edges and corners during facet formation and growth.
- Designing better materials: by simulating atomic arrangements and surface energies, researchers can engineer targeted crystal shapes (facet engineering) for better batteries, catalysts, and optical devices without relying purely on trial and error.

3. Design and features

3.1 Graphic design

CRYSP is designed to construction and visualization of the crystal (particle) shape and cleavage, and the crystal (particle) on a planar substrate. The graphic user interface (GUI) of CRYSP includes a drop-down menu, a menu bar, a display panel, and several operational dialogs. The drop-down menu provides access to all the operational dialogs, while the menu bar lists frequently used ones. Figure 1 shows the display panel with a menu bar. A control dialog of the crystal shape and other operational dialogs can be toggled on and off. The size of the CRYSP window, including the display panel, can be adjusted via the Auxiliary menu.

The menus and their functions are organized as follows:

- File Menu
 - i) Load crystal structure templates.
 - ii) Import a crystal structure or lattice file.
 - iii) Load a demo crystal structure.
 - iv) Exit the CRYSP application.
- Table Menu
 - i) Periodic table of elements.
 - ii) Table of space groups (standard settings).
 - iii) Table of space groups (non-standard settings).
- Shape Menu
 - i) Apply the BFDH law and its extensions (*see Figure 2*).
 - ii) Input dialog for crystallographic parameters.
 - iii) Input dialog for non-crystallographic shape parameters.
 - iv) Crystal shape settings dialog.
 - v) Background display options.
- Output Menu
 - i) Select a region of interest for output.
 - ii) Save output in various formats (JPG, PNG, GIF, TIF).
- Auxiliary Menu
 - i) Adjust display panel size.
 - ii) Toggle toolbar visibility.
 - iii) Customize appearance (fonts, themes).

- Help Menu
 - i) Serial number input dialog.
 - ii) Display current version information.
 - iii) Link to the Landyne website.

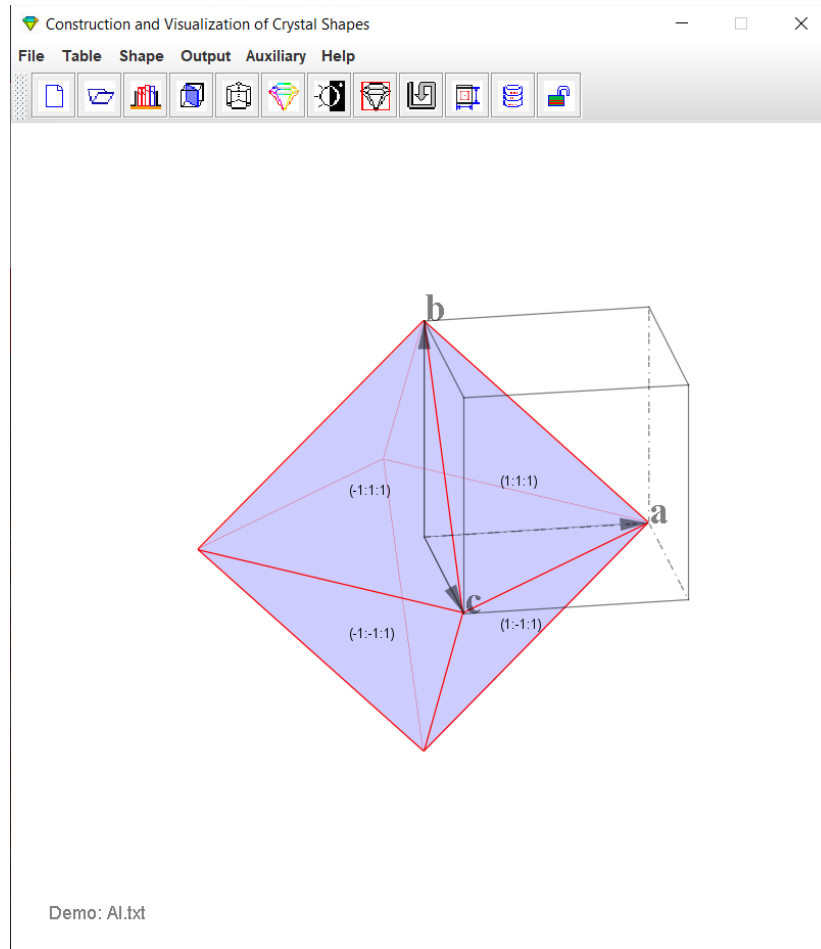


Figure 1. The GUI of CRYSP with an example of the FCC Al structure.

3.2 Function features

CRYSP combines ease of use with powerful functionality, making it a valuable tool for visualizing and analyzing crystal shapes. All operations are accessible from a single main window, which launches individual tool dialogs as needed. A file template is available to assist with preparing crystal structure data, and all structure files generated within the Landyne suite are fully compatible with CRYSP.

The software supports a wide range of symmetry groups, including:

- Conversion from 230 space groups to 32 point groups.
- Predefined decagonal and icosahedral groups.
- Extendable user-defined non-crystallographic types.

Users can construct crystal shapes by specifying surface energies for different facets. By adjusting these values, users can observe how the equilibrium shape evolves in real time—clearly demonstrating the influence of surface energy anisotropy. Users can also define cutting planes by selecting specific facets, enabling the analysis of sliced or sectioned crystals. Nearly all aspects of the crystal shape are customizable.

CRYSP provides detailed information about each generated crystal shape, including:

- Polyhedral volume.
- Facet areas.
- Facet orientations (hkl directions).
- Edge lengths.

CRYSP is a versatile and user-friendly tool ideal for use in crystallography, nanostructure research, and any other field where the analysis and visualization of crystal facets are important. Key features of CRYSP include, but are not limited to:

- Interactive 3D visualization, with support for both orthographic and perspective views.
- Display options for wireframe polyhedral or color-filled facets.
- Full rotation and scaling of crystal shapes for detailed inspection.
- Construction and visualization of crystal shapes in natural habit, cleavage surfaces, and crystals on planar substrates.
- Support for structure file preparation using 230 standard space groups, with automatic conversion to 32 point groups.
- Extension to non-crystallographic point groups, such as icosahedral and decagonal pillar symmetries.
- Application of the BFDH law and its extensions for morphology prediction.
- Calculation of edge lengths, facet areas, and polyhedral volume.
- Ability to save building procedures and color settings for quick reuse.
- Save the crystal shape in common image formats: JPG, PNG, and TIF.
- Display atomic models of the polyhedral and save a list of atom coordinates.

4. Usage

4.1 Preparation of a file of crystal structure

CRYSP allows users to load a file containing a crystal structure or crystal lattice to calculate crystal shapes using the Wulff construction. While the Wulff construction itself requires only the lattice parameters, the point group symmetry, and the surface energy or growth rate for each facet, full crystal structure data is supported for the application of BFDH law and its extensions, which rely on atomic positions and unit cell contents to predict the crystal morphology.

A structure data file can be prepared using the "Crystal Structure File" template, as shown in Figure 2. This window provides an automated assistant to help ensure the file format requirements are met. The template includes all 230 space groups in Hermann-Mauguin notation, as listed in the International Tables for Crystallography.

Additionally, the crystal file can be converted from previous data for modification or from a Crystallographic Information File (CIF). If a data file uses an alternative setting of space groups for triclinic, monoclinic, and orthorhombic systems, click on the alternative settings (1~74). A tool for transforming files from nonconventional notations to standard notations is provided, as shown in Figure 3.

Crystal Structure File

Description
New crystal structure

Space group
☒ The standard settings (1~230) ☐ The alternative settings (1~74)
 Number 1~230 Symbol ? Origin ▼

Lattice parameters
 a = (Å) b = (Å) c = (Å) α = (°) β = (°) γ = (°)

Coordinates of Atoms

atom	elem #	x	y	z	occ.
		0.0	0.0	0.0	1.0

Add Remove Clear View

Number of atom in the list: 0 Global isotropic temperature factor 0.0

Notes
References etc.

New Load Save Close

Figure 2. A template for preparing a crystal structure file.

From Alternative to Standard Setting

Description
new crystal structure

Triclinic, monoclinic and orthorhombic systems
 Space group number 3 Alternative symbols P 1 2 1 ▼

Lattice parameters
 a = (Å) b = (Å) c = (Å) α = 90.0 (°) β = (°) γ = 90.0 (°)

Coordinates of Atoms

atom	elem #	x	y	z	occ.
		0.0	0.0	0.0	1.0

Add Remove Clear View

Number of atom in the list: 0 Global isotropic temperature factor 0.0

Notes
References etc.

New Transform Back Close

Figure 3. A template for preparing a crystal structure file using an alternative setting in triclinic, monoclinic and orthorhombic systems.

4.2 Database of crystal structures

A collection of crystal structures is provided with the Landyne software suite. Part of the structural data comes from the list in Appendix 1. of the book by M. De Graef and M.E. McHenry, and the other part is from the author's research works.

Below is a list of the resources for crystal structures:

- Library of Crystallographic Prototypes: Part 1 edited by M.J. Mehl *et al.*, and Part 2 edited by D. Hicks *et al.*
- Crystallography Open Database.
<https://www.crystallography.net/cod/>
- American Mineralogist Crystal Structure Database.
<https://rruff.geo.arizona.edu/AMS/amcsd.php>
- The Pauling File: Inorganic Materials Database containing Phase Diagram, Crystal Structure and Physical Property entries
<https://paulingfile.com/>
- Appendix 1. Crystal Structure Descriptions in Structure of Materials by M. De Graef and M.E. McHenry, 2nd Edition, Cambridge University Press, 2012.
- Pearson's Handbook, *Crystallographic Data for Intermetallic Phases*, edited by P. Villars, ASM, 1998.

4.3 CRYSP

The usage of CRYSP is straightforward and intuitive. The best way to learn how to use CRYSP is through experimentation. For example, you can load demo crystallographic data from the File menu. Morphological Importance (MI) tool displays a list of crystal planes that are most likely to form the crystal shape, as shown in Figure 4. The plane with indices $h = 1, k = 1, l = 1$ ranks highest in the MI sequence. In the input parameters dialog (Figure 5), assign the index $h = 1, k = 1, l = 1$ with $x = 1.0$ and select the Surface button. Then, assign the index $h = 1, k = 0, l = 0$ with $x = 0.6$ and select the Interface button. There are two ways to assign the w value: either use d_{hkl} or a user-defined value; both are multiplied by x value. The value of w is inversely proportional to the free surface energy or the growth rate. Click the Shape button, and the crystal shape will appear on the display panel (see Figure 1). In the Crystal Shape dialog, clicking the Facet Color Table allows you to assign colors to each facet.

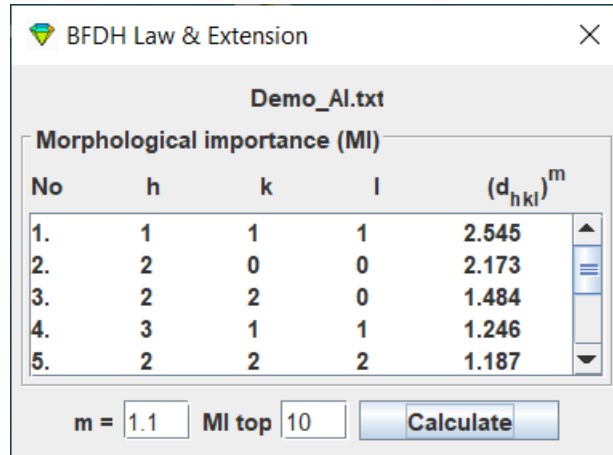
Display options can be toggled on or off. Selection Interface +P1 +P2 to show the cleavage and part of the polyhedral as Winterbottom construction in Figures 6 and 7. More examples are given in the next section. Region of Interest can be defined and then the display can be selected to JPG, PNG, GIF and TIF format.

Two applications are briefly described here: (1) inverse Wulff construction for surface energies of crystal particles (Lai, Chen & Guo, 2019) can be done by simulating shapes with a series of w values, the area ratio of two planes (indices) via the w value can be plotted a curve. An area ratio for a shape can be measured in experiment and then the w value can be calculated via the curve

obtained above; (2) as mentioned in the introduction section, the crystal (particle) shape on a planar substrate is characterized by the aspect ratio (AR), defined as $\beta_1 \equiv h_{\max}/S_{\text{base}}^{\frac{1}{2}}$, and $\beta_2 \equiv S_{\text{base}}/V_{\text{tot}}^{\frac{2}{3}}$. We should $\beta_2^3 \approx 1/\beta_1^2$. The definition as β_2 is recommended to characterize the aspect ratio (AR). CRYSP allows the users to measure the S_{base} and V_{tot} for the crystal (particle) shape on a planar substrate.

Here are a few tips for first-time users to familiarize themselves with CRYSP:

1. Load a crystal structure file or a crystal lattice file.
2. Open Input Parameters Dialog and enter some facets of interest with a spacing factor. Make sure that the facets form an enclosed polyhedral.
3. If you want to save your work, choose "Save (current work)" to save it to a work file. Load the crystal structure first, then reload the previous work of the same crystal structure.
4. Click Shape button. The Wulff shape should be generated and display.
5. Select and adjust the Region of Interest and then save the display as a file of .png, .jpg, .gif or .tif format.



No	h	k	l	$(d_{hkl})^m$
1.	1	1	1	2.545
2.	2	0	0	2.173
3.	2	2	0	1.484
4.	3	1	1	1.246
5.	2	2	2	1.187

m = 1.1 MI top 10 Calculate

Figure 4. BFDH law and extension for morphological importance of a crystal structure as a list of forms with central distances dependent on d spacing.

Input Parameters

Demo_Al.txt | 32. m-3m

Crystal plane and spacing factor

h k l : 0 0 1 x = 0.6

☒ $w = x \cdot d(hkl)$
☐ $w = x \cdot$

Surface Interface

S	-1	-1	-1	2.338
S	1	1	-1	2.338
S	1	-1	1	2.338
S	-1	1	1	2.338
T	0	0	2	2.4297

Number of planes in the list: 9

Clear Save Load Shape

Input Parameters (ext)

I 235 icosahedral a = 10 Å c/a = 1.0

Crystal plane and spacing factor

h k l : 1 0.618 0 x = 1.0

☒ $w = x \cdot d(hkl)$
☐ $w = x \cdot$

Surface Interface

S	1	0.618	0	8.5065
S	0	1	0.618	8.5065
S	-0.618	0	1	8.5065
S	0	-1	0.618	8.5065
S	1	-0.618	0	8.5065

Number of planes in the list: 12

Clear Save Load Shape

Figure 5. the input parameters for crystal structures and for non-crystallographic structures.

Figure 6. Crystal shape and cleavage as demo on the display panel.

14

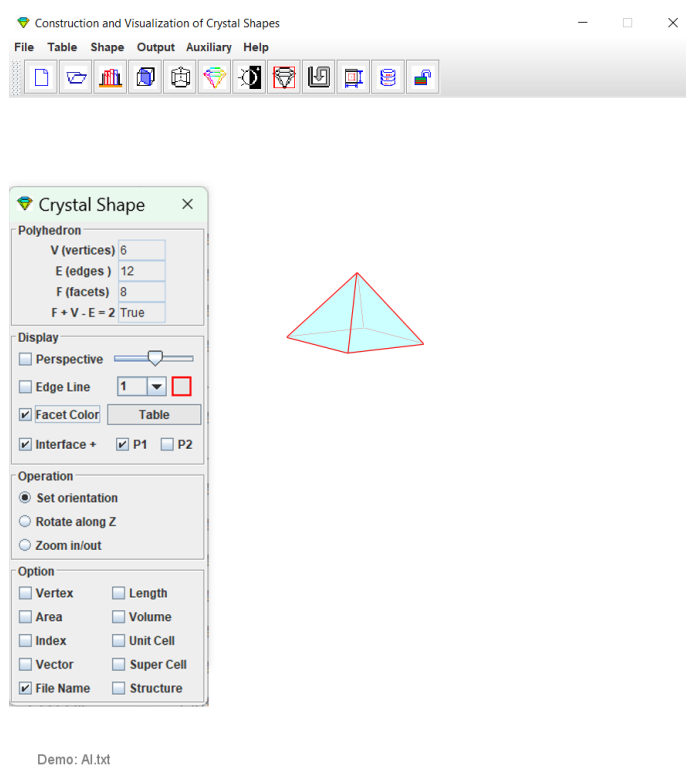


Figure 7. Part of crystal shape as demo on the display panel.

The atom cluster can be revealed by selecting the dialog as shown in Figure 8 and ticking the structure option in Crystal Shape dialog, inserted in Figures 6 and 7. The lattice range should be over the size of the polyhedral. The color and size of atoms can be adjusted.

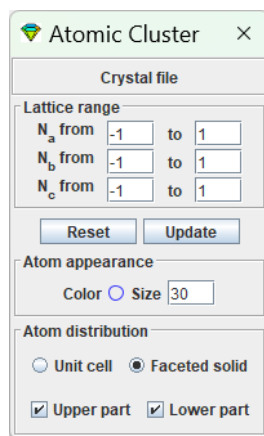


Figure 8. A dialog for an atom cluster.

5. Examples

5.1 Crystal shapes in natural habit and on planar substrate

An example of the Winterbottom construction with various $(\gamma_{sv} - \gamma_{sp})$ values in equation (3), which follows Figure 1. in the research paper by Zucker *et al.* (2012).

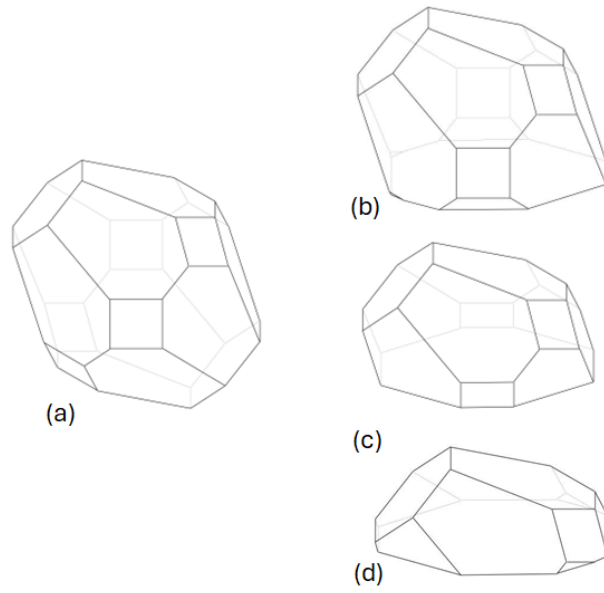
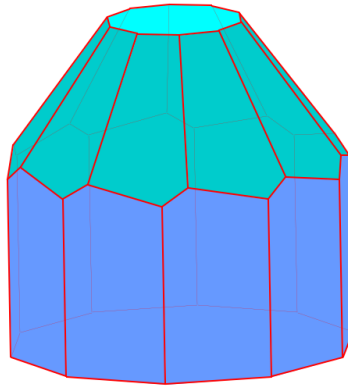


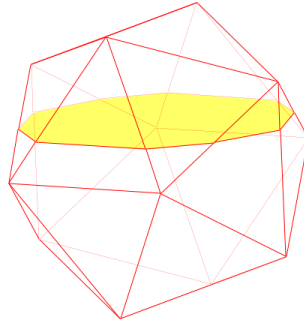
Figure 9. Left the Winterbottom construction begins with the Wulff shape of a particle and $(\gamma_{sv} - \gamma_{sp})$. Right the distance between the $\gamma = 0$ point in the Wulff shape and the substrate surface is equal to $(\gamma_{sv} - \gamma_{sp})$.

5.2 Non-crystallographic crystals



C10_tenfold

Figure 10. Decagonal column with a sharp end.



I235_icosahedral

Figure 11. I235 icosahedral crystal shape with a cleavage interface.

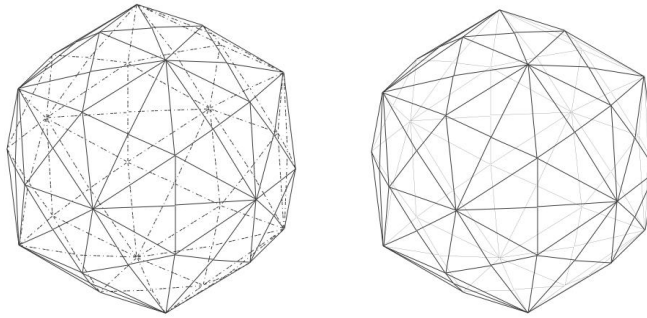
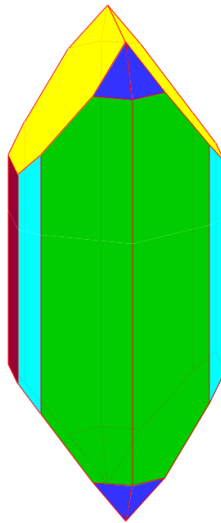


Figure 12. $I_h m \bar{3} 5$ icosahedral crystal shape.

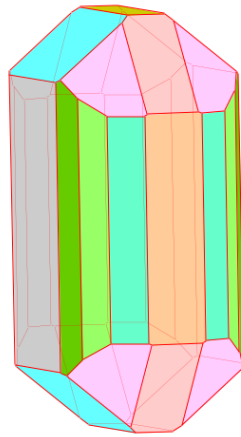


Aeschynite-Y.lat.txt

Figure 13. Aeschynite-Y.

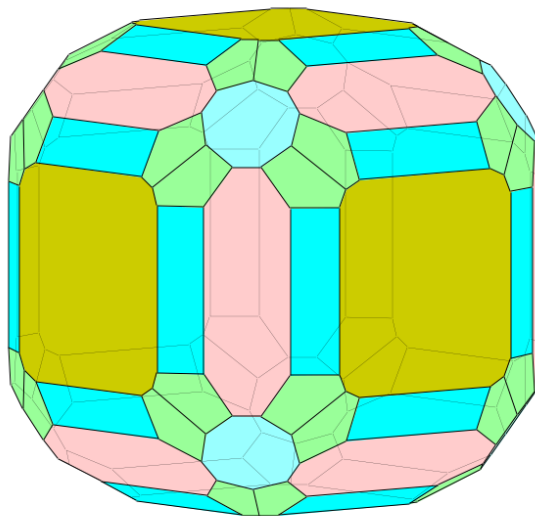
5.3 Mineral crystals

The crystal structure and shape parameters were referenced to the data set in KrystalShaper by S. Weber.



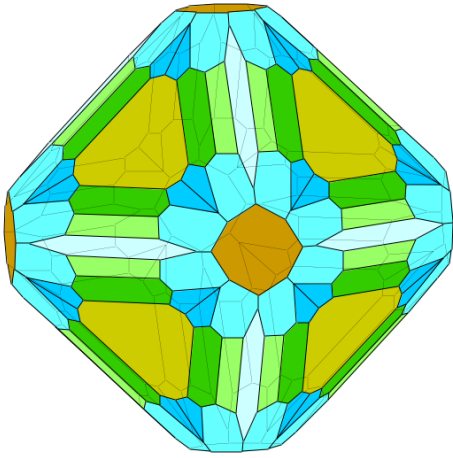
Anglesite.lat.txt

Figure 14. Anglesite.

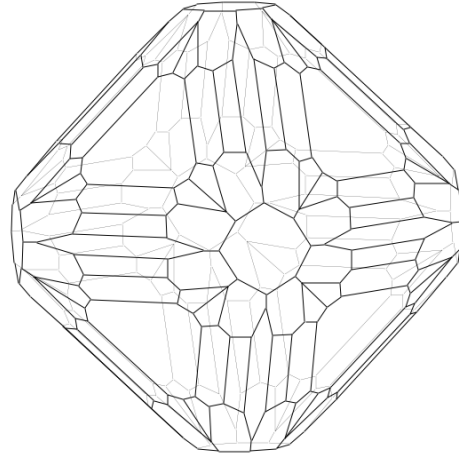


cubehex.lat.txt

Figure 15. Cubehex.

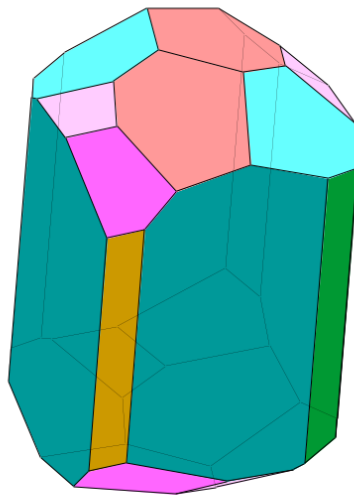


cubic-strang.iat.txt



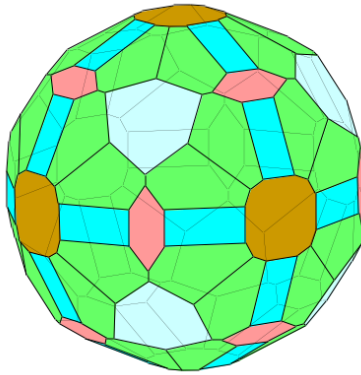
cubic-strang.iat.txt

Figure 16. Cubic-strang.



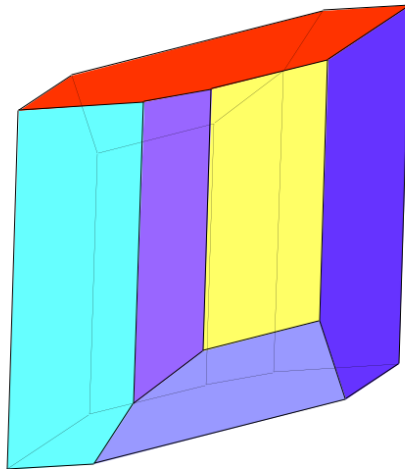
Epsomite.iat.txt

Figure 17. Epsomite.



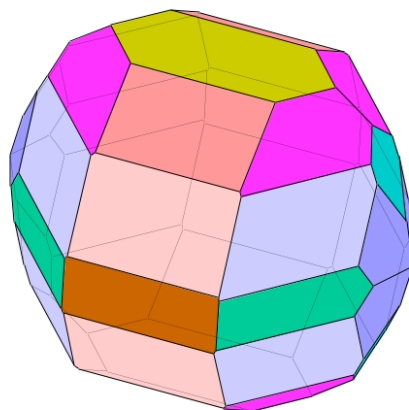
hexocta.iat.txt

Figure 18. Hexocta.



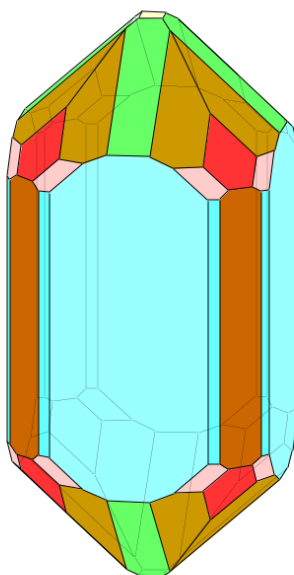
pentahydrate.iat.txt

Figure 19. Pentahydrate.



Sulfur.lat.bt

Figure 20. Sulfur.



zircon.lat.bt

Figure 21. zircon66.

5.4 Example of atom cluster

By gradually increasing the size of a cluster, the atom configuration on the facet layer may change for a compound, which the composition is more than one kind of atoms. The list of atom coordinates of the cluster can be saved and then reloaded into SVAT software to display in colors. Figure 22 shows an atom cluster of Al in CRYSP and in SVAT.

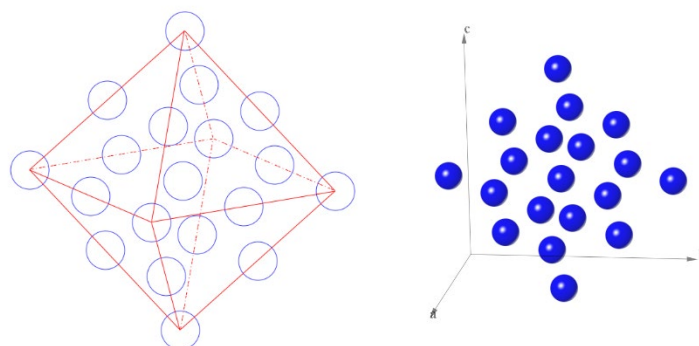


Figure 22. Atom cluster of Al in CRYSP and in SVAT.

6. Software

6.1 Landyne suite

Landyne (computer software & graphic design) was established in 2010 by X.Z. Li and Jane Li in Lincoln, NE. We have developed comprehensive software suited to electron diffraction simulation, electron microscopy image processing and crystallographic analysis. The suite serves as a valuable tool for TEM-related research and educational purposes in electron microscopy and crystallography.

6.2 Installation

OpenJDK21 must be installed for running CRYSP. The executable bytecodes, together with the data files for testing and this manual file, are available in compressed form (landyne6.7z)

<https://temsoftware.unl.edu/>
<https://landyne.com/>.

Decompress landyne6.7z in a user-defined directory, e.g., c:\landyne6\ and execute launcher.exe.

6.3 Licenses

The software is fully functional in demo mode but is limited to using the demo input file. Both periodic-time and perpetual licenses are available. For licensing information, please contact LANDYNE at jlandyne@gmail.com. Suggestions and comments are always welcome.

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