LANDYNE

User Manual

Structural Visualization and Analytical Tool

Structural Viewer and Analytical Tool

File Table Component Display Output Tools Auxiliary Help

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1. Introduction

The Landyne suite, developed by Dr. X.Z. Li, is a software package for electron diffraction simulation and electron microscopy image processing aimed at crystallography analysis. The suite serves both as research tools as well as educational aids. As the suite's software components and user base continue to expand, the necessity for a robust tool for structural visualization and analysis becomes increasingly evident.

Various software tools for structural building, visualization, and analysis are available online free or commercially. Some, like [CMX], are comprehensive with multipurpose functionality and advanced graphics. Others, such as [FCV], focus solely on displaying crystal structure without extensive analytical capabilities.

SVAT (Structure Visualization and Analysis Tool) was initially developed in 2011 for interactive 3D visualization and analysis of alloy and intermetallic structures. Over the years, SVAT has evolved with additional functions to meet user demands. SVAT4 was featured in a paper published in Journal of Applied Crystallography [xzli, 2020] and the current version, SVAT6, offers essential functions such as interactive 3D visualization of crystal structure within a unit-cell, including the chemical bonds and magnetic moments.

More functions of SVAT6 include, e.g.,

- Interactive 3D visualization with options for projections in user-selected [uvw] directions or layer-by-layer views.
- Analysis tools for local structures (polyhedral clusters) by defining a central atom and spherical radius.
- New data templates for structure file preparation using 230 standard space groups and alternative settings.
- Importing .xyz files for viewing molecular cluster structures.
- Calculation tools for bond lengths, angles, chemical compositions, and density.
- Saving the full list of atoms in a unit cell for structure modification.
- Animated display modes such as rotation or wobble for enhanced visualization.
- Capability to save work progress to files for quick access and continuation.
- Export structure displays as JPG, PNG, and TIF image formats.

More details of the features are described below.

2. Design and features

2.1 Graphic design
The graphic user design of SVAT6 includes a drop-down menu, a menu bar, a display panel, and several operational panels. The drop-down menu provides access to all the operational panels, while the menu bar lists frequently used ones. The display panel and a control panel are always

visible, whereas other operational panels can be taggled on and off, as shown in Figures 1 and 2. Users can adjust the software frame size, including the display panel, via the Auxiliary menu.

2.2 Function features

Visualization tools:

- Use the left mouse button for rotation along the x-y axes, the right mouse button for rotation along the z-axis, and the mouse wheel for zooming in/out. Zoom options are also available for laptops without a mouse wheel.
- The crystal structure can be interactively oriented using the mouse (1° steps) and arrow keys (0.1° steps).
- Crystal structures along [uvw] can be set up in the projection option and reselected in the 3D option.
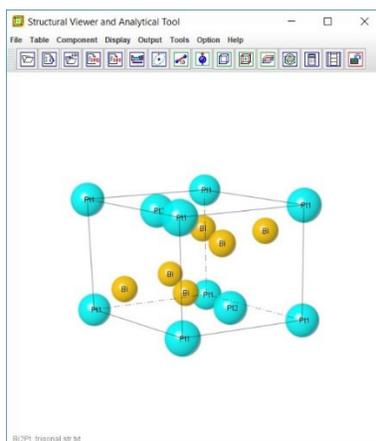- Atom sizes and colors can be defined by built-in data or customized by users.

Figure 1. The GUI of SVAT6 with an example of the Bi_2Pt structure.

- Atom sizes can be globally scaled up or down.
- Atoms can be displayed as circles, disks, or two sets of solid balls for fast changes.
- The background can be toggled between white and black.
- Both conventional and symmetric unit cells are available for hexagonal structures, and primitive unit cells for rhombohedral structures.
- Users can add bonds and magnetic moments to atoms.
- Animation for rotation or oscillation modes can be set up.
- Optional display of file name, unit cell, lattice vectors, and perspective view, with adjustable position, font size, and color.
- Crystal structures can be rotated along any axes and separately on screen.
- Zoom options for 3D display, projection, and layer display.
- Lattice-only option available for teaching crystallography.
- Import .xyz files to display molecular clusters.

Analysis tools:

- Atoms can be labeled with assigned labels, elements, identified numbers, occupancy factors, or no labels.
- Display atoms with partial occupancy.
- Show coordinates of any selected atom.
- Search and build atom clusters by defining the center atom and distance.
- Display structure projection along [uvw] or a slice of an atom layer.
- Save a full list of atoms in a unit cell for structure modification.
- Calculate and verify the composition of the crystal structure.
- Search for the shortest bond and list bonds in a crystal structure.
- Calculate bond distances and angles between bonds.
- Calculate the composition and density of crystal structures.
- Compare two crystal structures in the second run of SVAT6.
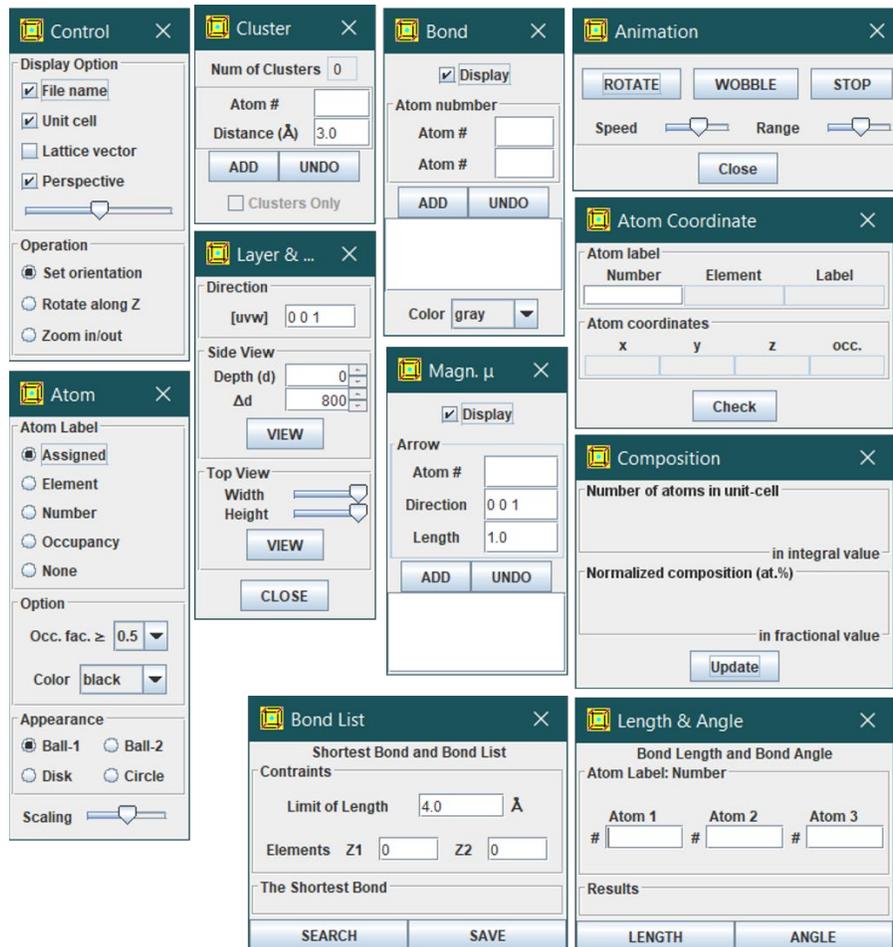
Figure 2. All the operational panels in the SVAT6.

Input and output features:

- Template available for preparing crystal structures.
- Save or load work on building crystal structure bonds.
- Access a periodic table of elements, including calculated and empirical atomic radii.
- Access a space group table.
- Define a region of interest for output.
- Output display options in .gif, .jpg, .png, or .tif formats.

3. Usage

3.1 Preparation of a new structure file

A structure data file can be prepared using the "New Crystal Structure File" dialog window, as shown in Figure 3. 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. However, for monoclinic systems, only the unique b-axis is used.

Two origin choices can be accepted as input parameters, but choice-2 will be converted to choice-1. To save the data structure, click the "Save" button. To create a new structure file, click the "New" button.

Figure 3. A template for preparing a crystal structure file.

Figure 4. A template for preparing a crystal structure file using an alternative setting in triclinic, monoclinic and orthorhombic systems.

Figure 5. The periodic table of the elements with the calculated and empirically measured atomic radii [3]. Both atomic radius and atom display color can be customized.

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 4.

Besides the structure file, there is a second type of input file containing previous work on a structure. A work file of the same crystal structure can be loaded to continue using the work done previously.

The periodic table of elements, showing calculated and empirically measured atomic radii (WAR), is depicted in Figure 5. Both the atomic radius and the atom display color can be customized for visualizing the crystal structure.

3.2 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 *Structure of Materials: An Introduction to Crystallography, Diffraction, and Symmetry* by Marc De Graef and Michael E. McHenry (2nd Edition, Cambridge University Press, 2012), while the other part is from the author's research works.

Below is a list of shared resources for the crystal structures:

- Pearson's Handbook, *Crystallographic Data for Intermetallic Phases*, edited by P. Villars, ASM.
- ICDD – International Centre for Diffraction Data.
- Appendix 1, *Crystal Structure Descriptions in Structure of Materials* by M. De Graef and M.E. McHenry [TSM].
- *Library of Crystallographic Prototypes*: Part 1 edited by M.J. Mehl et al., and Part 2 edited by D. Hicks et al. [ECP].

3.3 Guide

The usage of SVAT6 is straightforward and self-explanatory. For example, crystal structures can be displayed in 3D view with an adjustable perspective constant. Various options for atomic labels and appearances are available. Chemical bonds and magnetic moments can be added to numeric atomic labels. Here are a few tips for first-time users to familiarize themselves with SVAT6:

- Crystal structure files in CIF format can be uploaded and edited in the template for new crystal structures. Some CIF files may require manual editing for complete transfer.
- It is recommended to check the composition after preparing a new data file.
- Before setting bonds between atoms, select the atom label as a number.
- Before setting magnetic moments on atoms, select the atom label as a number.
- To save your work, choose "Save (current work)" to save it to a binary file. Load the crystal structure first, then reload the previous work of the same crystal structure.
- Atom radius and display color can be edited for the current work and saved into a work file. This customized data set can be reloaded for later use.
- Before saving the display, define the region of interest (ROI) and save it as a TIF file.

- To view the structure along a [uvw] direction, first select [uvw] in "Layer and Projection," then re-select "Structure." Users can switch the perspective factor on or off.
- Use arrow keys to fine-tune the orientation of the crystal structure. Ensure the mouse pointer is on the display panel.
- The Ball-2 atom appearance is slightly more transparent than Ball-1.
- A full list of atoms in a unit cell can be saved with the space group P1. Adjust the number of atoms in the data file when adding or deleting atoms.
- To save the display as a file of .jpg, .png or .tif format.

4. Examples

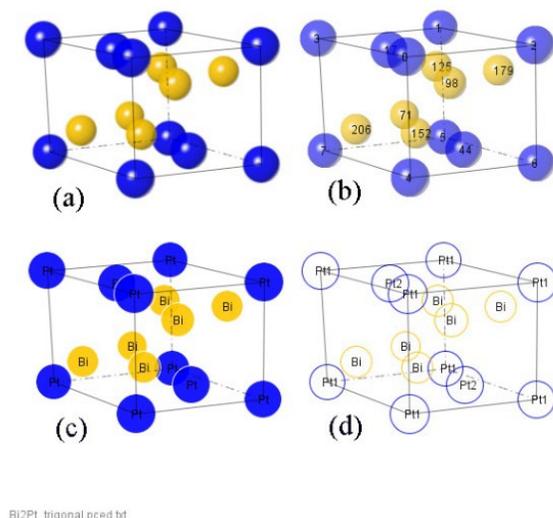A few examples are listed below, which are related to the author's previous research work.

Figure 6. The structure of Bi_2Pt with various appearances. Atoms in (a) solid ball, (b) transparent ball, (c) disk and (d) circle and labels in (a) off, (b) numerical, (c) element and (d) atom label.
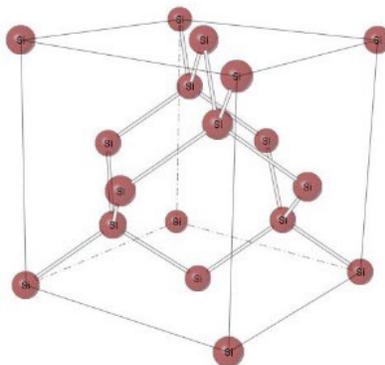

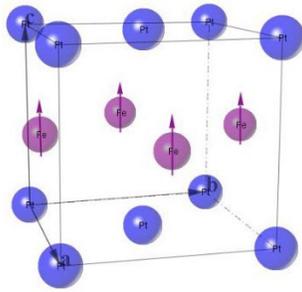Figure 7. The structure of Si with chemical bonds as balls-and-sticks.

Figure 8. The structure of FePt $L1_0$ phase with magnetic moments on Fe atoms.

(a)   (b)
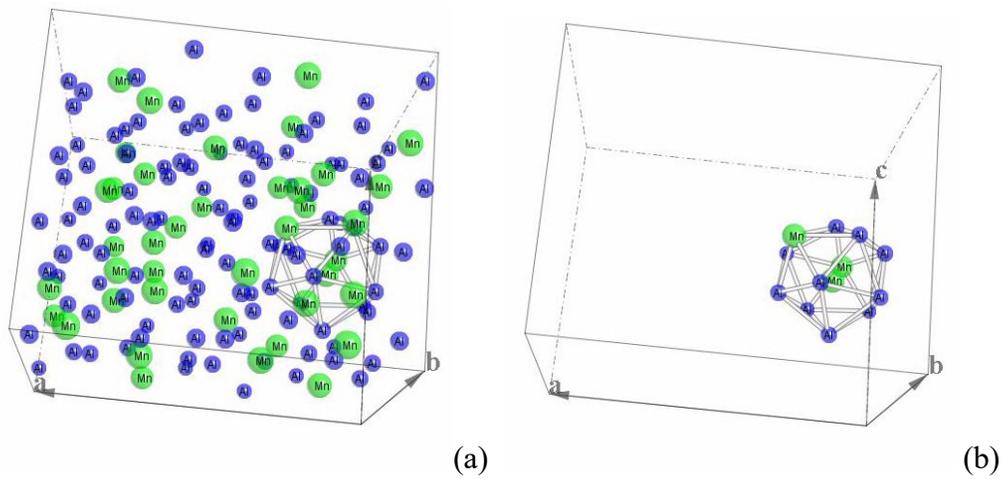
Figure 9. (a) Structure of the Al_3Mn phase - a crystalline approximant of Al-Mn decagonal quasicrystal and (b) a polyhedral cluster is shown in the structure.
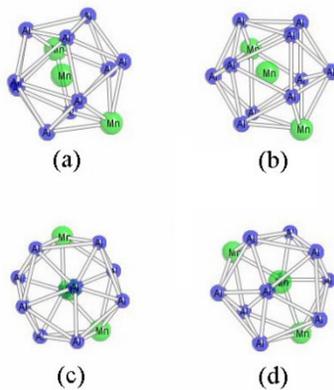

(a)   (b)

(c)   (d)
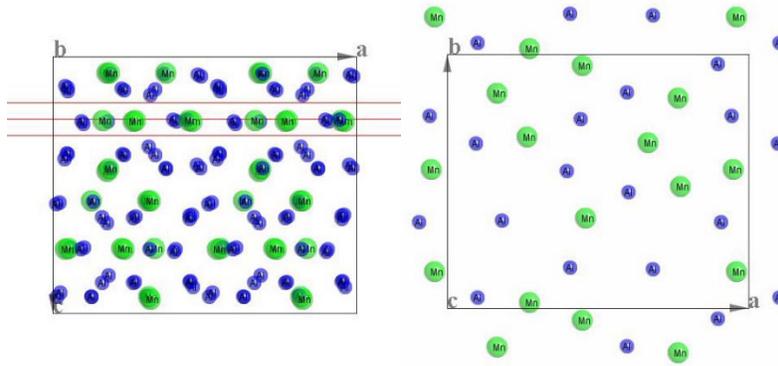
Figure 10. Four polyhedral clusters in the structure of the Al_3Mn phase.

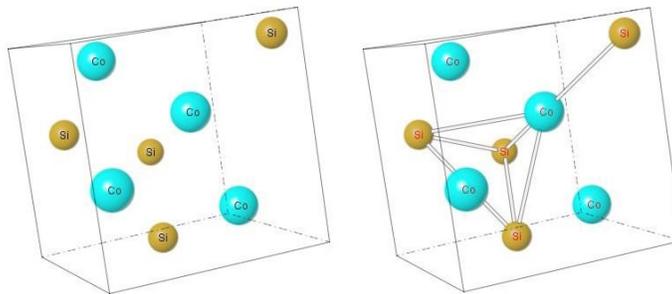Figure 11. Structural projection of Al₃Mn phase, and a slice of layer, side-view, and top-view.

Figure 12. Structure of CoSi B20 phase in the set I of atom coordinates.
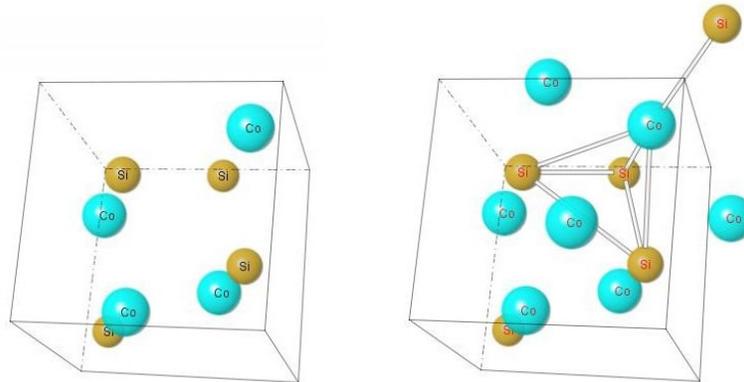

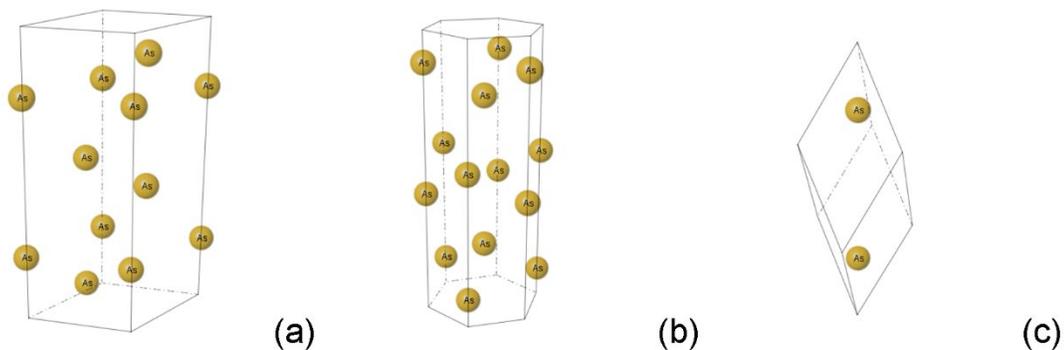Figure 13. Structure of CoSi B20 phase in the set II of atom coordinates.

Figure 14. Structure of the α-As phase in (a) conventional cell, (b) symmetric cell, and (c) primitive cell.

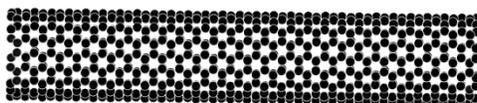
Figure 15. Section of carbon tube, data file in .xyz format.

5. Installation

5.1 Computer requirement

Java virtual machine, such as openJDK21, must be installed for running SVAT6. The 3D vision is calculated in a 3D geometry and Java2D functions, so the Java3D library is not needed.

5.2 Software installation

The executable bytecodes, together with the data files for testing and this specification file, are available in compressed form (landyne6.7z) *https://www.unl.edu/ncmn-enif/xzli/computer-programs* and *https://landyne.com/*. Decompress landyne6.7z in a user-defined directory, e.g., c:\landyne6\ and execute launcher.exe.

5.3 Licenses and feedback

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

6. References

Li, X.Z., SVAT4 – a computer program for crystal structure visualization and analysis, J. Appl. Cryst. 53(2020) 848-853.

CrystalMaker X [CMX], http://crystalmaker.com/crystalmaker/

Flash: 3D Crystal Viewer [FCV], http://www.dawgsdk.org/crystal/index.en

Wikipedia: Atomic radius [WAR], http://en.wikipedia.org/wiki/Atomic_radius

The Structure of Materials [TSM], http://som.web.cmu.edu/frames.html

Encyclopedia of Crystallographic prototypes [ECP], http://aflowlib.org/CrystalDatabase/