LANDYNE

User Manual

Structural Visualization and Analytical Tool

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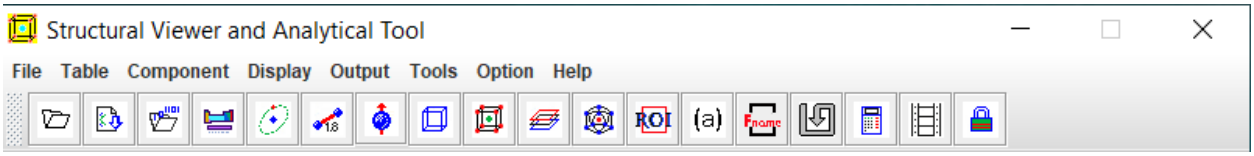

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1. Introduction

Landyne suite is a software package developed by Dr. X.Z. Li for electron diffraction simulation and crystallography analysis. The software package can be used as research tools as well as teaching aids. The need for a tool for structural visualization and analysis becomes obvious with the expansion of the software components and users' growth. The software for structural building, visualization, and analysis at various levels may be found on the internet. Some of them are complicated software with multi-purpose and advanced graphics, e.g., [CMX]. Others are simply programs for displaying crystal structure only, not many functions for analyzing crystal structure, e.g. [FCV]. The motivation of SVAT development is to provide a structure visualization tool and work as an analytical tool for the Landyne suite.

SVAT was developed for interactive 3D visualization and analysis of alloy and intermetallic structures in 2011. As requested during later applications over the years, more functions were gradually integrated into SVAT for visualization and analysis. A paper on SVAT4 was published in J. Applied Crystallography [xzli, 2020]. The current version is SVAT5. The essential functions are an interactive 3D visualization of crystal structure in a unit-cell, including the chemical bonds and magnetic moments. More functions are available, e.g., a projection in a user-selected [uvw] direction or layer by layer, and a local structure (or polyhedral clusters) by defining a center atom and a radius of spherical range. A new data template is available to prepare structure files using 230 standard space groups and the alternative settings. Tools for calculation of the bond length/angle and the examination of chemical composition are included. The full list of atoms in a unit cell can be saved. The list can be used to modify the structure. The structure can be displayed in animated modes of rotation or wobble. One important FEATURE is that user's work on the structure can be saved to a file, which can be reloaded for a quick display next time or continue on unfinished work. The display of a structure can be saved as files in JPEG and TIFF image formats. More details of the features are described below.

2. Design and features

2.1 Graphic design

The graphic user design of SVAT5 consists of a drop-down menu, a menu bar, a display panel, and several operational panels. The drop-down menu provides all the operational panels while the menu bar lists frequently used ones. The display panel and a control panel are always on screen, while other operational panels can be switched on and off, as shown in Figures 1 and 2.

2.2 Function features

Function features as a visualization tool are outlined below,

- Mouse left button for rotation along x-y axes, mouse right button for rotation along the z-axis, mouse wheel for lattice zoom in/out. Zoom option is also available for a laptop PC without a mouse wheel.
- The arbitrary orientation of crystal structure may be displayed interactively by mouse (step 1°) and arrow-key (step 0.1°).

- Display of crystal structure along [uvw] may be set up firstly in a projection option and then re-selecting the 3D option.
- Sizes and colors of atoms are defined in built-in data or modified by users.

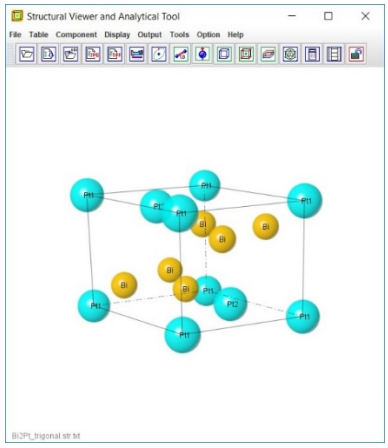


Figure 1. The GUI of the SVAT5 with an example of the Bi_2Pt structure.

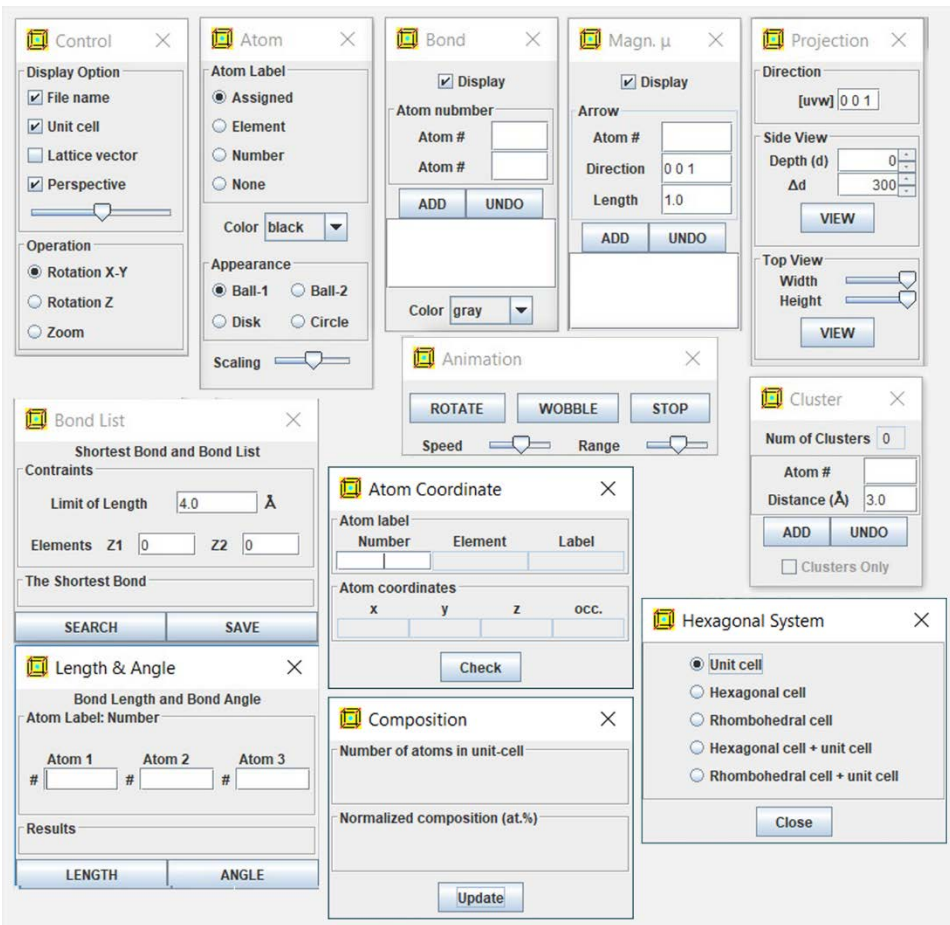


Figure 2. All the operational panels in the SVAT5.

- Overall sizes of all atoms can be scaling up or down.
- The appearance of atoms can be shown in circles or disks or two sets of solid balls for fast change of the crystal structure in the first two choices.
- Background can be tagged between white and black color.
- Conventional and symmetric unit cells are available for hexagonal structure. In addition, the primitive unit cell is available for rhombohedral structure.
- Users may add bonds between atoms or magnetic moments of atoms.
- Animation can be set up for rotation or oscillation modes.
- Display of file name, unit cell, lattice vectors, and perspective view is optional. The position, font size, and color can be adjusted in a filename dialog.
- The orientation of crystal structure may be rotated on any axes and also rotated on screen separately.
- The size of the crystal structure may be zoomed for 3D display and for projection and layer display.
- Lattice's only option is to teach crystallography.

Function features as an analysis tool are outlined below,

- Atoms can be tagged with assigned labels or elements or identified numbers or no labels for building bonds and display.
- Display the coordinate of any selected atom.
- Search and build atom clusters by defining the center atom and distance.
- Display of structure projection along [uvw] or a slice of atom layer.
- A full list of atoms in a unit cell can be saved. This function is useful for structure modification.
- The composition of the crystal structure can be calculated. It is a useful method to verify the correctness of the structure.
- To search the shortest bond and the bond list in a crystal structure.
- To calculate bond distance and the angle between the two bonds.
- To compare two crystal structures in the second run of the SVAT5.

Function features for input and output are outlined below,

- A template is available for the preparation of crystal structure.
- The work on building bonds of the crystal structure is allowed to save or load.
- A periodic table of elements is available. Data sets of calculated and empirical measured atomic radii are available.
- A space group table is available.
- Region of interest can be used for output.
- Output the display can be chosen in formats of .gif or .jpg or .tif.

3. Usage

3.1 Preparation of a new structure file

A structure data file can be prepared using the **New Crystal Structure File** dialogue window in Figure 3. The dialogue window provides an automatic assistant for the user and makes sure to meet the requirement of the file format. The template is embedded with the 230 space groups in the Hermann-Mauguin notation, which list in the international table for crystallography. However, only b unique axis will be used in a monoclinic system. 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; or make a new one click the **New** button.

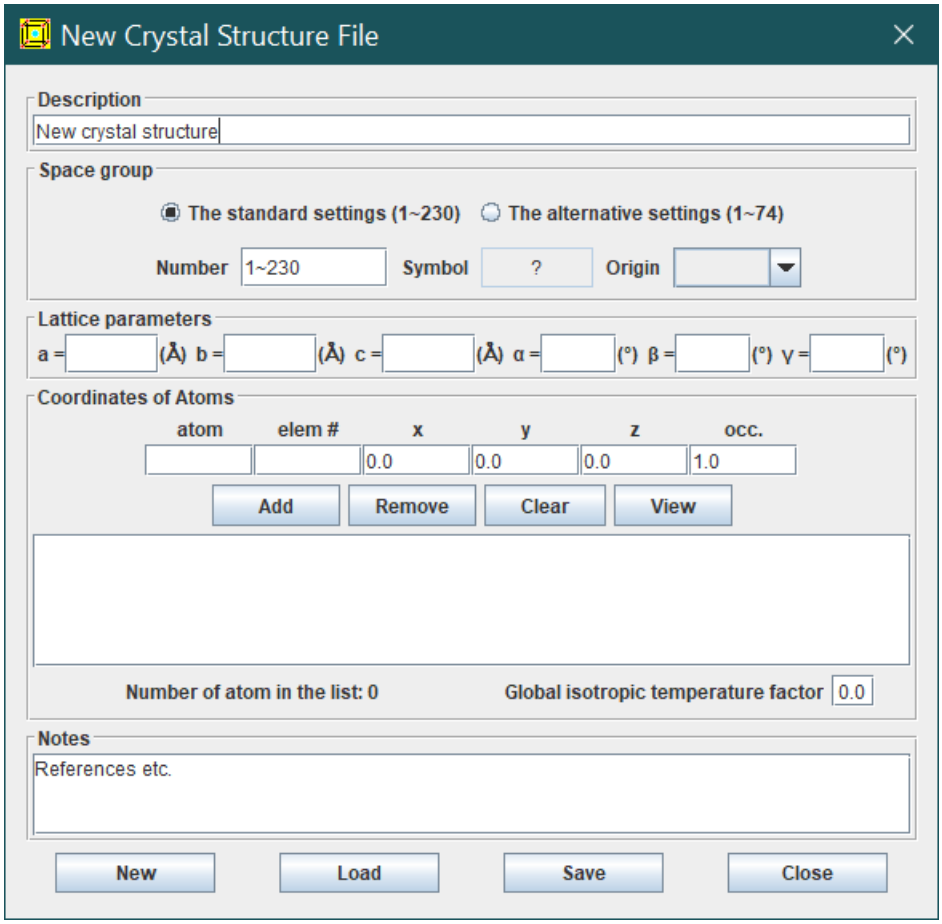


Figure 3. A template for preparing a crystal structure file.

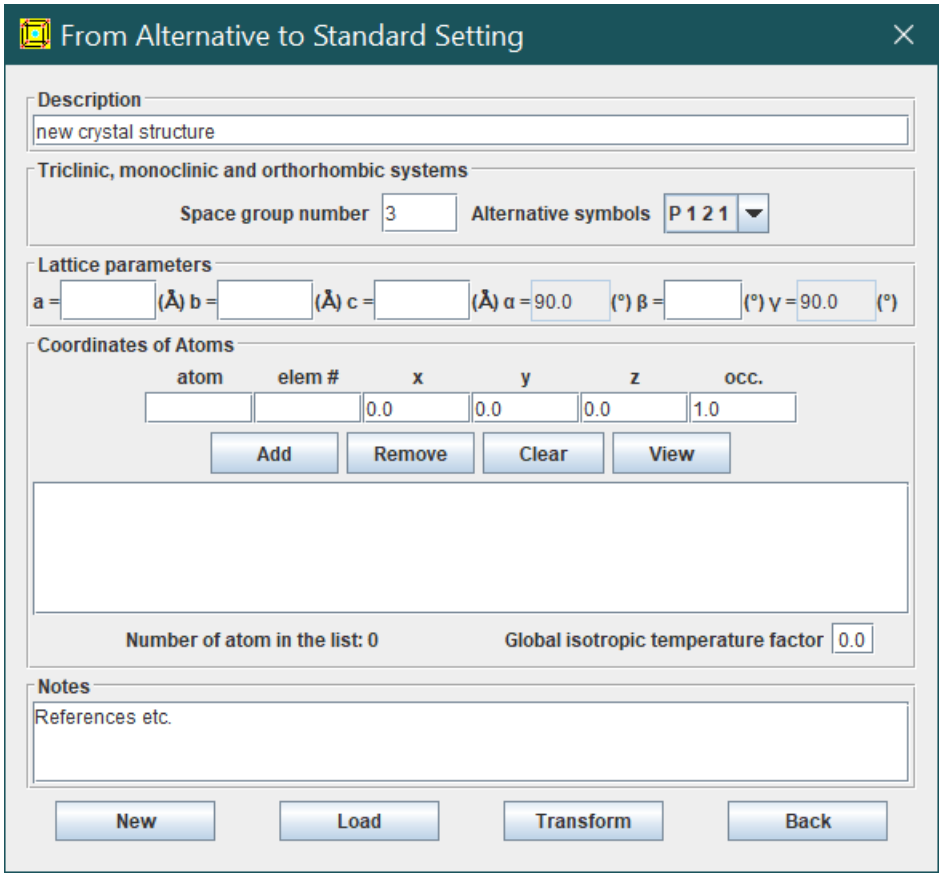


Figure 4. A template for preparing a crystal structure file using an alternative setting in triclinic, monoclinic and orthorhombic systems.

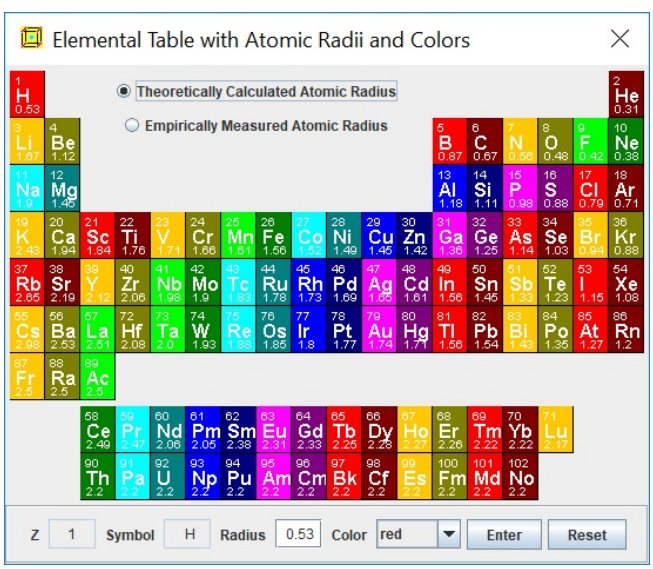


Figure 5. The periodic table of the elements with the calculated and empirically measured atomic radii [3]. Both atomic radius and atom display color can be customized.

The crystal file can be also converted from a previous data for modification or from a crystallographic information file (CIF). If a data file in an alternative setting of space group for triclinic, monoclinic and orthorhombic systems is used, please click on the alternative settings (1~74). A tool for the transformation of files in the nonconventional notations to the standard notations is provided, as shown in Figure 4.

In addition to the structure file, there is a second type of input file containing the previous work on a structure. A work file of the same crystal file can be loaded subsequently to use the work done previously.

The periodic table of the elements with the calculated and empirically measured atomic radii [WAR] is shown in Figure 5. Both atomic radius and atom display color can be customized for the visualization of the crystal structure.

3.2 Database of crystal structures

A collection of crystal structures is provided with Landyne software suite, a part of the structural data is from the list in the appendix1 in the Structure of Materials: An Introduction to Crystallography, Diffraction and Symmetry, by Marc De Graef and Michael E McHenry (2nd Edition, Cambridge university press 2012) and the other part is from in the author's research works.

Here we list the shared resources of the crystal structures.

- Pearson's Handbook, Crystallographic data for intermetallic phases. Ed. P. Villars. ASM.
- ICDD – International Centre for Diffraction Data.
- Appendix 1. Crystal Structure Descriptions in Structure of Material by M. De Graef and M.E. McHenry [TSM].
- Library of Crystallographic prototypes, part 1. Eds. M.J. Mehl *et al*., part2. Eds. D Hicks, *et al*. [ECP].

3.3 Guide

The usage of SVAT5 is straight-forward and self-explanatory. For example, crystal structure can be displayed in 3D view with an adjustable perspective constant. Various options for the atomic label and atomic appearance are available. Chemical bonds and magnetic moments can be added on for numeric atomic labels. Here we give a few hints for first-time users to familiarize themselves with the usage of the SAVT5.

- Crystal structure files in CIF can be uploaded and edited in the template for new crystal structures. Some CIF files may not be transferred entirely thus need manually edit.
- It is recommended to check the composition after a new data file is prepared.
- Before a user sets the bond between atoms, the user needs to choose the atom label as a number.
- Before a user sets the magnetic moment on atoms, the user needs to choose the atom label as a number.

- If a user wants to save the work, please choose Save (current work) to a binary file. The user needs the load the crystal structure first and reload (previous work) of the same crystal structure.
- Atom radius and atom displayed color can be edited by users for current work and can also be saved into a work file and reloaded as a customized data set for later works.
- Before a user saves the display, the user may define the region of interest using ROI and TIFF.
- To view the structure along a [uvw], the user first selects the [uvw] in Layer and Projection, then re-select Structure. Users may switch the perspective factor on or off.
- Using key arrows to fine adjust the orientation of crystal structure. Make sure the mouse arrow on the display panel.
- The atom appearance of Ball-2 is slightly more transparent than Ball-1.
- A user may save a full list of atoms in a unit cell with the space group of P1. The user needs to adjust the number of atoms in the data-file when they add or delete atoms.
- If a user wants to save (display in .tif), you need to make sure that JAI (jai_codec.jar and jai_core.jar) in the java direction, e.g., java\jre1.8.0_221\lib\ext\.

4. Examples

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

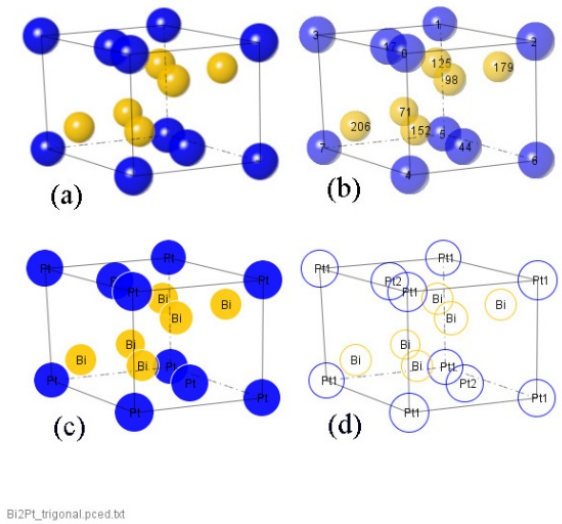


Figure 6. The structure of Bi_2Pt with various appearances. Atoms in (a) solid ball, (b) transparent ball, (c) disk and (d) circle and labels in (a) off, (b) numerical, (c) element and (d) atom label.

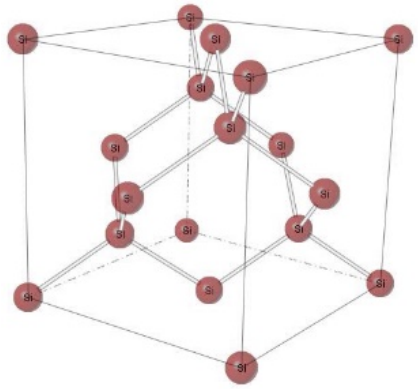


Figure 7. The structure of Si with chemical bonds as balls-and-sticks.

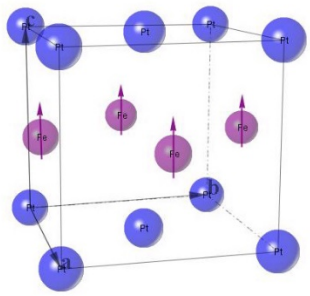
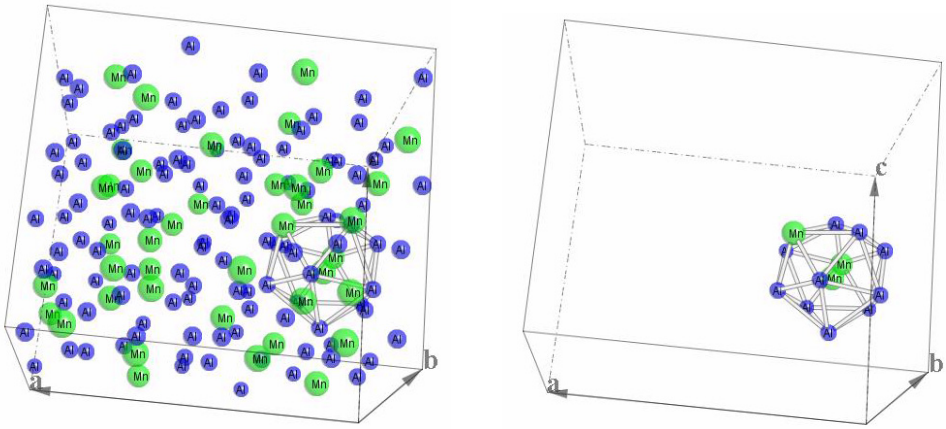


Figure 8. The structure of FePt $L1_0$ phase with magnetic moments on Fe atoms.



(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.

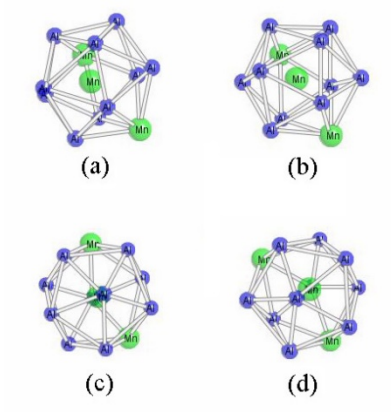


Figure 10. Four polyhedral clusters in the structure of the Al_3Mn phase.

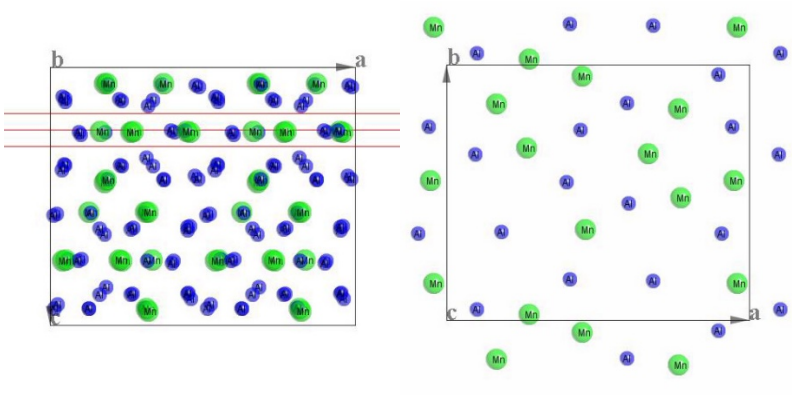


Figure 11. Structural projection of Al_3Mn phase, and a slice of layer, side-view, and top-view.

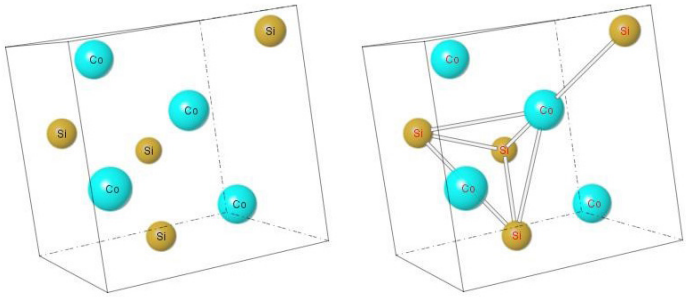


Figure 12. Structure of CoSi B20 phase in the set I of atom coordinates.

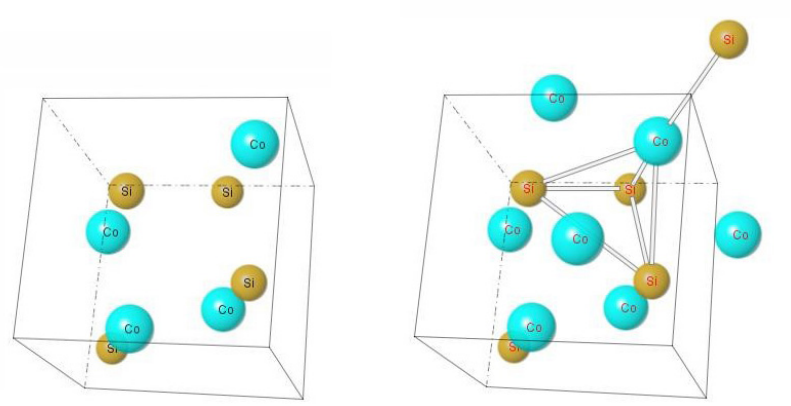


Figure 13. Structure of CoSi B20 phase in the set II of atom coordinates.

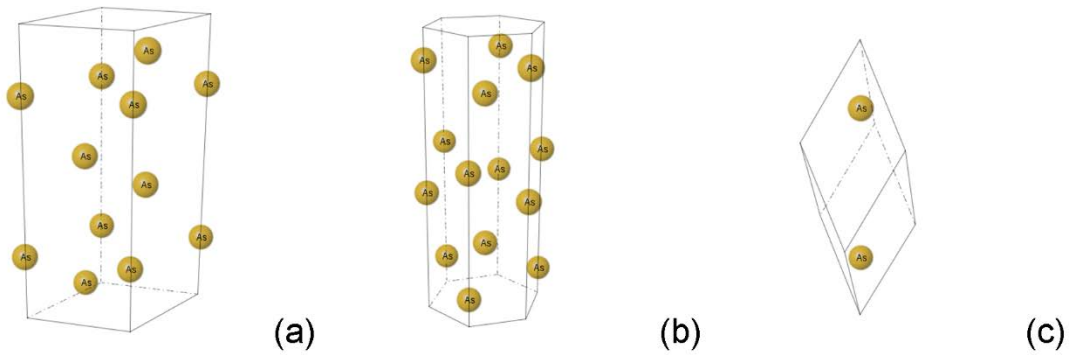


Figure 14. Structure of the α-As phase in (a) conventional cell, (b) symmetric cell, and (c) primitive cell.

5. Installation

5.1 Computer requirement

Java virtual machine, i.e., J2RE, must be installed for running SVAT5. The 3D vision is calculated in a 3D geometry and Java2D functions, so the Java3D library is not needed. Java Advance Image is needed for TIFF file, copy jai_codec.jar and jai_core.jar to, e.g., java\jre\lib\ext\ fold.

5.2 Software installation

The executable bytecodes, together with the data files for testing and this specification file, are available in compressed form (landyne5.7z) https://www.unl.edu/ncmn-enif/xzli/computer-programs and https://landyne.com/. Decompress landyne5.7z in a user-defined directory, e.g., c:\landyne5\ and execute launcher.exe.

5.3 Licenses and feedback

The software works in two modes, demo mode and license mode. The software is fully operational at demo mode but limited to the demo input file.

Both short-term and perpetual licenses are available in LANDYNE (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.

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

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