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SVAT4: a computer program for visualization and analysis of crystal structures

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SVAT4 is a computer program for interactive visualization of three-dimensional crystal structures, including chemical bonds and magnetic moments. A wide range of functions, *e.g.* revealing atomic layers and polyhedral clusters, are available for further structural analysis. Atomic sizes, colors, appearance, view directions and view modes (orthographic or perspective views) are adjustable. Customized work for the visualization and analysis can be saved and then reloaded. *SVAT4* provides a template to simplify the process of preparation of a new data file. *SVAT4* can generate high-quality images for publication and animations for presentations. The usability of *SVAT4* is broadened by a software suite for simulation and analysis of electron diffraction patterns.

1. Introduction

Visualization of crystal structures and interpretation of functional atomic clusters is essential in research and education on metallography, crystallography and other related research fields. Thus, various software is available for these purposes (see <http://www.ccp14.ac.uk/solution/structuredrawing/index.html> and https://www.rcsb.org/pages/thirdparty/molecular_graphics), either as commercial products or free for the scientific community, some of it in open-source forms.

SVAT was initially developed for visualization of crystal structures in 2011: the need for yet more software for such purposes was due to the growth of the software components and the number of users of the *Landyne* software suite for electron diffraction simulation and crystallographic analysis (Li, 2016, 2020*a,b*). More functions, as requested by users, were gradually integrated into *SVAT* for visualization and analysis of crystal structures. The current version is *SVAT4*, which exists as a component in the *Landyne* software suite and also works as standalone software.

SVAT and follow-up versions have been used for nearly ten years in the author's home institute and by users of the *Landyne* suite. So far, most applications of *SVAT4* involved alloys or intermetallic compounds in materials science research. Although *SVAT4* is lightweight, it provides some unique features beyond the standard functions as a structural visualization and analysis tool. The limitations of *SVAT4* are, for example, that it is not suitable for handling large molecules, and it has no functions to show atoms as ellipsoids or to create a stereo pair.

This paper reports on the current status of *SVAT4* and its relation to other components in the *Landyne* software suite. *SVAT4* was developed in Java. The Java Runtime Environment, or JRE, must be installed in order to run *SVAT4*. Java Advanced Imaging is needed for generating TIFF images. The *SVAT4* executable codes, a collection of input data and a user

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Figure 1
The GUI of *SVAT4*, with the Bi_2Pt structure as an example.

manual can be downloaded from the author's web pages (Li, 2020a,b).

2. Design and functions

2.1. Software design

The graphical user interface (GUI) of *SVAT4* was built from the Java Swing package. It consists of a drop-down menu, a menu bar, a display panel (as shown in Fig. 1) and multiple operational panels (as shown in Fig. 2). The drop-down menu provides access to all the operational panels, while the menu bar lists only frequently used ones. The display panel and a control panel are designed to be always on screen, while other operational panels can be switched on and off.

With the inclination toward lightweight software, 3D vision is generated using 3D geometrical calculation and Java2D functions instead of the Java3D library. In addition to the essential functions for an interactive 3D visualization of crystal structure in a unit cell, including chemical bonds and magnetic moments, a wide range of functions for analysis have been implemented, e.g. structural projection or layer-by-layer visualization along a user-defined $[uvw]$ direction and visualization as polyhedral clusters. Atoms in a central unit cell and adjacent unit cells are stored for the construction of the

Figure 2
Operational panels of *SVAT4* for visualization and analysis.

structural projection and the polyhedral clusters. Since the input data are the independent atoms in the unit cell, it is practical to save the full list of atoms in the unit cell for further structure modification. Another useful function is the ability to calculate the chemical composition of the crystal structure, which can be used for double-checking of the input data. Hexagonal and rhombohedral structures can be visualized in both conventional and symmetric unit cells. Additional functions are provided for calculation of the bond length/angle for an atom pair/triplet. The structure can be displayed in animated modes of rotation or sway. The crystal structures can be saved as JPEG and TIFF image formats. A unique feature is that the user's customized work on the structure for analysis can be saved to a file, which can be reloaded for a quick display next time or to continue unfinished work.

2.2. Selected functions

Details on the functions and usage of *SVAT4* are given in the user manual, and selected topics are outlined below:

In *SVAT4*, the crystal structure may be rotated around the horizontal and vertical axes and the screen normal separately. Thus, the crystal structure may be visualized in an arbitrary orientation by using a mouse (step 1°) and by using the arrow keys (step 0.1°) or along a specified orientation, *i.e.* $[uvw]$. Display of the file name, lattice frame, unit-cell vectors, lattice-only mode, or orthographic or perspective view is optional. A dialog is provided for adjusting the position, font size and color of the file name. Animation can be set up for rotation or sway modes. Crystal structures can be compared in multiple frames of *SVAT4* simultaneously.

Atoms can be displayed as circles or discs or two types of solid balls, either translucent or opaque. The radii of atoms are predefined according to the empirically measured and calculated data from Wikipedia (https://en.wikipedia.org/wiki/Atomic_radius). The radii and colors of atoms can also be revised by users. For example, users may replace atomic radii with ionic radii (https://en.wikipedia.org/wiki/Ionic_radius). Atoms can be tagged with assigned labels or elemental or numeric labels or no labels. The size of the unit cell and overall sizes of all atoms can be adjusted separately. Bonds between atoms or magnetic moments of atoms can be added to the crystal structure. Work on the customized appearance of the crystal structure can be saved and reloaded.

Crystal structures can be analyzed as a projection of the unit cell or a slice of atoms along a selected direction $[uvw]$ and polyhedral atomic clusters, each of them defined by a central atom and a bond distance. Other functions include (i) to calculate the shortest bond and a bond list in a crystal structure; (ii) to retrieve the coordinates of an individual atom; (iii) to calculate the bond distance and angle between two adjacent bonds; and (iv) to retrieve the chemical composition. Users may save the full list of atoms in a unit cell, which can be used for modification of the structure in a new model.

2.3. Usage

A template has been designed for the preparation of new structure data with computer assistance, as shown in Fig. 3. In

SVAT4, the standard notations of the 230 space groups in *International Tables for Crystallography* (Hahn, 2005) are built in, and the Hermann–Mauguin symbols are used. If the crystal structure is described in a non-conventional space-group notation, a transformation to the standard space-group notation is required. A function for deciphering CIF format is also available in the template. A collection of crystal structures, taken from De Graef & McHenry (2012) and from the author's work, was included in the *Landyne* software suite. The data set includes most of the typical prototypes of crystal phases, and a gallery of the crystal structures is shown online (Li, 2020b). Crystal structures of alloys and intermetallic phases can be retrieved from many resources, *e.g.* the AFLOW library of crystallographic prototypes (Mehl *et al.*, 2017; Hicks *et al.*, 2019; <http://aflowlib.org/CrystalDatabase/>), *Pearson's Handbook* (Villars, 1998) and the International Center for Diffraction Data's Powder Diffraction File (<http://www.icdd.com/>).

The use of *SVAT4* is mostly straightforward and self-explanatory. However, some operations may not be so obvious for first-time users. A few examples are listed below. The orientation and zoom operations of the crystal structure can be adjusted with 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 zoom in/out: or using the options for the three operations on the control dialog. The data for a rhombohedral structure can be prepared in two ways: as a hexagonal cell using the R lattice type in the trigonal system or as a conventional cell using the rhombohedral system. If two

Landyne Template for Crystal Structure File

Description: Magnetite

Bravais Lattice: Crystal system: Cubic, Lattice type: F: face-centered

Space group: ☒ For the 230 international notations, ☐ For the nonconventional notations
Number: 227, Symbol: F d-3 m, Origin: Choice 1

Lattice parameters: a = 8.3969 (Å), b = 8.3969 (Å), c = 8.3969 (Å), α = 90.0 (°), β = 90.0 (°), γ = 90.0 (°)

Coordinates of Atoms

atom	elem #	x	y	z	occ.
Fe1	26	0.25	0.25	0.25	1.0
Fe2	26	0.625	0.625	0.625	1.0
O	8	0.3799	0.3799	0.3799	1.0

Number of atom in the list: 3, Global isotropic temperature factor: 0.0

Notes: This file is edited from Magnetite.str_choice1.txt, Fe3O4 Magnetite

Buttons: New, Edit, Save, Close

Figure 3
Template for preparation of input data with computer assistance in *SVAT4*.

origin choices are available in a space group but the user is uncertain which one should be used, the user may check the chemical composition and bond distance of each structure for verification of the input data. In order to view the structure along a selected direction $[uvw]$, the direction in the 'Layer and Projection' dialog should be selected first, and then the structural view re-selected. When using the arrow keys to adjust the orientation of the crystal structure, make sure that the cursor is over the display panel. In order to display the previous analysis of a structure, the input data of the structure should be loaded first, and then the corresponding work file.

3. Examples

This section aims to highlight the use and features of *SVAT4* with examples that were chosen from the author's previous research and consulting work.

3.1. Si and FePt

Silicon has a diamond cubic crystal structure, $a = 0.357$ nm (Ashcroft & Mermin, 1976). Fig. 4(a) shows the crystal structure of silicon. The nearest-neighbor bonds between silicon atoms are shown to emphasize the structural features.

FePt films and FePt-based nanocomposite films containing the high-anisotropy tetragonal L_{10} ordered phase have significant potential for extremely high density perpendicular magnetic recording media (Li *et al.*, 2007). Fig. 4(b) shows the crystal structure of the FePt L_{10} tetragonal phase with the lattice parameters $a = 0.385$ nm and $c = 0.371$ nm; magnetic moments were added on Fe atoms along the $[001]$ zone axis to illustrate the magnetic anisotropy.

3.2. Al_3Mn

Al_3Mn is an orthorhombic intermetallic phase, space group 62 ($Pnma$), $a = 1.487$, $b = 1.247$, $c = 1.256$ nm, which is a crystalline approximant of the Al–Mn decagonal quasicrystal (DQC). The structural relationship between the Al_3Mn phase and the Al–Mn DQC has been reported in detail on the basis of selected-area electron diffraction (SAED) and high-resolution electron microscopy results (Li, 1995). Fig. 5 shows (a) the crystal structure of Al_3Mn , (b) a polyhedral cluster around an Mn atom, (c) a side view of the structure with lines marking a flat layer of atoms and

(d) a top view of the atom distribution in the flat layer as marked in (c). The polyhedral cluster shows slightly distorted icosahedral coordinates. The flat layer reveals locally fivefold symmetric features.

3.3. FeSi and CoSi

FeSi (CoSi) has the B20 prototype structure, one of the fascinating materials in modern condensed-matter physics. The B20 structure has a non-centrosymmetric space group, 198 ($P2_13$), which is achiral owing to the neutral 2_1 or 180°

Figure 4
(a) The crystal structure of the silicon phase and (b) the crystal structure of the FePt L_{10} tetragonal phase.

Figure 5
(a) The crystal structure of Al_3Mn , (b) a polyhedral cluster around an Mn atom, (c) a side view of the projection with a flat layer of atoms marked and (d) a top view of the atom distribution in the flat layer as marked in (c).

Table 1

Two sets of the atom coordinate for the FeSi B20 structure.

They are related by the transformation $1/4 + x$, $1/4 + y$, $1/4 + z$.

Data set	Fe $x (= y = z)$	Si $x (= y = z)$	Reference
1	0.38650	0.09262	Wilhelm <i>et al.</i> (2007)
2	0.13650	0.84262	Wartchow <i>et al.</i> (1997)

screw axis. The lattice parameter is $a = 0.4489$ nm for FeSi and $a = 0.4438$ nm for CoSi. A recent study shows that the chirality in $\text{Co}_{1-x}\text{Si}_x$ leads to nonzero Dzyaloshinskii–Moriya interactions, which create spin spirals and support skyrmions with broken helicity (Balasubramanian *et al.*, 2020).

Two sets of atom coordinates for the FeSi B20 structure were reported, as shown in Table 1. Fig. 6 shows the crystal structures of FeSi using (a) data set 1 and (c) data set 2. A tetrahedron of three Si and one Fe is outlined in Fig. 6(b) to emphasize the structural feature of the B20 structure. The same tetrahedron and three Fe atoms surrounding the tetrahedron are shown in Fig. 6(d), which was constructed using a periodic transformation of the atoms in Fig. 6(c), as indicated by arrows. The atomic coordinates in the two data sets are related by the transformation from (x, y, z) in set 2 to $(1/4 + x, 1/4 + y, 1/4 + z)$ in set 1.

3.4. As

Arsenic (α -As) has the A7 prototype structure, space group 166 ($R\bar{3}m$), $a = 0.3760$, $c = 1.0457$ nm. The coordinates of the only independent atom are $(0, 0, 0.2271)$. Other elements, Sb

Figure 6

The crystal structure of the FeSi B20 phase using (a) data set 1 and (c) data set 2 in Table 1. (b) A tetrahedron of three Si and one Fe is outlined, and (d) the same tetrahedron is shown, with three Fe atoms around the tetrahedron added by using a periodic transformation of the atoms in (c).

Table 2Two sets of atom coordinate for the Fe_3O_4 inverse spinel structure.

Data set 1 corresponds to the second origin choice. Data set 2 corresponds to the first origin choice.

Data set	Fe1 $x (= y = z)$	Fe2 $x (= y = z)$	O $x (= y = z)$	Reference
1	1/8	1/2	0.2549	Fleet (1981)
2	1/4	5/8	0.3799	Transformed data

and Bi, have the same type of structure. Fig. 7 shows the crystal structures of the α -As phase in the (a) conventional cell, (b) symmetric cell and (c) primitive cell. This example shows that *SVAT4* provides a variety of ways to display hexagonal and rhombohedral structure. Besides the single-cell mode, as shown in Fig. 7, a combination of two types of cells can also be visualized in *SVAT4*.

3.5. Fe_3O_4

The cubic inverse spinel Fe_3O_4 is ferromagnetic. The structure has space group 227 ($Fd\bar{3}m$), $a = 0.83941$ nm, and two origin choices, the first at $\bar{4}3m$ and the second at $\bar{3}m$. Table 2 lists the structure data of Fe_3O_4 in two data sets. They are related by the transformation from (x, y, z) with the second origin choice to $(1/8 + x, 1/8 + y, 1/8 + z)$ with the first origin choice.

Both origin choices can be used to prepare the input data in *SVAT4*. If the origin choice for the atomic coordinates is wrong, the error can be easily detected by checking the composition. For example, if the atom coordinates in data set 1 are used and the first origin is mistakenly chosen, the composition is Fe_{24}O_8 , a wrong composition. By contrast, if the atom coordinates in data set 1 are used and the second origin is correctly chosen, the composition is $\text{Fe}_{24}\text{O}_{32}$, a correct composition. This also works for the combination of data set 2 and the first origin choice.

It is expected that the usability of *SVAT4* can be broadened with other components in the *Landyne* suite. Here is a glimpse of such an extension. Fig. 8 shows (a) a $[001]$ projection of the Fe_3O_4 structure by using *SVAT4*, (b) a SAED pattern

Figure 7

Crystal structure of the α -As A7 phase in the (a) conventional cell, (b) symmetric cell and (c) primitive cell.

Figure 8

(a) A [001] projection of the Fe₃O₄ structure generated from *SVAT4*, (b) a simulated SAED pattern generated from the *SAED4* software, and (c) a projected atom potential map generated from the *PAPM* software.

simulated using the *SAED4* software and (c) a projected atomic potential map obtained using the *PAPM* software.

4. Related software

Data files of crystal structures for *SVAT4* are also used in other components in the *Landyne* suite for simulations and analyses, e.g. *SAED4*, *QSAED3*, *PCED4*, *SAKI4* and *PAPM*. Although the visualization of a crystal structure using *SVAT4* is not obligatory before using the data in other components in the *Landyne* suite, it is recommended to verify the data with *SVAT4* first, especially for new input data.

SAED4 is designed for SAED simulation from a single grain in the kinematical and Bloch wave dynamical theories (Li, 2019). Simulations are also possible for composited patterns of twins and multi-phases, and the tool is able to search for the zone axis of an experimental pattern. *PCED4* is designed for SAED simulation from polycrystals in the kinematic theory and also in the Blackman theory, a semi-dynamical theory, including peak profiles, textures and mass ratio (Li, 2010). *PCED4* provides a straightforward approach for pattern indexing and is very useful for phase identification. *SAKI4* is used for simulation and analysis of Kikuchi patterns (Li, 2020a,b). A tool in *SAKI4* allows determination of the precise orientation by using an experimental pattern with at least three Kikuchi pairs. *PAPM* is an extension of *SAED4* and *QSAED3* for simulation of projected atomic potential (difference) maps (Li, 2020a,b). The potential map can be used to correlate to experimental structural high-resolution electron microscopy images and annular bright-field scanning transmission electron microscopy images. The potential difference map can be used to improve the structural model.

5. Summary

SVAT4, a component in the *Landyne* software suite, was developed for visualization and analysis of crystal structures. One unique feature is that the work on structural characterization can be saved and reloaded together with a structure file. The design and functions of *SVAT4* have been elaborated, and the usage of *SVAT4* was illustrated with selected application examples. Other components in the *Landyne* software

suite can broaden the usability of *SVAT4*, which is proven to be a useful tool in research and education.

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