Stereographic Projection for Interactive Crystallographic Analysis

(SPICA3e)

User’s manual

X.Z. LI, Ph. D

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1. Introduction

Stereographic projection is a projection of points from the surface of a sphere onto its equatorial plane. The importance of the stereographic projection in crystallography derives from the fact that a set of points on the surface of the sphere provides a complete representation of a set of directions in three-dimensional space, the directions being the set of lines from the center of the sphere to the set of points. A complete stereographic projection of some particular set of points is usually called a stereogram. The mathematics behind the geometry of stereographic projection and the computer implementation are well documented in literature (e.g., Bennett, 1928; Young & Lytton, 1972) and can also be found in most books on electron microscopy and x-ray crystallography (e.g., Edington, 1975; Cullity, 1978; De Graef, 2003; Fultz & Howe, 2008).

Stereographic projections of crystal directions and planes are usually the essential modules in most commercial or public-domain computer programs for crystallography or electron microscopy; for example, CaRIne (Boudias & Monceau, 1998), Crystallographica (Siegrist, 1997), DIAMOND (Bergerhoff et al., 1996), CrystalMaker (Kohn, 2007), Crystal Studio (Crystal Studio, 2015), WebEMAP (Zuo & Mabon, 2004) and JEMS (Stadelmann, 1987). As program modules, they are sufficient for regular use to draw stereograms of crystal directions and planes; on the other hand, dedicated computer programs are available for the extended usages of the stereographic projections. A computer program for simulation of electron diffraction Kikuchi pattern was developed by Lee et al. (1994) on the basis of the work by Young & Lytton (1972). JECP/SP (Li, 2004) was developed for generating stereographic projections, applicable to specimen orientation adjustment in transmission electron microscope (TEM) experiments. SP2 (Chen & Chen, 2012) was developed for standard operation of stereographic projections and can also be used to make composite stereograms, which are necessary to explore the orientation relationships between two crystalline phases.

For crystallographic analysis in electron diffraction experiments, stereographic projection software is expected to include more functions; for example, not only the standard stereogram analysis, but also the composite stereogram for analyzing the relationship of two crystalline phases, the simulation of Kikuchi map and the prediction of tiling angles in selected-area electron diffraction (SAED) experiments. In the present work, a user-friendly SPICA3 has been developed as a dedicated software on stereographic projection, which includes all of the features mentioned above and a few more of its own. SPICA3 can be used as a teaching aid for students in crystallography as well as a practical tool for researchers performing TEM experiments and analysis of the experimental results.

2. Theory background

As mentioned above, the mathematics behind the geometry of stereographic projection can be found in most books for electron microscopy and x-ray crystallography. There are various ways to implement stereographic projections in computer programs. The implementation in SPICA3 is briefly described in this section.
2.1 Wulff net

Wulff net, or stereographic net, is a stereographic projection of the longitude and latitude curves on a sphere, which can be drawn as two series of circles with their center and radius shown in Figure 3.

Longitude arcs:

\[ y^2 + (x \pm \frac{r}{\tan(\varphi)})^2 = \left(\frac{r}{\sin(\varphi)}\right)^2 \]  

(1a)

Latitude arcs:

\[ (y \pm \frac{r}{\cos(\theta)})^2 + x^2 = \left(r \cdot \tan(\theta)\right)^2 \]  

(1b)

Here \( r \) is the radius of the sphere of stereogram. The coordinate \((x, y)\) is on the longitude or latitude circles. The above formulas can be derived on the basis of the definition of the Wulff net.
2.2 Stereographic projection

The Cartesian coordinate system for a crystal lattice is set up as follows: the $c$ axis of a crystal lattice is set up along the $z$ axis of the coordinate system, the $a$ axis is set up in the $x$-$z$ plane, and then the coordinates of the $a$ and $b$ axes are fixed up. A stereogram is firstly calculated using (001) or [001] as an initial direction of projection. The stereogram with a specific direction of projection, (hkl) or [uvw], is obtained by rotating the initial stereogram so that (hkl) or [uvw] becomes the direction of projection.

Figure 4 (a) shows a sphere with its center at D and a plane passing though O for stereographic projection. The projection from the north pole and through the equator of the sphere to the stereographic plane is NQ. It defines a circle with a radius of OQ on the stereographic plane. For any point $P$ on the stereographic plane, a line $NP$ intersects the sphere at one point $P'$. It defines the stereographic projection of $P'$ to $P$ on the stereographic plane. In Cartesian coordinates, the $(x, y, z)$ on the sphere and the $(X, Y)$ on the plane, the relation of the
projection point on the stereographic plane and the associated point on the sphere are given by the formula,

\[(X, Y) = \left(\frac{x}{1-z}, \frac{y}{1-z}\right)\]  \hspace{1cm} (2)

where the set of points \((x,y,z)\) are on unit sphere, so that \(x^2 + y^2 + z^2 = 1\).

2.3 Composite stereogram

SPICA3 allows two stereograms either from the same or different crystalline phases to be generated simultaneously; either the two single stereograms or the overlain stereogram can be displayed separately. Both of the stereogram and the Wulff net can be rotated in an increment step of 0.01° in order to analyze the crystallographic relationship. If the stereograms are generated from the same crystalline phase, different properties can be displayed, e.g., one with the selected plane indices shows trace curves, and the other shows the standard plane indices; one shows the plane \((hkl)\) pole and other shows the \([uvw]\) poles; or one shows Kikuchi map and the other shows the \([uvw]\) poles.

2.4 Kikuchi map and trace curve

Although the Kikuchi patterns obtained using a TEM are not truly stereographic projections, they are excellent approximations to it when the camera length is relatively large. Furthermore, the use of the stereographic projection in simulated patterns allows the display of all possible orientations on a single figure, which cannot be done easily with a photographic montage.

The coordinate system for generating the Kikuchi map in stereographic projection was adopted the work by Young & Lytton (1971). The geometry for the standard stereographic projection of a Kikuchi line pair is shown in Figure 4; (b) is the projection of (a) with the observer looking from \(N\) toward \(O\). Here the projected plane normal \(P(P_x, P_y)\) can be calculated from the following equations,

\[P_x = (2DO) \tan \left(\frac{1}{2} \gamma\right) P_x'/(P_x'^2 + P_y'^2)^{\frac{1}{2}}\]  \hspace{1cm} (3a)
\[P_y = (2DO) \tan \left(\frac{1}{2} \gamma\right) P_y'/(P_x'^2 + P_y'^2)^{\frac{1}{2}}\]  \hspace{1cm} (3b)
\[\gamma = \cos^{-1}\left[P_z'/(P_x'^2 + P_y'^2 + P_z'^2)^{\frac{1}{2}}\right]\]  \hspace{1cm} (3c)

where \(P_x', P_y',\) and \(P_z'\) are the coordinates of \(P' (r = (P_x'^2 + P_y'^2 + P_z'^2)^{\frac{1}{2}})\) referred to the standard basis for stereographic projection, and \(\gamma\) is the angle between the plane normal to \(DP'\) and \(DO\). The formulas above can be used to generate trace curves by applying \(\theta = 0°\).

The Kikuchi map is generated from the data set of the \((h k l)\) stereographic projection, and the distribution of the zone axes on the Kikuchi map can be found from the \([u v w]\) stereographic projection of the same crystal phase on the second stereogram. For a cubic crystal, a plane normal is parallel to the orientation with the same index as this plane, but it is necessary
to transform between the plane index and the plane normal index for non-cubic crystals. A function for the transformation from a plane \((h k l)\) to the plane normal \([u v w]\) is provided in SPICA3 on the basis of the matrix by (Liu & Liu, 2012).

### 2.5 Prediction of the tilt or rotation angles for a TEM holder

Computer-assisted specimen orientation adjustment in TEM experiments is possible for a crystalline specimen with known lattice parameters. The microscope can be kept in the image mode while the specimen is tilted to any zone axis within the range available for the TEM specimen holder under calculated guidance. The application of stereographic projection for specimen orientation adjustment was described in the paper by Chou (1987). A slightly different algorithm was adopted in JECP/SP and inherited in SPICA3.

The key point is to set up the positions of the TEM specimen holder and the crystal orientation in the stereographic projection sphere. The tilt angle of the TEM goniometer and the second tilt angle are assumed to be along longitude and latitude of the stereographic projection sphere. The crystal orientation can be obtained from the observed SAED pattern. Suppose that the SAED pattern with a zone axis \([uvw]\) is currently observed. For any diffraction spot \((hkl)\) on the SAED pattern, the azimuth \(\chi\) is between the line of \((000)-(hkl)\) and the projection of the TEM specimen holder (or goniometer axis) on the fluorescent screen, as shown in Figure 5. A stereographic projection map can be calculated using the above input parameters to provide all the zone axes with computer-predicted tilting or rotating angles. The tilting limitation of the TEM holder can also be drawn in the generated stereogram.

### 2.6 Modules for crystallographic calculation

One module mentioned above is for the transformation from the crystal plane \((h k l)\) to the plane normal \([u v w]\) for non-cubic crystalline phases. Other modules include the calculation of the angles between two crystal planes, between two zone axes or between a plane normal and a zone axis, the transformation between Miller and Miller-Bravais indices for the hexagonal system, and a calculated list of reflection \((hkl)\), together with the plane spacing and the kinematical intensity.

![Figure 4](image_url)  
*Figure 4. The geometric relation of the observed SAED pattern and the TEM specimen holder for a stereographic projection as a guidance in SAED experiments.*
Figure 5. SPICA3 with an (hkl) stereogram of a cubic structure as an example.

3. Program design and graphic user interface

SPICA3 was programmed using Java SE Development Kit 8 (JDK8u74) from Oracle. It has been successfully tested on Microsoft Windows 7 and 8 OS with a Java virtual machine, i.e. Java 2 Runtime Environment (J2RE). The software can be executed as a standalone program or as one component in the Landyne software package with a launcher, both of which can be downloaded at http://www.unl.edu/ncmn-cfem/xzli/computer-programs.

The graphical user interface (GUI) of SPICA3 fully utilizes Java Swing to provide a Windows-style operational environment. It consists of a scalable display panel of the stereogram and various dialogs for data input/output and graphic editing operations. Figure 1 shows the display panel of SPICA3 with a menu bar and an example of a cubic (hkl) stereogram with some main trace lines. Figure 2 shows three basic operational dialogs in SPICA3: (a) the calculation dialog, (b) the pole range dialog and (c) the orientation dialog for Wulff net and stereograms. More operational dialogs of SPICA3 for other purposes are available (not shown here).

SPICA3 is a fully functional tool for generating stereograms of crystal directions and planes. To generate a stereogram, the user needs to provide the crystalline lattice parameters, \( a, b, c, \alpha, \beta, \gamma \), and the direction of projection, \([uvw]\) or \((hkl)\). As an option, the Wulff net can be drawn and rotated on top of the generated stereogram. Crystal lattice parameters can be loaded from a data file and readjusted in the calculation dialog (see Figure 2(a)). Two stereograms from two
crystalline phases can be generated and overlain into a composite stereogram for analyzing their structural relationship. The list of (hkl) can be edited to show trace curves of selected (hkl) poles. Kikuchi maps can be displayed from the generated data of (hkl) poles and the wavelength of the incident beam. The zone axes for the Kikuchi maps can be generated from the same crystalline phase on the second stereogram and then overlain with the Kikuchi map. The additional application is to predict tilt/rotation angles of zone axes for both double and rotation TEM holders.

![Figure 6. Three basic operational dialogs in SPICA3, (a) the calculation dialog, (b) the pole range dialog and (c) the orientation dialog for Wulff net and stereograms.](image)

4. Usage of SPICA3

SPICA3 is coded mainly in Java and partially coded for PC with Microsoft windows only. To run the software, a recent version of Java Runtime Environment (e.g., JRE 1.8.0_60), must be installed on a PC for all versions of Microsoft window. The executable bytecodes (SPICA3.jar) with Landyne launcher and this file are packed in .z7 form. The compressed file is available at [http://www.unl.edu/ncmn-cfem/xzli/computer-programs](http://www.unl.edu/ncmn-cfem/xzli/computer-programs). For the latest updates and news about SPICA3 and other Landyne programs, please visit in this website.

Uncompress the installation file SPICA3.z7 in a selected directory and execute SPICA3.jar by double click or use Landyne launcher.
The basic steps for using SPICA3,

- FePt L10 and MgO FCC as default input lattices for phase 1 and phase 2.
- Crystal lattice can be loaded from Crystal/phase and modified via input fields.
- Click Calculation/Stereogram to generate stereographic projection map.
- Click right mouse button to modify the display options.
- Calculate hkl stereogram and select Show trace to display trace.
- Calculate hkl stereogram and select Show Kikuchi to display Kikuchi map.
- Load the other the same phase and calculate uvw to display zone axes.
- Press left mouse button and drag to zoom the stereogram.
- Hold Ctrl and click left mouse botton to set the viewpoint center.
- Click stereogram/pole list, selected pole can be removed or added on.
- Click stereogram/orientation, Wulff net and stereograms can be rotated.
- The overlayed stereographic projections give the crystallographic relation of two phases.
- Click Calculation/Goniometer to generate TEM holder information.
- Click Option to change color, label size and tilt label.
- Click Tool to calculate the angle of two [uvw]s or two (hkl)s.
- Click Help/Current drive to obtain the serial number of current driver.

5. Examples

Some application examples are given here to show the proof of validity and practicability of SPICA3. The basic usage steps are introduced here, more details are given in the user manual of SPICA3.

5.1 Stereogram and Wulff net

The input parameters to generate a stereogram include the lattice parameters of a crystalline phase and a direction of projection. The lattice parameters can be loaded using the menu bar from the input file of a crystal structure and the lattice parameters can be readjusted in the calculation dialog, if necessary. The range of the poles is controlled by a set of preset values in the pole range dialog. When a list of the poles is generated, the pole in the list can be deleted or a new one can be added to the list. The stereogram and the Wulff net can be rotated separately. The display of the stereogram can be zoomed in or out. Figure 6 shows (a) the (h k l) stereogram and (b) the [u v w] stereogram of the hexagonal structure of Zn, \(a = 0.26649\) nm, \(b = 0.226649\) nm, \(c = 0.49468\) nm, \(\alpha = 90^\circ\), \(\beta = 90^\circ\) and \(\gamma = 120^\circ\). In order to display all indices clearly, the maximum indices were chosen as \(h \leq 2\), \(k \leq 2\), \(l \leq 2\), \(u \leq 3\), \(v \leq 3\) and \(w \leq 1\). The Miller index was labelled in the stereogram; the Miller-Bravais index can be transformed from Miller index using a module in SPICA3. Wulff net, as a tool for measurement, can be applied to the stereogram by users. Wulff net is applied in Figure 1 and not applied in Figure 6.

5.2 Composite stereogram
An example is taken from our recent work on Mn$_2$CrGa$_{1-x}$Al$_x$ alloy, $x=0.0$, 0.2, 0.5 (Li et al., 2016). A spinodal decomposition of the alloys ($x=0.2$, 0.5) generates two crystalline phases with a fixed orientation relationship after an annealing treatment at 500 °C for 2 hrs. The lattice parameters of the two phases in Mn$_2$CrGa$_{0.5}$Al$_{0.5}$ alloy are listed in Table 1. Figure 8 (a) shows a TEM image of the two crystalline phases in Mn$_2$CrGa$_{0.5}$Al$_{0.5}$ alloy, the cubic phase in light grey has a composition of Mn$_{65}$Cr$_{11}$Ga$_{13}$Al$_{13}$ and the tetragonal phase with strip shape in dark grey has a composition of Mn$_{45}$Cr$_{31}$Ga$_{13}$Al$_{11}$. Figure 8 (b-d) show the SAED patterns to reveal the orientation relationship of the two crystalline phases. Figure 9 shows the composite stereograms of (a) the index labels on the cubic phase and (b) the index labels on the tetragonal phase. The fixed orientation relationship of the two crystalline phases are,

$\begin{align*}
(001)_t &/ (100)_c \\
[100]_t &/ [012]_c \\
[310]_t &/ [011]_c \\
[120]_t &/ [010]_c
\end{align*}$

Figure 7. Two crystalline phases in Mn$_2$CrGa$_{0.5}$Al$_{0.5}$ alloy as the result of a spinodal decomposition: (a) a TEM image of the two phases, cubic phase in light grey and tetragonal phase with strip shape in dark grey, and (b-d) the electron diffraction patterns taken from the two crystalline phases.
Figure 8. Composite stereogram with (a) the index labels for the cubic phase and (b) the index labels for the tetragonal phase.

Figure 9. Kikuchi maps of a primitive cubic structure with [111] zone axis in the center, (a) generated using the method described by Liu & Liu (2012) and (b) generated using the formula by Young & Lytton (1971) with the wave length of 0.0251 Å (200kV).
Figure 10. A new tetragonal phase in Co-Fe-Cr-Ge alloy. (a) TEM image of the tetragonal phase with the grain size about 150 nm, (b-d) the SAED patterns of the tetragonal phase.

5.3 Kikuchi map and trace curve

The Kikuchi map is displayed by first generating a stereogram of \((h k l)\) and then selecting the corresponding display mode in SPICA3. The additional parameter for the Kikuchi map is the wavelength of the incident beam or the high voltage on TEM. Figure 10 shows the Kikuchi maps of a primitive cubic structure with the \([111]\) zone axis in the center, (a) generated using the method described by Liu & Liu (2012) and (b) generated using the formula by Young & Lytton (1971) with the wavelength of 0.0251 Å (200kV). The overlain distribution of the \([uvw]\) zone axes is shown in Figure 10(b) as the result of a composite stereogram.

Similar to the Kikuchi map, the Kossel map in x-ray diffraction and the electron backscatter diffraction (EBSD) map can also be simulated with SPICA3 by selecting an appropriate wavelength. The trace curve is displayed by generating a stereogram of \((h k l)\) and then selecting the corresponding mode; one example was shown in Figure 1.
Figure 11. A new tetragonal phase in Co-Fe-Cr-Ge alloy as an example using SPICA3 to predict the tilt angles for all zone axes within the tilt limitation of the TEM specimen holder. Two of the SAED patterns of [103] and [115] zone axes were selected and displayed in Figure 11 (c) and (d).

5.4 Tilt-angle prediction for a TEM holder

This function is very useful in many situations, for example, (a) when a severely stained specimen is observed and the visibility of Kikuchi line pairs is thus poor; (b) when a beam-sensitive specimen is examined, and it is essential to shorten the time spent on specimen tilting while the electron beam is on the specimen area of interest; (c) when a small grain-size specimen is investigated, for which even a slight orientation adjustment may cause the corresponding diffraction pattern to disappear due to a lateral sample shift; and (d) when a crystalline specimen is used in acquiring electron diffraction intensities of reachable zone-axis patterns for structure determination.

An example is the electron diffraction experiment on a new tetragonal phase in the composition of Co₃₀Fe₄₂Cr₇Ge₁₀ in our recent work (Jin et al., 2016), the lattice parameters are listed in Table 1. Figure 11 shows (a) a TEM image of the new tetragonal phase with a grain size about 150 nm, and (b-d) SAED diffraction patterns of the new tetragonal phase. In the experiment, the [001] SAED pattern in Figure 11(b) was obtained at tilt angles of (17.1°, 0.0°) with a double-tilt TEM holder. The angle between the vector (000)-(010) and the holder axis is about 14.9°. Figure 12 was generated using SPICA3 with the above parameters to predict the tilt angles for all zone axes within the tilt limitation of the TEM holder. The TEM specimen was tilted according to the predicted tilt angles and all SAED patterns were obtained. Two of the
SAED patterns of [103] and [115] zone axes were displayed in Figure 11 (c) and (d). It should be pointed out that the forbidden reflection, e.g. (010), in Figure 11 (c) appears in Figure 11(d) due to the double diffraction effect.

6. Installation of SPICA3

6.1 JRE and JAI
Download and install the most recent JRE from Java official site. Download and install the JAI, which is also available in [http://www.unl.edu/ncmn-cfem/xzli/download](http://www.unl.edu/ncmn-cfem/xzli/download).

6.2 Installation
Create a dedicated fold for LANDYNE software suit. Copy and decompress the package. If you have a license file, copy the license to the same fold with the program (qsaed3a.jar or qsaed3a.exe).

6.3 Run SPICA3 as a stand-alone software
To run SPICA3, double click the icon of SPICA3.exe or type: java -jar (-Xmx512m) SPICA3.jar in command line. -Xmx512m is an option to locate the memory of Java virtual machine up to 512 MB.

6.4 Run SPICA3 in the Landyne suite
Click the SPICA3 in Landyne launcher to start the software.

6.5 Get a license
A license file is needed to unlock the program for loading new file data. Without the license file the program is locked up in demo mode. License can be purchased from LANDYNE computer software.

7. Reference
Li, X.Z., Zhang, W.Y. and Sellmyer D.J. (2016). A TEM Study of the Spinodal Decomposition in Mn2CrGa0.5Al0.5 Alloy, to be published.