Journal of
Applied
Crystallography
ISSN 0021-8898

Received 15 August 2011
Accepted 20 November 2011

SP2: a computer program for plotting stereographic projection and exploring crystallographic orientation relationships

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Stereographic projection is one of the most powerful research tools for crystallography in materials science. A new program for full operation of stereographic projections and in-depth exploration of crystallographic orientation relationships is described. It is specifically designed for materials researchers who are in need of tools for extensive crystallographic analysis. The difference from other popular commercial software for crystallography is that this program provides new options for users to plot and fully control stereographic projections of an arbitrary pole centre for an arbitrary crystal structure and to illustrate composite stereographic projections, which are necessary to explore the orientation relationships between two phases. The program is able to perform a range of essential crystallographic calculations.

1. Introduction

Stereographic projection has long been one of the most powerful research tools for crystallographers in astronomy, physics, mechanical engineering, geography and materials science since its use was popularized by Federov, inventor of the universal microscope stage, and by the introduction of the Wulff net (Howarth, 1996). Stereographic projection enables crystallographers to explore the three-dimensional crystal planes and orientations of a crystal with an arbitrary crystal structure on a two-dimensional plane. Much commercial crystallographic software has been developed to provide powerful functions for plotting crystal structures in three dimensions, illustrating the atomic distribution for a given crystal plane. These programs include *CaRIne* (Boudias & Monceau, 1998), *Crystallography* (Siegrist, 1997), *DIAMOND* (Brandenburg, 2011), *CrystalMaker* (Kohn, 2007) and *Crystal Studio* (Crystal Studio, 1999). Most of these programs are able to draw stereographic projections. Some software packages for high-resolution transmission electron microscopy simulation, such as *WebEMAP* (Zuo & Mabon, 2004) and *JEMS* (Stadelmann, 1987), also have similar features. While the functionality for plotting superimposed electron diffraction patterns of two different phases is available (*e.g. JEMS* and *Crystal Studio*), the same functionality for stereographic projection is not yet available, to our best knowledge, in crystallographic software packages (*CaRIne* provides some functionality but it is not user friendly). However, besides the interest in such a stereographic projection, a superimposed stereographic projection of two phases with different crystal structures is frequently required by materials researchers in order to explore the complicated orientational relationships between the two phases.

Our aim is thus to develop a computer program to create composite stereographic projections which meets the particular requirements of researchers in materials science and other related sciences and offers new options *via* a user-friendly interface.

2. Program design

This program, *SP2*, can run directly in Windows XP and Windows 7 operating systems (32 bit or 64 bit). It has been registered at the Copyright Protection Centre of China and the source code for the program is available if required. The source code has been written with the object-oriented language Visual Basic 6.0 and compiled on the Microsoft platform with the help of Microsoft Visual Studio 2008. The program has been packaged as green software and can be executed without installation or registration.

Multiple parameters for a stereographic projection, such as crystal lattice parameters, the pole centre of a plane or an orientation, interplanar distance, the magnitude of the orientation vector, the rotation angle around a given basal coordinate and the spacing angle of a Wulff net, are available. Other features, including fine-controlled stereographic projection, are based on mathematical theory and designed by the present authors.

SP2 is ongoing development software and is therefore a work in progress.

3. Modules and methods

The program includes several core modules that are important for the output of composite stereographic projections. All of the modules are based on crystallographic and mathematical theory, the details of which can be readily found in many classic crystallography-related textbooks.

3.1. Stereographic projection

The main program core is completely based on the crystallographic theory for stereographic projection. We denote the three angles between an arbitrary orientation (*hkl*) and the three basal coordinates *X*, *Y* and *Z* as α, β and γ, respectively. Then it can be easily deduced with basic geometric knowledge that the position (x, y) of this orientation (*hkl*) in a stereographic projection with a radius *R* can be defined as

$$x = \frac{\cos\alpha}{1+\cos\gamma}R, \quad y = \frac{\cos\beta}{1+\cos\gamma}R, \tag{1}$$

and

$$\cos\alpha = h/(h^2+k^2+l^2)^{1/2}, \quad \cos\beta = k/(h^2+k^2+l^2)^{1/2}, \quad \cos\gamma = l/(h^2+k^2+l^2)^{1/2}. \tag{2}$$

Here, *R* is the radius of the equator of the stereographic projection. All orientation projections can be illustrated on a Wulff net and a stereographic projection of a given pole centre can be plotted.

The goal of the program *SP2* is not simply to plot a stereographic projection as this functionality has long been realized in many other commercial software packages. For the convenience of crystallographers, this program is specifically designed to plot two stereographic projections independently and superimpose them in one Wulff net so as to provide the function of exploring the mutual orientation relationship between two phases.

3.2. Wulff net

A Wulff net can be regarded as a group of orientation poles in stereographic projection which are lying on the same plane parallel or perpendicular to the equatorial plane with a given distance interval or a given angular spacing interval. The interplanar distance can be expressed as the departure angle of any pole in this plane from the equatorial plane.

Any pole in the plane has cylindrical coordinates

$$P_x = R\cos\alpha, \quad P_y = R\sin\alpha\cos\beta, \quad P_z = R\sin\alpha\sin\beta. \tag{3}$$

The three cosine components can be calculated by inputting the pole coordinates shown in equation (3) into equation (2). Then the coordinates of the pole in the stereographic projection can be deduced by using equation (1).

3.3. Coordinate transformation

The Cartesian coordinate system is used for the reference coordinate system. A crystal with an arbitrary crystal structure, such as a triclinic crystal, must be described in the Cartesian coordinate system by coordinate transformation.

If the *a* axis of a triclinic crystal lies parallel to the *X* axis of the Cartesian coordinate system, there exists a coordinate transformation matrix $\boldsymbol{T}(3\times 3)$, where

$$\boldsymbol{T}(3\times 3) = \begin{bmatrix} a\sin\beta & b(\cos\gamma-\cos\alpha\cos\beta)/\sin\beta & 0 \\ 0 & b\sin\alpha(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2} & 0 \\ a\cos\beta & b\cos\alpha & c \end{bmatrix}. \tag{4}$$

Any crystal can be expressed in the Cartesian coordinate system, which means that it is possible to plot a stereographic projection for all kinds of crystals.

3.4. Transformation between plane index and orientation index

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 plane index and plane normal index for noncubic crystals. The matrix is as follows:

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} \frac{\sin^2\alpha}{a^2V} & \frac{\cos\alpha\cos\beta-\cos\gamma}{abV} & \frac{\cos\gamma\cos\alpha-\cos\beta}{acV} \\ \frac{\cos\alpha\cos\beta-\cos\gamma}{abV} & \frac{\sin^2\beta}{b^2V} & \frac{\cos\beta\cos\gamma-\cos\alpha}{bcV} \\ \frac{\cos\gamma\cos\alpha-\cos\beta}{acV} & \frac{\cos\beta\cos\gamma-\cos\alpha}{bcV} & \frac{\sin^2\gamma}{c^2V} \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}. \tag{5}$$

Here, [*uvw*] is the plane normal of plane (*hkl*). When applied to the cubic phase, the normal [*uvw*] of a plane (*hkl*) is equal to [*hkl*] as the lattice parameters $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$.

3.5. Trace of a plane

The method for plotting the trace of a plane is similar to but easier than that for Wulff net plotting and will not be repeated here.

3.6. Rotation of stereographic projection

Composite stereographic projections must be rotated around a given axis and a given angle so as to illustrate the orientation relationships between two phases. On the other hand, if the pole centre of a stereographic projection is not [001] or (001) then all poles in the projection must be rotated accordingly. Let the unit rotation axis **u** be denoted as $[p_1, p_2, p_3]$ and the rotation angle as θ; then the rotation matrix $\boldsymbol{R}$ of an arbitrary axis **u** is as follows:

$$\boldsymbol{R} = \begin{bmatrix} p_1^2(1-\cos\theta)+\cos\theta & p_1p_2(1-\cos\theta)-p_3\sin\theta & p_1p_3(1-\cos\theta)+p_2\sin\theta \\ p_2p_1(1-\cos\theta)+p_3\sin\theta & p_2^2(1-\cos\theta)+\cos\theta & p_2p_3(1-\cos\theta)-p_1\sin\theta \\ p_3p_1(1-\cos\theta)-p_2\sin\theta & p_3p_2(1-\cos\theta)+p_1\sin\theta & p_3^2(1-\cos\theta)+\cos\theta \end{bmatrix}. \tag{6}$$

4. Main functions and features

4.1. Kikuchi lines

Kikuchi lines are produced by thick crystal samples when inelastic electron diffraction coexists with elastic electric diffraction patterns. Kikuchi lines were first reported by Kikuchi (1928). Kikuchi lines occur on the basis of strictly Bragg diffraction and are very sensitive to crystalline orientation. In transmission electron microscopes, they are easily observed in diffraction from regions of the specimen thick enough for multiple scattering. One of the applications of Kikuchi lines is the determination of crystal orientation, which can be achieved with a precision of 0.1°.

Kikuchi lines can be plotted on a stereographic projection of a pole centre of orientation and can serve as 'roads in orientation space' for microscopists. Kikuchi bands mark orientation space with well defined intersections (called zones or poles). All crystalline orientations falling into a Kikuchi band belong to a certain plane. Thus a Kikuchi line is similar to a planar trace on a stereographic projection. If the stereographic projection of an orientation is plotted with high-index orientation vector [*uvw*], say larger than 10, the plotted vectors will coincide with the shape of the Kikuchi band corresponding to the planar trace. This is the theoretical background

of the geometric method used to plot Kikuchi lines on a stereographic projection.

An example is shown in Fig. 1. A cubic crystal with a lattice parameter of 0.5 nm was used for plotting a stereographic projection of a pole centre of orientation [111]. The maximum orientation vector index [*uvw*] was set at 15. It was found that numerous poles coincide with the Kikuchi pattern for the [111] orientation and the threefold symmetry of the [111] orientation has been illustrated very well.

4.2. Wulff net

The Wulff net is a stereographic projection of a group of longitude lines and latitude lines of a sphere. It is named after the Russian mineralogist George Wulff (1902). Given an angular interval of the longitude and latitude lines of 1°, the Wulff net can be plotted at the same resolution of angular intervals. A high-resolution Wulff net is useful for measuring the angles between planes or orientations. Fig. 2 illustrates an example of a Wulff net at a resolution of 1°. This is realized by superimposing two sets of Wulff nets in the same orientation but with different angle intervals, *i.e.* 1 and 5°.

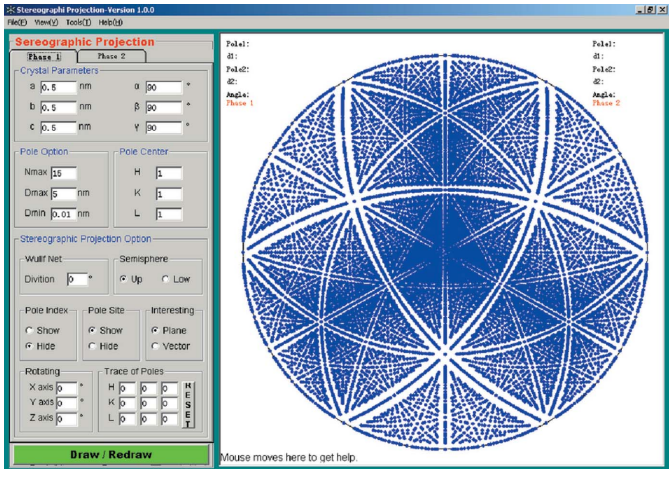

Figure 1
A screenshot of the program to plot Kikuchi lines in a planar projection with a pole centre of [111] orientation for a cubic structure. When the planar index is larger than nine, all planar poles will lie along the Kikuchi line and thus delineate the Kikuchi line pattern. The Kikuchi line patterns share the same crystallographic symmetry as the stereographic projection of the [111] pole centre.

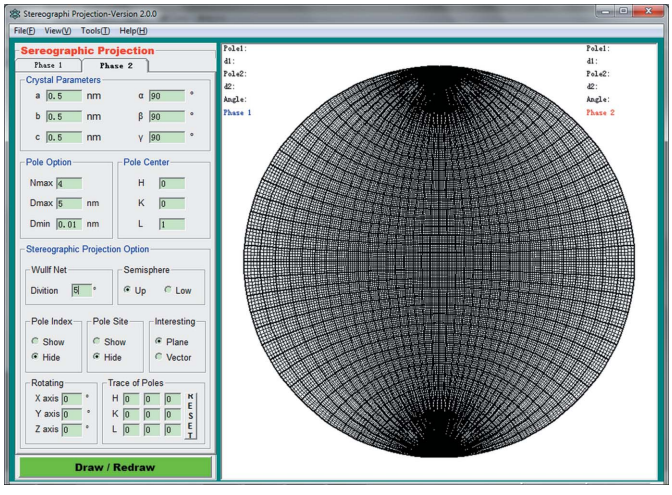

Figure 2
A typical Wulff net with a step size of 1°. This pattern is realized by combining two sets of Wulff nets, one with a step of 5° and the other 1°.

4.3. Composite stereographic projections for orientation relationships

Unlike a texture pole figure, which plots the orientations of many crystals in one projection (Hielscher & Schaeben, 2008), or an orientation analysis for a single crystal, which can be done by the program *MTEX* (Hielscher & Schaeben, 2010), composite stereographic projections for orientation relationships focus on the mutual orientation relationship between two phases. This relationship is unique; it is determined by crystallographic phase transformations and is possible to predict by the theory of phase transformations. It is important to explore all possible good matching pairs between the planes or orientations for both phases. Thus, composite stereographic projections will be useful to explore all possible orientation relationships, which will be a valuable guide for users to measure habit plane and growth orientation.

Fig. 3 shows a typical Burgers orientation relationship between a hexagonal closed-packed (h.c.p.) matrix and a body-centred cubic (b.c.c.) precipitate in the α-Mg/γ-$Mg_{17}Al_{12}$ precipitation system. The Burgers (1934) orientation relationship can be expressed as

$$(0001)_\alpha \parallel (110)_\gamma, \quad [2\bar{1}\bar{1}0]_\alpha \parallel [\bar{1}11]_\gamma, \quad [01\bar{1}0]_\alpha \parallel [\bar{1}\bar{1}2]_\beta. \qquad (7)$$

Here the subscripts 'α' and 'γ' represent the matrix α-Mg and the precipitate γ-$Mg_{17}Al_{12}$, respectively. The composite stereographic projections are plotted by drawing stereographic projections viewed at [0001] and [110] orientations for the matrix and precipitate, respectively. One of these projections is then rotated around the pole centre by 35.26°. For one of the pairs of orientations, $[01\bar{1}0]_\alpha \parallel [\bar{1}\bar{1}2]_\beta$, the index of the poles, the interplanar distance/orientation-vector magnitude and the angle between the two poles selected are shown.

Another example is the (111)/70.5° twin relationship in a cubic crystal, which is shown in Fig. 4. The rotation axis is [110] for both crystals while one of the projections has been rotated around the pole

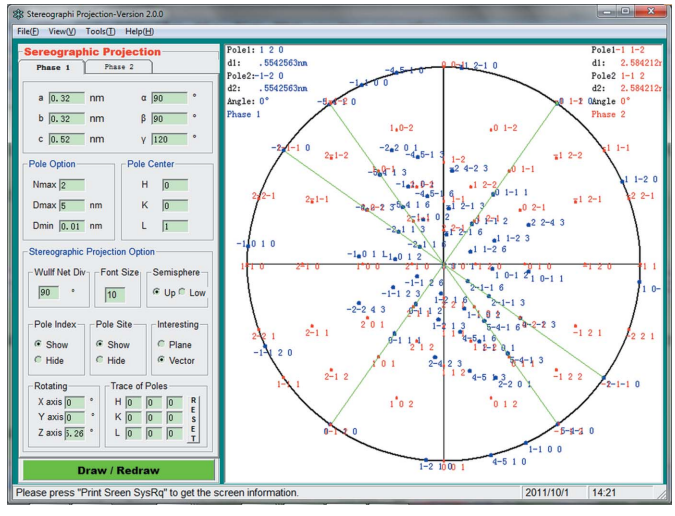

Figure 3
A typical Burgers orientation relationship between the h.c.p. matrix and the b.c.c. precipitate in the Mg/$Mg_{17}Al_{12}$ precipitation system.

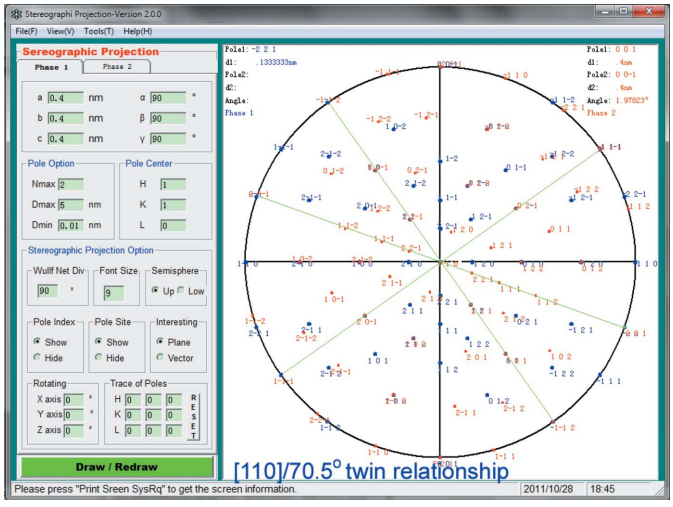

Figure 4
A typical [110]/70.5° twinning relationship in cubic crystals.

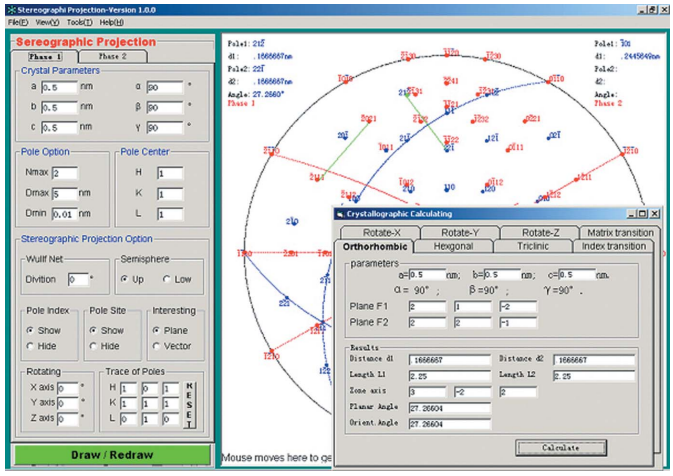

Figure 6
A useful crystallographic calculation toolkit is provided for calculating interplanar distance, orientation-vector magnitude, the angles between planes and orientations, and the zone axis of any two planes.

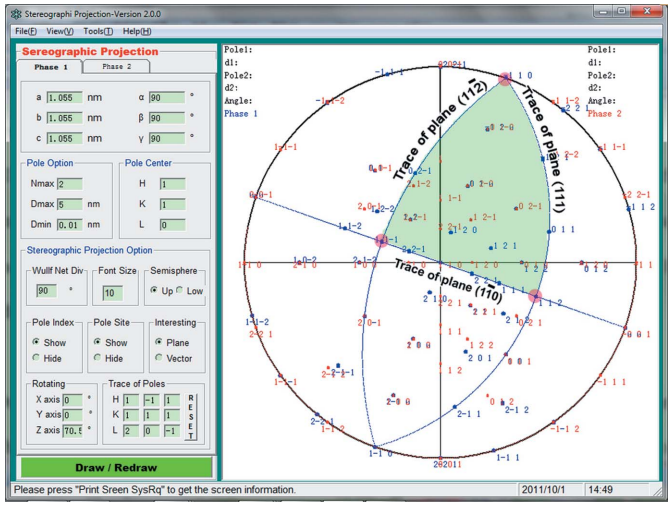

Figure 5
The triangular zone of a pole figure enclosed by three plane traces, plotted in a stereographic projection.

centre by 70.5°. The twinning plane is $(1\bar{1}1)$, which is the mirror plane of the two parts of the twin structure.

4.4. Triangular zone of a pole figure

Most Kikuchi lines are plotted in a triangular zone of the pole figure. This triangular zone contains three vertices, each pair of which has an angle between the planes of 90° or some other value defined by the user. An important aspect is that the triangular zone of the pole figure is often plotted on a stereographic projection and used with Kikuchi lines as an orientation map when microscopists are looking for the orientation of a given crystal.

The triangular zone of a pole figure is very easy to define, although none of the commercial programs include a function for this purpose. Given that any two of the vertices in a triangular zone belong to a certain plane group (exactly the cross product of the two vertices), three planar traces can be defined by the three vertices and then plotted on a projection (Fig. 5).

4.5. Crystallographic calculation toolkit

It is convenient for the purpose of crystallographic analysis to combine all necessary crystallographic calculation toolkits into a single interface. All of the most widely used theoretical methods for calculating interplanar distance, orientation-vector magnitude, the angle between planes or orientations, the zone axis, and the index conversion between plane and plane normal, as well as between different coordinate systems, have been incorporated into *SP2* (Fig. 6).

5. Program requirements and availability

The program is available as green software containing a single executable file which can be used without installation. The expected hardware configuration is as follows: more than 32 Mb of free RAM memory, 16 Mb of HDD, Pentium M processor or higher. The main software can work on most modern computers running Windows. The software is free for academic purposes and is available as supplementary material[1] or from the authors on request.

This work was financially supported by projects sponsored by (1) the National Natural Science Foundation of China under grant No. 50971047 and (2) the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry. Enlightening discussions with Dr Yong Yuan (Chinese Academic Society) and Dr Hongmei Zhu (PhD at South China University of Technology, China) are greatly appreciated. HL thanks Mr James Pering at the Centre of English Testing at The University of Sydney for his revision of grammar and spelling.

References

Boudias, C. & Monceau, D. (1998). *CaRIne Crystallography*. Verison 3.1. Software CaRIne Crystallography, Senlis, France.
Brandenburg, K. (2011). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Burgers, W. (1934). *Physica*, **1**, 561–586.

[1] The executable file and reference manuals are also available from the IUCr electronic archives (Reference: AJ5181). Services for accessing this material are described at the back of the journal.

Crystal Studio (1999). *Crystal Studio*, http://www.crystalsoftcorp.com/index.html.
Hielscher, R. & Schaeben, H. (2008). *J. Appl. Cryst.* **41**, 1024–1037.
Hielscher, R., Schaeben, H. (2010). *Math. Geosci.* **42**, 359–375.
Howarth, R. J. (1996). *Terra Nova*, **8**, 499–513.
Kikuchi, S. (1928). *Jpn. J. Phys.* **5**, 83–96.
Kohn, S. C. (2007). *Terra Nova*, **7**, 554–556.
Siegrist, T. (1997). *J. Appl. Cryst.* **30**, 418–419.
Stadelmann, P. (1987). *Ultramicroscopy*, **21**, 131–146.
Wulff, G. (1902). *Z. Kristallogr.* **36**, 1–28.
Zuo, J. M. & Mabon, J. C. (2004). *Microsc. Microanal.* **10**, 1000–1001.