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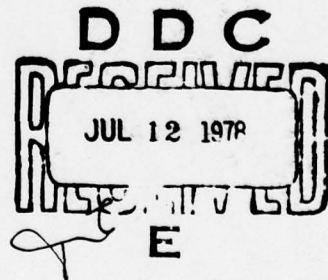
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MATERIALS NOTE 119

**COMPUTER-GENERATED STANDARD  
STEREOGRAPHIC PROJECTIONS**

by  
M. E. PACKER



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SUMMARY

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16. *ABSTRACT*  
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## NOTATION

$a, b, c$	lattice parameters (translations)
$\alpha, \beta, \gamma$	lattice parameters (angles)
$a^*, b^*, c^*$	reciprocal lattice parameters (translations)
$\alpha^*, \beta^*, \gamma^*$	reciprocal lattice parameters (angles)
$V$	volume of unit cell
$Q, Q'$	arbitrary directions in the lattice
$P$	the point on the projection representing direction $Q$
$u, v, w$	Miller indices of direction $Q$
$u', v', w'$	Miller indices of direction $Q'$
$D, D'$	lattice repeat distances for directions $Q$ and $Q'$
$u_0, v_0, w_0$	values of the parameters $u, v$ and $w$ which give local maxima in the value of $D$
$n$	an integer
$Dn$	lattice repeat distances defining the various ranges within which $D$ may fall
$u_n, v_n, w_n$	Miller indices of a direction which has a repeat distance $Dn$
$Q_1, Q_2, Q_3$	orthogonal directions in the lattice
$u_1, v_1, w_1$	Miller indices of direction $Q_1$
$u_2, v_2, w_2$	Miller indices of direction $Q_2$
$u_3, v_3, w_3$	Miller indices of direction $Q_3$
$O$	centre of reference sphere and of projection
$R$	radius of reference sphere
$\phi, \psi, \chi$	angles made by direction $Q$ with directions $Q_1, Q_2, Q_3$ respectively
$r, \theta$	polar coordinates of point $P$ on the projection

The Miller indices  $u_n, v_n, w_n$  are distinct from  $u_0, v_0, w_0, u_1, v_1, w_1$  etc. No confusion should arise since the former are used only in the context of subroutine LIMITS.

## 1. INTRODUCTION

The stereographic projection offers a convenient method for mapping certain types of crystallographic information in two dimensions and for determining angular relationships between various features in a crystal. Particularly useful are "standard projections" of a crystal. These are stereographic projections showing the relative positions of certain lattice plane normals and/or crystal directions for given orientations of the crystal, especially orientations of high symmetry. Use of the stereographic projection in crystal physics is described by Barrett [1].

## 2. PROGRAMS FOR STEREOGRAPHIC PROJECTIONS

Many projections have been published over the years but, except for the simplest crystal classes, a projection produced for one situation is unlikely to be of use in another, and the need frequently arises for projection along some unusual direction in the crystal, for a projection of a crystal which has non-cubic symmetry and for which a projection is not already available, or for a projection in some particular format.

Two computer programs have been written to fulfil these needs. One program determines the coordinates of the points on a standard projection in a format specified by input parameters. The other, using output from the first, plots the projection on a graph-plotting terminal.

Similar programs have been written and published in the past [2,3,4,5] and the present programs perform basically the same function as these. However, the options written into the present programs provide a combination of features which the author has found convenient in deformation, texture and electron diffraction/microscopy studies. The programs have been developed and tested over a period of many years and include several novel features.

The programs are written in FORTRAN-IV as implemented on a DECsystem-10. The coding has been largely optimised in the most deeply nested sections of the programs. The coordinates program, SPC, should be readily adaptable to any system with a FORTRAN-IV compiler since an attempt was made to conform to ASA Standard FORTRAN [6] as far as possible. Specific areas where the code is known to depart from Standard FORTRAN are:

- (1) The use of subscripted integer variables as subscripts
- (2) The 'OPEN' instruction, which sets up disc files for input and output
- (3) The 'TYPE' statement, which is used to output diagnostic information directly to a terminal.

In addition, certain tests to allow for rounding errors involve constants appropriate to a 36-bit processor.

The plotting program, SPP, on the other hand, is rather more dependent on the software available at this particular installation. In particular, it makes use of system subroutines which drive a digital incremental plotter.

On the DECsystem-10 with a KI processor, run times are about 2 sec. to calculate the coordinates for a 200-point projection, and of the order of 10 sec. to create the plot file.

Program listings have been deposited with the ARL Computer Centre and are available within the ARL system from DECTape D/933.

## 3. THEORY

For a lattice with parameters  $a, b, c, \alpha, \beta, \gamma$ , the angle  $\phi$  between directions  $uvw$  and  $u'v'w'$  is [7]

$$\cos \phi = [uu'a^2 + vv'b^2 + ww'c^2 + (vw' + wt')bc \cos \alpha + (wu' + uw')ca \cos \beta + (uv' + vu')ab \cos \gamma] / DD' \quad (1)$$



where

$$D = (u^2a^2 + v^2b^2 + w^2c^2 + 2vwb \cos \alpha + 2wuca \cos \beta + 2uvab \cos \gamma)^{\frac{1}{2}} \quad (2)$$

is the repeat distance along the direction  $uvw$ , and  $D'$ , correspondingly defined, the repeat distance along the direction  $u'v'w'$ .

Because of the relationship between directions in the real lattice and planes in the reciprocal lattice, and vice-versa,  $\phi$  is also the angle between the normals to lattice planes  $uvw$  and  $u'v'w'$  in the reciprocal lattice. Conversely, by replacing the parameters  $a, b, c, \alpha, \beta, \gamma$  by the reciprocal lattice parameters  $a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*$ ,  $\phi$  becomes the angle between the normals to the planes  $uvw$  and  $u'v'w'$  in the real lattice.

The reciprocal lattice parameters are defined by

$$\begin{aligned} a^* &= (bc \sin \alpha)/V & \cos \alpha^* &= (\cos \beta \cos \gamma - \cos \alpha)/(\sin \beta \sin \gamma) \\ b^* &= (ca \sin \beta)/V & \cos \beta^* &= (\cos \gamma \cos \alpha - \cos \beta)/(\sin \gamma \sin \alpha) \\ c^* &= (ab \sin \gamma)/V & \cos \gamma^* &= (\cos \alpha \cos \beta - \cos \gamma)/(\sin \alpha \sin \beta) \end{aligned}$$

where

$$V = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)^{\frac{1}{2}}$$

is the volume of the unit cell [8].

From equation (2), it can be shown to be necessary (but not sufficient) that

(1) For  $D$  to be a maximum,

$$w = 0 \quad (3a)$$

(2) For  $w$  fixed,  $D$  will be a maximum for

$$v = (wc/b)(\cos \beta \cos \gamma - \cos \alpha)/(\sin^2 \gamma) \quad (3b)$$

(3) For  $w$  and  $v$  fixed,  $D$  will be a maximum for

$$u = (vb \cos \gamma + wc \cos \beta)/a \quad (3c)$$

Consider a reference sphere centred at the origin of the lattice (Figure 1a). A point  $Q$  on the surface of the sphere uniquely represents a lattice direction passing through the origin and is represented stereographically on the horizontal plane through the centre of the sphere by the point  $P$ , which is the point where this plane is intersected by the line connecting  $Q$  to the south pole. This plane is the projection plane (Figure 1b).

Consider three reference directions  $Q1$ ,  $Q2$  and  $Q3$ , defined by Miller indices  $u1, v1, w1$ ,  $u2, v2, w2$  and  $u3, v3, w3$ , respectively.  $Q1$  defines the north pole and becomes the central pole on the projection.  $Q2$  and  $Q3$  are perpendicular to  $Q1$  and to each other and therefore lie on the perimeter of the projection. We may define a coordinate system  $R, \theta, \phi$  using these directions as coordinate axes:  $Q1$  ( $\phi = 0^\circ$ ),  $Q2$  ( $\phi = 90^\circ$ ,  $\theta = 0^\circ$ ),  $Q3$  ( $\phi = 90^\circ$ ,  $\theta = 90^\circ$ ). The arbitrary direction  $Q$ ,  $u, v, w$ , makes angles of  $\phi$ ,  $\psi$  and  $\chi$  with  $Q1$ ,  $Q2$  and  $Q3$ . These angles may be determined using equation (1). The coordinate  $\theta$  in the system defined above is then given by

$$\cos \theta = (\cos \psi)/(\sin \phi)$$

the positive or negative value of  $\theta$  being taken depending on whether  $\chi$  is greater or less than  $90^\circ$ .

The coordinate  $r$  is the distance of the point  $P$  from the centre of the projection and has the value  $R \tan \phi/2$ , where  $R$  is the radius of the reference sphere.

#### 4. PROGRAM SPC—STEREOGRAPHIC PROJECTION COORDINATES

The program is written as a collection of subroutines, which are called by the main program in the appropriate order. Extensive use is made of COMMON to minimise data transfers and core storage. The program allows data to be determined for up to 222 points. This number of points has been found ample for most applications. However, the combination of digits '222' is unique to this context and the program can be edited to handle any desired maximum by globally changing '222' to the desired figure before compiling.

The program basically considers crystal directions, but an appropriate request in the input

data causes the lattice to be replaced by the corresponding reciprocal lattice. Operation of the program on the reciprocal lattice then gives data which relate to lattice plane normals in the direct lattice. In this documentation of the program, all reference is to directions. A corresponding description applies, however, for lattice plane normals. It is not possible to consider both planes and directions simultaneously.

#### **4.1. Description of the Program**

##### **4.1.1. Main Program**

Subroutines are called in sequence.

##### **4.1.2. Subroutine INPUT**

Disc files are opened for input and output. Input data are read from file and their plausibility checked. The main data required are:

- (1) Title
- (2) Lattice parameters
- (3) Information defining the centre of the projection
- (4) Information defining the range of points to be accepted
- (5) Whether planes or directions are required
- (6) Radius of projection
- (7) Maximum number of points allowed.

The input data are also used to specify whether stereographic, polar, or cartesian coordinates are required for the output. Detailed specifications for the data required are included as comments in the subroutine.

##### **4.1.3. Subroutine RECLAT**

The reciprocal lattice is set up corresponding to the direct lattice specified. The direct lattice is replaced by the reciprocal lattice if lattice plane normals are to be considered. Constants to be used in other subroutines are determined.

##### **4.1.4. Subroutine ORTHOG**

From the input data defining the orientation of the projection, the program sets up reference directions at the centre of the projection ( $Q1$ ), and on the circumference at  $\theta = 0^\circ$  and  $90^\circ$  ( $Q2, Q3$ , respectively). The following cases are distinguished:

If only one direction is given, it is taken as  $Q1$ . If two directions are given and they are perpendicular to one another, they are taken as  $Q1$  and  $Q2$ , respectively. If two directions are given and they are not perpendicular,  $Q1$  is set up perpendicular to them both, i.e. these two directions are regarded as lying on the perimeter of the projection.

##### **4.1.5. Subroutine RATNL**

An attempt is made to rationalise indices of directions set up within subroutine ORTHOG. Additional constants to be used in other subroutines are determined.

##### **4.1.6. Subroutine LIMITS**

It was originally envisaged that 'low-index' directions could usefully be displayed more prominently on a projection, since these are usually of greater importance. In generalising to non-cubic lattices, this criterion was no longer satisfactory and a new rule-of-thumb was adopted, viz. that the smaller the repeat distance,  $D$ , along a given direction, the more 'important' it was likely to be. Thus, it was decided to classify the points obtained into groups depending on their  $D$ -parameters.

A series of  $n$  sets of Miller indices may be specified in the input ( $1 \leq n \leq 10$ ). The repeat distance  $D_n$  is calculated for each set. A candidate pole is then included in the output if its repeat

distance  $D$  lies within the range  $D_1 \leq D \leq D_n$ . Acceptable values of  $D$ , moreover, may be separated into  $n-1$  groups, depending on the value of  $D$ .

This structure facilitates obtaining a projection with a convenient number of points, especially for low-symmetry lattices. If the range of calculation is defined as a multiple range (i.e.  $n > 2$ ), and the number of points requested is exceeded during computation, the program deletes the uppermost range and starts again. Since non-integral indices may be used here, it is possible to define a very narrow range, so that only a single type of direction is included. This facility is used for preparing ideal-texture pole figures (Section 5.12).

#### 4.1.7. Subroutine GENUVW

This subroutine constitutes the core of the program. Sets of indices  $u, v, w$  are generated, tested to see whether they fall within the desired constraints, and the coordinates of the direction represented are calculated in relation to the three reference directions. An algorithm was required for generating suitable sets of indices  $u, v, w$ . For orthogonal lattices, simple stepping of  $u, v$  and  $w$  on either side of zero would be efficient, but for crystals of lower symmetry, various problems arise and the following procedure was developed.

As discussed above, the repeat distance is used as the criterion for inclusion in the output. For given values of  $v$  and  $w$ , there will be some value  $u_0$  which will lead to a minimum of  $D$ . This can be determined by differentiating the expression for  $D$  (Equation 3c). For these values of  $v$  and  $w$ , values of  $u$  can then be stepped out on either side of  $u_0$ , the procedure terminating when the combinations of  $u, v$  and  $w$  cease to be acceptable. A similar process occurs for each combination of  $v$  and  $w$ . A related procedure is used for each  $w$  to determine a value  $v_0$  from which values of  $v$  are stepped (Equation 3b). Values of  $w$  are simply stepped about zero (Equation 3a).

The coordinates of the point  $u, v, w$  are determined as  $\theta$  and, depending on the input parameters,  $r$  or  $\phi$ .

As acceptable points are found, the related data are stored. Because values of  $\theta$  greater than  $180^\circ$  are specially considered in the program, the results are conveniently stored in two blocks, thereby reducing the sorting required later. If the available storage becomes full, execution terminates unless a multiple range has been defined for the range of calculation (see Section 4.1.6), in which case, the least significant range is discarded and the calculation repeated with the reduced range.

#### 4.1.8. Subroutine ORDER

The stored data are sorted into increasing order with respect to  $\theta$ , and, for each  $\theta$ , in decreasing order with respect to  $r$  or  $\phi$ .

#### 4.1.9. Subroutine HEAD

General information is presented on a title page.

#### 4.1.10. Subroutine OUTPUT

If required, all relevant data are dumped on a binary file. Hard-copy output is initially sent to file in a form determined by the input parameters.

### 4.2. Operation of the Program

Detailed specifications for the data required for program SPC are given as comments in Subroutine INPUT. Table 1 gives a sample set of input data. It requests a 111 projection of lattice planes for a hexagonal lattice,  $c/a = 1.59$ . All planes are to be included whose interplanar spacing is greater than that of the 400 planes. The output will give stereographic coordinates  $\phi$ ,  $\theta$ , and a binary file will be produced for the plotting program.

The teletype record when running the program is shown in Table 2. The number of points specified (222 by default) was exceeded. However, since a multiple range was specified, the least significant range (300-400) was discarded and computation repeated.

Part of the output is shown in Table 3.



## 5. PROGRAM SPP—Stereographic Projection Plotter

### 5.1. Description of the Program

#### 5.1.1. Standard Projections

This program accepts as input the coordinate data produced by program SPC and plots the projection on a digital incremental plotter. Other parameters are input separately to determine the detailed format.

The program makes extensive use of a suite of system subroutines which draw lines and symbols on the plotter. Such subroutines are available at most installations which use graph-plotting facilities. However, the coding in SPP may need to be modified before the program can be used on some other system.

A specification of the operations performed by these subroutines is given in the Appendix.

The program permits standard projections up to 21 inches in diameter, although for diameters greater than 11 inches, or if requested specifically, the projection is plotted as two semi-circles. These restrictions are necessitated by the limited plotter width. If requested, only the first quadrant will be plotted.

For hexagonal lattices, it is more convenient to use the Miller-Bravais 4-index notation. The conversion is executed as the default option, but may be suppressed if desired.

#### 5.1.2. Ideal Sheet Textures

An additional facility is the plotting of pole figures of so-called "ideal" sheet textures of rolled, or rolled and recrystallised, metal sheets [9]. Because of the symmetry of the rolling process, the pole figure of such a sheet is symmetrical about the rolling direction. For reversed-rolling at least, it is also symmetrical about the transverse direction. Accordingly, an ideal texture can be simulated by reflecting the pole figure through the radii representing the rolling and transverse directions.

The program arranges for all points in the pole figure to be reflected into the first quadrant. By adding a rotation to the source data beforehand, the rolling direction can be varied. The program produces a set of quadrant pole figures for a specified set of rotations.

The procedure, although somewhat naive, is simple in concept and can be of great use in identifying texture components.

### 5.2. Operation of the Program

#### 5.2.1. Data Required

File SPC.BIN—binary output file from program SPC.

File SPP.DAT—auxiliary data defining the format of the projection:

- (1) Diameter of reference circle
- (2) A code defining the size indices are to be plotted
- (3) A code requesting that a circle, two semi-circles, or a quadrant be drawn
- (4) A code limiting the number of data points to be plotted
- (5) A code defining the angle at which the indices are to be plotted
- (6) A code suppressing the conversion to Miller-Bravais indices
- (7) Three parameters defining a sequence of angles for generating ideal-texture pole figures.

Detailed descriptions of the data required, and their format, are included as comments in the program.

#### 5.2.2. Examples

The results from the earlier test (shown in Table 3) were plotted with all zeros for the auxiliary data (thereby implementing default settings throughout). The resulting plot is shown in Figure 2.

As an example of the ideal-texture facility, the 5th line of the data (Table 1) was changed to read

0.99 0 0 1.01 0 0

i.e. so as to restrict the output to include only 1 0 0 planes. After processing with programs SPC and SPP, and with the auxiliary data

0 0 0 0 0 15 0 80

the set of ideal textures shown in Figure 3 was obtained. (Note that when the ideal-texture option is being used, many of the auxiliary data items need not be set because they are reset to standard values by the program.)

## 6. CONCLUSION

Two FORTRAN programs have been written for generating the points on standard stereographic projections for the most general of cases and for plotting these projections. The programs have operated reliably over several years and have been used for drawing projections for use in studies on deformation, texture, and electron microscopy and diffraction. Idealised pole figures of sheet textures may also be prepared.

## 7. ACKNOWLEDGMENT

The author is grateful to Mr. R. A. Coyle for assistance in writing the plotting program SPP.



## APPENDIX

Specification of subroutines used to drive the CALCOMP digital incremental plotter. Only those facilities are described which are invoked by the program SPP. The specification has been adapted from the complete specification of the set of plotting subroutines ALLPLT [10].

### Subroutine PLOT

Purpose: To provide the basic movements of the plotter pen.

Usage: CALL PLOT(LU,X,Y,N)

Description of Parameters:

LU: Integer input. Logical unit number.

X,Y: Real inputs. X and Y coordinates of the point to be plotted.

N: Integer input.

N = 1: X,Y are scaling factors (default: 1.,1.).

N = 2: Reset origin. The current position of the pen is defined as (X,Y).

N = 3: Pen is lifted, moved to X,Y and dropped (not used).

N = 4: Pen is dropped and moved to X,Y.

N = 5: Pen is lifted, moved to X,Y, but not dropped.

Remarks: The positive X-direction is along the paper towards the feed roll. The positive Y-direction is from right to left parallel to the drum axis when looking at the plotter. The initial position of the pen is at the centre of the paper and this is initially defined as the origin.

### Subroutine WHERE

Purpose: To return the current position of the pen relative to the current origin (in units consistent with the current scale factors).

Usage: CALL WHERE (LU,X,Y).

Description of Parameters:

LU: Integer input. Logical unit number.

X,Y: Real output. X and Y coordinates of current pen position.

### Subroutine SYMBOL

Purpose: To draw characters on the plotter.

Usage: CALL SYMBOL(LU,X,Y,HEIGHT,ASCII,THETA,N)

Description of Parameters:

LU: Integer input. Logical unit number.

X,Y: (1)  $N > 0$ : coordinates of the lower left hand corner of the character string to be plotted. On exit, the pen is left at the lower left-hand corner of the *next* character to be plotted (pen up).

(2)  $N < 0$ : Coordinates of centre of special symbol. On exit, the pen is left at X,Y (pen up).

X and Y may be *real or integer*, indicating, respectively, coordinates in inches with respect to the current origin, or coordinates in 0.01 inch increments with respect to the current position of the pen.

HEIGHT: Real input. The height in inches of the characters to be drawn.

ASCII: (1)  $N > 0$ : ASCII is the first word of the string of characters to be plotted.

(2)  $N < 0$ : ASCII must be an integer. The only values called here are  $N = -1$ ,  $ASCII = 0$ , which request a square with a diagonal cross.

THETA: Real input. Angle (in degrees) the string of characters is to make with the X-axis.

THETA increases in the anticlockwise direction.

- N: (1)  $N > 0$ : N characters are plotted.  
(2)  $N < 0$ : The special symbol specified in 'ASCII' is to be drawn.

**Subroutine NUMBER**

Purpose: To draw the value of a real number on the plotter.

Usage: Call NUMBER(LU,X,Y,HEIGHT,FLOAT,THETA,N)

Description of Parameters:

LU,X,Y,HEIGHT,THETA: As for subroutine SYMBOL.

FLOAT: the real number whose value is to be drawn.

N: Number of decimal places to be retained. The special case  $N = -1$  prints only the integral part of N, without a decimal point.

Remarks: Leading zeros are omitted and the number is left-justified. If FLOAT is less than 0.5, a single zero is drawn.

## REFERENCES

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**TABLE 1**

**Sample data for program SPC**

ALPHA TITANIUM  
2.950 2.950 4.683  
90. 90. 120.  
1 1 1 -1 1 0  
0 0 0 2 0 0 3 0 0 4 0 0  
PLANES

**TABLE 2**

**Teletype record for running program SPC**

RUN SPC

STORAGE EXHAUSTED  
RESTARTED WITH REDUCED RANGE  
104 POINTS

end of execution  
CPU time: 1.40 elapsed time: 2.78  
exit





Table 3—continued

180·00	1 -1 0 90·00	3 -1 1 47·76	2 0 1 28·84
185·94	3 -2 0 71·81		
189·84	2 -1 0 61·52		
194·58	3 -1 0 51·36		
197·34	3 -2 -1 75·81		
207·49	3 -2 -2 79·97	2 -1 -1 68·62	3 -1 -1 56·57 1 0 0 34·31 2 1 1 12·04
217·97	3 -1 -2 62·44		
220·93	2 -1 -2 75·91		
226·14	2 0 -1 44·12		
230·52	2 -1 -3 81·93		
237·36	2 -1 -4 86·49	1 0 -1 54·46	2 1 0 20·51
244·34	2 0 -3 63·32		
248·98	1 0 -2 70·33	2 1 -1 31·06	
254·65	1 0 -3 79·96	2 1 -2 41·29	
257·95	1 0 -4 85·93		
260·09	1 0 -5 89·87		
270·00	1 1 -4 69·04	1 1 -3 60·86	1 1 -2 49·69 1 1 -1 34·97 1 1 0 17·48
279·91	0 1 -5 89·87		
282·05	0 1 -4 85·93		
285·35	0 1 -3 79·96	1 2 -2 41·29	
291·02	0 1 -2 70·33	1 2 -1 31·06	
295·66	0 2 -3 63·32		
302·64	-1 2 -4 86·49	0 1 -1 54·46	1 2 0 20·51
309·48	-1 2 -3 81·93		
313·86	0 2 -1 44·12		
319·07	-1 2 -2 75·91		
322·03	-1 3 -2 62·44		
332·51	-2 3 -2 79·97	-1 2 -1 68·62	-1 3 -1 56·57 0 1 0 34·31 1 2 1 12·04
342·66	-2 3 -1 75·81		
345·42	-1 3 0 51·36		
350·16	-1 2 0 61·52		
354·06	-2 3 0 71·81		

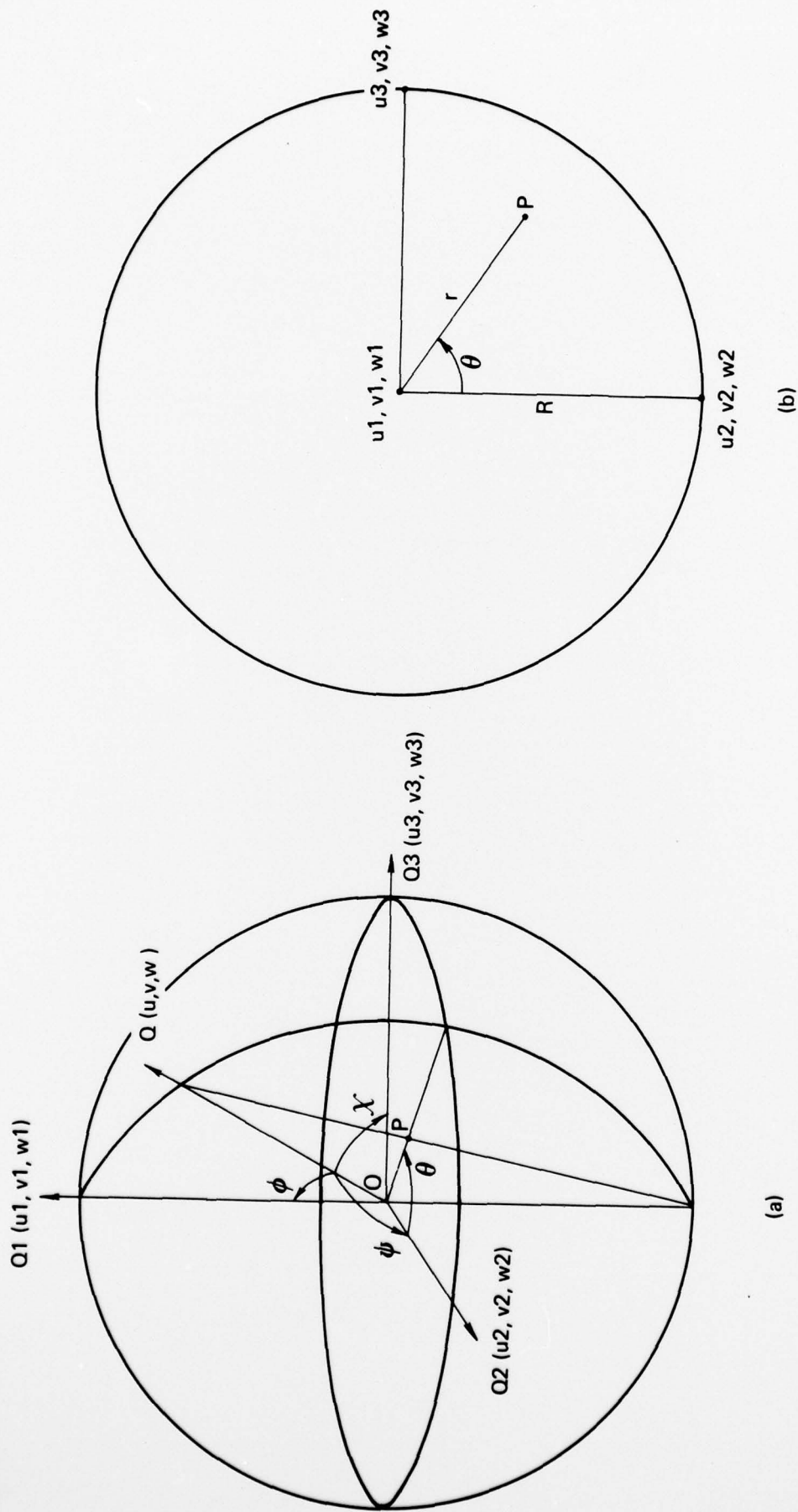


FIGURE 1. BASIC GEOMETRY FOR LOCATING A DIRECTION  $uvw$  ON A STEREOGRAPHIC PROJECTION. FIGURE 1a SHOWS THE REFERENCE SPHERE AND FIGURE 1b THE PROJECTION.

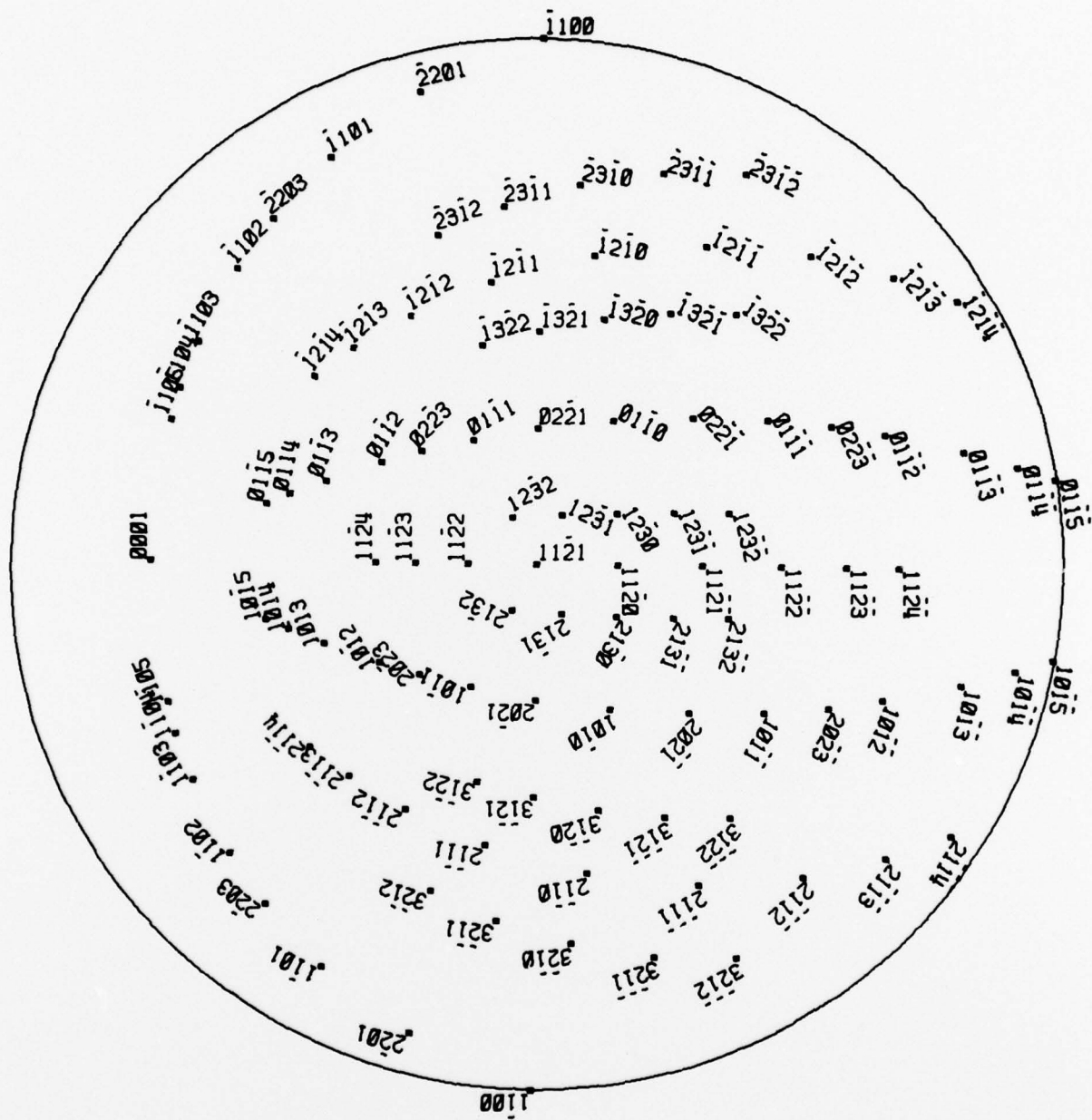


FIGURE 2. STANDARD 1121 PROJECTION FOR LATTICE PLANES IN TITANIUM.

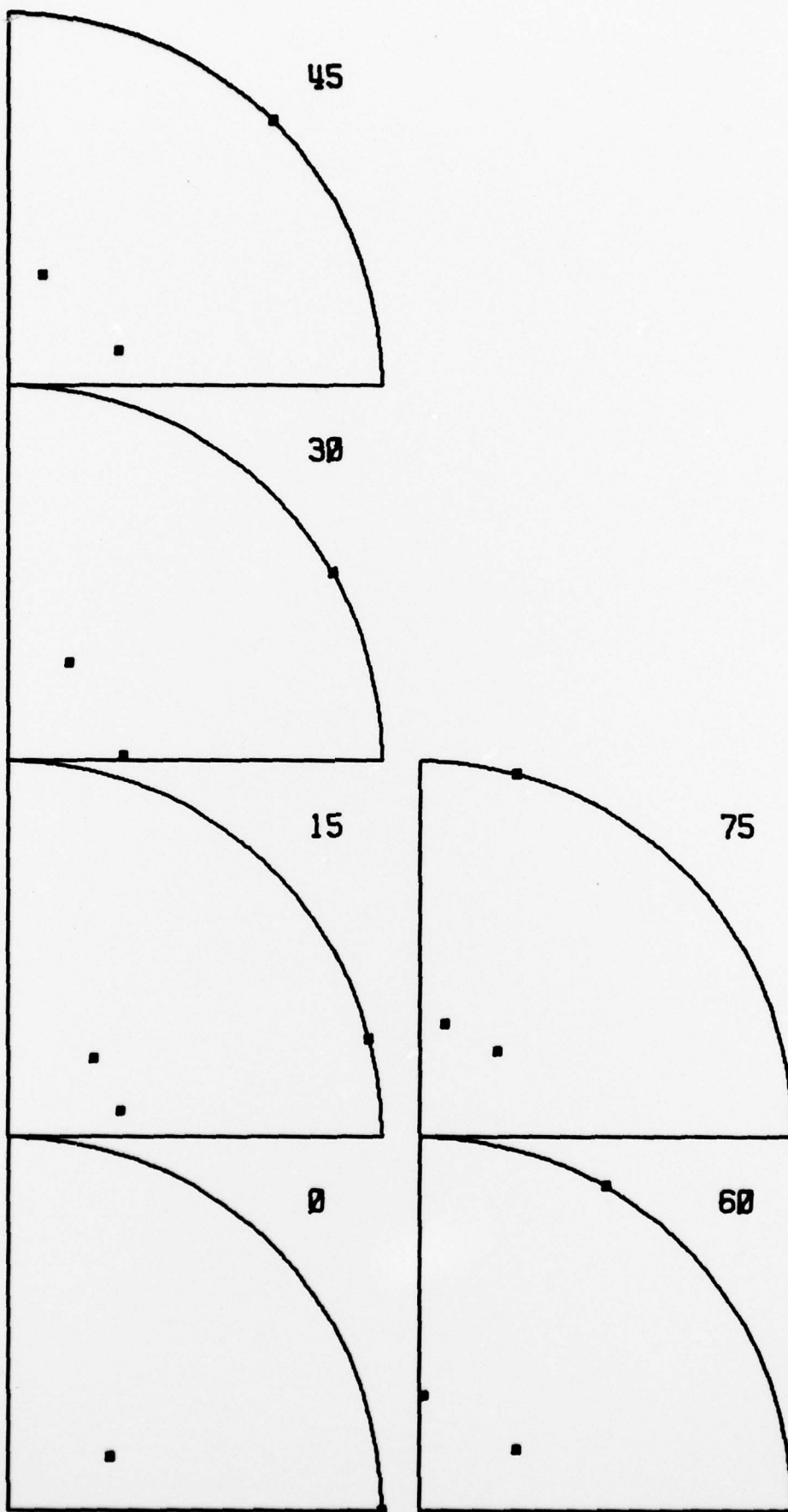


FIGURE 3. SIMULATED 100 POLE FIGURE FOR TITANIUM LATTICE. SEVERAL TEXTURES OF THE TYPE (111) [UVW] ARE REPRESENTED.

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