NRL Report 6919

Computer-Plotted Stereographic Projections

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July 7, 1969

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CONTENTS

ABSTRACT

Stereographic projections for materials having hexagonal symmetry depend on the axial (c/a) ratio. Thus, each material requires its individual set of stereographic projections. The facilities of the NRL Research Computation Center have been used to calculate and plot standard stereographic projections for seven hexagonal close-packed metals with different axial (c/a) ratios. The stereographic projections and the computer program are included in this report.

PROBLEM STATUS

This completes one phase of the problem; work on other phases is continuing.

AUTHORIZATION

NRL Problem M01-08
Project RR 007-01-46-5406

Manuscript submitted March 28, 1969.

COMPUTER-PLOTTED STEREOGRAPHIC PROJECTIONS

INTRODUCTION

The stereographic projection is a device for condensing three-dimensional angular relationships onto a plane. By preserving the angular relationships, the stereographic projection becomes most useful in crystal-structure studies. The interpretation of electron diffraction patterns and transmission electron micrographs is especially aided by the stereographic projection. Standard stereographic projections (a stereographic projection with a plane of low indices as the plane of projection) greatly facilitate solving problems in trace analysis, twinning, and crystal orientation.

A standard stereographic projection for the cubic crystal system gives the angles between planes (or normals to planes), the angles between directions, and the angles between planes and directions for all materials that belong to the cubic crystal system. For materials belonging to the hexagonal crystal system a different stereographic projection is needed for each material, because the formulas which represent either angles between planes, angles between directions, or angles between planes and directions depend on the axial (c/a) ratio of the material (1).

Standard stereographic projections of normals of planes of hexagonal close-packed (hcp) crystals with different axial (c/a) ratios have been published (2-13). The standard stereographic projections in this report have been calculated and plotted by means of a computer program. The materials and the axial (c/a) ratios of the projections are: beryllium (1.5677), cadmium (1.8856), hafnium (1.5811), magnesium (1.6235), titanium (1.5873), zinc (1.8562), and zirconium (1.5931). The lattice constants or axial ratios used in these calculations were taken from either Barrett and Massalski (13) or Pearson (14). The standard stereographic projections that were calculated and plotted for each material are the (0001), the $(10\bar{1}0)$, and the $(10\bar{1}2)$ projections. The program could easily be modified to calculate other standard projections or different axial (c/a) ratios.

METHOD

To plot a stereographic projection of radius R, the indices of the plane of the projection $(h_1k_1i_1\ell_1)$ must be chosen. Another pole $(h_3k_3i_3\ell_3)$, known to be 90 degrees from the $(h_1k_1i_1\ell_1)$ pole, is used to establish a y axis, while a third pole $(h_2k_2i_2\ell_2)$, known to be 90 degrees from the $(h_3k_3i_3\ell_3)$ pole, is used to establish an x axis, as in Fig. 1. The angle α between the $(h_1k_1i_1\ell_1)$ and $(h_2k_2i_2\ell_2)$ poles is then calculated.

Any (defg) pole can now be plotted on this projection. The angles between the (defg) and the $(h_1k_1i_1\ell_1)$, $(h_2k_2i_2\ell_2)$, and $(h_3k_3i_3\ell_3)$ poles are then calculated. These angles are ψ, ϕ, and χ, respectively. The radial polar coordinate (15) of the (defg) pole can now be found to be $R_1 = R \tan(\psi/2)$. The angular polar coordinate for the (defg) pole can also be calculated from the relationship (16) between the three sides of the spherical triangle and one included angle. The three sides of the spherical triangle between the $(h_1k_1i_1\ell_1)$, $(h_2k_2i_2\ell_2)$, and (defg) poles are α, ϕ, and ψ. The included angle θ is the angular polar coordinate and can be expressed as

$$\cos\theta = \frac{\cos\phi - \cos\psi\cos\alpha}{\sin\psi\sin\alpha} .$$

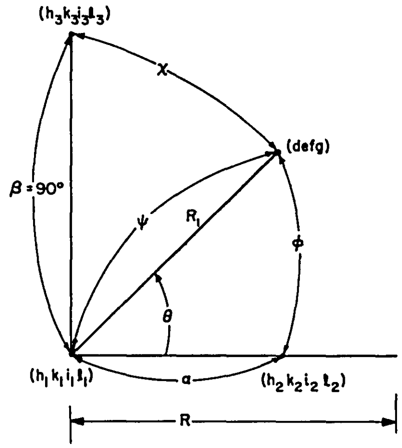

Fig. 1 - Representation of the poles and angles used in the plotting of the (defg) pole

The angular polar coordinate, having been calculated from the inverse cosine function, is restricted to values between 0 and π. The correct quadrant for the angle must be determined.

The angle χ between the (defg) and the $(h_3k_3i_3\ell_3)$ pole is calculated and compared to β, which equals 90 degrees. If χ is equal to or less than β, θ lies in the first or second quadrant ($0 \leq \theta \leq \pi$), but if χ is greater than β, θ lies in the third or fourth quadrant ($\pi < \theta < 2\pi$).

The polar (R_1, θ) coordinates can now be transformed to cartesian (x,y) coordinates without any ambiguity. The (x,y) position of the (defg) pole is then plotted to an accuracy of ±0.01 in. The error in the plotted point, determined by superimposing a 1-degree Wulff net, is less than 0.5 degrees for a 10-in.-diameter net.

Standard stereographic projections of the (0001), $(10\bar{1}0)$, and $(10\bar{1}2)$ poles are shown for beryllium (1.5677) in Figs. 2 through 4,* for cadmium (1.8856) in Figs. 5 through 7, for hafnium (1.5811) in Figs. 8 through 10, for magnesium (1.6235) in Figs. 11 through 13, for titanium (1.5873) in Figs. 14 through 16, for zinc (1.8562) in Figs. 17 through 19, and for zirconium (1.5931) in Figs. 20 through 22.

The angles between the (0001), $(10\bar{1}0)$, and $(10\bar{1}2)$ poles and the poles of the planes used in the stereographic projections are given in Tables 1, 2, and 3, respectively.

A flow chart of the computer program used to do the calculations and plotting is given in Appendix A. The program itself is given in Appendix B.

*Figures 2 through 22 appear on pages 5 through 25.

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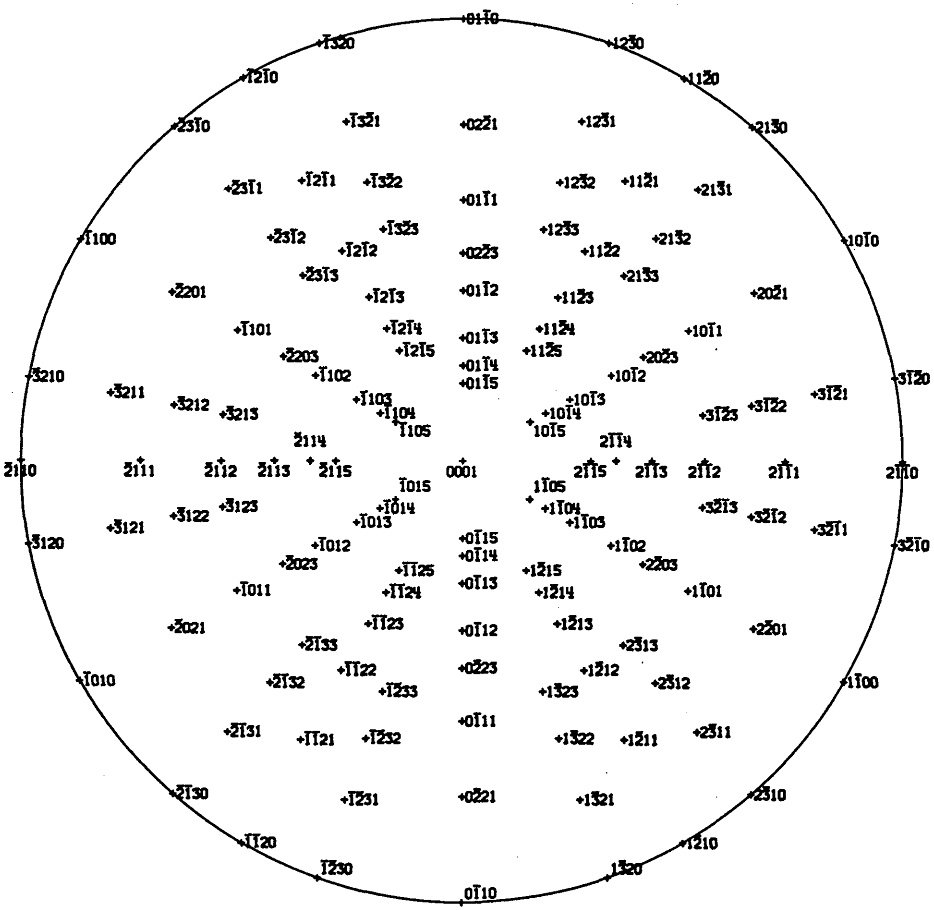


Fig. 2 - (0001) Stereographic projection of beryllium (1.5677)

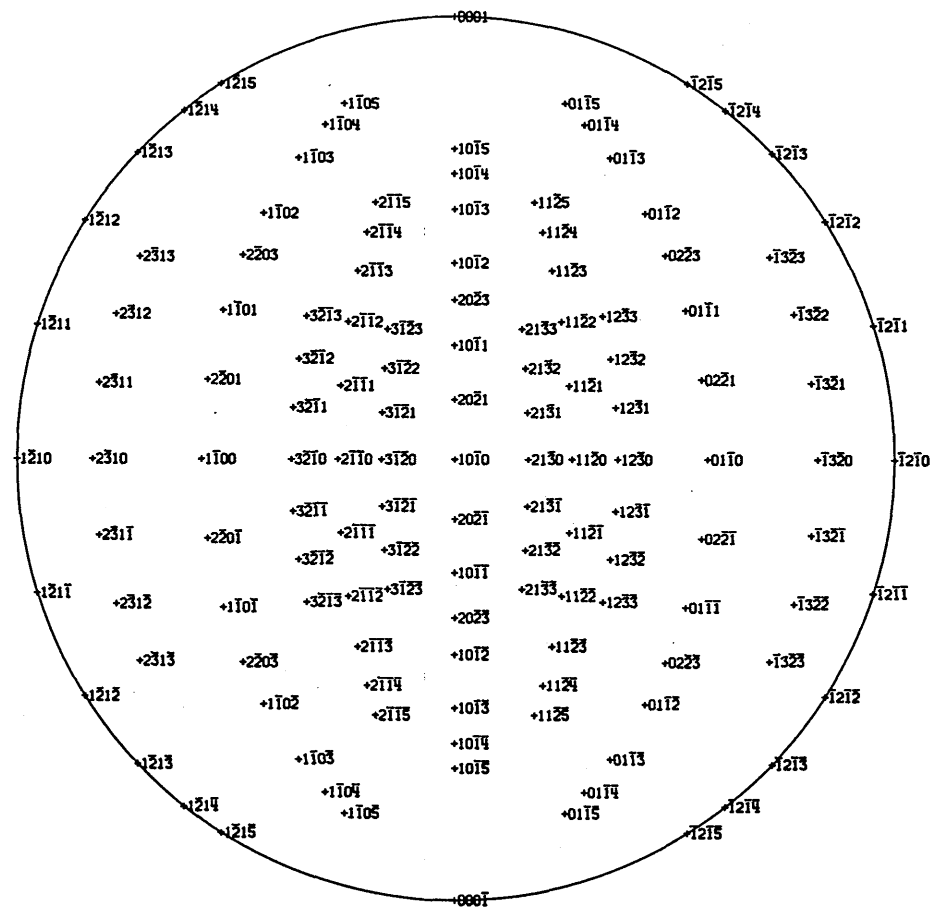


Fig. 3 - (10$\bar{1}$0) Stereographic projection of beryllium (1.5677)

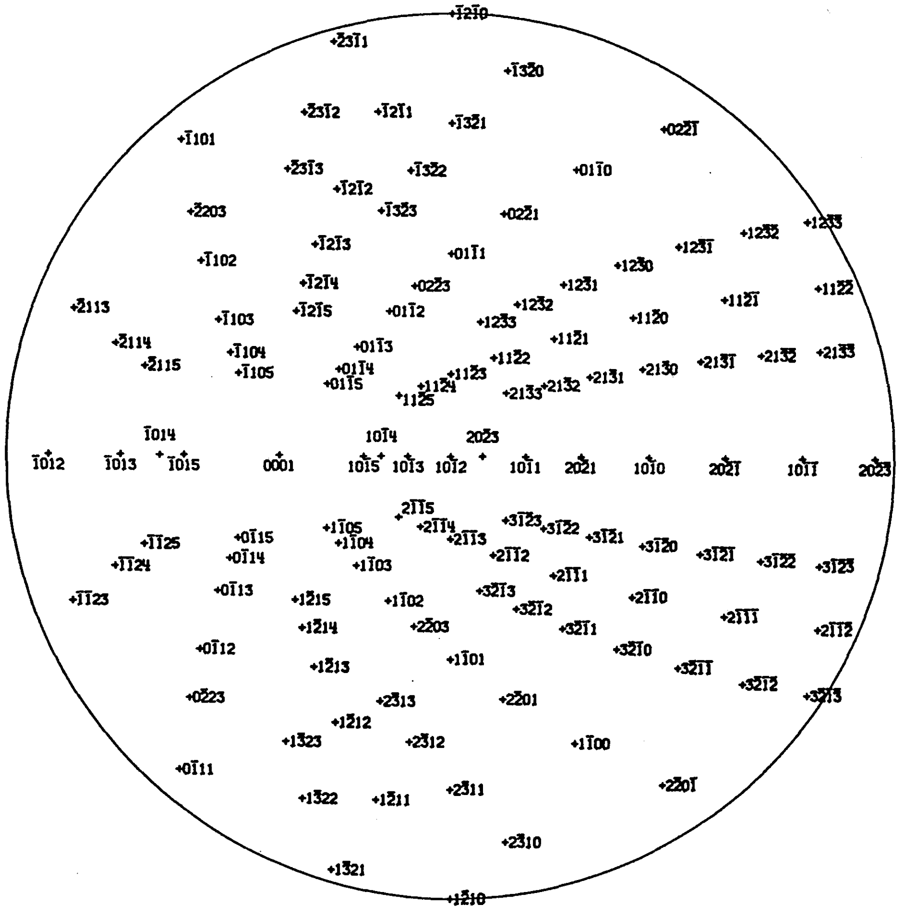


Fig. 4 - (10$\bar{1}$2) Stereographic projection of beryllium (1.5677)

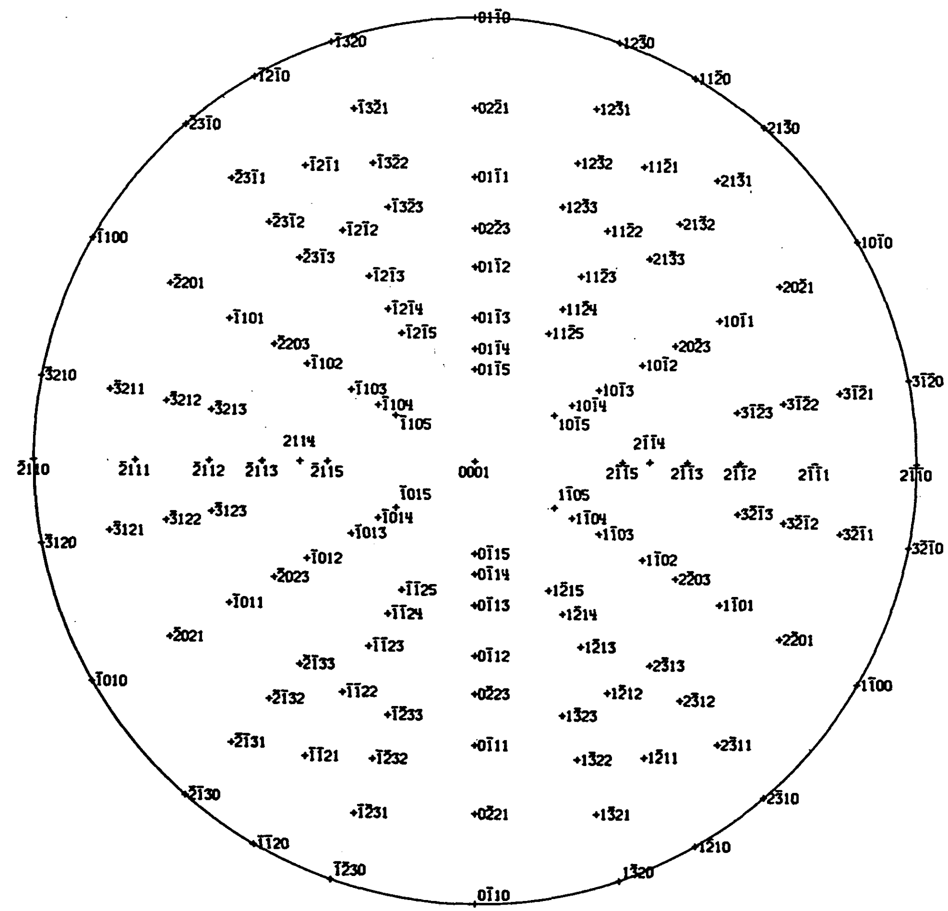


Fig. 5 - (0001) Stereographic projection of cadmium (1.8856)

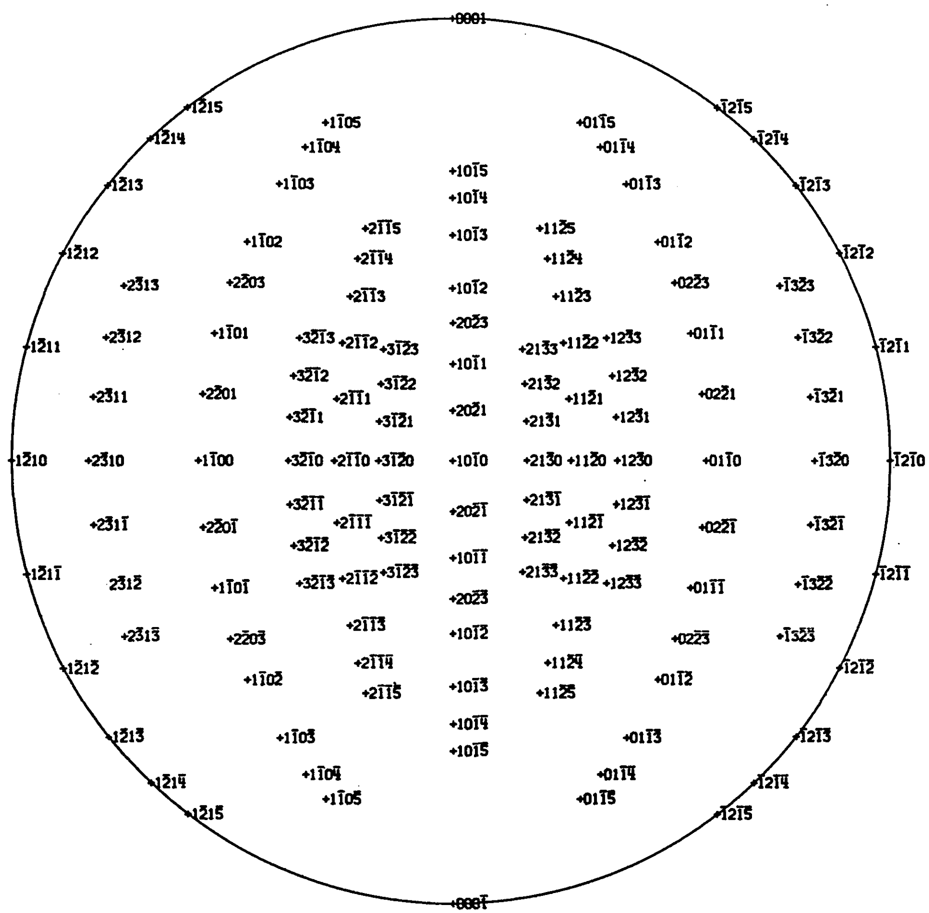


Fig. 6 - (10$\bar{1}$0) Stereographic projection of cadmium (1.8856)

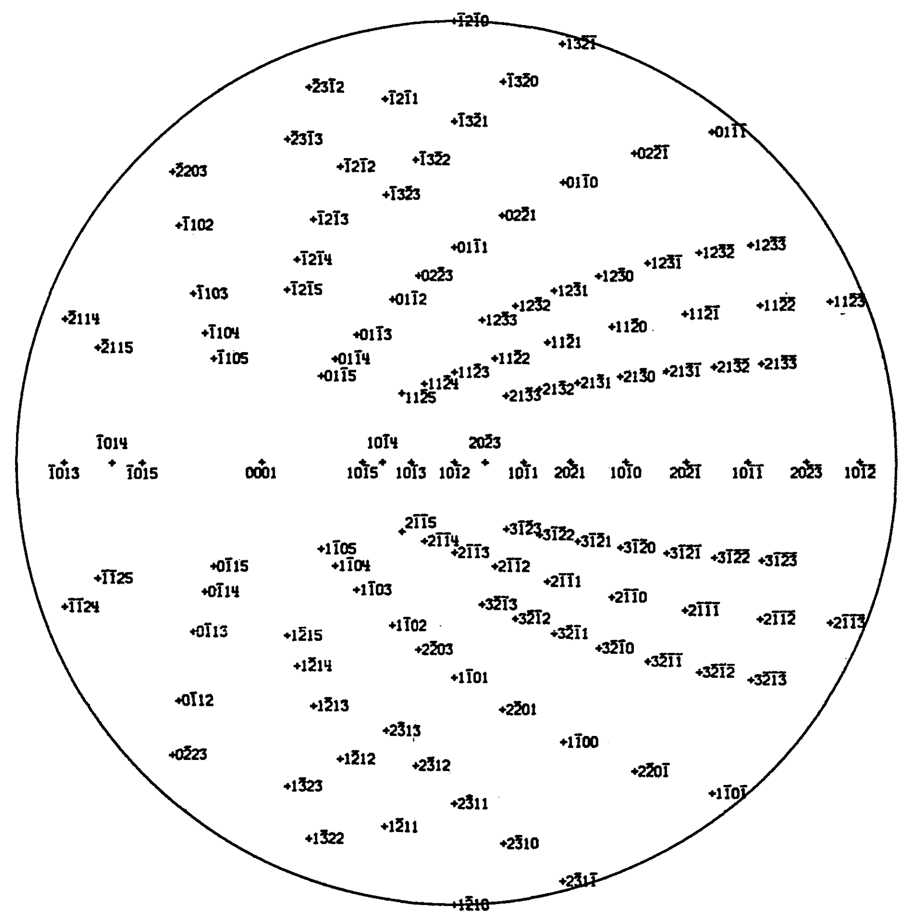


Fig. 7 - (10$\bar{1}$2) Stereographic projection of cadmium (1.8856)

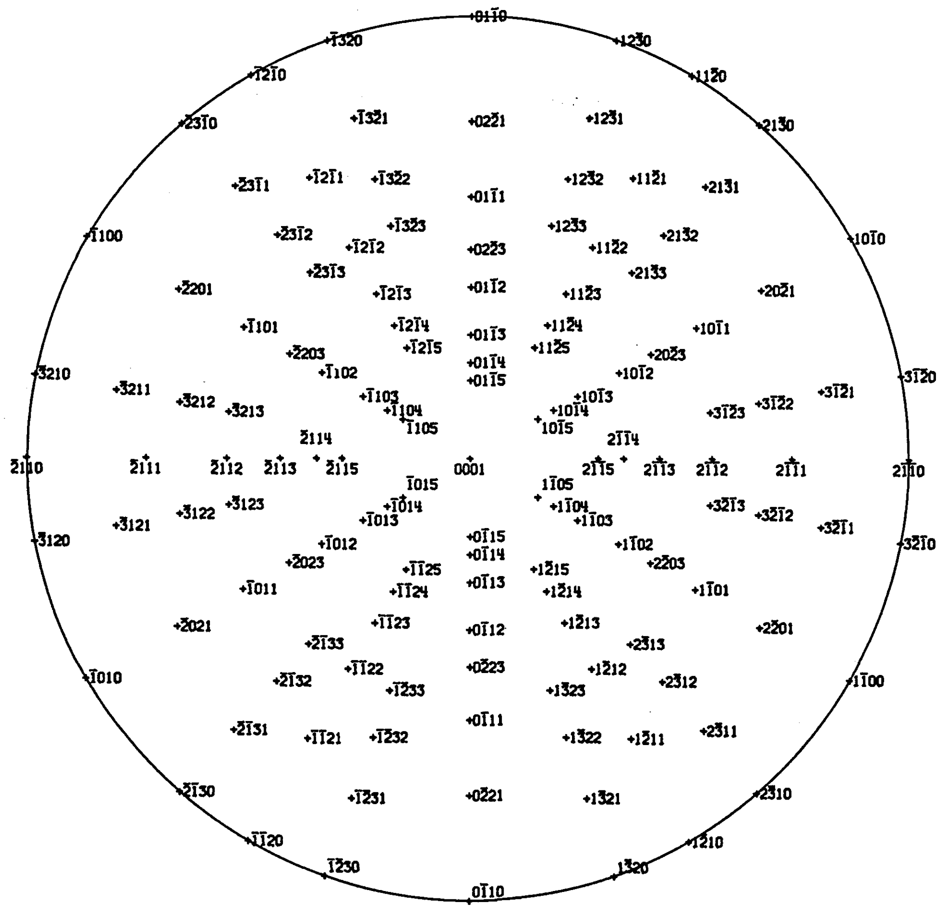


Fig. 8 - (0001) Stereographic projection of hafnium (1.5811)

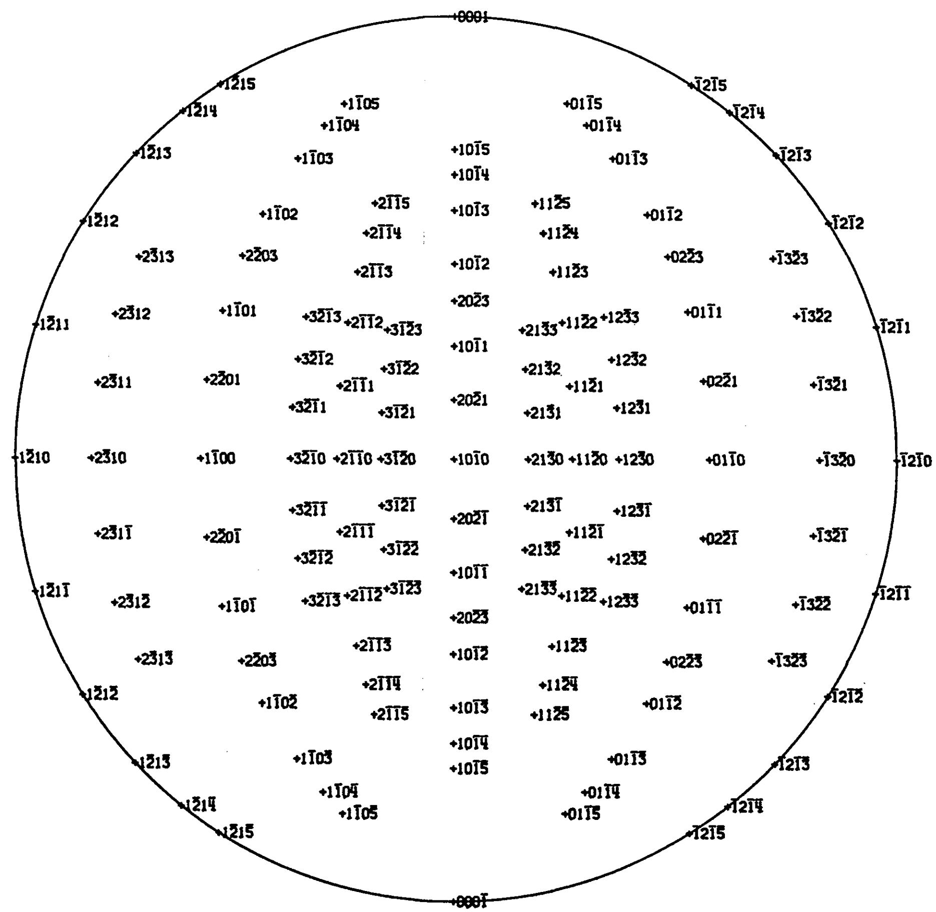


Fig. 9 - (10$\bar{1}$0) Stereographic projection of hafnium (1.5811)

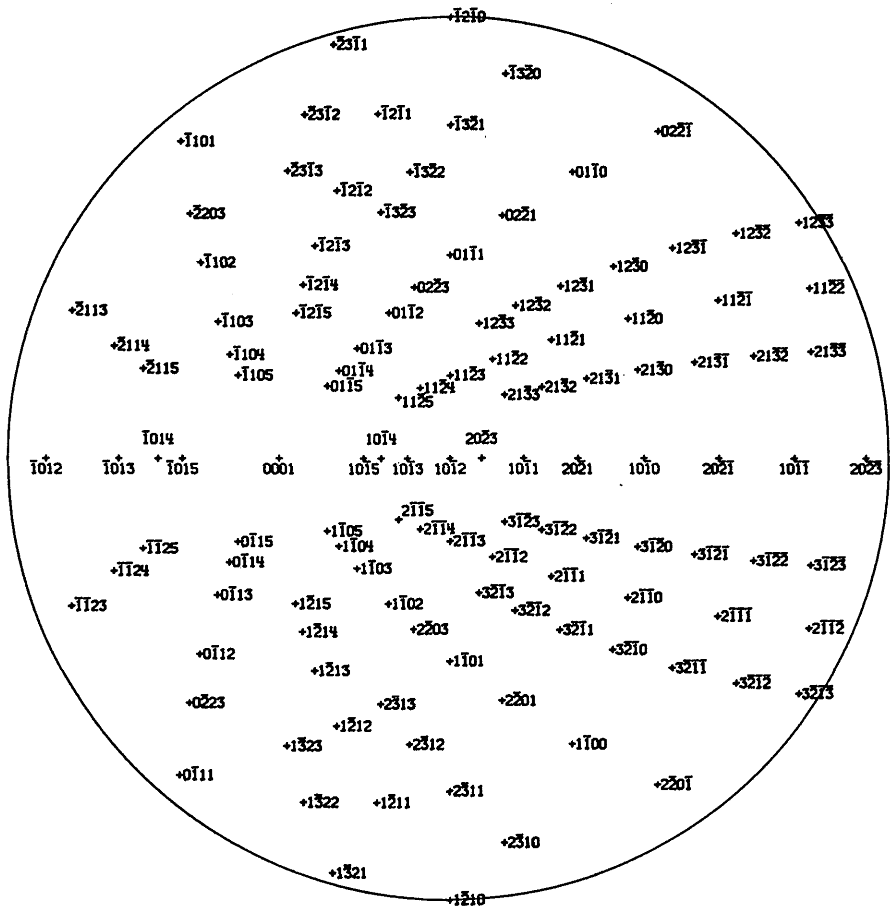


Fig. 10 - (10$\bar{1}$2) Stereographic projection of hafnium (1.5811)

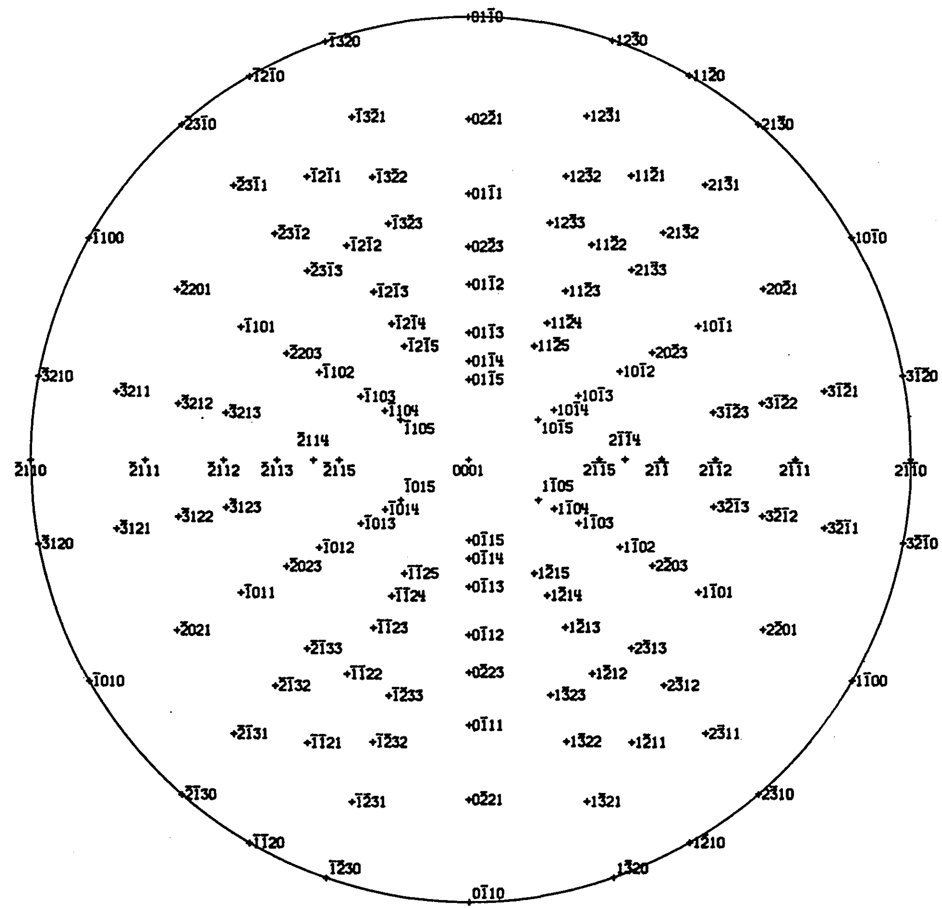


Fig. 11 - (0001) Stereographic projection of magnesium (1.6235)

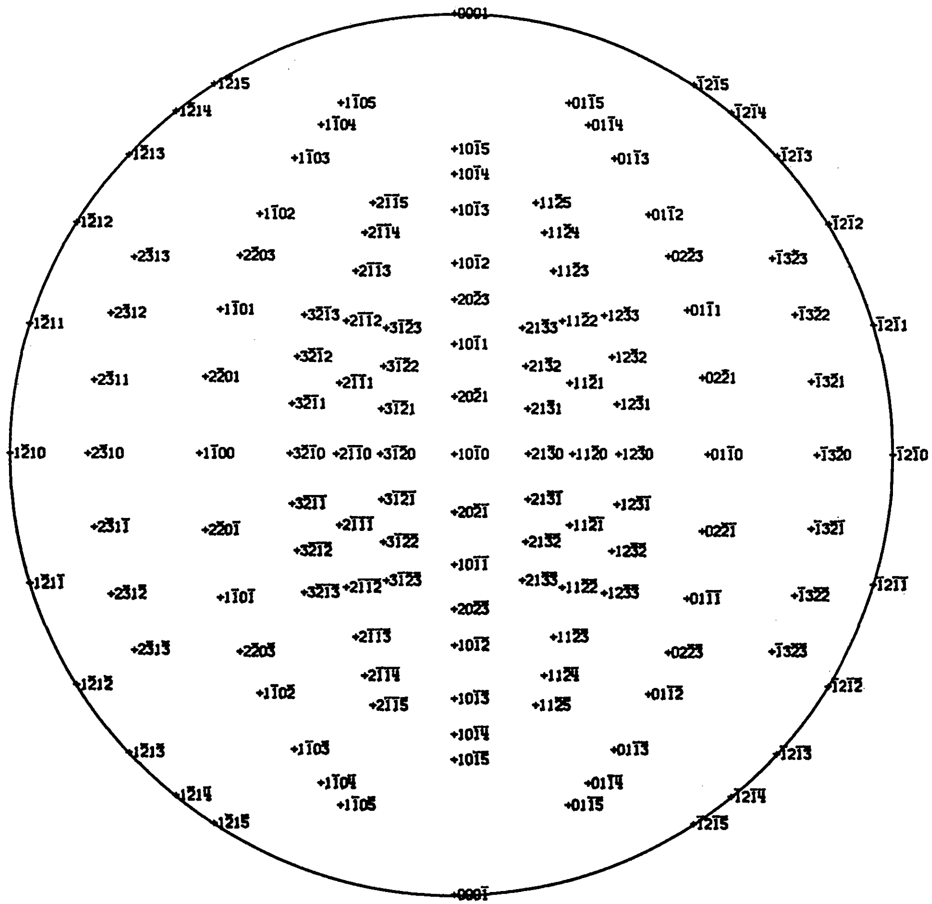


Fig. 12 - (10$\bar{1}$0) Stereographic projection of magnesium (1.6235)

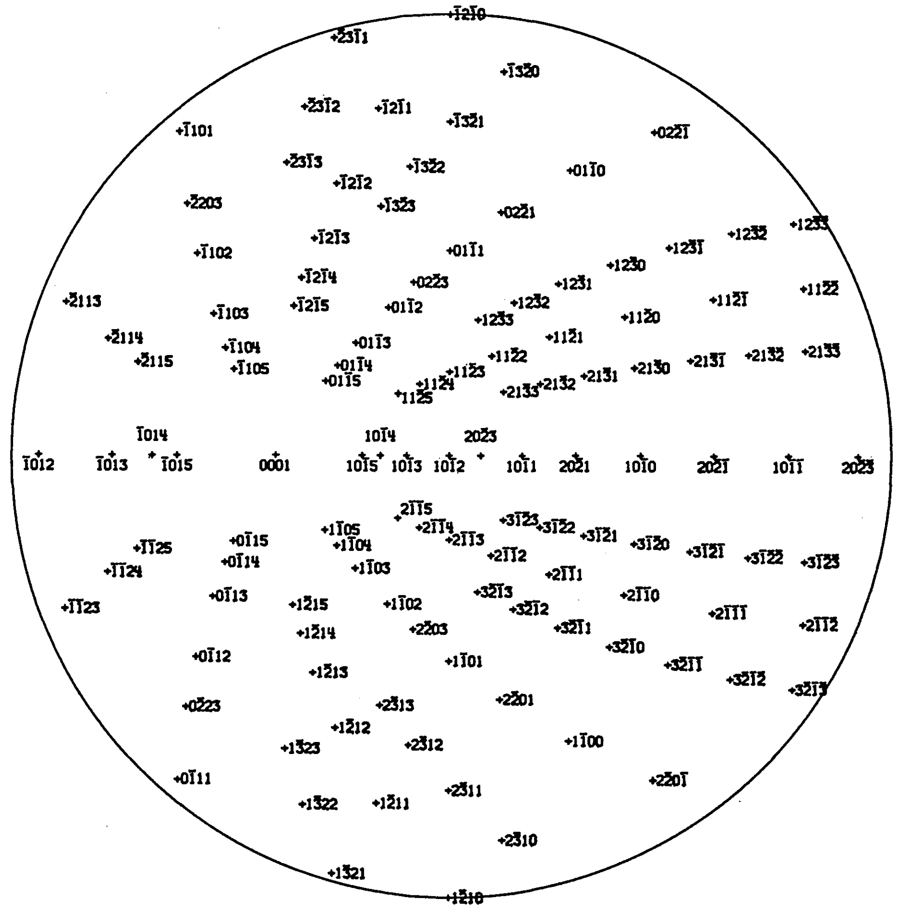


Fig. 13 - (10$\bar{1}$2) Stereographic projection of magnesium (1.6235)

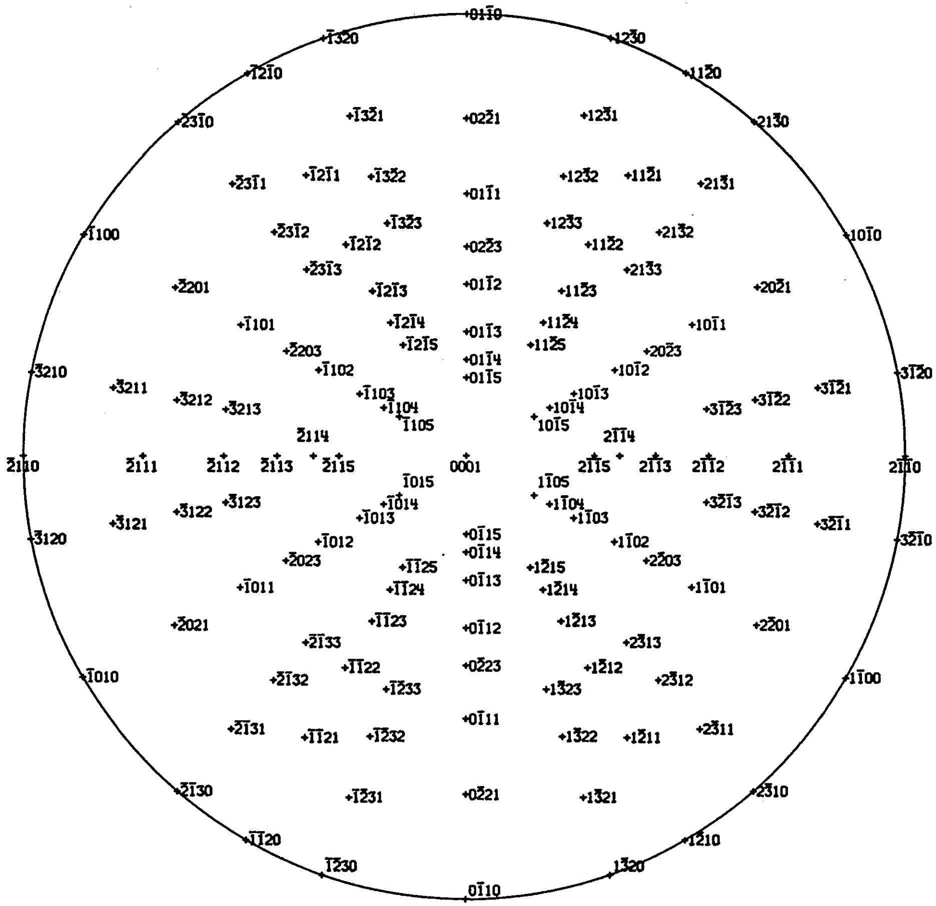


Fig. 14 - (0001) Stereographic projection of titanium (1.5873)

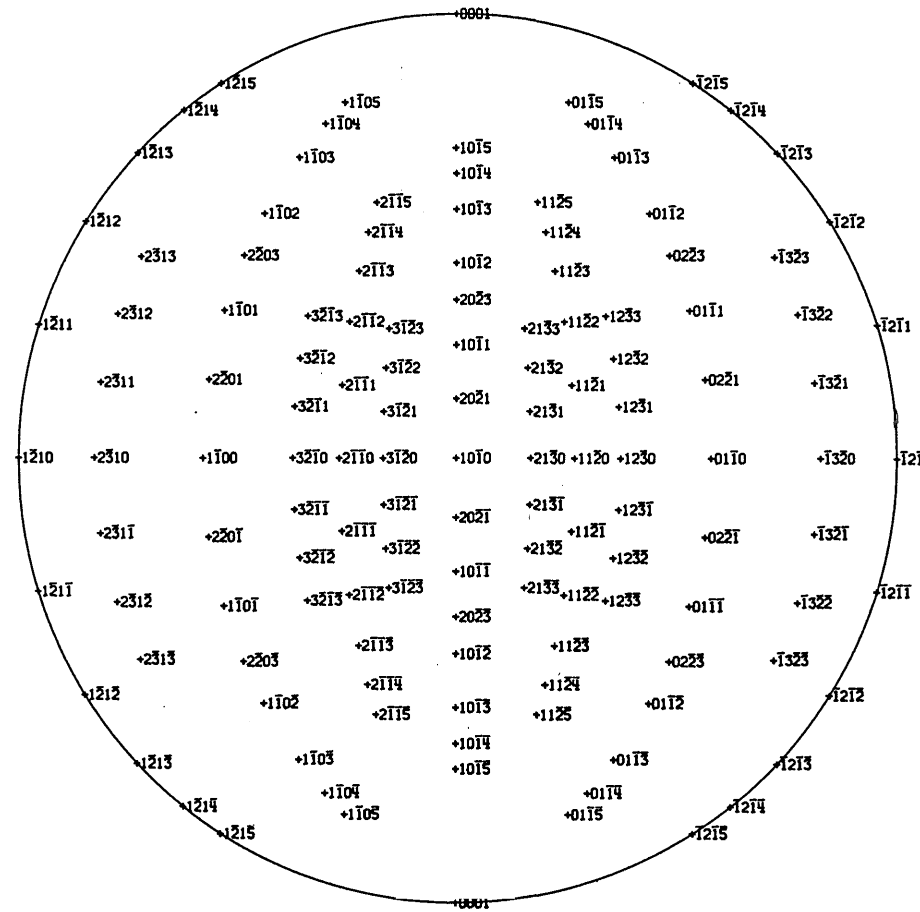


Fig. 15 - (10$\bar{1}$0) Stereographic projection of titanium (1.5873)

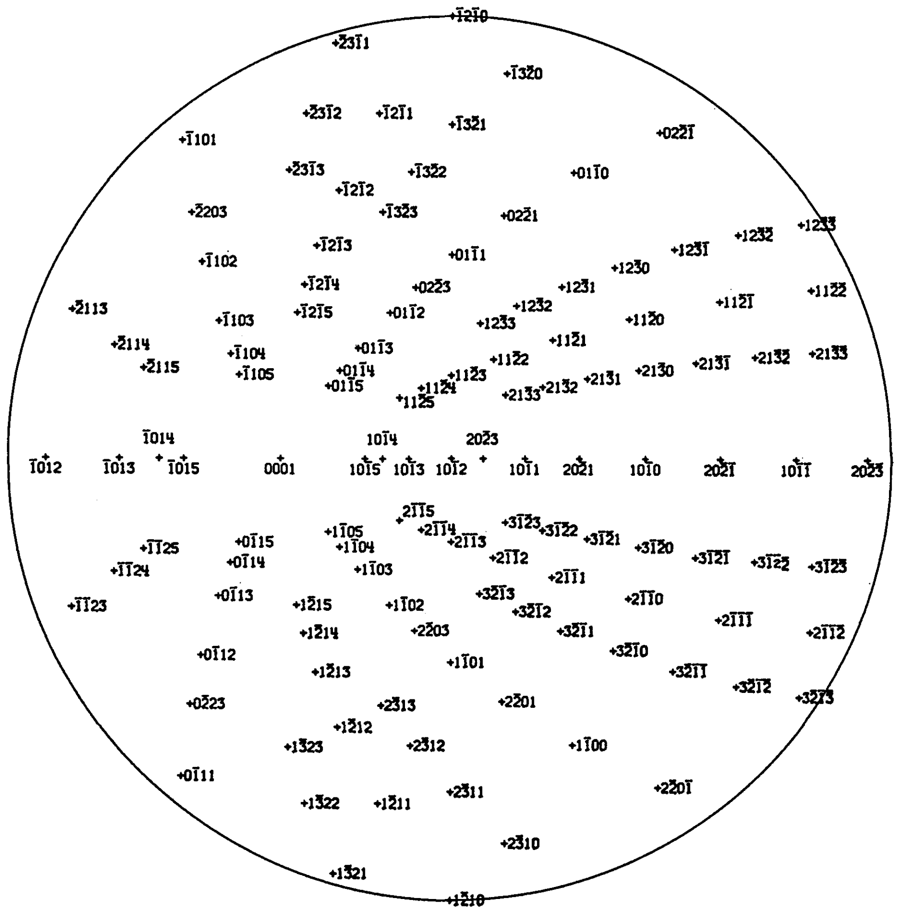


Fig. 16 - ($10\bar{1}2$) Stereographic projection of titanium (1.5873)

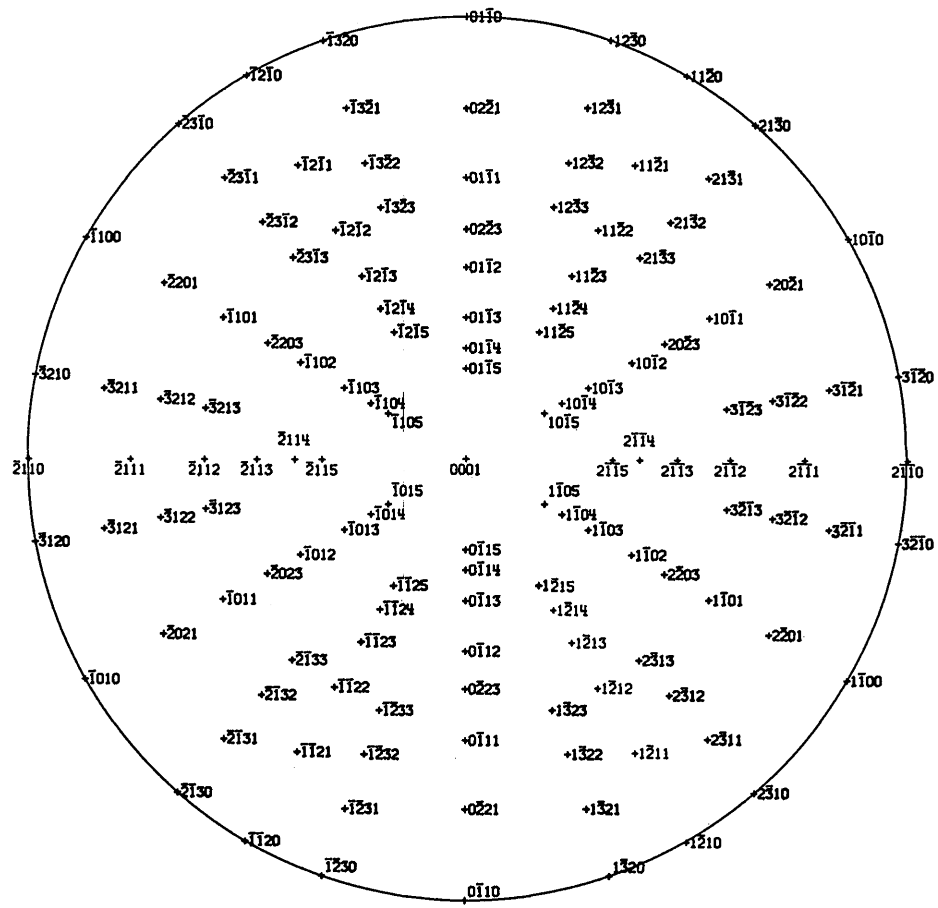


Fig. 17 - (0001) Stereographic projection of zinc (1.8562)

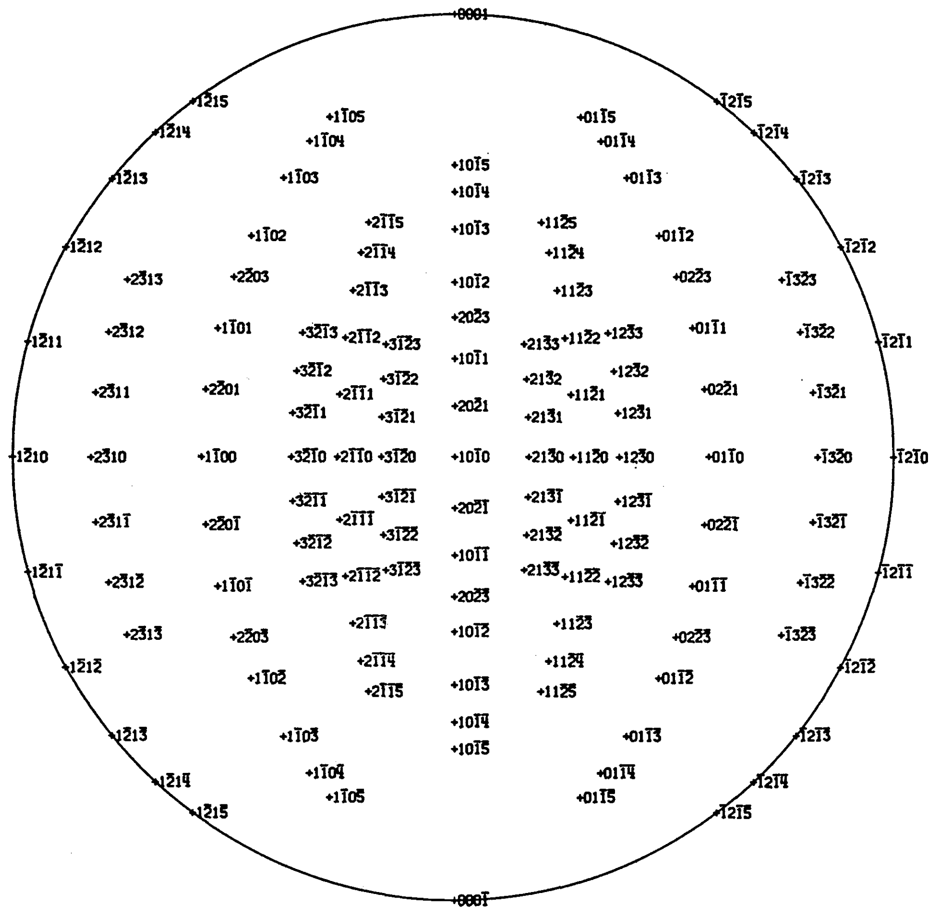


Fig. 18 - (10$\bar{1}$0) Stereographic projection of zinc (1.8562)

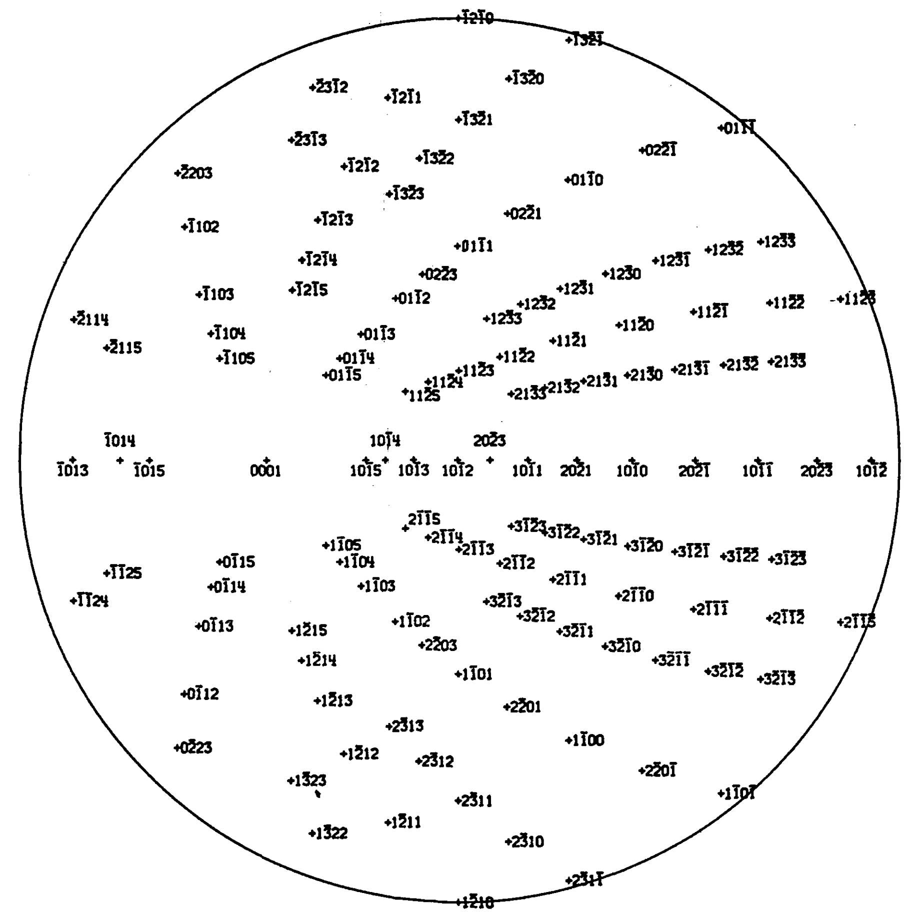


Fig. 19 - (10$\bar{1}$2) Stereographic projection of zinc (1.8562)

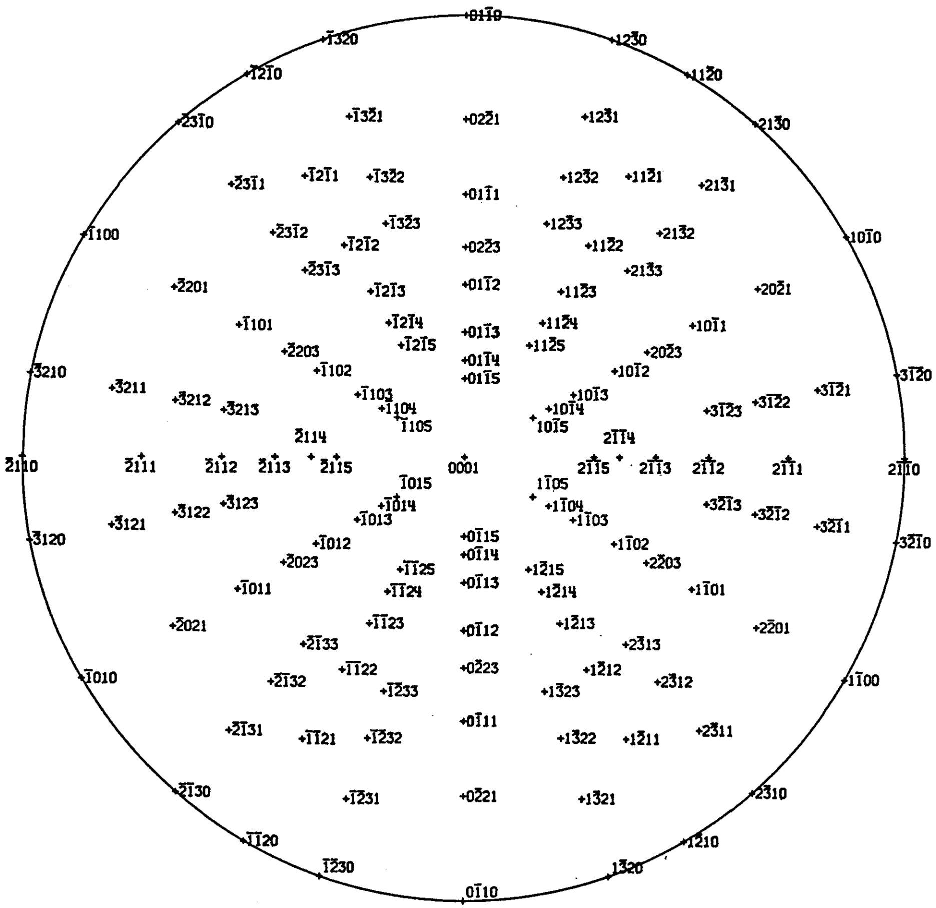


Fig. 20 - (0001) Stereographic projection of zirconium (1.5931)

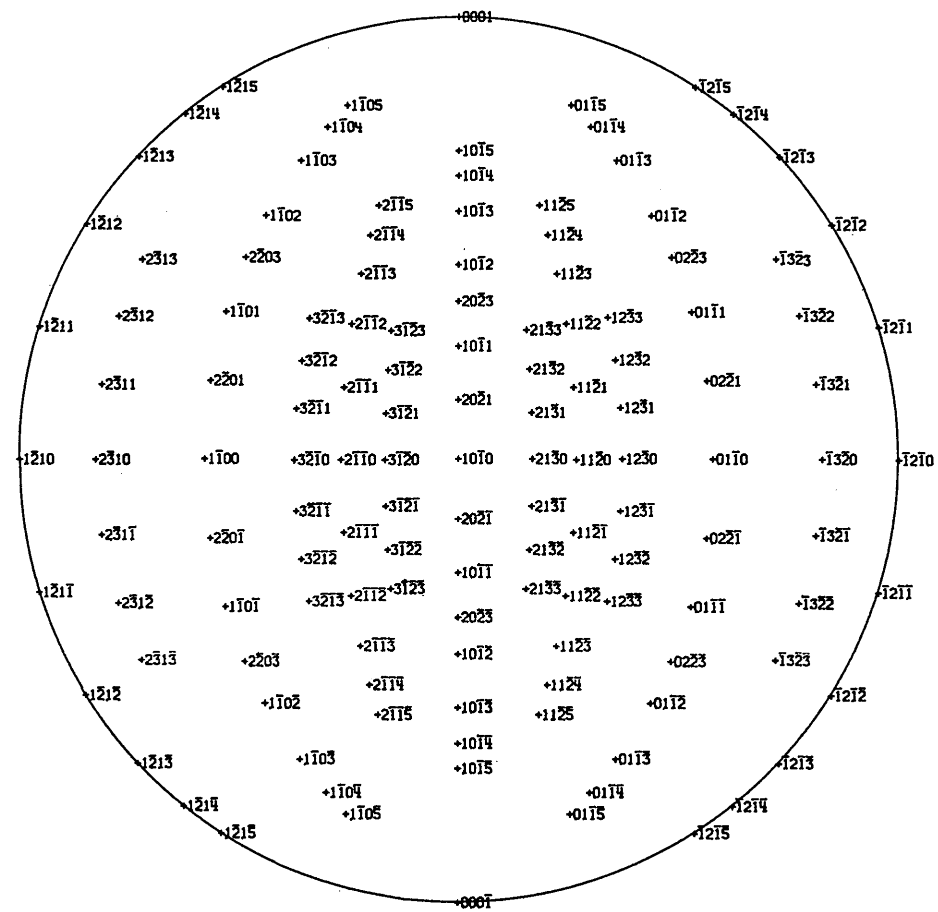


Fig. 21 - (10$\bar{1}$0) Stereographic projection of zirconium (1.5931)

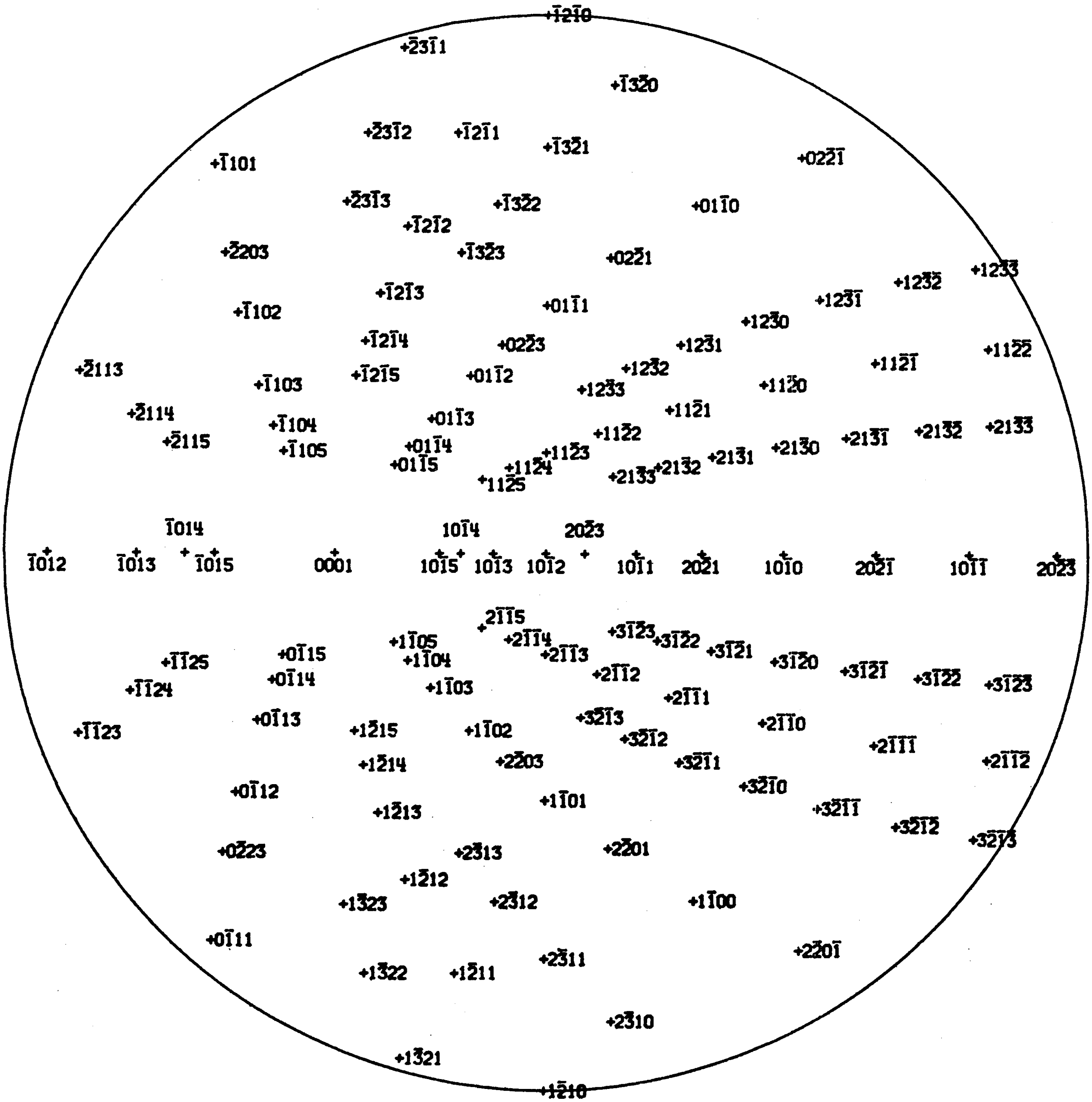


Fig. 22 - (101̅2) Stereographic projection of zirconium (1.5931)

Table 1
Angles Between Planes for Selected Hexagonal Metals

$h_1k_1i_1\ell_1$	$h_2k_2i_2\ell_2$	Axial (c/a) Ratio						
		Be (1.5677)	Cd (1.8856)	Hf (1.5811)	Mg (1.6235)	Ti (1.5873)	Zn (1.8562)	Zr (1.5931)
0001	0001	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	$10\bar{1}0$	90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$20\bar{2}1$	74.56	77.07	74.68	75.07	74.74	76.87	74.79
	$10\bar{1}1$	61.08	65.33	61.29	61.92	61.38	64.99	61.47
	$20\bar{2}3$	50.35	55.44	50.59	51.34	50.70	55.01	50.81
	$10\bar{1}2$	42.15	47.43	42.39	43.15	42.50	46.98	42.61
	$10\bar{1}3$	31.11	35.97	31.32	32.00	31.42	35.54	31.52
	$10\bar{1}4$	24.35	28.56	24.53	25.11	24.62	28.18	24.70
	$10\bar{1}5$	19.90	23.53	20.06	20.55	20.13	23.20	20.20
	$11\bar{2}0$	90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}1$	72.31	75.15	72.45	72.88	72.52	74.92	72.58
	$11\bar{2}2$	57.47	62.06	57.69	58.37	57.79	61.69	57.88
	$11\bar{2}3$	46.26	51.50	46.51	47.26	46.62	51.06	46.72
	$11\bar{2}4$	38.09	43.31	38.33	39.07	38.44	42.86	38.54
	$11\bar{2}5$	32.09	37.03	32.31	33.00	32.41	36.59	32.51
	$12\bar{3}0$	90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$12\bar{3}1$	78.21	80.15	78.30	78.60	78.35	80.00	78.39
	$12\bar{3}2$	67.34	70.85	67.51	68.04	67.59	70.57	67.66
	$12\bar{3}3$	57.94	62.49	58.16	58.83	58.26	62.12	58.35

Table 2
Angles Between Planes for Selected Hexagonal Metals

$h_1k_1i_1\ell_1$	$h_2k_2i_2\ell_2$	Axial (c/a) Ratio						
		Be (1.5677)	Cd (1.8856)	Hf (1.5811)	Mg (1.6235)	Ti (1.5873)	Zn (1.8562)	Zr (1.5931)
$10\bar{1}0$	0001	90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$10\bar{1}0$	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		60.00	60.00	60.00	60.00	60.00	60.00	60.00
	$20\bar{2}1$	15.44	12.93	15.32	14.93	15.26	13.13	15.21
		61.19	60.84	61.67	61.11	61.16	60.86	61.15
	$10\bar{1}1$	28.92	24.67	28.71	28.08	28.62	25.01	28.53
		64.05	62.98	63.99	63.82	63.96	63.06	63.94
	$20\bar{2}3$	39.65	34.56	39.41	38.66	39.30	34.99	39.19
		67.36	65.69	67.27	67.02	67.24	65.82	67.20
	$10\bar{1}2$	47.85	42.57	47.61	46.85	47.50	43.02	47.39
		70.40	68.39	70.30	70.01	70.26	68.56	70.22
	$10\bar{1}3$	58.89	54.03	58.68	58.00	58.58	54.46	58.48
		75.03	72.92	74.93	74.64	74.89	73.10	74.85
	$10\bar{1}4$	65.65	61.44	65.47	64.89	65.38	61.82	65.30
		78.10	76.17	78.02	77.75	77.98	76.34	77.94
	$10\bar{1}5$	70.10	66.47	69.94	69.45	69.87	66.80	69.80
		80.20	78.48	80.13	79.89	80.09	78.64	80.06
	$11\bar{2}0$	30.00	30.00	30.00	30.00	30.00	30.00	30.00
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}1$	34.40	33.17	34.34	34.14	34.31	33.26	34.28
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}2$	43.10	40.08	42.95	42.49	42.88	40.32	42.82
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}3$	51.26	47.33	51.08	50.50	50.99	47.66	50.91
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}4$	57.71	53.55	57.52	56.92	57.43	53.90	57.35
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}5$	62.61	58.57	62.43	61.86	62.34	58.92	62.26
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$12\bar{3}0$	19.11	19.11	19.11	19.11	19.11	19.11	19.11
		40.89	40.89	40.89	40.89	40.89	40.89	40.89
		79.11	79.11	79.11	79.11	79.11	79.11	79.11

(Table Continues)

Table 2 (Continued)
Angles Between Planes for Selected Hexagonal Metals

$h_1k_1i_1\ell_1$	$h_2k_2i_2\ell_2$	Axial (c/a) Ratio						
		Be (1.5677)	Cd (1.8856)	Hf (1.5811)	Mg (1.6235)	Ti (1.5873)	Zn (1.8562)	Zr (1.5931)
	$12\bar{3}1$	22.34	21.41	22.29	22.14	22.27	21.48	22.24
		42.27	41.86	42.25	42.18	42.24	41.89	42.23
		79.34	79.27	79.34	79.32	79.33	79.27	79.33
	$12\bar{3}2$	29.32	26.79	29.19	28.80	29.13	26.99	29.07
		45.77	44.43	45.70	45.49	45.67	44.53	45.64
		79.96	79.72	79.94	79.91	79.94	79.73	79.93
	$12\bar{3}3$	36.79	33.06	36.61	36.05	36.53	33.36	36.45
		50.16	47.90	50.05	49.70	49.99	48.07	49.95
		80.78	80.35	80.76	80.69	80.75	80.38	80.74

Table 3
Angles Between Planes for Selected Hexagonal Metals

$h_1k_1i_1\ell_1$	$h_2k_2i_2\ell_2$	Axial (c/a) Ratio						
		Be (1.5677)	Cd (1.8856)	Hf (1.5811)	Mg (1.6235)	Ti (1.5873)	Zn (1.8562)	Zr (1.5931)
$10\bar{1}2$	0001	42.15	47.43	42.39	43.15	42.50	46.98	42.61
	$10\bar{1}0$	47.85	42.57	47.61	46.85	47.50	43.02	47.39
		70.40	68.39	70.30	70.01	70.26	68.56	70.22
	$20\bar{2}1$	32.41	29.64	32.29	31.92	32.24	29.89	32.19
		58.61	55.50	58.65	58.77	58.67	56.15	58.69
		63.29	59.32	62.92	61.79	62.76	59.27	62.60
		82.76	78.03	82.53	81.82	82.42	78.40	82.32
	$10\bar{1}1$	18.93	17.90	18.90	18.78	18.88	18.01	18.86
		49.29	51.91	49.42	49.83	49.48	51.70	49.54
		76.77	67.24	76.32	74.93	76.11	68.03	75.92
		86.28	87.00	86.61	87.61	86.76	87.55	86.90
	$20\bar{2}3$	8.21	8.01	8.20	8.19	8.20	8.03	8.20
		43.00	46.61	43.17	43.71	43.25	46.32	43.33
		77.60	77.13	77.97	79.11	78.14	78.00	78.30
		87.50	85.38	87.02	85.52	86.79	84.74	86.59
	$10\bar{1}2$	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		39.21	43.21	39.40	39.99	39.49	42.88	39.57
		71.06	79.25	71.45	72.63	71.62	78.57	71.79
		84.30	85.14	84.78	86.29	85.01	86.04	85.21
	$10\bar{1}3$	11.04	11.46	11.07	11.15	11.08	11.44	11.09
		36.09	40.20	36.28	36.88	36.37	39.86	36.45
		62.52	70.66	62.89	64.05	63.06	69.96	63.22
		73.26	83.40	73.71	75.15	73.93	82.53	74.12
	$10\bar{1}4$	17.80	18.87	17.86	18.04	17.89	18.80	17.91
		35.53	39.63	35.72	36.32	35.81	39.29	35.69
		57.51	65.28	57.87	58.97	58.03	64.62	58.18
		66.50	75.99	66.92	68.26	67.12	75.17	67.30
	$10\bar{1}5$	22.25	23.90	22.33	22.59	22.37	23.78	22.41
		35.77	39.89	35.96	36.56	36.05	39.55	36.14
		54.34	61.76	54.68	55.73	54.84	61.12	54.98
		62.50	70.96	62.45	63.70	62.63	70.18	62.81

(Table Continues)

Table 3 (Continued)
Angles Between Planes for Selected Hexagonal Metals

$h_1k_1i_1\ell_1$	$h_2k_2i_2\ell_2$	Axial (c/a) Ratio						
		Be (1.5677)	Cd (1.8856)	Hf (1.5811)	Mg (1.6235)	Ti (1.5873)	Zn (1.8562)	Zr (1.5931)
	$11\bar{2}0$	54.47	50.37	54.28	53.68	54.19	50.71	54.11
		90.00	90.00	90.00	90.00	90.00	90.00	90.00
	$11\bar{2}1$	38.83	37.83	38.80	38.67	38.78	37.92	38.76
		70.83	63.07	70.49	69.43	70.33	64.28	70.19
		76.98	80.02	77.13	77.60	77.20	79.78	77.27
	$11\bar{2}2$	27.29	28.31	27.35	27.51	27.37	28.24	27.40
		66.50	71.52	66.75	67.50	66.86	71.12	66.96
		84.76	75.73	84.34	83.01	84.14	76.48	83.96
	$11\bar{2}3$	21.18	23.03	21.27	21.55	21.31	22.89	21.35
		59.17	65.09	59.45	60.32	59.58	64.61	59.70
		84.68	85.53	85.14	86.55	85.35	86.35	85.54
	$11\bar{2}4$	19.60	21.61	19.70	19.99	19.74	21.44	19.78
		54.30	60.51	54.59	55.50	54.73	60.00	54.85
		77.00	86.86	77.45	78.86	77.66	86.02	77.85
	$11\bar{2}5$	20.47	22.46	20.56	20.86	20.61	22.30	20.65
		51.09	57.31	51.38	52.27	51.51	56.79	51.63
		71.37	81.02	71.81	73.18	72.02	80.19	77.20
	$12\bar{3}0$	50.65	45.90	50.43	49.74	50.33	46.30	50.23
		59.52	56.17	59.36	58.87	59.29	56.45	59.22
		82.71	82.00	82.68	82.57	82.66	82.06	82.65
	$12\bar{3}1$	39.44	36.74	39.33	38.95	39.27	36.98	39.22
		49.60	48.38	49.55	49.39	49.53	48.49	49.50
		62.02	55.25	61.70	60.71	61.55	55.81	61.42
		69.82	64.35	69.55	68.74	69.43	64.80	69.32
		74.00	75.36	74.07	74.28	74.10	75.25	74.13
		88.43	88.77	88.57	89.00	88.63	88.99	88.69
	$12\bar{3}2$	29.45	28.45	29.41	29.29	29.39	28.55	29.38
		41.08	41.60	41.11	41.21	41.13	41.57	41.14
		66.25	64.18	66.41	66.88	66.48	64.87	66.54
		72.58	69.31	72.18	70.95	72.00	69.07	71.83

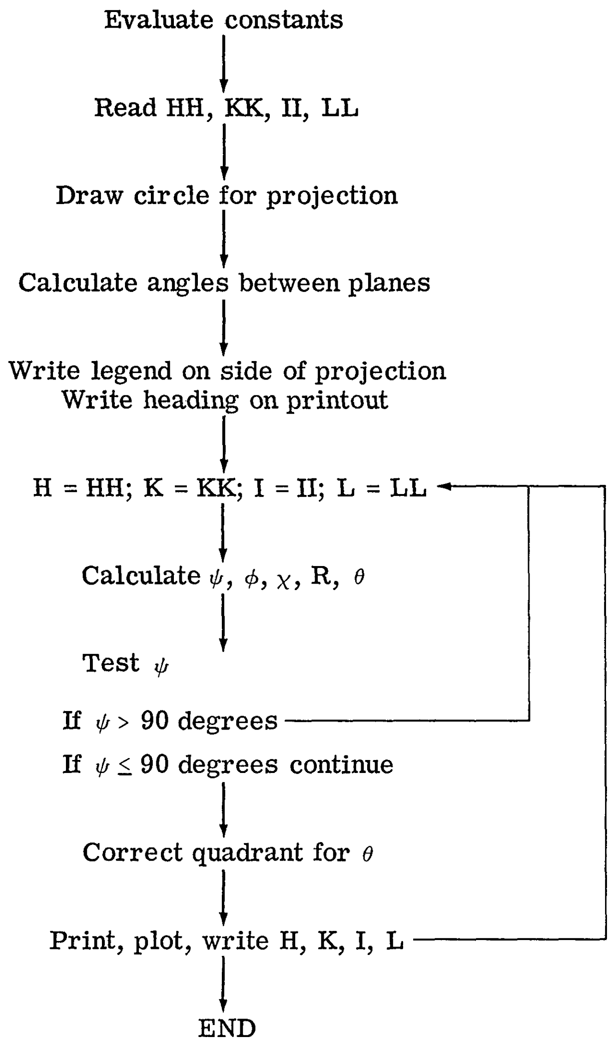
(Table Continues)

Table 3 (Continued)
Angles Between Planes for Selected Hexagonal Metals

$h_1k_1i_1\ell_1$	$h_2k_2i_2\ell_2$	Axial (c/a) Ratio						
		Be (1.5677)	Cd (1.8856)	Hf (1.5811)	Mg (1.6235)	Ti (1.5873)	Zn (1.8562)	Zr (1.5931)
		79.49	72.30	79.14	78.08	78.99	72.88	78.84
		80.29	84.81	80.51	81.20	80.62	84.46	80.71
	$12\bar{3}3$	21.42	21.62	21.44	21.48	21.44	21.61	21.45
		34.57	36.27	34.65	34.92	34.69	36.14	34.73
		59.93	64.16	60.14	60.78	60.23	63.82	60.32
		73.38	72.26	73.65	74.51	73.78	73.04	73.90
		81.73	79.10	81.29	79.90	81.08	78.64	80.89
		87.92	79.55	87.52	86.29	87.34	80.24	87.17

Appendix A

COMPUTER PROGRAM FLOW CHART



Appendix B

COMPUTER PROGRAM FOR STEREOGRAPHIC PROJECTIONS AND ANGLES BETWEEN PLANES

```
      PROGRAM PROJECT
      EXTERNAL ABSF
      TYPE INTEGER H,K,I,L,HH(220),KK(220),II(220),LL(220)
      DIMENSION ABUFFER(254),BBUFFER(254),CBUFFER(254)
C
C     C AND A VALUES SPECIFY C/A RATIO
C
      C = 1.5873  $  A = 1.0000                                         TI
C
C     CONSTANTS USED LATER IN THE PROGRAM
C
      RADIUS = 5. $ ADDX = 10. $ ADDY = 5.
      CONV = 57.29577
      CON = SQRT(0.75*(A/C)**2)
      COM = SQRT(1.)
      COP = SQRT(1. + 3.*(A/C)**2)
      COR = SQRT(3.)
      COT = SQRT(4.+(27./4.)*(A/C)**2)
      COMP = 1.5708
      NN = 0
      IJ = 0
   50 IJ = IJ + 1
  100 READ 101,HH(IJ),KK(IJ),II(IJ),LL(IJ)
  101 FORMAT(4I3)
      NN = NN + 1
      IF(EOF,5) 51,50
   51 CONTINUE
      DO 1 IJK = 1,3
      GO TO (60,61,62),IJK
   60 CALL PLOTS(ABUFFER,254,1)
      GO TO 65
   61 CALL PLOTS(BBUFFER,254,1)
      CALL PLOT(0.,0.,-3)
      GO TO 65
   62 CALL PLOTS(CBUFFER,254,1)
      CALL PLOT(0.,0.,-3)
   65 CONTINUE
C
C     DRAW A CIRCLE OF RADIUS 5.0 ABOUT X = 10.,Y = 5.
C
      CALL PLOT(5.,5.,3)
      DELX = .01
      XR = 5.
  900 XR = XR + DELX
      IF(15.-XR) 901,902,902
  902 ARGU=ABSF(RADIUS**2-(XR-ADDX)**2)
      ARG = SQRT(ARGU)
  905 YR = ARG + ADDY
      CALL PLOT(XR,YR,2)
      GO TO 900
  901 CALL PLOT(15.,5.,2)
      XR = 15.
  909 XR = XR - DELX
  910 IF(XR-5.) 911,912,912
  912 ARGU = ABSF(RADIUS**2 - (XR-ADDX)**2)
```

```
      ARG = SQRT(ARGU)
  915 YR = ADDY - ARG
      CALL PLOT(XR,YR,2)
      GO TO 909
  911 CONTINUE
      CALL PLOT(5.,5.,2)
C
C     BETA1 = ANGLE BETWEEN THE  0 0 0 1 AND THE  2-1-1 0 PLANES
C     BETA2 = ANGLE BETWEEN THE  1 0-1 0 AND THE -1 2-1 0 PLANES
C     BETA3 = ANGLE BETWEEN THE  1 0-1 2 AND THE  2 0-2-3 PLANES
C
      ARGBETA1 = 0.0
      ARGBETA2 = 0.0
      ARGBETA3 = (2.-4.5*(A/C)**2)/(COT*COP)
      IF(ABSF(ARGBETA1)-1.) 310,310,311
  311 IF(ARGBETA1) 312,310,313
  312 ARGBETA1 = -1.
      GO TO 310
  313 ARGBETA1 = 1.
  310 BETA1 = ACOS(ARGBETA1)
      IF(ABSF(ARGBETA2)-1.) 315,315,316
  316 IF(ARGBETA2) 317,315,318
  317 ARGBETA2 = -1.
      GO TO 315
  318 ARGBETA2 = 1.
  315 BETA2 = ACOS(ARGBETA2)
      IF(ABSF(ARGBETA3)-1.) 320,320,321
  321 IF(ARGBETA3) 322,320,323
  322 ARGBETA3 = -1.
      GO TO 320
  323 ARGBETA3 = 1.
  320 BETA3 = ACOS(ARGBETA3)
C
C     RHO1 = ANGLE BETWEEN THE  0 0 0 1 AND THE  0 1-1 0 PLANES
C     RHO2 = ANGLE BETWEEN THE  1 0-1 0 AND THE  0 0 0 1 PLANES
C     RHO3 = ANGLE BETWEEN THE  1 0-1 2 AND THE -1 2-1 0 PLANES
C
      ARGRHO1 = 0.0
      ARGRHO2 = 0.0
      ARGRHO3 = 0.0
      IF(ABSF(ARGRHO1)-1.) 325,325,326
  326 IF(ARGRHO1) 327,325,328
  327 ARGRHO1 = -1.
      GO TO 325
  328 ARGRHO1 = 1.
  325 RHO1 = ACOS(ARGRHO1)
      IF(ABSF(ARGRHO2)-1.) 330,330,331
  331 IF(ARGRHO2) 332,330,333
  332 ARGRHO2 = -1.0
      GO TO 330
  333 ARGRHO2 = 1.
  330 RHO2 = ACOS(ARGRHO2)
      IF(ABSF(ARGRHO3)-1.) 335,335,336
  336 IF(ARGRHO3) 337,335,338
  337 ARGRHO3 = -1.
      GO TO 335
  338 ARGRHO3 = 1.
  335 RHO3 = ACOS(ARGRHO3)
      ABETA1 = CONV*BETA1  $ ABETA2 = CONV*BETA2
```

```
      ABETA3 = CONV*BETA3
      ARHO1 = CONV*RHO1    $ ARHO2 = CONV*RHO2
      ARHO3 = CONV*RHO3
      PRINT 40,ABETA1,ABETA2,ABETA3
   40 FORMAT(1H1,4X,9H BETA1 = ,F9.5,9H BETA2 = ,F9.5,9H BETA3 = ,
     1 F9.5//)
      PRINT 41, ARHO1,ARHO2,ARHO3
   41 FORMAT(5X,8H RHO1 = ,F9.5,8H RHO2 = ,F9.5,8H RHO3 = ,F9.5//)
C
C     LEGEND WRITTEN ON SIDE OF PROJECTION
C
      GO TO (98,198,298) , IJK
   98 CALL SYMBOL(0.5,6.1,0.280,15HSTANDARD (0001),0.0,15)
      GO TO 10
  198 CALL SYMBOL(0.5,6.1,0.280,15HSTANDARD (1010),0.0,15)
  199 CALL SYMBOL(3.38,6.3,0.280,1H-,0.0,1)
      GO TO 10
  298 CALL SYMBOL(0.5,6.1,0.280,15HSTANDARD (1012),0.0,15)
  299 CALL SYMBOL(3.38,6.3,0.280,1H-,0.0,1)
   10 CONTINUE
      CALL SYMBOL(0.5,5.4,0.280,13HPROJECTION OF,0.0,13)
      CALL SYMBOL(0.5,4.7,0.280,6HPLANES,0.0,6)
      CALL SYMBOL(0.5,4.0,0.280,14H(C/A = 1.5873),0.0,14)
C
C     HEADING WRITTEN ON TOP OF PAGE
C
      GO TO (399,1399,2399) , IJK
  399 PRINT 411,C
  411 FORMAT(1H1,38H STANDARD PROJECTION ( 0 0 0 1) C/A = ,F6.4//)
      GO TO 11
 1399 PRINT 1412,C
 1412 FORMAT(1H1,38H STANDARD PROJECTION ( 1 0-1 0) C/A = ,F6.4//)
      GO TO 11
 2399 PRINT 2413,C
 2413 FORMAT(1H1,38H STANDARD PROJECTION ( 1 0-1 2) C/A = ,F6.4//)
   11 CONTINUE
C
      IK = 0
   90 IK = IK + 1
      H = HH(IK)
      K = KK(IK)
      I = II(IK)
      L = LL(IK)
      AH = H $AK = K $ AI = I $ AL = L
      UNEED = SQRT(AH**2 + AK**2 + AH*AK + 0.75*AL*AL*(A/C)**2)
C
C     PSI1 = ANGLE BETWEEN 0001 AND HKIL PLANE
C     PSI2 = ANGLE BETWEEN 10-10 AND HKIL PLANE
C     PSI3 = ANGLE BETWEEN 10-12 AND HKIL PLANE
C
      ARGPSI1 = (.75*AL*(A/C)**2)/(CON*UNEED)
      ARGPSI2 = (AH+.5*AK)/(COM*UNEED)
      ARGPSI3 = (AH+.5*AK+1.5*AL*(A/C)**2)/(COP*UNEED)
      IF(ABSF(ARGPSI1)-1.) 355,355,356
  356 IF(ARGPSI1) 357,355,358
  357 ARGPSI1 = -1.
      GO TO 355
  358 ARGPSI1 = 1.
  355 PSI1 = ACOS(ARGPSI1)
```

```
      IF(ABSF(ARGPSI2)-1.) 360,360,361
  361 IF(ARGPSI2) 362,360,363
  362 ARGPSI2 = -1.
      GO TO 360
  363 ARGPSI2 = 1.
  360 PSI2 = ACOS(ARGPSI2)
      IF(ABSF(ARGPSI3)-1.) 365,365,366
  366 IF(ARGPSI3) 367,365,368
  367 ARGPSI3 = -1.
      GO TO 365
  368 ARGPSI3 = 1.
  365 PSI3 = ACOS(ARGPSI3)
C
C     PHI1 = ANGLE BETWEEN THE HKIL AND THE  2-1-1 0 PLANES
C     PHI2 = ANGLE BETWEEN THE HKIL AND THE -1 2-1 0 PLANES
C     PHI3 = ANGLE BETWEEN THE HKIL AND THE  2 0-2-3 PLANES
C
      ARGPHI1 = (2.*AH-AK+0.5*(2.*AK-AH))/(COR*UNEED)
      ARGPHI2 = (-AH+2.*AK+0.5*(2.*AH-AK))/(COR*UNEED)
      ARGPHI3 = (2.*AH+AK-(9./4.)*AL*(A/C)**2)/(COT*UNEED)
      IF(ABSF(ARGPHI1)-1.) 370,370,371
  371 IF(ARGPHI1) 372,370,373
  372 ARGPHI1 = -1.
      GO TO 370
  373 ARGPHI1 = 1.
  370 PHI1 = ACOS(ARGPHI1)
      IF(ABSF(ARGPHI2)-1.) 375,375,376
  376 IF(ARGPHI2) 377,375,378
  377 ARGPHI2 = -1.
      GO TO 375
  378 ARGPHI2 = 1.
  375 PHI2 = ACOS(ARGPHI2)
      IF(ABSF(ARGPHI3)-1.) 380,380,381
  381 IF(ARGPHI3) 382,380,383
  382 ARGPHI3 = -1.
      GO TO 380
  383 ARGPHI3 = 1.
  380 PHI3 = ACOS(ARGPHI3)
C
C     CHI1 = ANGLE BETWEEN THE HKIL AND THE  0 1-1 0 PLANES
C     CHI2 = ANGLE BETWEEN THE HKIL AND THE  0 0 0 1 PLANES
C     CHI3 = ANGLE BETWEEN THE HKIL AND THE -1 2-1 0 PLANES
C
      ARGCHI1 = (AK+0.5*AH)/(COM*UNEED)
      ARGCHI2 = (0.75*AL*(A/C)**2)/(CON*UNEED)
      ARGCHI3 = (-AH+2.*AK+0.5*(2.*AK-AH))/(COR*UNEED)
      IF(ABSF(ARGCHI1)-1.) 340,340,341
  341 IF(ARGCHI1) 342,340,343
  342 ARGCHI1 = -1.
      GO TO 340
  343 ARGCHI1 = 1.
  340 CHI1 = ACOS(ARGCHI1)
      IF(ABSF(ARGCHI2)-1.) 345,345,346
  346 IF(ARGCHI2) 347,345,348
  347 ARGCHI2 = -1.
      GO TO 345
  348 ARGCHI2 = 1.
  345 CHI2 = ACOS(ARGCHI2)
      IF(ABSF(ARGCHI3)-1.) 350,350,351
```

```
  351 IF(ARGCHI3) 352,350,353
  352 ARGCHI3 = -1.
      GO TO 350
  353 ARGCHI3 = 1.
  350 CHI3 = ACOS(ARGCHI3)
C
C     CONVERT ANGLES FROM RADIANS TO DEGREES
C
      APHI1 = CONV*PHI1    $ APHI2 = CONV*PHI2
      APHI3 = CONV*PHI3
      ACHI1 = CONV*CHI1   $  ACHI2 = CONV*CHI2
      ACHI3 = CONV*CHI3
      APSI1 = CONV * PSI1  $   APSI2 = CONV * PSI2
      APSI3 = CONV * PSI3
C
C     R1 IS THE RADIAL POLAR COORDINATE OF THE HKIL POLE IN A 0001
C     STANDARD PROJECTION
C     R2 IS THE RADIAL POLAR COORDINATE OF THE HKIL POLE IN AN 10-10
C     STANDARD PROJECTION
C     R3 IS THE RADIAL POLAR COORDINATE OF THE HKIL POLE IN AN 10-12
C     STANDARD PROJECTION
C     ARTHETA1 IS THE ARGUMENT OF THE INVERSE COSINE OF THE ANGLE THETA1
C     WHICH IS THE ANGULAR POLAR COORDINATE OF THE HKIL POLE IN THE
C     0001 STANDARD PROJECTION
C     ARTHETA2 IS THE ARGUMENT OF THE INVERSE COSINE OF THE ANGLE THETA2
C     WHICH IS THE ANGULAR POLAR COORDINATE OF THE HKIL POLE IN THE
C     10-10 STANDARD PROJECTION
C     ARTHETA3 IS THE ARGUMENT OF THE INVERSE COSINE OF THE ANGLE THETA3
C     WHICH IS THE ANGULAR POLAR COORDINATE OF THE HKIL POLE IN THE
C     10-12 STANDARD PROJECTION
C
      R1 = RADIUS * TANF(PSI1/2.)
      R2 = RADIUS * TANF(PSI2/2.)
      R3 = RADIUS * TANF(PSI3/2.)
      ARTHETA1 = (COS(PHI1)-COS(BETA1)*COS(PSI1))/(SIN(BETA1)*SIN(PSI1))
      ARTHETA2 = (COS(PHI2)-COS(BETA2)*COS(PSI2))/(SIN(BETA2)*SIN(PSI2))
      ARTHETA3 = (COS(PHI3)-COS(BETA3)*COS(PSI3))/(SIN(BETA3)*SIN(PSI3))
      GO TO (12,13,14),IJK
   12 CONTINUE
C
C     IF PSI1 IS GREATER THAN 90 DEGREES,HKIL POLE WILL NOT BE ON
C     (0001) PROJECTION
C
  203 IF(COMP - PSI1) 206,209,209
  209 CONTINUE
C
C     CORRECT QUADRANT FOR THETA1
C
      IF(ABSF(ARTHETA1)-1.)  700, 700, 701
  701 IF(ARTHETA1) 702, 700, 703
  702 ARTHETA1 = -1.
      GO TO 700
  703 ARTHETA1 = 1.
  700 THETA1 = ACOS(ARTHETA1)
      IF(RHO1 - CHI1) 501,502,502
  501 THETA1 = 2.*3.14159 - THETA1
      GO TO 502
C
C     CONVERT FROM POLAR COORDINATES (R1,THETA1) TO CARTESIAN
```

```
C       COORDINATES (X,Y)
C
  502 X = R1*COS(THETA1)
      Y = R1 * SIN(THETA1)
      ATHETA1 = CONV * THETA1
C
C     X1,Y1 ARE THE COORDINATES OF THE HKIL POLE AND WILL BE PLOTTED
C     ON THE (0001) PROJECTION
C
      X1 = X + ADDX  $ Y1 = Y + ADDY
      GO TO 15
   13 CONTINUE
C
C     IF PSI2 IS GREATER THAN 90 DEGREES,HKIL POLE WILL NOT BE ON
C     (10-10) PROJECTION
C
 1203 IF(COMP - PSI2) 206,1209,1209
 1209 CONTINUE
C
C     CORRECT QUADRANT FOR THETA2
C
      IF(ABSF(ARTHETA2)-1.) 1700,1700,1701
 1701 IF(ARTHETA2) 1702,1700,1703
 1702 ARTHETA2 = -1.
      GO TO 1700
 1703 ARTHETA2 = 1.
 1700 THETA2 = ACOS(ARTHETA2)
      IF(RHO2 - CHI2) 1501,1502,1502
 1501 THETA2 = 2.*3.14159 - THETA2
C
C     CONVERT FROM POLAR COORDINATES (R2,THETA2) TO CARTESIAN
C     COORDINATES (X,Y)
C
 1502 X = R2*COS(THETA2)
      Y = R2*SIN(THETA2)
      ATHETA2 = CONV * THETA2
C
C     X2,Y2 ARE THE COORDINATES OF THE HKIL POLE AND WILL BE PLOTTED
C     ON THE (10-10) PROJECTION
C
      X2 = X + ADDX   $  Y2 = Y + ADDY
      GO TO 15
   14 CONTINUE
C
C     IF PSI3 IS GREATER THAN 90 DEGREES,HKIL POLE WILL NOT BE ON
C     (10-12) PROJECTION
C
 2203 IF(COMP - PSI3) 206,2209,2209
 2209 CONTINUE
C
C     CORRECT QUADRANT FOR THETA3
C
      IF(ABSF(ARTHETA3)-1.) 2700,2700,2701
 2701 IF(ARTHETA3) 2702,2700,2703
 2702 ARTHETA3 = -1.
      GO TO 2700
 2703 ARTHETA3 = 1.
 2700 THETA3 = ACOS(ARTHETA3)
      IF(RHO3 - CHI3) 2501,2503,2503
```

```
 2501 THETA3 = 2.*3.14159 - THETA3
C
C     CONVERT FROM POLAR COORDINATES (R3,THETA3) TO CARTESIAN
C     COORDINATES (X,Y)
C
 2503 X = R3 * COS(THETA3)
      Y = R3*SIN(THETA3)
      ATHETA3 = CONV * THETA3
C
C     X3,Y3 ARE THE COORDINATES OF THE HKIL POLE AND WILL BE PLOTTED
C     ON THE (10-12) PROJECTION
C
      X3 = X + ADDX  $  Y3 = Y + ADDY
   15 CONTINUE
      IHX = ABSF(100.*X)
      IHY = ABSF(100.*Y)
      GO TO (398,1398,2398) , IJK
  398 PRINT 401,H,K,I,L,APSI1,APHI1,ACHI1,ATHETA1,X,Y,IHX,IHY
      CALL SYMBOL(X1,Y1,0.06,3,0.,-1)
  401 FORMAT(5X,4I3,8H PSI1 = ,F8.3,8H PHI1 = ,F8.3,8H CHI1 = ,F8.3,
     1 10H THETA1 = ,F8.3,5H X = ,F5.2,5H Y = ,F5.2,2I6/)
C
C     IN ORDER TO AVOID WRITING THE HKIL VALUES ON TOP OF EACH OTHER
C     THIS SERIES OF COMMANDS MOVES THE ORIGIN OF THE TROUBLESOME
C     HKIL VALUES
C
      IF(L-5) 920,820,920
  820 IF(H-1) 830,821,920
  821 IF(K) 822,823,920
  822 IF(K+1) 920,824,920
  824 IF(I) 920,840,920
  823 IF(I+1) 920,840,920
  830 IF(H+1) 920,831,920
  831 IF(K) 920,832,833
  832 IF(I-1) 920,840,920
  833 IF(K-1) 920,834,920
  834 IF(I) 920,840,920
  840 IF(Y) 841,920,842
  841 Y1Y = Y1 + 0.10
      X1X = X1 + 0.05
      GO TO 939
  842 Y1Y = Y1 - 0.15
      X1X = X1 + 0.05
      GO TO 939
  920 IF(IHY) 930,931,930
  931 IF(I  - 4) 932,933,932
  932 Y1Y = Y1 - 0.17
      X1X = X1 - 0.17
      GO TO 939
  933 Y1Y = Y1 + 0.17
      X1X = X1 - 0.17
      GO TO 939
  930 IF(Y1 - 0.50) 934,935,935
  934 Y1Y = Y1 + 0.05
      GO TO 936
  935 Y1Y = Y1 - 0.05
  936 X1X = X1 + 0.05
      GO TO 16
 1398 PRINT 402,H,K,I,L,APSI2,APHI2,ACHI2,ATHETA2,X,Y,IHX,IHY
```

```
      CALL SYMBOL(X2,Y2,0.06,3,0.,-1)
  402 FORMAT(5X,4I3,8H PSI2 = ,F8.3,8H PHI2 = ,F8.3,8H CHI2 = ,F8.3,
     1 10H THETA2 = ,F8.3,5H X = ,F5.2,5H Y = ,F5.2,2I6/)
      Y1Y = Y2 - 0.05
      X1X = X2 + 0.05
      GO TO 16
 2398 PRINT 403,H,K,I,L,APSI3,APHI3,ACHI3,ATHETA3,X,Y,IHX,IHY
      CALL SYMBOL(X3,Y3,0.06,3,0.,-1)
  403 FORMAT(5X,4I3,8H PSI3 = ,F8.3,8H PHI3 = ,F8.3,8H CHI3 = ,F8.3,
     1 10H THETA3 = ,F8.3,5H X = ,F5.2,5H Y = ,F5.2,2I6/)
      IF(IHY) 1920,1921,1920
 1921 IF(L-4) 1922,1923,1924
 1923 Y1Y = Y3 + 0.17
      X1X = X3 - 0.17
      GO TO 939
 1922 IF(L-3) 1924,1925,1924
 1925 IF(H-2) 1924,1923,1924
 1924 Y1Y - Y3 - 0.17
      X1X = X3 - 0.17
      GO TO 939
 1920 IF(L-5) 1930,1931,1930
 1931 IF(H-2) 1932,1933,1930
 1933 IF(K+1) 1930,1934,1930
 1934 IF(I+1) 1930,1935,1930
 1935 Y1Y = Y3 + 0.05
      X1X = X3 + 0.05
      GO TO 939
 1932 IF(H-1) 1930,1936,1930
 1936 IF(K-1) 1930,1937,1930
 1937 IF(I+2) 1930,1938,1930
 1938 Y1Y = Y3 - 0.10
      X1X = X3 + 0.05
      GO TO 939
 1930 Y1Y = Y3 - 0.05
      X1X = X3 + 0.05
      GO TO 939
   16 CONTINUE
C
C     THE FOLLOWING SERIES OF COMMANDS WRITES THE VALUES OF H,K,I, AND L
C     NEAR THE HKIL POLE
C
  939 IF(H) 940,941,941
  940 XX1 = X1X
      YY1 = Y1Y + 0.09
      CALL SYMBOL(XX1,YY1,0.105,1H-,0.0,1)
  941 CALL NUMBER(X1X,Y1Y,0.105,H,0.,2HI1)
      X2X = X1X + 0.09
      Y2Y = Y1Y
      IF(K) 950,951,951
  950 XX2 = X2X
      YY2 = Y2Y + 0.09
      CALL SYMBOL(XX2,YY2,0.105,1H-,0.0,1)
  951 CALL NUMBER(X2X,Y2Y,0.105,K,0.0,2HI1)
      X3X = X2X + 0.09
      Y3Y = Y2Y
      IF(I) 960,961,961
  960 XX3 = X3X
      YY3 = Y3Y + 0.09
      CALL SYMBOL(XX3,YY3,0.105,1H-,0.0,1)
```

```
      Y4Y = Y3Y
      IF(L) 970,971,971
  970 XX4 = X4X
      YY4 = Y4Y + 0.09
      CALL SYMBOL(XX4,YY4,0.105,1H-,0.0,1)
  971 CALL NUMBER(X4X,Y4Y,0.105,L,0.,2HI1)
  206 IF((NN-1)-IK) 2,2,90
    2 CALL PLOT(10.,5.,3)
      CALL PLOTS(0,0)
    1 CONTINUF
      CALL STOPPLOT
  301 FND
             SCOPE
'LOAD
'RUN,2,2500
  0  0  0  1
  1  0 -1  0
  1  0 -1  1
  1  0 -1  2
  1  0 -1  3
  1  0 -1  4
  1  0 -1  5
  1  0  1  5
  1  0  1  4
  1  0  1  3
  1  0  1  2
  1  0  1  1
  1  0  1  0
  0  1 -1  0
  0  1 -1  1
  0  1 -1  2
  0  1 -1  3
  0  1 -1  4
  0  1 -1  5
  0 -1  1  5
  0 -1  1  4
  0 -1  1  3
  0 -1  1  2
  0 -1  1  1
  0 -1  1  0
 -1  1  0  0
 -1  1  0  1
 -1  1  0  2
 -1  1  0  3
 -1  1  0  4
 -1  1  0  5
  1 -1  0  5
  1 -1  0  4
  1 -1  0  3
  1 -1  0  2
  1 -1  0  1
  1 -1  0  0
  2  0 -2  1
  2  0 -2  3
 -2  0  2  3
 -2  0  2  1
  0 -2  2  1
  0 -2  2  3
  0 +2 -2  3
  0  2 -2  1
```

-2	2	0	1
-2	2	0	3
2	-2	0	3
2	-2	0	1
2	1	-3	0
2	1	-3	1
2	1	-3	2
2	1	3	3
2	-1	3	3
2	-1	3	2
2	-1	3	1
2	-1	3	0
1	2	-3	0
1	2	-3	1
1	2	-3	2
1	2	-3	3
-1	-2	3	3
-1	-2	3	2
-1	-2	3	1
-1	-2	3	0
-1	3	-2	0
-1	3	-2	1
-1	3	-2	2
-1	3	-2	3
1	-3	2	3
1	-3	2	2
1	-3	2	1
1	-3	2	0
-2	3	-1	0
-2	3	-1	1
-2	3	-1	2
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2	-3	1	2
2	-3	1	1
2	-3	1	0
-3	2	1	0
-3	2	1	1
-3	2	1	2
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3	-2	-1	3
3	-2	-1	2
3	-2	-1	1
3	-2	-1	0
3	1	2	0
-3	1	2	1
-3	1	2	2
-3	1	2	3
3	-1	-2	3
3	-1	-2	2
3	-1	-2	1
3	-1	-2	0
1	1	-2	0
1	1	-2	1
1	1	-2	2
1	1	-2	3
1	1	-2	4
1	1	-2	5
-1	-1	2	5
-1	-1	2	4

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-1	-1	2	2
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-1	2	-1	0
-1	2	-1	1
-1	2	-1	2
-1	2	-1	3
-1	2	-1	4
-1	2	-1	5
1	-2	1	5
1	-2	1	4
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1	-2	1	2
1	-2	1	1
1	-2	1	0
-2	1	1	0
-2	1	1	1
-2	1	1	2
-2	1	1	3
-2	1	1	4
-2	1	1	5
2	-1	-1	5
2	-1	-1	4
2	-1	-1	3
2	-1	-1	2
2	-1	-1	1
2	-1	-1	0
0	0	0	-1
-1	2	-1	-5
-1	2	-1	-4
-1	2	-1	-3
-1	2	-1	-2
-1	2	-1	-1
0	1	-1	-5
0	1	-1	-4
0	1	-1	-3
0	1	-1	-2
0	1	-1	-1
0	2	-2	-3
0	2	-2	-1
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1	2	-3	-3
1	2	-3	-2
1	2	-3	-1
1	1	-2	-5
1	1	-2	-4
1	1	-2	-3
1	1	-2	-2
1	1	-2	-1
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2	1	-3	-2
2	1	-3	-1
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1	0	-1	-4
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2	0	-2	-1
3	-1	-2	-3
3	-1	-2	-2
3	-1	-2	-1

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2	-1	-1	-4
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3	-2	-1	-3
3	-2	-1	-2
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2	-3	1	-3
2	-3	1	-2
2	-3	1	-1
1	-2	1	-5
1	-2	1	-4
1	-2	1	-3
1	-2	1	-2
1	-2	1	-1

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Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY *(Corporate author)* Naval Research Laboratory Washington, D. C. 20390	2a. REPORT SECURITY CLASSIFICATION Unclassified 2b. GROUP

3. REPORT TITLE

COMPUTER-PLOTTED STEREOGRAPHIC PROJECTIONS

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*
A final report on one phase of the problem.

5. AUTHOR(S) *(First name, middle initial, last name)*

E. A. Metzbower

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
July 7, 1969	50	16

8a. CONTRACT OR GRANT NO. NRL Problem M01-08 b. PROJECT NO. RR 007-01-46-5406 c. d.	9a. ORIGINATOR'S REPORT NUMBER(S) NRL Report 6919 9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*

10. DISTRIBUTION STATEMENT

This document has been approved for public release and sale; its distribution is unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Department of the Navy (Office of Naval Research), Washington, D. C. 20360

13. ABSTRACT

Stereographic projections for materials having hexagonal symmetry depend on the axial (c/a) ratio. Thus, each material requires its individual set of stereographic projections. The facilities of the NRL Research Computation Center have been used to calculate and plot standard stereographic projections for seven hexagonal close-packed metals with different axial (c/a) ratios. The stereographic projections and the computer program are included in this report.

DD FORM 1 NOV 65 1473 (PAGE 1)

S/N 0101-807-6801

Security Classification

Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Stereographic projection Hexagonal symmetry Computer program						