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THE ACCURATE DETERMINATION OF D(10)  
SPACINGS FROM LEED PHOTO-  
GRAPHIC MEASUREMENTS

C. E. Holcombe, Jr

**UNION CARBIDE CORPORATION**  
**NUCLEAR DIVISION**  
**OAK RIDGE Y-12 PLANT**

*operated for the* **ATOMIC ENERGY COMMISSION** *under* **U. S. GOVERNMENT** **Contract W-7405 eng 26**



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C. E. Holcombe, Jr

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ABSTRACT

A computer program, expressed in BASIC programming language, was written to enable the accurate calculation of  $D(10)$  spacings from low energy electron diffraction (LEED) of single crystal surfaces from film and camera distance measurements. Thus, a poorly aligned specimen (of any two-dimensional structure) which gives a LEED pattern can be used to obtain accurate d-spacing data by using this method.

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## SUMMARY

By use of a computer program, expressed in BASIC programming language, the accurate calculation of  $D(10)$  spacings from low-energy electron diffraction (LEED) of single crystal surfaces from film and camera distance measurements is possible. Since the LEED data are corrected for magnification differences caused by the curvature of the fluorescent screen, for near-normal incidence of the electron beam, and for crystal position, accurate d-spacing data can be obtained from poorly aligned specimens which give a LEED pattern.

## INTRODUCTION

In order to enable the accurate calculation of  $D(10)$  spacings from low-energy electron diffraction (LEED) of single crystal surfaces from film and camera distance measurements, a method of calculation from geometric considerations was sought. A computer program (GELEED), expressed in BASIC programming language, was written to correct LEED data for magnification differences caused by the curvature of the fluorescent screen, for near-normal incidence of the electron beam (which causes the center of the LEED pattern not to coincide with the center of the fluorescent screen), and for crystal position (when its position is not at the geometric center of curvature of the fluorescent screen). Thus, a poorly aligned specimen which gives a LEED pattern can be used to obtain accurate  $d$ -spacing data by using this computer program.

## DETERMINATION OF THE D(10) SPACINGS

### GEOMETRICAL ANALYSIS

#### Magnification Correction

Because of the curvature of the screen and because the LEED pattern may not be exactly centered on the screen, magnification corrections are different at each LEED spot. Thus, the geometric analysis that follows shows how the magnification factor is computed.

From Figure 1, it is seen that:

$$Q = \sqrt{R_1^2 - Y_1^2} \quad , \quad (1)$$

$$\left( \frac{Y_1}{Q + X_2} \right) = \frac{Y_2}{X_1} \quad , \quad \text{and} \quad (2a)$$

$$X_1 Y_1 = X_2 Y_2 + Y_2 Q = X_2 Y_2 + Y_2 \left( \sqrt{R_1^2 - Y_1^2} \right) \quad . \quad (2b)$$

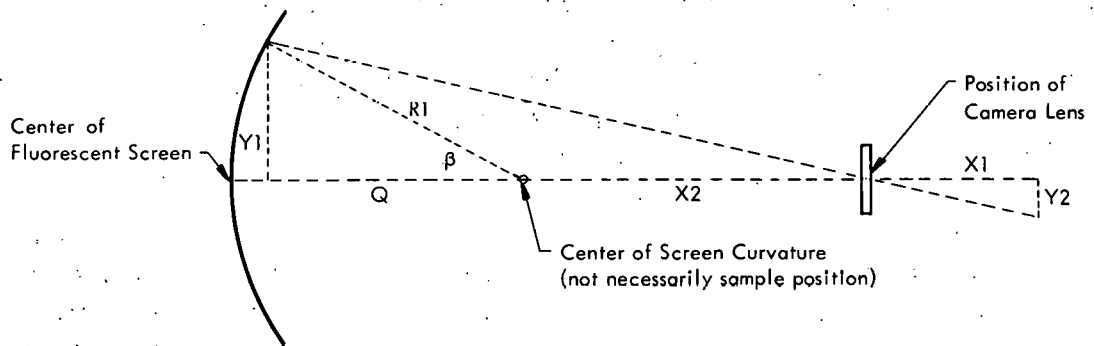


Figure 1. GEOMETRY OF THE "LEED" SYSTEM.

Collecting terms and squaring gives:

$$Y_2 \left( \sqrt{R_1^2 - Y_1^2} \right) = X_1 Y_1 - X_2 Y_2 \quad , \quad (2c)$$

$$\left( \sqrt{R_1^2 - Y_1^2} \right)^2 = \left( \frac{X_1 Y_1}{Y_2} - X_2 \right)^2 \quad , \quad (2d)$$

$$R1^2 - Y1^2 = \frac{X1^2 Y1^2}{Y2^2} - \frac{2X1X2Y1}{Y2} + X2^2, \quad (2e)$$

$$\left(\frac{X1^2}{Y2^2} + 1\right) Y1^2 - \left(\frac{2X1X2}{Y2}\right) Y1 + \left(X2^2 - R1^2\right) = 0, \text{ and} \quad (2f)$$

$$\left(X1^2 + Y2^2\right) Y1^2 - (2X1X2Y2) Y1 + \left[Y2^2 \left(X2^2 - R1^2\right)\right] = 0, \quad (2g)$$

which can be solved by the quadratic formula to yield:

$$Y1 = \frac{2X1X2Y2 \pm \sqrt{4X1^2 X2^2 Y2^2 - 4Y2^2 (X2^2 - R1^2) (X1^2 + Y2^2)}}{2 (X1^2 + Y2^2)}, \quad (2h)$$

which reduces to:

$$Y1 = \left[ \frac{Y2}{(X1^2 + Y2^2)} \right] \left[ X1X2 \pm \sqrt{(X1X2)^2 - (X2^2 - R1^2) (X1^2 + Y2^2)} \right], \quad (2i)$$

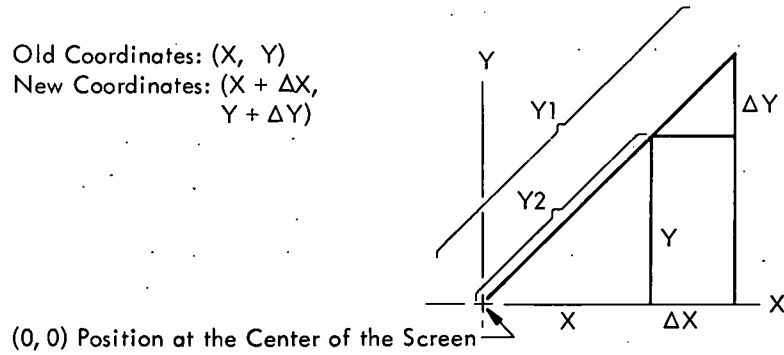
and it can be shown that the positive root is applicable.

Thus, from the analysis it is seen that, in order to calculate the magnification correction, the center of the fluorescent screen must be used as the (0,0) coordinate when the positions of the LEED spots are defined by an X-Y coordinate system (with distances given in centimeters). The center of the screen on the photographs can be found by taking a photograph of the LEED system with illumination from the sample heater and by geometric determination (with a compass) of the position of the center of the screen on the photographs. Since this position of the center of the screen is the same for all photographs taken, it can be located and used as the center of the X-Y coordinate system by placing graph paper (10 x 10 to 1 cm ruled) over the photographs, using an illumination reader to aid in marking the positions of the LEED spots on the graph paper.

#### Determination of the New Coordinates after the Magnification Correction

After the  $Y1$  is calculated (Equation 2i), its coordinates are changed because of a change in magnitude. However, since its direction is the same after the magnification correction, the following geometry applies:

Old Coordinates:  $(X, Y)$   
 New Coordinates:  $(X + \Delta X,$   
 $Y + \Delta Y)$



where the following equations:

$$(X + \Delta X) = \frac{Y1X}{\sqrt{X^2 + Y^2}}, \text{ and} \quad (3)$$

$$(Y + \Delta Y) = \frac{Y1Y}{\sqrt{X^2 + Y^2}}$$

are derived from the solution of these simultaneous equations:

$$Y1 = \sqrt{(X + \Delta X)^2 + (Y + \Delta Y)^2}, \text{ and} \quad (4a)$$

$$\left( \frac{Y + \Delta Y}{X + \Delta X} \right) = \frac{Y}{X}. \quad (4b)$$

### Translation of Axes of the Coordinate System

Next, it is necessary to find the center of the photographic LEED pattern which can be accomplished by summing the X and Y coordinates respectively of the (10) LEED spots and dividing by the number of the (10) LEED spots, giving the coordinate  $(S1, S2)$  of the center of the LEED pattern with respect to the  $(0,0)$  position at the center of the screen.

To translate the axes of the coordinate system to the position of the center of the LEED pattern  $(S1, S2)$ , the following formulae are used:

$$X_n = X_o - S1, \text{ and} \quad (5)$$

$$Y_n = Y_o - S2, \quad (6)$$

where subscript "n" represents the new axes and "o" the old axes.  $X_o$  and  $Y_o$  are the coordinates of any LEED spot after the magnification correction.

### M (off-centering) Correction

Because the position of the crystal usually does not coincide exactly with the center of curvature of the screen, it is necessary to determine the amount of off centering in order to calculate correctly the  $d(10)$  values. The geometric analysis that follows shows how the  $M$  correction is computed.

From Figure 2, it is seen that:

$$\sin \theta = Y1/L \quad , \quad (7)$$

$$P = Q - M \quad , \quad (8)$$

$$Q = \sqrt{R1^2 - Y1^2} \quad , \text{ and} \quad (9a)$$

$$P = \sqrt{R1^2 - Y1^2} - M \quad . \quad (9b)$$

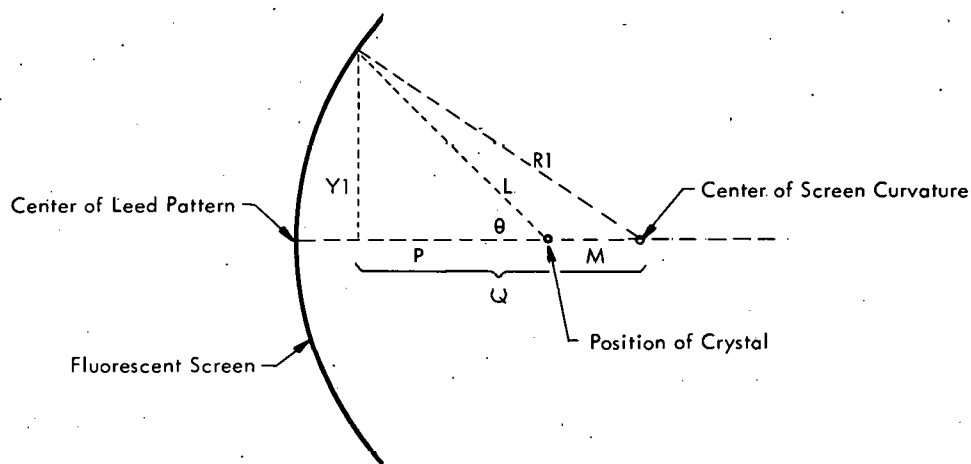


Figure 2. GEOMETRY OF A "LEED" PATTERN.

Note:  $Y1$  is now the corrected  $Y1$ ; therefore,  $Q$  is not the same value as in Figure 1 if the center of the LEED pattern does not coincide with the center of the screen.

$$L = \sqrt{Y1^2 + P^2} \quad , \quad (10a)$$

$$P^2 = R1^2 - Y1^2 - 2M \sqrt{R1^2 - Y1^2} + M^2 \quad , \text{ or} \quad (10b)$$

$$P^2 = R1^2 - Y1^2 - M \left( 2 \sqrt{R1^2 - Y1^2 - M} \right) , \text{ and} \quad (10c)$$

$$L = \sqrt{R1^2 - M \left( 2 \sqrt{R1^2 - Y1^2 - M} \right)} .$$

Thus:

$$\sin \theta = \frac{Y1}{\sqrt{R1^2 - M \left( 2 \sqrt{R1^2 - Y1^2 - M} \right)}} \quad (10d)$$

From electron diffraction theory:

$$d \sin \theta = \lambda , \text{ and} \quad (11)$$

$$\lambda = \sqrt{\frac{150.4}{V}} \quad (\lambda \text{ is in angstroms when } V \text{ is in volts}) \quad (12)$$

Therefore:

$$d = \frac{\lambda}{\sin \theta} = \frac{\sqrt{\left(\frac{150.4}{V}\right) \left[ R1^2 - M \left( 2 \sqrt{R1^2 - Y1^2 - M} \right) \right]}}{Y1} \quad (13)$$

Since there is a relation between  $d(10)$  and  $d(11)$ , whereby  $d(11)$  can be multiplied by some factor,  $F1$ , to be equal to  $d(10)$ , it is possible to solve a set of simultaneous equations for  $M$ , the amount of off centering. For example, a square point group type (explained in the input data instructions) has a factor of  $\sqrt{2}$  and a hexagonal point group type has a factor of  $\sqrt{3}$ . The designation  $Y2$  will be used for the average corrected distance from the center of the LEED pattern to the (11) LEED spots, and  $Y1$  is the average corrected distance to the (10) LEED spots. The designation  $Y2$  here is in no way related to the  $Y2$  used in calculating the magnification correction. The calculation of  $M$  is shown as:

$$d(10) = F1 d(11) , \quad (14)$$

where:

$Y1$  and  $V1$  are used to calculate  $d(10)$ , and

$Y2$  and  $V2$  are used to calculate  $d(11)$ .

Thus:

$$\frac{\sqrt{\left(\frac{150.4}{V1}\right) \left[ R1^2 - M \left( 2 \sqrt{R1^2 - Y1^2} - M \right) \right]}}{Y1} = F1 \frac{\sqrt{\left(\frac{150.4}{V2}\right) \left[ R1^2 - M \left( 2 \sqrt{R1^2 - Y2^2} - M \right) \right]}}{Y2} \quad (15)$$

Squaring both sides and dividing out terms gives:

$$\left[ R1^2 - M \left( 2 \sqrt{R1^2 - Y1^2} - M \right) \right] Y2^2 = F1^2 Y1^2 \left[ R1^2 - M \left( 2 \sqrt{R1^2 - Y2^2} - M \right) \right] \quad (16)$$

Getting the equation in the form of a quadratic yields:

$$\left( Y2^2 - F1^2 Y1^2 \right) M^2 + \left( 2F1^2 Y1^2 \sqrt{R1^2 - Y2^2} - 2Y2^2 \sqrt{R1^2 - Y1^2} \right) M + \left( R1^2 Y2^2 - R1^2 F1^2 Y1^2 \right) = 0 \quad (17)$$

Solving for M by the quadratic formula gives:

$$\begin{aligned} A &= \left( Y2^2 - F1^2 Y1^2 \right) , \\ B &= \left( 2F1^2 Y1^2 \sqrt{R1^2 - Y2^2} - 2Y2^2 \sqrt{R1^2 - Y1^2} \right) , \\ C &= \left( R1^2 Y2^2 - R1^2 F1^2 Y1^2 \right) , \text{ and} \\ M &= \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} ; \end{aligned} \quad (18)$$

and, it can be shown that the negative root is applicable.

#### Calculation of D(10)

After the average M value is calculated from several photographs which contain both (10) and (11) LEED spots, d(10) is calculated from Equation 13,



using the average  $M$  value. The  $d(10)$  values can be calculated from several photographs taken at different electron beam voltages. The magnification correction and the center of the LEED pattern are calculated as previously described before the  $d(10)$  values are computed. The computer program, entitled GELEED (for general LEED calculation program for square, hexagonal, and rectangular-point group types), is written in BASIC programming language for a teletype computer system. The final  $d(10)$  printout includes the average corrected  $Y1$  value (with respect to the center of the LEED pattern), the  $d(10)$  spacing, the electron beam voltage, the wavelength of the electron beam ( $\lambda$ ), and the sine of the angle of diffraction ( $\theta$ ). The average value of  $d(10)$  is also printed.

### PROGRAM INFORMATION

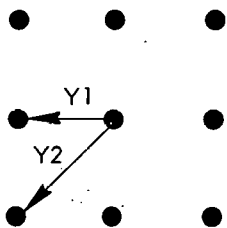
The operations carried out in the program are as just described. Following are the directions for inputting the data for GELEED, a copy of the program, and an example of a determination of the data and printout for a hexagonal point group type (beryllium).

Input Data for GELEED (general LEED calculation program for square, hexagonal, and rectangular point group types)

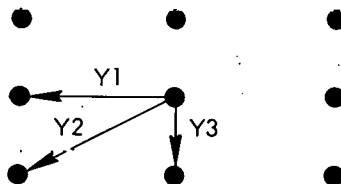
815 DATA G1, Q2, Q1, A1, X1, X2

G1 is the point group type. There are three point group types as follows:

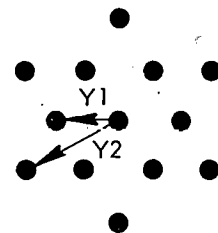
G1 = 0 (square)



G1 = 2 (rectangular)



G1 = 1 (hexagonal)



Q2 is a directive number:

1. If  $Q2 = 0$ , the average corrected  $Y1$  values, the corresponding average corrected  $Y2$  values, and  $M$  values are printed, along with the average  $M$  value.

2. If  $Q2 = 1$  (or any integral number greater than 1), there will be a more complete printout, showing all  $Y1$  and  $Y2$  values, their respective averages, and the  $M$  value calculated from the average  $Y1$  and  $Y2$  values for each film, along with the average  $M$  value. It is best to use this directive for all cases where there may be a chance of error in assigning coordinates for the spots on the films. If all the  $Y1$  or  $Y2$  values are not nearly equal respectively, then an error in coordinates is probable.

Q1 is the number of films used in the calculation of the  $M$  value.

A1 is the number of films used in the calculation of  $d(10)$ , after the  $M$  value has been calculated.

X1 is the distance from the lens of the camera to the back plate of the camera (where the film is loaded).

X2 is the distance from the lens of the camera to the center of curvature of the screen (ie, the distance from the camera lens to the back of the LEED system minus the radius of curvature of the screen).

820 DATA N, P, U1, W1, U2, W2 . . . U(N), W(N)

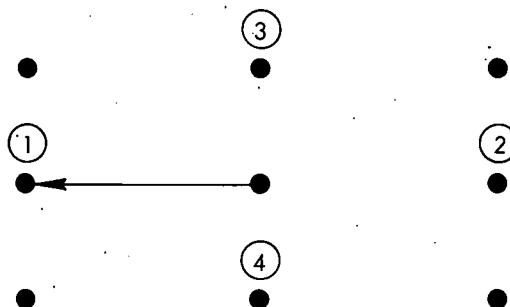
N is the total number of LEED spots to be used in the  $M$  calculation for one particular film.

P is the number of (11) LEED spots to be used in the  $M$  calculation for one particular film.

U1, W1, . . . , U(N), W(N) are the coordinates (in centimeters) of the LEED spots, with the center of the coordinate system placed on the center of the screen (determined geometrically from a photograph of the screen taken with illumination from the specimen heater).

Notes:

1. In all cases the (10) LEED spots must be listed first. There must be 4 for a square point group type, 6 for a hexagonal point group type, and 4 for a rectangular point group type. For a rectangular point group type, the coordinates would be entered as follows:



in that sequence for the (10) spots. The  $d(10)$  finally calculated would be from the average distance to Points 1 and 2. For square and hexagonal point group types, the coordinates of the (10) LEED spots may be entered in any order.

2. The coordinates of the (11) LEED spots must be entered after the (10) spots. Any number of (11) spots can be used.

#### 825 DATA - 840 DATA

Same as the 820 DATA for as many films as are available to calculate the average  $M$  value (the amount of off centering from the center of curvature of the screen), given in centimeters.

#### 845 DATA $V, X_1, Z_1, X_2, Z_2, \dots, X(A_2), Z(A_2)$

$V$  is the electron beam voltage where the film was taken.

$X_1, Z_1, \dots, X(A_2), Z(A_2)$  are the coordinates (in centimeters) of the (10) LEED spots, with the center of the coordinate system placed on the center of the screen. Note 1 applies here. Since the average  $M$  is calculated from the data in Statements 820 - 840, no coordinates of (11) LEED spots are used. The average  $d(10)$  is calculated from the data here.

#### 850 DATA - 910 DATA

Same as the 845 DATA for as many films as are available to calculate  $d(10)$ , given in angstroms.

#### Notes about the Program:

1. The radius of curvature of the fluorescent screen is defined in Statement 45 LET  $R1 = 7$ . If the radius differs from 7 centimeters, it is necessary to modify this statement.

2. The maximum amount of off centering (M value) is set in the program with limits of  $\pm 3$  centimeters, with a + symbol indicating that the off centering is toward the screen.

### Listing of GELEED

```

5 PRINT "LOW ENERGY ELECTRON DIFFRACTION CALCULATIONS"
10 PRINT
15 PRINT
20 DIM R(80),U(80),W(80),Y(80),T(60),X(60),Z(60),S(20),L(20)
25 DIM Q(20),E(20),G(20),D(20),V(20)
30 DEF FNO(D) = ((-B)+D*SQR(B*B-4.*A*C))/(2.*A)
35 READ G1,Q2,Q1,A1,X1,X2
40 LET M=0
45 LET R1=7.
50 IF Q2>0 THEN 60
55 PRINT "AV.CORR.Y1","AV.CORR.Y2","M VALUE"
60 FOR K=1 TO Q1
65 READ N,P
70 IF G1>0 THEN 90
75 LET N1=4
80 LET N2=0
85 GO TO 120
90 IF G1>1 THEN 110
95 LET N1=6
100 LET N2=0
105 GO TO 120
110 LET N1=2
115 LET N2=2
120 FOR J=1 TO N
125 READ U(J),W(J)
130 LET R(J)=SQR(U(J)2+W(J)2)
135 LET A=((X1*X1)+(R(J)*R(J)))
140 LET B=(-2.*X1*X2*R(J))
145 LET C=((X2*X2)-(R1*R1))*(R(J)*R(J))
150 LET R(J) = FNO(1.)
155 LET D1=SQR((U(J)2)+(W(J)2))
160 LET U(J)=(R(J)*U(J))/D1
165 LET W(J)=(R(J)*W(J))/D1
170 NEXT J
175 LET S1=0
180 LET S2=0
185 FOR J=1 TO (N-P)
190 LET S1=S1+U(J)
195 LET S2=S2+W(J)
200 NEXT J
205 LET S1=S1/(N-P)
210 LET S2=S2/(N-P)
215 LET Y1=0
220 LET Y2=0
225 LET Y3=0
230 FOR J=1 TO N
235 LET U(J)=U(J)-S1
240 LET W(J)=W(J)-S2
245 LET Y(J)=SQR((U(J)2)+(W(J)2))
250 IF J=>(N-(P+N2)+1) THEN 265
255 LET Y1=Y1+Y(J)
260 GO TO 285
265 IF J=>(N-P+1) THEN 280

```

```

270 LET Y3=Y3+Y(J)
275 GO TO 285
280 LET Y2=Y2+Y(J)
285 NEXT J
290 LET Y1=(Y1/(N-(N2+P)))
295 LET Y2=(Y2/(N-(N1+N2)))
300 IF N2=0 THEN 310
305 LET Y3=(Y3/(N-(N1+P)))
310 IF Q2=0 THEN 400
315 PRINT "OBSERVED Y1 VALUES AFTER CORRECTION"
320 FOR J=1 TO N1
325 PRINT Y(J)
330 NEXT J
335 PRINT "AVERAGE Y1 =" Y1
340 IF N2=0 THEN 370
345 PRINT "OBSERVED Y3 VALUES AFTER CORRECTION"
350 FOR J=(N1+1) TO (N1+N2)
355 PRINT Y(J)
360 NEXT J
365 PRINT "AVERAGE Y3 =" Y3
370 PRINT "OBSERVED Y2 VALUE(S) AFTER CORRECTION"
375 FOR J=(N-P+1) TO N
380 PRINT Y(J)
385 NEXT J
390 PRINT "AVERAGE Y2 =" Y2
395 PRINT "AV.CORR.Y1", "AV.CORR.Y2", "M VALUE"
400 IF G1>0 THEN 410
405 LET Y3=Y1
410 IF G1=1 THEN 425
415 LET F1=(SQR(Y1+2+Y3+2))/Y1
420 GO TO 430
425 LET F1=SQR(3.)
430 LET A=((Y2*Y2)-(F1*F1*Y1*Y1))
435 LET B=(2.*F1+2*Y1+2*SQR(R1+2-Y2+2))-(2.*Y2+2*SQR(R1+2-Y1+2))
440 LET C=(R1*R1*Y2*Y2)-(R1*R1*F1*F1*Y1*Y1)
445 LET M2 = FNO(-1.)
450 PRINT Y1, Y2, M2
455 IF Q2=0 THEN 465
460 PRINT
465 IF M2>=-3 THEN 475
470 GO TO 480
475 IF M2<3 THEN 485
480 PRINT "NO SUITABLE M SOLUTION"
485 LET M=M+M2
490 NEXT K
495 LET M2=(M/Q1)
500 PRINT
505 PRINT "SOLUTION FOR BEST M VALUE (AVERAGE) =" M2
510 PRINT
515 PRINT
520 LET T=0
525 FOR K=1 TO A1
530 IF G1>0 THEN 545
535 LET A2=4
540 GO TO 570
545 IF G1>1 THEN 560
550 LET A2=6
555 GO TO 570
560 LET A2=4
565 LET A3=2
570 READ V(K)
575 LET S3=0

```

```

580 LET S4=0
585 FOR I=1 TO A2
590 READ X(I),Z(I)
595 LET T(I)=SQR(X(I)2+Z(I)2)
600 LET A=((X1*X1)+(T(I)*T(I)))
605 LET B=(-2.*X1*X2*T(I))
610 LET C=((X2*X2)-(R1*R1))*(T(I)*T(I))
615 LET T(I) = FNO(1.)
620 LET D2=SQR((X(I)2)+(Z(I)2))
625 LET X(I)=(T(I)*X(I))/D2
630 LET Z(I)=(T(I)*Z(I))/D2
635 LET S3=S3+X(I)
640 LET S4=S4+Z(I)
645 NEXT I
650 LET S3=S3/A2
655 LET S4=S4/A2
660 LET T1=0
665 FOR I=1 TO A2
670 LET X(I)=X(I)-S3
675 LET Z(I)=Z(I)-S4
680 LET T(I)=SQR(X(I)2+(Z(I)2))
685 IF G1<=1 THEN 705
690 IF I>=A3 THEN 710
695 LET T1=T1+T(I)
700 GO TO 710
705 LET T1=T1+T(I)
710 NEXT I
715 IF G1<=1 THEN 730
720 LET T1=T1/A3
725 GO TO 735
730 LET T1=(T1/A2)
735 LET S(K)=T1
740 LET L(K)=SQR(150.4/V(K))
745 LET Q(K)=SQR((R1*R1)-(S(K)*S(K)))
750 LET E(K)=SQR((R12-(M2*((2.*Q(K))-M2))))
755 LET G(K)=S(K)/E(K)
760 LET D(K)=L(K)/G(K)
765 LET T=T+D(K)
770 NEXT K
775 LET H=T/A1
780 PRINT "CORRECTED Y", "D(10) SPAC", "VOLTAGE", "LAMBDA", "SIN THETA"
785 PRINT
790 FOR K=1 TO A1
795 PRINT S(K), D(K), V(K), L(K), G(K)
800 NEXT K
805 PRINT
810 PRINT "AVERAGE VALUE OF D(10) =" H
815 DATA
820 DATA
825 DATA
830 DATA
835 DATA
840 DATA
845 DATA
850 DATA
855 DATA
860 DATA
865 DATA
870 DATA
875 DATA
880 DATA
885 DATA

```

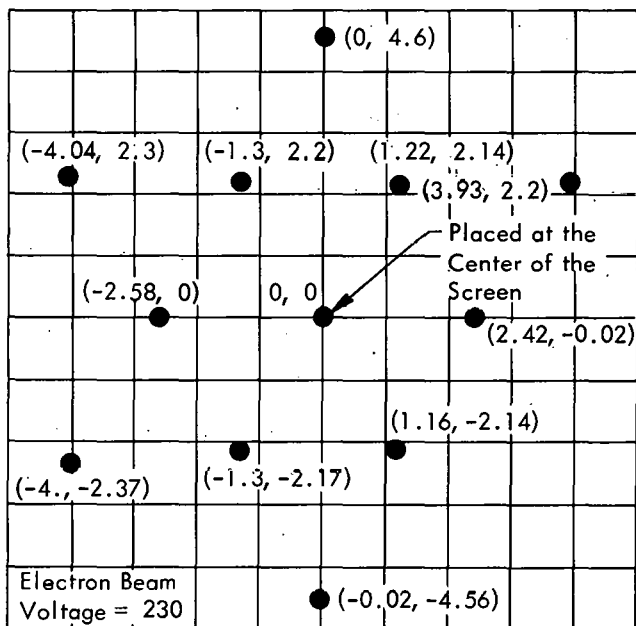
```

890 DATA
895 DATA
900 DATA
905 DATA
910 DATA
915 IF G1>0 THEN 930
920 PRINT "SQUARE POINT GROUP TYPE"
925 GO TO 950
930 IF G1>1 THEN 945
935 PRINT "HEXAGONAL POINT GROUP TYPE"
940 GO TO 950
945 PRINT "RECTANGULAR POINT GROUP TYPE"
950 STOP
955 END

```

Example of Determination of Data and Printout for a Hexagonal Point Group (beryllium)

Graphical Representation of Beryllium Data -



Calculations for a Single Crystal of Beryllium - The input data for one film of a beryllium crystal (1000 plane) is as follows:

```

815 DATA 1,1,1,1,24.6,20.5
820 DATA 1,5,-2.58,0,-1.3,2.2,1.22,2.14,2.42,-.02,1.16,-2.14,-1.3,-2.17
825 DATA -4.04,2.3,0,4.6,3.93,2.2,-.02,-4.56,-4.,-2.37
845 DATA 230,-2.58,0,-1.3,2.2,1.22,2.14,2.42,-.02,1.16,-2.14,-1.3,-2.17

```

With the directive number, Q2, equal to 1, the printout is as follows:

03/02/71. 09.30.39.  
PROGRAM GELEED

LOW ENERGY ELECTRON DIFFRACTION CALCULATIONS

OBSERVED Y1 VALUES AFTER CORRECTION

2.7544  
2.76113  
2.73229  
2.72143  
2.70288  
2.73631

AVERAGE Y1 = 2.73474

OBSERVED Y2 VALUE(S) AFTER CORRECTION

4.77204  
4.78717  
4.76082  
4.75433  
4.77462

AVERAGE Y2 = 4.7698

| AV.CORR.Y1 | AV.CORR.Y2 | M VALUE |
|------------|------------|---------|
| 2.73474    | 4.7698     | .243829 |

SOLUTION FOR BEST M VALUE (AVERAGE) = .243829

| CORRECTED Y | D(10) SPAC | VOLTAGE | LAMBDA  | SIN THETA |
|-------------|------------|---------|---------|-----------|
| 2.73474     | 2.0037     | 230     | .808649 | .403579   |

AVERAGE VALUE OF D(10) = 2.0037  
HEXAGONAL POINT GROUP TYPE

With the directive number, Q2, equal to 0, the data input is

B15 DATA 1,0,1,1,24.6,20.5

and the printout is the following:

03/02/71. 09.33.21.  
PROGRAM GELEED

LOW ENERGY ELECTRON DIFFRACTION CALCULATIONS

| AV.CORR.Y1 | AV.CORR.Y2 | M VALUE |
|------------|------------|---------|
| 2.73474    | 4.7698     | .243829 |

SOLUTION FOR BEST M VALUE (AVERAGE) = .243829



| CORRECTED Y | D(10) SPAC | VOLTAGE | LAMBDA  | SIN THETA |
|-------------|------------|---------|---------|-----------|
| 2.73474     | 2.0037     | 230     | .808649 | .403579   |

AVERAGE VALUE OF D(10) = 2.0037  
HEXAGONAL POINT GROUP TYPE

The program (GELEED) has been verified for square, hexagonal, and rectangular point group types.