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Research and Development Report

A FORTRAN PROGRAM FOR THE
CALCULATION OF DISLOCATION
IMAGE PROFILES ACCORDING TO
THE DYNAMICAL THEORY OF
ELECTRON DIFFRACTION

by

H. J. Leamy and R. Trivedi

EASTER

October 1967

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TABLE OF CONTENTS

	Page
ABSTRACT	1
INTRODUCTION	1
FORMULATION OF THE PROBLEM	2
NUMERICAL METHODS AND FORTRAN PROGRAM	5
IMAGE PROFILE CALCULATION EXAMPLES	8
CONCLUDING REMARKS	10
REFERENCES	13

IS-1696

A FORTRAN PROGRAM FOR THE CALCULATION OF
DISLOCATION IMAGE PROFILES ACCORDING TO THE
DYNAMICAL THEORY OF ELECTRON DIFFRACTION

H. J. Leamy and R. Trivedi

ABSTRACT

A simple FORTRAN program for the routine calculation of the intensity distributions produced by dislocation arrays as observed by transmission electron microscopy under either bright or dark field conditions is presented. The programmed calculations are based upon the dynamical theory of electron diffraction in the two beam approximation.

INTRODUCTION

The availability of modern electron microscopes and the existence of suitable theories of electron transmission contrast effects has greatly influenced the general field of crystal defect study.¹ In particular, the study of dislocation arrangements on the slip planes of deformed crystals has been shown to be of great value.²⁻⁴ Surprisingly, however, the dynamical theory of electron diffraction has not been applied to many of the simple dislocation configurations which might be observed in such studies. The purpose of this report is to present a short FORTRAN program which hopefully will facilitate the routine application

of the theory, and to demonstrate the application of the program by means of a few examples.

FORMULATION OF THE PROBLEM

Howie and Whelan⁵ first applied the dynamical theory of Bethe⁶ to the case of electron diffraction. The coupled, first order differential equations given by these authors form the base for the considerations which follow. They may be written:

$$\begin{aligned}\frac{dT}{dz} + \pi i (s + d\alpha'/dz)T &= i\pi \left(\frac{1}{t_e} + \frac{i}{\tau_e}\right)S \\ \frac{dS}{dz} - \pi i (s + d\alpha'/dz)S &= i\pi \left(\frac{1}{t_e} + \frac{i}{\tau_e}\right)T\end{aligned}\tag{1}$$

where S and T are the amplitudes of the scattered and transmitted beams, respectively, t_e and τ_e are the extinction and absorption lengths, respectively, and s is the interference error. The equations given above are identical to those given by Amelinckx⁷ (9.157, p. 191) except that $\left(\frac{1}{t_e} + \frac{i}{\tau_e}\right)$ has been substituted for $1/t_e$ in order to account for the anomalous absorption effect. The reader is encouraged to consult the review by Amelinckx for the derivation of these equations and for a detailed explanation of the various terms.

The derivation of Eqs. (1) involves the invocation of the column approximation and, for purposes of this report, Eqs. (1) are restricted to the two beam case. Utilization of the column approximation may be accomplished with the coordinate system shown in Fig. 1.

Fig. 1. Illustrating the notation used in calculating the contrast due to a screw dislocation parallel to the foil plane. The dislocation is along the y axis. The z axis is perpendicular to the foil.

The z -coordinate axis in this figure is that given in Eqs. (1). The α' factor in the same equations is the well-known phase angle which is given by:

$$\alpha' = \alpha/2\pi = \bar{g} \cdot \bar{R}(x, z) \quad (2)$$

where $\bar{g}$ is a diffraction vector and $\bar{R}(x, z)$ describes the atomic displacements in the foil produced by the imperfection.

Application of Eqs. (1) to the calculation of image profiles for the experimentally important case of dislocations parallel to the foil surface is a relatively simple procedure. First, the displacement functions of the dislocations must be incorporated into the α' terms. These may be written in the isotropic elasticity approximation as:

$$\bar{R}(x, z) = \frac{\bar{b}}{2\pi} \Phi$$

$$\bar{R}(x, z) = \frac{1}{2\pi} \left[\bar{b} \Phi + \bar{b} \frac{\sin \Phi}{4(1-\nu)} + (\bar{b}x\bar{u}) \left[\frac{1-2\nu}{2(1-\nu)} \ln \frac{\cos 2\Phi}{4(1-\nu)} \right] \right] \quad (3)$$

for screw and edge dislocations, respectively, where $\bar{u}$ is a unit vector tangent to the dislocation and directed in its positive sense, ν is Poisson's ratio, and Φ is as defined in Fig. 1. For observation of dislocations in foils oriented as described above, the term $\bar{g} \cdot (\bar{b} \times \bar{u})$ in α' is zero so that the expression for edge dislocations is considerably simplified. The appropriate derivatives for substitution into Eqs. (1) are thus:

$$\left[\frac{d\alpha'}{dz} \right]_{\text{screw}} = \frac{\bar{g} \cdot \bar{b}}{2\pi} \left[\frac{x-x_0}{(x-x_0)^2 + (z-z_0)^2} \right]$$

$$\left[\frac{d\alpha'}{dz} \right]_{\text{edge}} = \frac{\bar{g} \cdot \bar{b}}{2\pi} \left[\frac{x-x_0}{(x-x_0)^2 + (z-z_0)^2} \right] \left[1 + \frac{3}{4} \cos 2\Phi \right]$$

where x_0 and z_0 are the coordinates of the dislocation and ν has been taken equal to 1/3. Equations (1) must, after substitution of Eqs. (3), be integrated over the foil thickness at several column positions for the generation of a complete image profile. This is most easily accomplished if they are transformed according to the substitution:

$$\begin{aligned} T &= T(\text{real}) + iT(\text{imaginary}) = T_R + iT_I \\ S &= S(\text{real}) + iS(\text{imaginary}) = S_R + iS_I \end{aligned} \quad (5)$$

This yields:

$$\begin{aligned} \frac{dT_R}{dz} - \pi(s + d\alpha'/dz)T_I &= -\frac{\pi}{t_e} S_I - \frac{\pi}{\tau_e} S_R, \\ \frac{dT_I}{dz} + \pi(s + d\alpha'/dz)T_R &= -\frac{\pi}{\tau_e} S_I + \frac{\pi}{t_e} S_R, \\ \frac{dS_R}{dz} + \pi(s + d\alpha'/dz)S_I &= -\frac{\pi}{t_e} T_I - \frac{\pi}{\tau_e} T_R, \\ \frac{dS_I}{dz} - \pi(s + d\alpha'/dz)S_I &= -\frac{\pi}{\tau_e} T_I + \frac{\pi}{t_e} T_R. \end{aligned} \quad (6)$$

and

Finally, the simultaneous numerical integration of Eqs. (6) is most conveniently accomplished when all of the variables are converted to dimensionless parameters by appropriate division or multiplication by either t_e or τ_e .

NUMERICAL METHODS AND FORTRAN PROGRAM

The intensities of the transmitted and diffracted beams which emerge from the bottom surface of the foil at any given column position are the desired quantities. Thus, the integration must be performed over the foil thickness from top to bottom. Since only the boundary conditions at the top of the foil, $T_R = 1$, $T_I = 0$, $S_R = 0$, and $S_I = 0$, are known, the first integration step must be accomplished by the forward difference method.⁸ The remaining steps may then be performed by the central difference method.⁸ Since the accuracy of these methods depends upon the interval over which the finite differences are taken, the foil thickness must be divided into a large number of intervals and the required computation is a task fit only for an electronic computer.

A FORTRAN program for the simultaneous integration of Eqs. (6) for the case of screw dislocations is given in Fig. 2. The initial portion of the program (statements 1-17) is written so that profiles for any number of dislocations in any array may be calculated, an especially useful feature if large numbers of image force dislocations are required. The column positions employed in the generation of the complete profile are dictated by statements 23-24. In Fig. 2 a particularly simple arrangement is employed for calculation of a profile of width $3t_e$. The amount of computation time per profile could be decreased by a more

```

BEGIN COMPILATION
C      ELECTRON MICROSCOPICAL IMAGE PROFILE CALCULATIONS FOR SCREW DISLOCATIONS
C
C
C      VARIABLE DEFINITIONS.....
C
C      'DEL' = INTEGRATION INCREMENT = 0.0025 EXTINCTION DISTANCES
C      'N' = NUMBER OF INTEGRATION INCREMENTS REQUIRED TO TRAVERSE FOIL THICKNESS
C      'M' = PROFILE WIDTH INDEX (SEE STATEMENTS 25 - 34)
C      'NUMBER' = THE NUMBER OF DISLOCATIONS IN THE ARRAY
C      'NUMB(INK)' = INDEX NUMBER OF THE INK'TH DISLOCATION
C      'BSIGN(INK)' = THE SIGN OF THE INK'TH DISLOCATION IN THE ARRAY
C      'XD(INK)' = THE X COORDINATE OF THE INK'TH DISLOCATION IN THE ARRAY
C      'Y(INK)' = THE Z COORD OF THE INK'TH DISLOCATION IN THE ARRAY
C      'EN' = THE IMAGE ORDER = G.B
C      'RA' = RATIO OF EXTINCTION DISTANCE TO ABSORPTION DISTANCE
C      'YS' = INTERFERENCE ERROR, S, TIMES THE EXTINCTION DISTANCE
C      TR, TI, SR, AND SI ARE THE REAL AND IMAGINARY PARTS OF THE TRANSMITTED
C      AND SCATTERED BEAM AMPLITUDES, RESPECTIVELY
C      LABEL 1 IS FOR THE INPUT DATA COLUMNS...NUMB, BSIGN, X COORD, AND Z COORD
C      LABEL 2 IS A DESCRIPTIVE LABEL WHICH MUST BE SUPPLIED WITH EACH DATA SET
C
C      .....
C
S.0001      DIMENSION X(500),TI(500),SI(500),XLAB(5),YLAB(5),GLAB(5),
2AE(100),NUMB(100),BSIGN(100),XD(100),Y(100),ANUM(100),AK(100),
3DENOM(100),PHI(100),HLAB(5),YLAB1(5),LABEL1(20),LABEL2(20)
S.0002      READ (1,1000) LABEL1
S.0003      READ (1,1000) XLAB,YLAB,YALB1
S.0004      1      READ(1,120) N,M,NUMBER
S.0005      120      FORMAT (3I5)
S.0006      IF(N) 155,155.2
S.0007      121      FORMAT (4E10.0)
S.0008      2      READ(1,121) EN,RA,DEL,YS
S.0009      READ (1,1000) GLAB, HLAB
S.0010      READ (1,1000) LABEL2
S.0011      1000      FORMAT (20A4)
S.0012      DO 2000 INK=1,NUMBER
S.0013      2000      READ (1,1001) NUMB(INK),BSIGN(INK),XD(INK),Y(INK)
S.0014      1001      FORMAT (4F10.2)
S.0015      WRITE (3,122) EN,RA,DEL,YS
S.0016      122      FORMAT(1H1,4HEN =F8.4,7X,4HRA =F8.4,7X,5HDEL =F6.4,7X,3HY =F8.4)
S.0017      WRITE (3,1000) LABEL1
S.0018      DO 2001 INK=1,NUMBER
S.0019      2001      WRITE (3,1001) NUMB(INK),BSIGN(INK),XD(INK),Y(INK)
S.0020      WRITE (3,1000) LABEL2
S.0021      AN=N
S.0022      TH=AN*DEL
S.0023      WRITE (3,125) TH
S.0024      125      FORMAT (1X,11HTHICKNESS =F8.4)
S.0025      PI=4.*ATAN(1.)
S.0026      EPS1=0.2E00
S.0027      EPS2=0.02E00
S.0028      K=2.*M
S.0029      DO 100 J=1,K
S.0030      IF(J-5) 3,3,4
S.0031      3      X(J)=-1.5+J*EPS1
S.0032      GO TO 11

```

Fig. 2: FORTRAN program for the calculation of image profiles of screw dislocations.

```

BEGIN COMPILATION
C      ELECTRON MICROSCOPICAL IMAGE PROFILE CALCULATIONS FOR SCREW DISLOCATIONS
C
C
C      VARIABLE DEFINITIONS.....
C
C      'DEL' = INTEGRATION INCREMENT = 0.0025 EXTINCTION DISTANCES
C      'N' = NUMBER OF INTEGRATION INCREMENTS REQUIRED TO TRAVERSE FOIL THICKNESS
C      'M' = PROFILE WIDTH INDEX (SEE STATEMENTS 25 - 34)
C      'NUMBER' = THE NUMBER OF DISLOCATIONS IN THE ARRAY
C      'NUMB(INK)' = INDEX NUMBER OF THE INK'TH DISLOCATION
C      'BSIGN(INK)' = THE SIGN OF THE INK'TH DISLOCATION IN THE ARRAY
C      'XD(INK)' = THE X COORDINATE OF THE INK'TH DISLOCATION IN THE ARRAY
C      'Y(INK)' = THE Z COORD OF THE INK'TH DISLOCATION IN THE ARRAY
C      'EN' = THE IMAGE ORDER = G.B
C      'RA' = RATIO OF EXTINCTION DISTANCE TO ABSORPTION DISTANCE
C      'YS' = INTERFERENCE ERROR, S, TIMES THE EXTINCTION DISTANCE
C      TR, TI, SR, AND SI ARE THE REAL AND IMAGINARY PARTS OF THE TRANSMITTED
C      AND SCATTERED BEAM AMPLITUDES, RESPECTIVELY
C      LABEL 1 IS FOR THE INPUT DATA COLUMNS...NUMB, BSIGN, X COORD, AND Z COORD
C      LABEL 2 IS A DESCRIPTIVE LABEL WHICH MUST BE SUPPLIED WITH EACH DATA SET
C
C      .....
C
S.0001      DIMENSION X(500),TI(500),SI(500),XLAB(5),YLAB(5),GLAB(5),
          2AE(100),NUMB(100),BSIGN(100),XD(100),Y(100),ANUM(100),AK(100),
          3DENOM(100),PHI(100),HLAB(5),YLAB1(5),LABEL1(20),LABEL2(20)
S.0002      READ (1,1000) LABEL1
S.0003      READ (1,1000) XLAB,YLAB,YALB1
S.0004      1 READ(1,120) N,M,NUMBER
S.0005      120 FORMAT (3I5)
S.0006      IF(N) 155,155.2
S.0007      121 FORMAT (4E10.0)
S.0008      2 READ(1,121) EN,RA,DEL,YS
S.0009      READ (1,1000) GLAB, HLAB
S.0010      READ (1,1000) LABEL2
S.0011      1000 FORMAT (20A4)
S.0012      DO 2000 INK=1,NUMBER
S.0013      2000 READ (1,1001) NUMB(INK),BSIGN(INK),XD(INK),Y(INK)
S.0014      1001 FORMAT (4F10.2)
S.0015      WRITE (3,122) EN,RA,DEL,YS
S.0016      122 FORMAT(1H1,4HEN =F8.4,7X,4HRA =F8.4,7X,5HDEL =F6.4,7X,3HY =F8.4)
S.0017      WRITE (3,1000) LABEL1
S.0018      DO 2001 INK=1,NUMBER
S.0019      2001 WRITE (3,1001) NUMB(INK),BSIGN(INK),XD(INK),Y(INK)
S.0020      WRITE (3,1000) LABEL2
S.0021      AN=N
S.0022      TH=AN*DEL
S.0023      WRITE (3,125) TH
S.0024      125 FORMAT (1X,11HTHICKNESS =F8.4)
S.0025      PI=4.*ATAN(1.)
S.0026      EPS1=0.2E00
S.0027      EPS2=0.02E00
S.0028      K=2.*M
S.0029      DO 100 J=1,K
S.0030      IF(J-5) 3,3,4
S.0031      3 X(J)=-1.5+J*EPS1
S.0032      GO TO 11

```

Fig. 2: FORTRAN program for the calculation of image profiles of screw dislocations.

```

S.0033      4      IF(J-55) 5,5,6
S.0034      5      X(J)=(J-M)*EPS2
S.0035      GO TO 11
S.0036      6      X(J)=1.5-(60-J)*EPS1
S.0037      GO TO 11
S.0038      11     DO 2002 INK=1,NUMBER
S.0039      AE(INK)=X(J)-XD(INK)
S.0040      IF(AE(INK)) 2002,201,2002
S.0041      201     TI(J)=0.0
S.0042      SI(J)=0.0
S.0043      GO TO 179
S.0044      2002    ANUM(INK)=EN*BSIGN(INK)*AE(INK)/(2.*PI)
S.0045      TR1=1.
S.0046      TI1=0.
S.0047      SR1=0.
S.0048      SI1=0.
S.0049      DO 200 I=1,N
S.0050      IF (I-1) 10,10,20
S.0051      10      AI=0.5
S.0052      DO 2003 INK=1,NUMBER
S.0053      DENOM(INK)=(AE(INK))**2+((AI-Y(INK))*DEL)**2
S.0054      2003    PHI(INK)=ANUM(INK)/DENOM(INK)
S.0055      PHIT=0
S.0056      DO 2004 INK=1,NUMBER
S.0057      2004    PHIT=PHIT+PHI(INK)
S.0058      YAP=YS+PHIT
S.0059      TR2=TR1+(YAP*TI1-SI1-RA*SR1)*PI*DEL
S.0060      TI2=TI1+(-YAP*TR1+SR1-RA*SI1)*PI*DEL
S.0061      SR2=SR1+(-YAP*SI1-TI1-RA*TR1)*PI*DEL
S.0062      SI2=SI1+(YAP*SR1+TR1-RA*TI1)*PI*DEL
S.0063      GO TO 200
S.0064      20      AI=I-1
S.0065      TR0=TR1
S.0066      TI0=TI1
S.0067      SR0=SR1
S.0068      SI0=SI1
S.0069      TR1=TR2
S.0070      TI1=TI2
S.0071      SR1=SR2
S.0072      SI1=SI2
S.0073      DO 2005 INK=1,NUMBER
S.0074      DENOM(INK)=(AE(INK))**2+((AI-Y(INK))*DEL)**2
S.0075      2005    PHI(INK)=ANUM(INK)/DENOM(INK)
S.0076      PHIT=0
S.0077      DO 2006 INK=1,NUMBER
S.0078      2006    PHIT=PHIT+PHI(INK)
S.0079      YAP=YS+PHIT
S.0080      TR2=TR0+(YAP*TI1-SI1-RA*SR1)*2.*PI*DEL
S.0081      TI2=TI0+(-YAP*TR1+SR1-RA*SI1)*2.*PI*DEL
S.0082      SR2=SR0+(-YAP*SI1-TI1-RA*TR1)*2.*PI*DEL
S.0083      SI2=SI0+(YAP*SR1+TR1-RA*TI1)*2.*PI*DEL
S.0084      200     CONTINUE
S.0085      TI(J)=(TR2*TR2)+(TI2*TI2)
S.0086      SI(J)=(SR2*SR2)+(SI2*SI2)
S.0087      179     WRITE (3,I50) X(J),TI(J),SI(J)
S.0088      150     FORMAT (1X,3HX =F10.4,10X,4HT1 =E14.6,10X,4HSI =E14.6)
S.0089      100     CONTINUE
S.0090      CALL GRAPH (J,X,TI,3,7,12.,8.,0.508,-1.7,2.54,-2.0,XLAB,YLAB,
S.0091      2GLAB,HLAB)
      CALL GRAPH (J,X,SI,3,7,12.,8.,0.508,-1.7,2.54,-2.0,XLAB,YLAB1,
      2GLAB,HLAB)

```

Fig. 2: (Continued).

```

S.0033      4      IF(J-55) 5,5,6
S.0034      5      X(J)=(J-M)*EPS2
S.0035              GO TO 11
S.0036      6      X(J)=1.5-(60-J)*EPS1
S.0037              GO TO 11
S.0038      11     DO 2002 INK=1,NUMBER
S.0039              AE(INK)=X(J)-XD(INK)
S.0040              IF(AE(INK)) 2002,201,2002
S.0041      201     TI(J)=0.0
S.0042              SI(J)=0.0
S.0043              GO TO 179
S.0044      2002    ANUM(INK)=EN*BSIGN(INK)*AE(INK)/(2.*PI)
S.0045              TR1=1.
S.0046              TI1=0.
S.0047              SR1=0.
S.0048              SI1=0.
S.0049              DO 200 I=1,N
S.0050              IF (I-1) 10,10,20
S.0051      10      AI=0.5
S.0052              DO 2003 INK=1,NUMBER
S.0053              DENOM(INK)=(AE(INK))**2+((AI-Y(INK))*DEL)**2
S.0054      2003    PHI(INK)=ANUM(INK)/DENOM(INK)
S.0055              PHIT=0
S.0056              DO 2004 INK=1,NUMBER
S.0057      2004    PHIT=PHIT+PHI(INK)
S.0058              YAP=YS+PHIT
S.0059              TR2=TR1+(YAP*TI1-SI1-RA*SR1)*PI*DEL
S.0060              TI2=TI1+(-YAP*TR1+SR1-RA*SI1)*PI*DEL
S.0061              SR2=SR1+(-YAP*SI1-TI1-RA*TR1)*PI*DEL
S.0062              SI2=SI1+(YAP*SR1+TR1-RA*TI1)*PI*DEL
S.0063              GO TO 200
S.0064      20      AI=1-1
S.0065              TR0=TR1
S.0066              TI0=TI1
S.0067              SR0=SR1
S.0068              SI0=SI1
S.0069              TR1=TR2
S.0070              TI1=TI2
S.0071              SR1=SR2
S.0072              SI1=SI2
S.0073              DO 2005 INK=1,NUMBER
S.0074              DENOM(INK)=(AE(INK))**2+((AI-Y(INK))*DEL)**2
S.0075      2005    PHI(INK)=ANUM(INK)/DENOM(INK)
S.0076              PHIT=0
S.0077              DO 2006 INK=1,NUMBER
S.0078      2006    PHIT=PHIT+PHI(INK)
S.0079              YAP=YS+PHIT
S.0080              TR2=TR0+(YAP*TI1-SI1-RA*SR1)*2.*PI*DEL
S.0081              TI2=TI0+(-YAP*TR1+SR1-RA*SI1)*2.*PI*DEL
S.0082              SR2=SR0+(-YAP*SI1-TI1-RA*TR1)*2.*PI*DEL
S.0083              SI2=SI0+(YAP*SR1+TR1-RA*TI1)*2.*PI*DEL
S.0084      200     CONTINUE
S.0085              TI(J)=(TR2*TR2)+(TI2*TI2)
S.0086              SI(J)=(SR2*SR2)+(SI2*SI2)
S.0087      179     WRITE (3,150) X(J),TI(J),SI(J)
S.0088      150     FORMAT (1X,3HX =F10.4,10X,4HTI =E14.6,10X,4HSI =E14.6)
S.0089      100     CONTINUE
S.0090              CALL GRAPH (J,X,TI,3,7,12.,8.,0.508,-1.7,2.54,-2.0,XLAB,YLAB,
S.0091              2GLAB,HLAB)
S.0091              CALL GRAPH (J,X,SI,3,7,12.,8.,0.508,-1.7,2.54,-2.0,XLAB,YLAB1,
S.0091              2GLAB,HLAB)

```

Fig. 2: (Continued).

judicious choice of column positions. For the case of screw dislocations, the numerator of the expression for $d\alpha'/dz$ is independent of z and thus need be calculated only once for a given column (statements 35-41). Equations (4) show that, for columns which contain dislocations, $d\alpha'/dz$ is indeterminate when evaluated at the dislocation. Intensity values at such column positions are therefore not calculated (statements 37-40). Finally, statements 48-60 and 61-81 provide for the calculation of the first forward difference and the remaining central difference values, respectively.

Calculation of image profiles for the case of edge dislocations requires only the substitution of $(d\alpha'/dz)$ edge into the program of Fig. 2 as shown in Fig. 3. Indeed, both displacement functions may easily be combined in a single program according to the relation: $\alpha = \alpha_{\text{screw}} \cos\theta + \alpha_{\text{edge}} \sin\theta$, for calculation of pure screw, edge, or mixed dislocations. However, since the computation time for the screw dislocation case is nearly half that for the edge case, and since edge dislocations qualitatively give the same contrast as screw dislocations, such a general program is not given here.

IMAGE PROFILE CALCULATION EXAMPLES

The effect of the size of DEL, the integration interval, upon the accuracy of a typical profile is shown in Fig. 4. The profiles in this figure were calculated for the case of a single screw dislocation located in the center of a $6t_e$ foil with image order, $\bar{g} \cdot \bar{b}$, equal to two and an interference error value of zero ($X = st_e = 0$). The top profile was

```

BEGIN COMPILATION
S.0001      DIMENSION X(500),T(500),S(500),XLAB(5),YLAB(5),GLAB(5),
           2HLAB(5),YLAR(5),LABEL1(20),LABEL2(20),NUMB(100),BSIGN(100),
           3XD(100),Y(100),AE(100),ANUM(100),DENOM(100),PHI(100)
S.0002      READ (1,1000) LABEL1
S.0003      READ (1,1000) XLAB, YLAB
S.0004      1 READ(1,120) N,M,NUMBER
S.0005      120 FORMAT (3I5)
S.0006      IF(N) 155,155,2
S.0007      2 READ(1,121) EN,RA,DEL,YS
S.0008      121 FORMAT (4E10.0)
S.0009      READ (1,1000) GLAB, HLAB
S.0010      READ (1,1000) LABEL2
S.0011      1000 FORMAT (20A4)
S.0012      DO 2000 INK=1,NUMBER
S.0013      2000 READ (1,1001) NUMB(INK),BSIGN(INK),XD(INK),Y(INK)
S.0014      1001 FORMAT (4F10.2)
S.0015      WRITE (3,122) EN,RA,DEL,YS
S.0016      122 FORMAT(1H1,4HEN =F8.4,7X,4HRA =F8.4,7X,5HDEL =F6.4,7X,3HY =F8.4)
S.0017      WRITE (3,1000) LABEL1
S.0018      DO 2001 INK=1,NUMBER
S.0019      2001 WRITE (3,1001) NUMB(INK),BSIGN(INK),XD(INK),Y(INK)
S.0020      WRITE (3,1000) LABEL2
S.0021      AN=N
S.0022      TH=AN*DEL
S.0023      WRITE (3,125) TH
S.0024      125 FORMAT (1X,11HTHICKNESS =F8.4)
S.0025      PI=4.*ATAN(1.)
S.0026      EPS1=0.2E00
S.0027      EPS2=0.02E00
S.0028      K=2.*M
S.0029      DO 100 J=1,K
S.0030      IF(J-5) 3,3,4
S.0031      3 X(J)=-1.6+J*EPS1
S.0032      GO TO 11
S.0033      4 IF(J-65) 5,5,6
S.0034      5 X(J)=(J-M)*EPS2
S.0035      GO TO 11
S.0036      6 X(J)=1.6-(70-J)*EPS1
S.0037      GO TO 11
S.0038      11 DO 2002 INK=1,NUMBER
S.0039      AE(INK)=X(J)-XD(INK)
S.0040      IF(AE(INK)) 2002,201,2002
S.0041      201 TI(J)=0.0
S.0042      SI(J)=0.0
S.0043      GO TO 2678
S.0044      2002 CONTINUE
S.0045      TR1=1.
S.0046      T11=0.
S.0047      SR1=0.
S.0048      S11=0.
S.0049      DO 200 I=1,N
S.0050      IF (I-1) 10,10,30
S.0051      10 AI=0.5
S.0052      DO 2003 INK=1,NUMBER
S.0053      ANUM(INK)=(EN*AE(INK)*BSIGN(INK)/(2.*PI))*(1.+75*COS(2.*ATAN
           2(DEL*(AI-Y(INK))/AE(INK))))
           DENOM(INK)=(AE(INK))*2+((AI-Y(INK))*DEL)**2
S.0054      2003 PHI(INK)=ANUM(INK)/DENOM(INK)
S.0055      PHIT=0
S.0056      DO 2004 INK=1,NUMBER
S.0057      PHIT=PHIT+PHI(INK)
S.0058      2004 YAP=YS+PHIT
           TR2=TR1+(YAP*T11-S11-RA*SR1)*PI*DEL
           T12=T11+(-YAP*TR1+SR1-RA*S11)*PI*DEL
           SR2=SR1+(-YAP*S11-T11-RA*TR1)*PI*DEL
           S12=S11+(YAP*SR1+TR1-RA*T11)*PI*DEL
           GO TO 200
S.0059      30 AI=1-1
           TRO=TR1
           TJO=T11
           SRO=SR1
           SJO=S11
           TR1=TR2
           T11=T12
           SR1=SR2
           S11=S12
           DO 2005 INK=1,NUMBER
           ANUM(INK)=(EN*AE(INK)*BSIGN(INK)/(2.*PI))*(1.+75*COS(2.*ATAN
           2(DEL*(AI-Y(INK))/AE(INK))))
           DENOM(INK)=(AE(INK))*2+((AI-Y(INK))*DEL)**2
S.0060      2005 PHI(INK)=ANUM(INK)/DENOM(INK)
S.0061      PHIT=0
S.0062      DO 2006 INK=1,NUMBER
S.0063      PHIT=PHIT+PHI(INK)
S.0064      2006 YAP=YS+PHIT
           TR2=TRO+(YAP*T11-S11-RA*SR1)*2.*PI*DEL
           T12=TJO+(-YAP*TR1+SR1-RA*S11)*2.*PI*DEL
           SR2=SRO+(-YAP*S11-T11-RA*TR1)*2.*PI*DEL
           S12=SJO+(YAP*SR1+TR1-RA*T11)*2.*PI*DEL
S.0065      200 CONTINUE
           TI(J)=(TR2*TR2)+(T12*T12)
           SI(J)=(SR2*SR2)+(S12*S12)
S.0066      2678 WRITE (3,150) X(J),TI(J),SI(J)
S.0067      150 FORMAT (1X,3HX =F10.4,10X,4HTI =E14.6,10X,4HSI =E14.6)
S.0068      100 CONTINUE
           CALL GRAPH (J,X,TI,3,7,12.,8.,0.508,-1.7,2.54,-2.0,XLAB,YLAB,
           2GLAB,HLAB)
           CALL GRAPH (J,X,SI,3,7,12.,8.,0.508,-1.7,2.54,-2.0,XLAB,YLAB,
           2GLAB,HLAB)
S.0069      GO TO 1
S.0070      155 STOP
S.0071      END

```

Fig. 3: FORTRAN program for the calculation of image profiles of edge dislocations.

calculated with a DEL value of $0.0025t_e$ and is identical to that given by other authors.⁵ As the remaining profiles of this figure show, increasing the value of DEL progressively degrades the accuracy of the computed profile. Thus, the appropriate DEL value is best determined by trial calculations of the sort shown in Fig. 4. However, routine calculations of both edge and screw array profiles for dislocations located near the center of a $6t_e$ thick foil may be accomplished with a DEL value of 0.0025 for image order values of 1 and 2. In addition, the use of a $6t_e$ foil thickness value obviates the need for surface relaxation corrections if the dislocations are situated close to the center.

Figure 5 shows the profiles computed for a single edge dislocation at various diffraction conditions. These results are in agreement with those reported by others⁵ and illustrate the effect of changes in X and the image order upon the calculated intensity distribution.

CONCLUDING REMARKS

Although the FORTRAN program presented here is not as generally applicable as might be desired, it may easily be modified for calculation of the intensity distributions expected for more complicated experimental situations by substitution of the appropriate $d\alpha'/dz$ factors. In fact, a large number of calculations for the specific cases of ordinary and superlattice dislocation dipoles have been performed and will be presented in a future report.⁹

Figure 4

Fig. 4

Fig. 4: Image profiles calculated for edge dislocations of various diffraction conditions.

Figure 5

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Fig. 5: Image profiles of a single screw dislocation with $\bar{g} \cdot \bar{b} = 2$ for various values of the integration interval, DEL .

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