TEMACI

A Computer Program for
TEM Amplitude Contrast Imaging.

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1 Introduction

This manual will give a brief description of the computer program for simulations of TEM amplitude contrast images using the Howie-Basinski equations (1). The program was written fully in Fortran 90 format. The program has been compiled and run successfully on UNIX, Linux and Microsoft Windows systems. However, the precompiled version can only run under LINUX systems. It can run under a text mode or a graphic-user interface. The GUI part of the program calls some Fortran libraries, which have been staticly included in the executable file *TEMACI*, so that it is not necessary to install the libraries used in the code in your own machines, except to copy the file *pgxwin_server* into your working directory. All variables are defined using a flexible data type, which can be changed according to the accuracy required in calculations, the running platforms and machines. The source code of the program can be obtained from the author, Zhongfu Zhou (e-mail: z.zhou@st-hughs.oxon.org) or Dr. M. L. Jenkins, Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK, E-mail: mike.jenkins@materials.ox.ac.uk.

2 Running *TEMACI*

The program *TEMACI*can be invoked under either text mode or graphic-user interface (GUI) mode. To run the program in GUI mode, just simple type the command:
/home/myaccount/systemdir/temaci.
The directory **/home/myaccount/systemdir/** is where the executable file “temaci” locates.
In order to run the program with text mode, an option parameter *-t* should be used, for example:
temaci **-t** *[input file] [defect configuration file]*

Before carrying out any simulation using the text mode, some files (described below) need to be generated/modified. These files should be put into your current working directory. If the program is running under the GUI mode, all parameters necessary for running calculations can be inputted in the GUI. Screen snapshots below show three examples for imaging of a screw, an edge dislocation and dislocation loop.

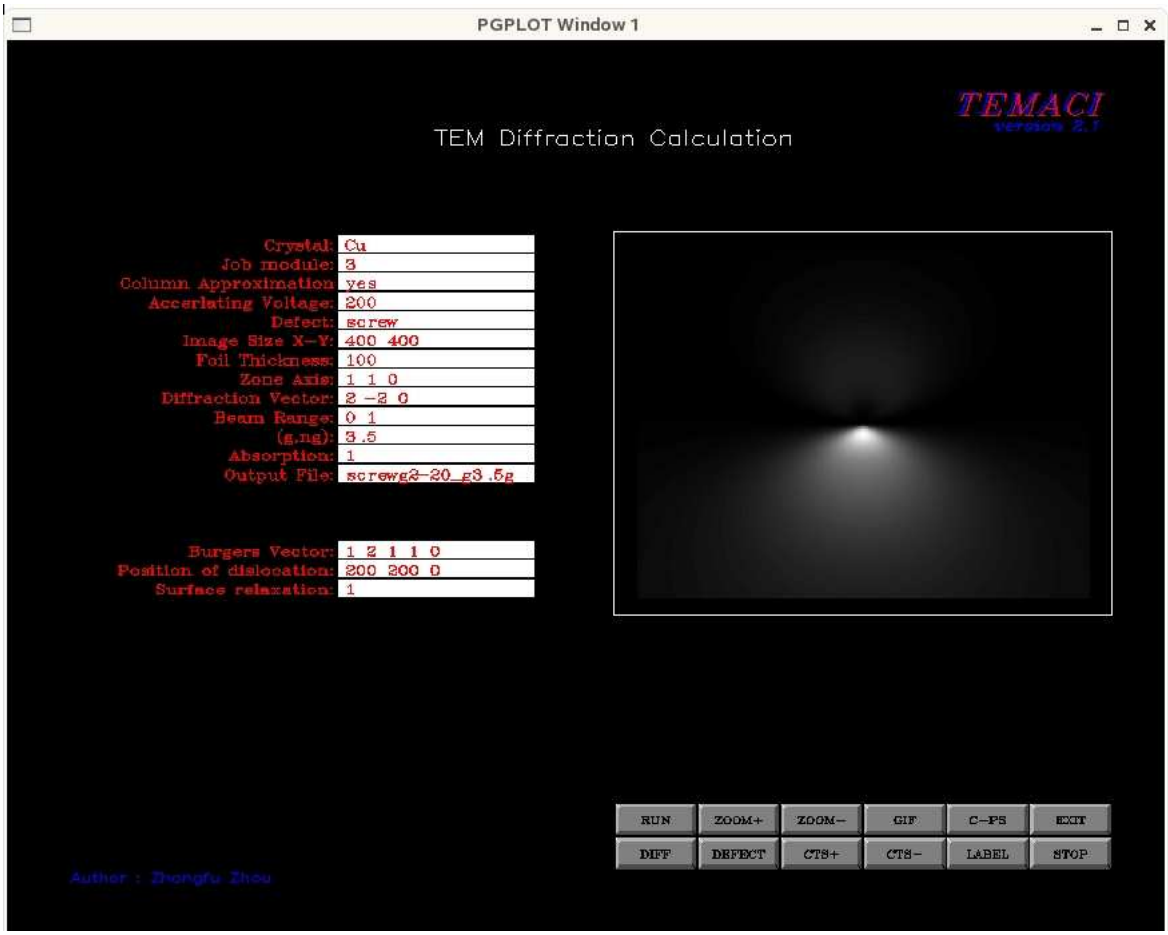

Figure 1: GUI demo 1 - screw dislocation (with surface relaxation)

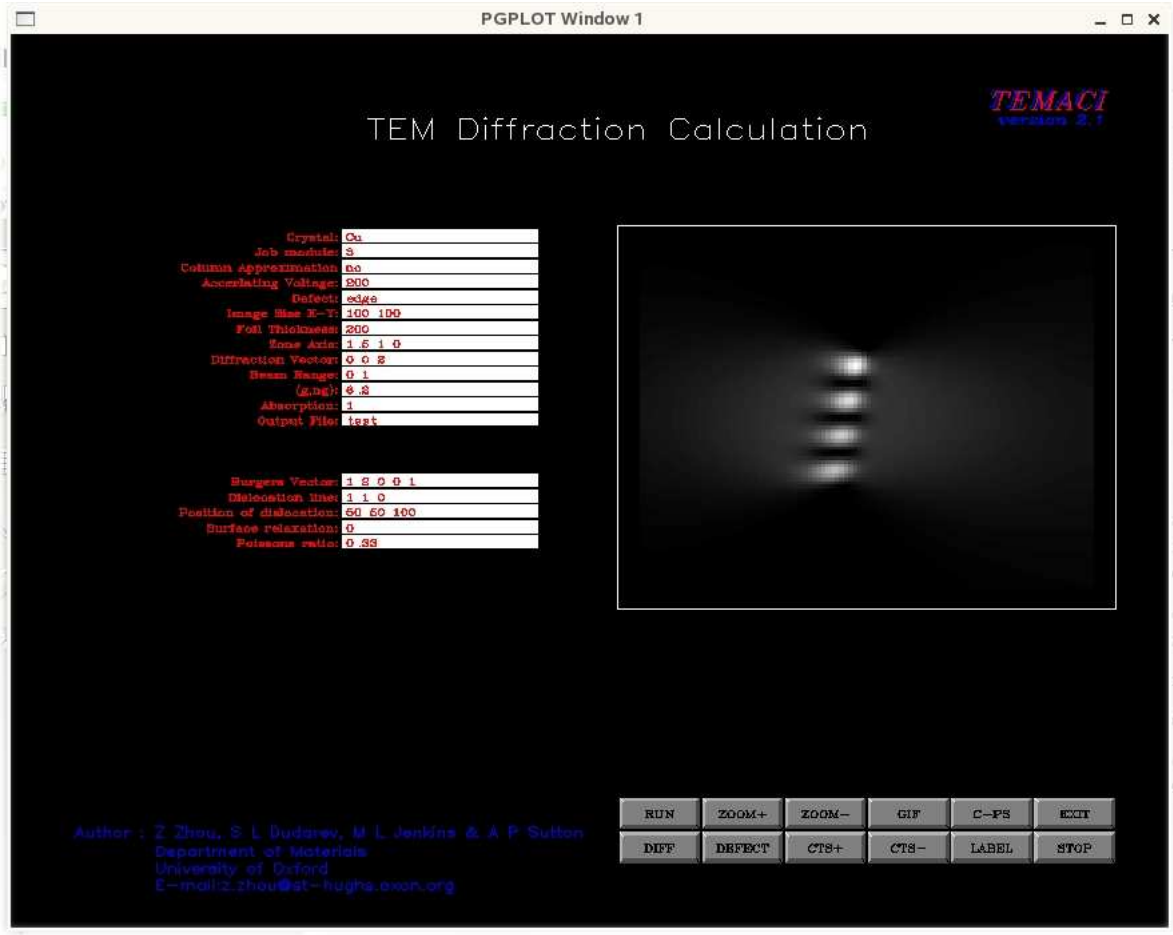

Figure 2: GUI demo 2 - edge dislocation (inclined)

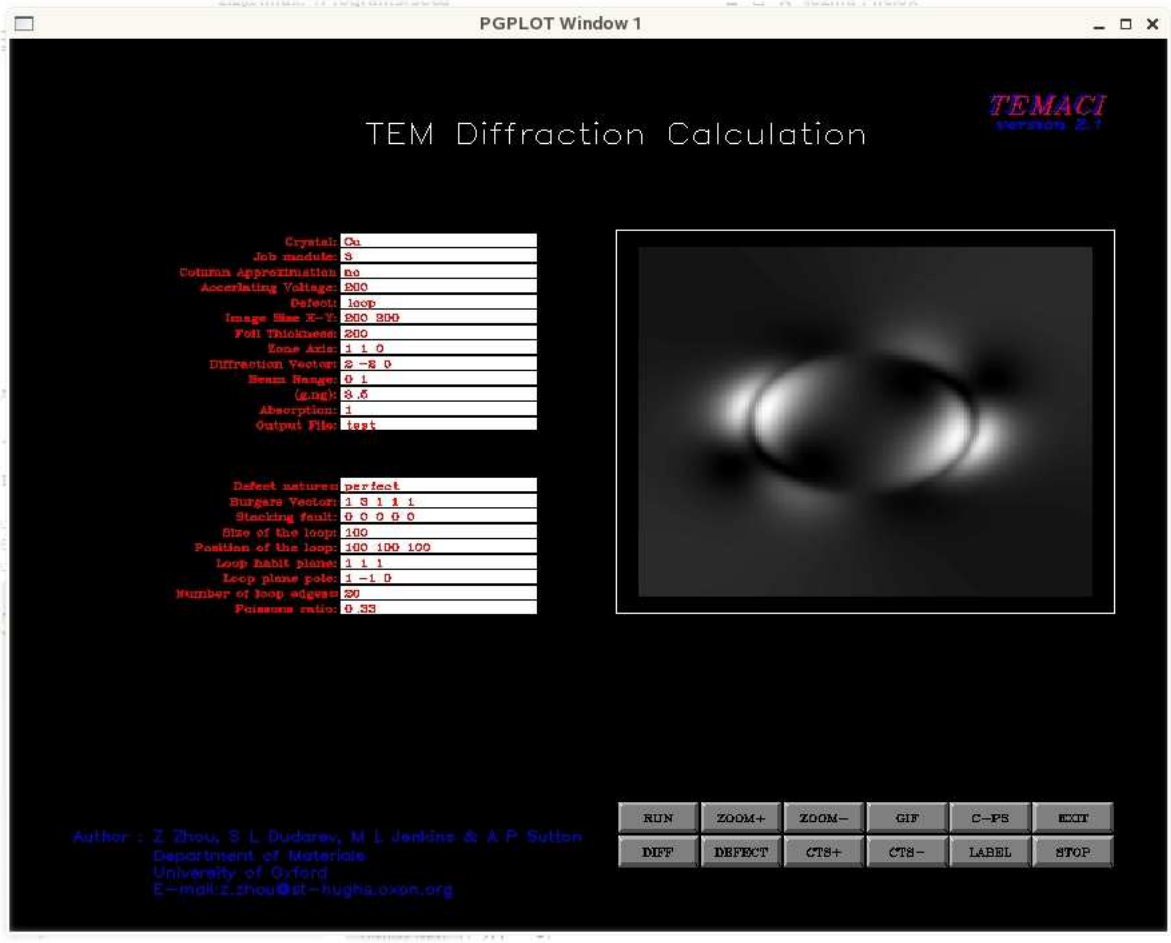

Figure 3: GUI demo 3 - inclined dislocation loop

NOTE:

- Under the GUI running environment, the input for *defect* should be
  - *screw* : screw dislocation
  - *edge* : edge dislocation
  - *loop* : polygonal dislocation loop
  - *no* : no defect
- Please only click the button RUN to run calculations, the button C-PS to generate an dark-field image of Postscript format and EXIT to exit the program. All other buttons are reserved and cannot be activated in the current version.

- If the projection of the sample in the x-y plane is not square, the images shown in the GUI image window will be stretched to fit in the window, which influences the appearance of the defect image. **Also it is important to know that the images formed by the GUI module might not represent the real contrast and sample shape for the following two reasons: 1) The contrast of images automatically generated are always extended into 256 grey levels no matter how small the actual contrast is. 2) The width and height of the image do not reflect the actual shape of the sample. It is recommended to form images using the intensity data array for publishing.**

- If you intend to use the text mode, all three files described below are necessary. The formats of these files is outlined below. In order to avoid errors, it is advisable to stick to the formats specified in the examples.

3 Input files for the text mode

3.1 Main Input File Format.

If the program is running under text mode, the input file containing all the necessary control parameters for the simulation should be given prior to all calculations. In this file the parameters which control the operation of the program, such as sample, diffraction conditions. Shown below is a typical input file. Input parameters are give underneath a set of keywords, which will be explained shortly. However, in order to avoid errors, it is preferable for the general format of input files to be the same as that given below.

```
sample number
'Cu'
crystal
'Cu'
Job Module (1:amplitude contrast images, 2:thickness fringes, 3:multi layber i
3
CA (The Column Approximation: yes or no)
'no'
Accelerating voltage (KV)
100.0
Defect (edge, screw, pg_loop, void, tetrahedron, 3D-strain or no)
'screw'
size of sample in x direction
50
```

```
size of sample in y direction
50
size of sample in z direction (foil thickness)
300
zone axis (z direction perpendicular to the foil)
1,0,1
Diffraction vector g
0 2 0
Range of beams considered
0,1
Strong Diffracted position (i.e. g, 2g, 3.5g ... )
4.5
Anomalous absorption (0 : without, 1 : with absorption)
1
```

3.2 Input description and Keywords

In this section, the various parameters in the main input file will be explained.

(i) **Keyword**: *Sample number*

Allowed values: characters

This keyword is used to just give a label to the sample, the value does NOT influence simulations.

(ii) **Keyword**: *crystal*

Allowed values: element (e.g. Fe, Au, Si ...)

In the current version, only single element crystals are accepted by the program.

(iii) **Keyword**: *job module*

Allowed values: $1 \cdots 3$

This parameter controls which kind of calculation will be performed. 1: general amplitude contrast images according to all beams will be calculated and given out when simulation finishes; 2: Calculation of thickness fringes (beware that for this module, the thickness of sample must be identical with the sample size along the x direction; 3: A set of images according to beam g will be recorded layer by layer, so that you can get a set of dark filed images according to different foil thickness. Also intensities according to other beams at the exit surface of the sample are recorded (same as job module 1).

(iv) **Keyword**: *The column approximation*

Allowed values: yes / no

This keyword is used to switch between the column approximation or non-column approximation.

(v) **Keyword**: *Accelerating voltage*

Allowed values: integer

This keyword is used to give out the accelerating voltage of TEM, please note the unit is kV.

(vi) **Keyword**: *Defect*

Allowed values: characters

This keyword is used to specify the type of defect in the sample. *edge*: edge dislocation; *screw*: screw dislocation; *pg_loop*: polygonal dislocation loops; *void*: a spherical void; *tetrahedron*: a stacking fault tetrahedron; *3D-strain*: any 3-dimensional distortion field, for example, the distortion field converted from atomistic configuration (this is a little bit complicated, please discuss with the program developer if you want to use this module); *no*: perfect crystal, no defect (this is mainly used for calculations of thickness fringes).

(vii) **Keyword**: *Size of sample in x direction*

Allowed values: real number

Size of the sample along x direction, unit $\mathring{A}$.

(viii) **Keyword**: *Size of sample in y direction*

Allowed values: real number

Size of the sample along y direction, unit $\mathring{A}$.

(ix) **Keyword**: *Size of sample in z direction*

Allowed values: real number

Size of the sample along z direction, unit $\mathring{A}$. This is the foil thickness.

(x) **Keyword**: *zone axis*

Allowed values: integers

The zone axis in the form of $\{hkl\}$ is necessary here for giving out the orientation of the sample foil. In the current version, it is essential to set this direction perpendicular to the diffraction vector g.

(xi) **Keyword**: *Diffraction vector*

Allowed values: integers

Please give the diffraction vector here.

(xii) **Keyword**: *Range of beams*

Allowed values: two integers

These two integers define the range of beams along the systematic row taken account in the calculation, i.e. 0, 1 - for a two-beam calculation, in which only transmitted and diffraction beam **g** are considered.

(xiii) **Keyword**: *Strong diffraction position*

Allowed values: a real number

It defines the diffraction conditions (**g**,t**g**), t here is the position of the systematic row and Ewald sphere crossed. For example, $t = 1.0$ defines the two-beam dynamical condition.

(xiv) **Keyword**: *A normalous absorption*

Allowed values: 0/1

0 : without absorption; 1 : with absorption.

4 Defect configuration files for *TEMACI*

In order to run the program for the simulations of the TEM amplitude contrast of defects under the text mode, a defect configuration file must be present in the command line. The following are examples of such files for the defect models which can be simulated using the program:

4.1 Edge dislocation

```
            {Data for edge dislocation in Crystal}
=================================================================
1,3,1,1,1                       - Burgers vector b (m/n[u,v,w])
200.0,200.0,3.0                 - Position of the dislocation in the foil
-2,1,1                          - Dislocation line direction
0.42                            - Poissons ratio
0.5                             - Factor for avoiding the singularity
                                  of strain field
```

4.2 Screw dislocation

```
            {Data for a screw dislocation in Crystal}
=================================================================
1,2,1,1,0                       - Burgers Vector b (m/n[u,v,w])
25  25  0                       - Position of the dislacation
0,0,1                           - cut plane (=b//z x x) must perpediculat to b
1                               - surface relaxation
```

4.3 void

```
            {Data for a spherical void in crystal}
=======================================================
250                             - Radius of the spherical void
300,300,300                     - Position of the centre of the void
```

4.4 Polygonal loop

```
            {Data for polygonal dislocation loop in Crystal}
=================================================================
'faulted'                        - perfect, faulted, or pureSF
1,3,1,1,1                        - Burgers vector b (m/n[u,v,w])
1,6,-2,1,1                       - Burgers vector of stacking fault
50.0                             - Radius of the loop
100.0,100.0,150.0                - Position of the centre of the loop
1,1,1                            - loop plane normal
-2,1,1                           - loop plane polar
4                                - Number of sides of the polygon
0.34                             - Poissons ratio
0.5                              - Factor for avoiding the singularity
                                   of strain field close to dislocation edges
```

4.5 Stacking-fault tetrahedron

```
            {Data for stacking-fault tetrahedra in Crystal}
=================================================================
'faulted'               - pure stacking fault ('pureSF') or faulted
100.0,100.0,150.0       - Position of the centroid
200.0                   - length of edges
0.23                    - Poissons ratio
8                       - Factor for avoiding the singularity
                          of strain field close to the dislocation edges
```

4.6 Atomistic configuration

```
            {Name of the input file of the distortoin field}
=================================================================
Fe_3M_111_110_43atoms_AD_z111_x1-10  - File name for strain field
```

4.7 Output of the program

The intensities according to each beam are written into file named as *input_main_filenameXXg*.

XX represents one of the beams considered in the calculations, for example, it can be 00 and 01

for a calculation under the two-beam approximation. Following is the head of such a output file which gives out the 2D array of intensity at the exit surface of the sample.

```
width
         20
height
         20
unit of width
  1.00000000000000
unit of height
  1.00000000000000
  8.420E-02   8.447E-02   8.476E-02   8.505E-02   8.536E-02   8.567E-02   8.6
  8.429E-02   8.458E-02   8.487E-02   8.518E-02   8.549E-02   8.582E-02   8.6
  8.439E-02   8.468E-02   8.498E-02   8.530E-02   8.563E-02   8.597E-02   8.6
  8.447E-02   8.478E-02   8.509E-02   8.542E-02   8.576E-02   8.611E-02   8.6
  8.456E-02   8.487E-02   8.520E-02   8.554E-02   8.589E-02   8.626E-02   8.6
  8.464E-02   8.496E-02   8.530E-02   8.565E-02   8.602E-02   8.640E-02   8.6
```

Also a file named as *input_main_filename.par* is generated, which records the parameters of the calculation and some other useful information, as in the following:

```
++++++ PARAMETERS for result file, "test" ++++++


Date:           14 -3 - 2007     Time:           17 : 20


**********************
PROCESSING TIME
0 : 1 : 53  (hours:minutes:seconds)
**********************


LIST OF PARAMETERS

---------------------------------------

Sample NO: Cu
---------------------------------------

Sample: Cu
---------------------------------------
Job performed
Multilayer contrast images
---------------------------------------
the Column Approximation
not used
---------------------------------------
Interpolation Method:
```

```
 linear
 ----------------------------------------

 ----------------------------------------

 Crystal structure:
 ----------------------------------------
 Accelerating voltage
   100.000000000000       kv
 ----------------------------------------
 Magnitude of wave vector k
   27.0263227870029
 ----------------------------------------
 The lattice constant of sample
   3.61000000000000
 ----------------------------------------
 The spacing of diffraction crystal planes
   1.80500000000000
 ----------------------------------------
 size of sample (x*y*z in Angstrom)
   20.0000000000000       *    20.0000000000000       *    50.0000000000000
 ----------------------------------------
 number of beams considered
           2
 ----------------------------------------
 number of grids
          20  *           20  *           50
 ----------------------------------------
 size of each grid (in Angstrom)
   1.00000000000000       *    1.00000000000000       *    1.00000000000000
 ----------------------------------------
 Fourier components of periodical potentials (U(0)-U(           1
 g), in Angstrom E(-2))
U(  0)=0.1516
U( 1g)=0.0701
 ----------------------------------------
 The ratio of immaginary and real parts of periodical potentials
0.00
 ----------------------------------------
 Z direction of sample
 [   1.00000000000000      ,  0.000000000000000E+000 ,   1.00000000000000
 ----------------------------------------
 X direction of sample
 [  0.000000000000000E+000 ,   2.00000000000000      ,  0.000000000000000E+000
 ----------------------------------------
 Optical axis
 [  0.000000000000000E+000 ,  0.000000000000000E+000 ,  0.000000000000000E+000
 ----------------------------------------
 Diffraction vector g
 [  0.000000000000000E+000 ,   2.00000000000000      ,  0.000000000000000E+000
 ----------------------------------------
```

```
Bemas considered
          0 g ~            1 g
---------------------------------------
Diffraction condition
  2.50000000000000      g strongly excited
---------------------------------------
Diffraction condition
 s_g=   8.5191065285989 96E-003   1/A
---------------------------------------
Style of defect
pg_loop
---------------------------------------
Loop style
          6 -sided polygonal loop
---------------------------------------
Burgers Vector
  1.00000000000000      /   3.00000000000000      [   1.00000000000000      ,
  1.00000000000000      ,   1.00000000000000      ]
---------------------------------------
Loop size (twice of distance from the centroid to a vertex)
  50.0000000000000       Angstrom
---------------------------------------
Position of the loop centre (in Angstrom)
(   50.0000000000000      ,   50.0000000000000      ,   25.0000000000000
---------------------------------------
Loop normal
[   1.00000000000000      ,   1.00000000000000      ,   1.00000000000000
---------------------------------------
---------------------------------------
Loop polar
[   1.00000000000000      ,  -1.00000000000000      ,  0.000000000000000E+000
---------------------------------------
g.b
 0.666666666666667
---------------------------------------
Correction factor for avoiding the singularity of strain
  1.00000000000000       A
---------------------------------------
```

5 The structure of the program

The structure of the program for TEM diffraction contrast calculations is shown in figure 4. First the program reads sample information, diffraction condition and other control parameters from an initial file. Then the wave vector, Fourier components of potential and deviation parameters are calculated according to the input information. The calculations of amplitudes of each beam are then carried out slice by slice. Each slice is divided into small rectangular cells parallel to

the x and y axes. The *modified* Howie-Whelan equations (equation (2)) are solved for each cell with a given distortion field. The amplitudes at the exit surface of the slice are then calculated using the interpolation procedure described in section 7.

The distortion fields of dislocations can be calculated using elasticity theory or atomistic simulation. Subroutines for calculating the distortion fields of polygonal dislocation loops using isotropic elasticity theory have been developed. The program can be used to simulate TEM diffraction contrast images of straight dislocations, planar dislocation loops, stacking faults and stacking-fault tetrahedra.

The program has been optimised to save CPU time and memory. It can handle the simulations of amplitude diffraction contrast images with up to 99 beams taken into account. The maximum imaging resolution depends on the memory of machines. It can be 2500×2500 in mesh for machines more than 512 MB RAM. There is no limit in the number of slices. For typical simulations of weak-beam images of resolution 200×200 for a sample cut into 1000 slices, the CPU time required for PCs with CPU frequency of 1.7 KHz running Linux system is about 20 minutes. This capability makes systematic simulations possible.

The outputs of the program are 2-dimensional data arrays of the intensities of diffraction contrast. Any software package capable for 2D data plotting can be used to generate images with small modification to the output file accordingly. The authour of the **TEMACI** has also developed two codes to produce images using the data arrays. One program can produces images of TIFF format with the use of LibTiff library. Another program is more flexible, and is based on PGPLOT. Both programs are able to generate a batch of images using a single command, which is useful for the systematic study of images under various sample or diffraction conditions. These two programs are not integrated with the main program, only can be obtained by request to the authour.

5.1 Solving the Howie-Basinski equations

For simulations of weak-beam images, we have to solve the Howie-Basinski equations for many beams, including at least several beams in the systematic row. The equations (1) are partial

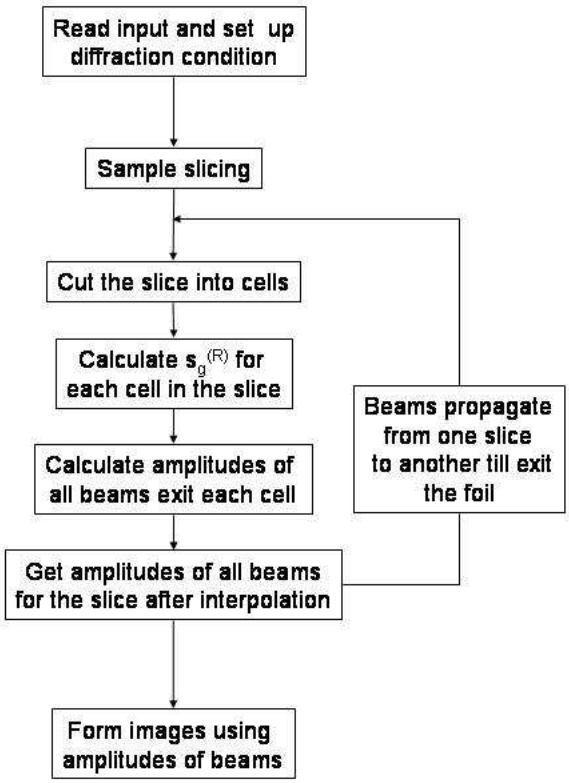

Figure 4: Summary of the steps involved in carrying out a simulation of amplitude diffraction contrast images of an individual dislocation loop.

differential equation sets, which cannot be solved directly even by numerical procedures.

$$\begin{aligned}(\mathbf{k}+\mathbf{g}+\mathbf{s_g})\cdot\nabla\Phi_{\mathbf{g}} &= 2\pi i(\mathbf{k}+\mathbf{g}+\mathbf{s_g})\cdot\mathbf{s}_{\mathbf{g}}^{(\mathbf{R})}\Phi_{\mathbf{g}} \\ &\quad -\pi i\sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'})U_{\mathbf{g}-\mathbf{g}'}e^{i\pi\frac{U_0}{(\mathbf{k}+\mathbf{g}+\mathbf{s_g})_z}z-i\pi\frac{U_0}{(\mathbf{k}+\mathbf{g}'+\mathbf{s}_{\mathbf{g}'})_z}z}\Phi_{\mathbf{g}'} \qquad (1)\end{aligned}$$

where $\mathbf{s}_{\mathbf{g}}^{(\mathbf{R})} = \mathbf{s_g} + \nabla\left[\mathbf{g}\cdot\mathbf{R}(\mathbf{r})\right]$ is an effective local deviation parameter that varies spatially when the distortion field $\partial R_i/\partial x_j$, ($i$, j = 1, 2, 3) changes with position.

One possible approach is to first neglect the derivatives with respect to x and y and solve the ordinary differential equation set (equation (2)),which is similar to the Howie-Whelan equations, except the strain field with respect to x and y are retained, we call it *modified* Howie-Whelan equations.

$$\frac{\partial\Phi_{\mathbf{g}}}{\partial z} = \frac{2\pi i}{\beta_{\mathbf{g}}}(\mathbf{k}+\mathbf{g}+\mathbf{s_g})\cdot\mathbf{s}_{\mathbf{g}}^{(\mathbf{R})}\Phi_{\mathbf{g}} - \pi i\sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'})\frac{U_{\mathbf{g}-\mathbf{g}'}}{\beta_{\mathbf{g}}}\Phi_{\mathbf{g}'}. \qquad (2)$$

where $\beta_{\mathbf{g}} = (\mathbf{k}+\mathbf{g}+\mathbf{s_g})_z$. These equations take into account the full three-dimensional nature of lattice distortions $\partial R_i/\partial x_j$ but still make the column approximation.

Generally, there are two ways to solve numerically the modified Howie-Whelan equations: namely, the matrix eigensystem method and the Runge-Kutta method. Only the matrix eigensystem method is used in the program.

6 Solving the modified HW equations by an eigensystem method

In matrix notation, equation set (2) can be rewritten as

$$\frac{\partial}{\partial z}\mathbf{\Phi} = \pi i\mathbf{H}\mathbf{\Phi} \qquad (3)$$

Here $\mathbf{\Phi}$ is a column vector $\{\mathbf{\Phi}\} = \Phi_{\mathbf{g}}$. $\mathbf{H}$ is a general matrix with elements

$$\{\mathbf{H}\}_{\mathbf{g}\mathbf{g}'} = \frac{2}{\beta_{\mathbf{g}}}(\mathbf{k}+\mathbf{g}+\mathbf{s_g})\cdot\mathbf{s_g}^{(\mathbf{R})} - \sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'})\frac{U_{\mathbf{g}-\mathbf{g}'}}{\beta_{\mathbf{g}}} \qquad (4)$$

If we consider n beams which associate with n different diffraction vectors along a systematic row, $\mathbf{H}$ is a $n\times n$ matrix.

Using standard matrix diagonalization programs, we can find the eigenvalues ω of $\mathbf{H}$, from which we form a diagonal matrix $\mathbf{\Omega}$ with elements $\{\mathbf{\Omega}\}_i, (i = 1, 2, \cdots n)$. From the corresponding eigenvectors, which are column vectors, we form a square matrix $\mathbf{C}$ which satisfies the equation

$$\mathbf{C^{-1}HC} = \mathbf{\Omega} \tag{5}$$

Here $\mathbf{C^{-1}}$ is the reciprocal matrix of $\mathbf{C}$.

Then we have

$$\frac{\partial}{\partial z}\mathbf{\Phi} = \pi i \mathbf{H\Phi} = \pi i \mathbf{C\Omega C^{-1}\Phi} \tag{6}$$

$$\frac{\partial}{\partial z}\left(\mathbf{C^{-1}\Phi}\right) = \pi i \mathbf{\Omega C^{-1}\Phi} \tag{7}$$

Now we know that $\mathbf{C^{-1}\Phi}$ is a column vector with n elements. We define it as $\mathbf{C^{-1}\Phi} = \mathbf{\Gamma} = \begin{pmatrix} \Gamma_1 \\ \Gamma_2 \\ \cdots \\ \Gamma_n \end{pmatrix}$. Then we have

$$\frac{\partial}{\partial z}\mathbf{\Gamma} = \pi i \mathbf{\Omega\Gamma} \tag{8}$$

The matrix expression (equation (8)) can be written in the form of an equation set as below

$$\frac{\partial \Gamma_i}{\partial z} = \pi i \omega_i \Gamma_i, \quad (i = 1, 2, \cdots, n) \tag{9}$$

which has solution

$$\Gamma_i = \Gamma_i(0) e^{\pi i \omega_i z}, \quad (i = 1, 2, \cdots, n) \tag{10}$$

Equation (10) may be written in a matrix form as

$$\mathbf{\Gamma} = \mathbf{E\Gamma_0} \tag{11}$$

where $\mathbf{E}$ is a diagonal matrix with elements $\{\mathbf{E}\}_i = e^{\pi i \omega_i z}, \quad (i = 1, 2, \cdots, n)$; $\mathbf{\Gamma_0}$ is a column vector, $\{\mathbf{\Gamma_0}\}_i = \Gamma_i(0)$ for $i = 1, 2, \cdots, n)$. From the definition of matrix $\mathbf{\Gamma}$, we know that

$$\mathbf{C^{-1}\Phi} = \mathbf{EC^{-1}\Phi_0} \tag{12}$$

$$\mathbf{\Phi} = \mathbf{CEC^{-1}\Phi_0} = \mathbf{P\Phi_0} \tag{13}$$

Here $\mathbf{\Phi_0}$ is a column vector with $\{\mathbf{\Phi_0}\}_i = \Phi_i(0), \quad (i = 1, 2, \cdots, n)$. We define the scattering matrix $\mathbf{P} = \mathbf{CEC^{-1}}$. Equation (13) gives the required solution for Φ.

7 The Validity of the Interpolation Procedure

Here we show that a solution obtained using the interpolation procedure outlined in Section 3 is an exact solution of the Howie-Basinski equations (1) in the limit of an infinitesimal cell size. To illustrate the numerical solution we consider a weak-beam condition in which **g** is selected from a systematic row of reflections $\mathbf{g}' = \mathbf{g},\ 2\mathbf{g},\ 3\mathbf{g},\ ...,\ n\mathbf{g}$, where n is an integer. We choose the x-axis to be parallel to the systematic row of $\mathbf{g}'$-vectors. The amplitudes of diffracted beams in this case are independent of coordinate y and the diffraction problem is two-dimensional.

Our approach is to use the modified Howie-Whelan equations (2) to propagate the diffracted beams along the zone axis, and to take account of the inclined propagation by equating beam amplitudes entering a slice normal the zone axis to linear combinations of beam amplitudes exiting adjacent cells in the previous slice. Let $\Phi_{g'}^{(in)}(\nu, z)$ and $\Phi_{g'}^{(out)}(\nu, z + \Delta z)$ denote the amplitudes of the diffracted beam $\mathbf{k} + \mathbf{g}'$ entering and exiting the ν'th cell of the slice at z of thickness Δz. Within each slice there are rows of cells along the x-axis and ν increases along each row and from one row to the next along the y-axis. Let θ'_g denote the angle between the diffracted beam $\mathbf{k} + \mathbf{g}'$ and the zone axis (see Figure 5). The angle θ'_g is in the (x, z) plane, and

$$\tan\theta_{g'} = \frac{(\mathbf{k}+\mathbf{g}')_x}{(\mathbf{k}+\mathbf{g}')_z} \approx \frac{(\mathbf{k}+\mathbf{g}')_x}{(\mathbf{k}+\mathbf{g}'+\mathbf{s}'_{\mathbf{g}})_z}, \tag{14}$$

since $(\mathbf{s}_{g'})_z \ll (\mathbf{k}+\mathbf{g}')_z$.

In the column approximation the amplitude $\Phi_{g'}^{(out)}(\nu, z+\Delta z)$ exiting the ν'th cell of a given slice equals the amplitude $\Phi_{g'}^{(in)}(\nu, z+\Delta z)$ entering the ν'th cell of the next slice. But for the inclined propagation considered here the amplitude entering the ν'th cell of the next slice is set equal to a weighted average of the amplitudes exiting the cell directly above and an adjacent cell:

$$\Phi_{g'}^{(in)}(\nu, z+\Delta z) = \left(1 - \frac{\Delta z}{W}\tan\theta_{g'}\right)\Phi_{g'}^{(out)}(\nu, z+\Delta z) + \left(\frac{\Delta z}{W}\tan\theta_{g'}\right)\Phi_{g'}^{(out)}(\nu-1, z+\Delta z), \tag{15}$$

if $\theta_{g'}$ is positive and

$$\Phi_{g'}^{(in)}(\nu, z+\Delta z) = \left(1 + \frac{\Delta z}{W}\tan\theta_{g'}\right)\Phi_{g'}^{(out)}(\nu, z+\Delta z) - \left(\frac{\Delta z}{W}\tan\theta_{g'}\right)\Phi_{g'}^{(out)}(\nu+1, z+\Delta z), \tag{16}$$

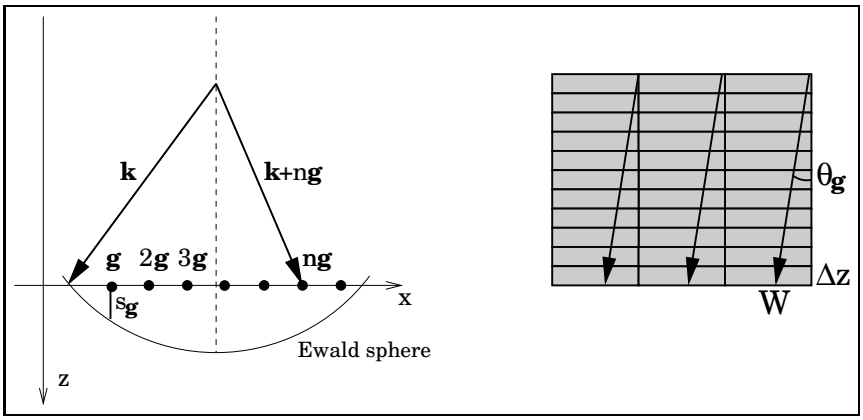

Figure 5: Schematic diagram to illustrate the geometry of the assumed diffraction conditions. The vertical broken line represents the zone axis, **g** is a reciprocal lattice vector and **k** is the wave vector of the incident beam of electrons. The geometry of diffraction illustrated in this figure corresponds to a weak-beam condition typically used in electron microscope imaging where the Ewald sphere *does not* pass through a reciprocal lattice point.

if $\theta_{g'}$ is negative. Here W is the length of a cell along x. The geometry is illustrated in Figure 5. The slices are assumed to be sufficiently thin for all the reflections $\mathbf{g}'$ that $|(\Delta z/W)\tan\theta_{g'}| \ll 1$.

We now show the equivalence between the interpolation method and the original set of differential equations (1). We write the derivative $\partial\Phi_g/\partial z$ as

$$\frac{\partial\Phi_{g'}(x,z)}{\partial z} = \lim_{\Delta z\to 0}\frac{\Phi_{g'}^{(in)}(x,z+\Delta z)-\Phi_{g'}^{(in)}(x,z)}{\Delta z}, \tag{17}$$

where the point x is located within the ν'th cell. The calculation of $\Phi_{g'}^{(in)}(x,z+\Delta z)$ involves two steps. First, starting from the amplitude $\Phi_{g'}^{(in)}(x,z)$ incident on a given slice and integrating equations (2), we find the amplitude $\Phi_{g'}^{(out)}(x,z+\Delta z)$ of the wave coming out of the slice. Second, by using the interpolation formulae (15) and (16) we find the amplitude $\Phi_{g'}^{(in)}(x,z+\Delta z)$ of the wave incident on the next slice.

Substituting equation (15) into equation (17), we find that

$$\begin{aligned}
\frac{\partial\Phi_{g'}(\nu,z)}{\partial z} &= \lim_{\Delta z\to 0}\frac{1}{\Delta z}\left\{\left(1-\frac{\Delta z}{W}\tan\theta_{g'}\right)\Phi_{g'}^{(out)}(\nu,z+\Delta z)\right. \\
&+ \left.\left(\frac{\Delta z}{W}\tan\theta_{g'}\right)\Phi_{g'}^{(out)}(\nu-1,z+\Delta z)-\Phi_{g'}^{(in)}(\nu,z)\right\} \\
&= \lim_{\Delta z\to 0}\frac{1}{\Delta z}\left\{\Phi_{g'}^{(out)}(\nu,z+\Delta z)-\Phi_{g'}^{(in)}(\nu,z)\right. \\
&- \left.\left(\frac{\Delta z}{W}\tan\theta_{g'}\right)\left[\Phi_{g'}^{(out)}(\nu,z+\Delta z)-\Phi_{g'}^{(out)}(\nu-1,z+\Delta z)\right]\right\}.
\end{aligned} \tag{18}$$

The difference

$$\lim_{\Delta z\to 0}\frac{1}{\Delta z}\left\{\Phi_{g'}^{(out)}(\nu,z+\Delta z)-\Phi_{g'}^{(in)}(\nu,z)\right\}$$

describes the effect of propagation of electrons through a slice in the direction of the zone axis and is given by the modified Howie-Whelan equations (2)

$$\begin{aligned}&\lim_{\Delta z\to 0}\tfrac{1}{\Delta z}\left\{\Phi_{g'}^{(out)}(\nu,z+\Delta z)-\Phi_{g'}^{(in)}(\nu,z)\right\}\\&=\tfrac{2\pi i}{\beta_{\mathbf{g}}}(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})\cdot\mathbf{s}_{\mathbf{g}}^{(\mathbf{R})}\Phi_{\mathbf{g}}-\pi i\textstyle\sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'})\frac{U_{\mathbf{g}-\mathbf{g}'}}{\beta_{\mathbf{g}}}\Phi_{\mathbf{g}'}.\end{aligned}\tag{19}$$

The second term in the right-rand side of (18) in the limit of small width W of a cell is given by

$$\lim_{\Delta z\to 0}\lim_{W\to 0}\frac{1}{\Delta z}\left\{\left(\frac{\Delta z}{W}\tan\theta_{g'}\right)\left[\Phi_{g'}^{(out)}(\nu,z+\Delta z)-\Phi_{g'}^{(out)}(\nu-1,z+\Delta z)\right]\right\}=\tan\theta_{g'}\frac{\partial\Phi_{g'}(x,z)}{\partial x},$$

and hence the combined effect of propagation through a slice *and* the subsequent application of the interpolation formulae is equivalent to a differential equation

$$\frac{\partial\Phi_g(x,z)}{\partial z}+\tan\theta_g\frac{\partial\Phi_g(x,z)}{\partial x}=\frac{2\pi i}{\beta_{\mathbf{g}}}(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})\cdot\mathbf{s}_{\mathbf{g}}^{(\mathbf{R})}\Phi_{\mathbf{g}}-\pi i\sum_{\mathbf{g}'}(1-\delta_{\mathbf{g}\mathbf{g}'})\frac{U_{\mathbf{g}-\mathbf{g}'}}{\beta_{\mathbf{g}}}\Phi_{\mathbf{g}'}.\tag{20}$$

Taking into account the fact that $\tan\theta_g=(\mathbf{k}+\mathbf{g})_x/(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})_z$ and that $\beta_g=(\mathbf{k}+\mathbf{g}+\mathbf{s}_{\mathbf{g}})_z$ we see that the equation set (20) is equivalent to the Howie-Basinski equations.

8 Relevant papers:

- Z. Zhou, S. L. Dudarev, M. L. Jenkins and A. P. Sutton (2003), 'A comparison of the Column Approximation and the Howie-Basinski approach in simulations of TEM images under weak-beam conditions', *Inst. Physics Conf. Ser.* **179**, 203.

- Z. Zhou, S. L. Dudarev, M. L. Jenkins, A. P. Sutton (2004), 'Simulations of electron diffraction contrast images of nanometer-sized dislocation loops', *MRS Proceedings* **792**, 491.

- Z. Zhou, A. P. Sutton, S. L. Dudarev, M. L. Jenkins and M. A. Kirk (2005), 'Simulations of electron elastic diffuse scattering patterns from individual nanometre-sized dislocation loops: I. Kinematical methodology', *Proc. R. Soc. London A* **461**, 3935.

- Z. Zhou, M. L. Jenkins, S. L. Dudarev, A. P. Sutton and M. A. Kirk (2006), 'Simulations of weak-beam diffraction contrast images of dislocation loops by the many-beam Howie-Basinski equations', *Phil. Mag.*, **86**, 4851.

- M. L. Jenkins, Z. Zhou, S. L. Dudarev, A. P. Sutton and M. A. Kirk (2006), 'Electron microscope weak-beam imaging of stacking fault tetrahedra: observations and simulations', *J. Mater. Sci.*, **41**, 4445.