

Calculation, Simulation, and Screen Graphic Display of Complex TED Patterns with the PC Program "Pattern"

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It is well known to electron microscopists working in the field of materials structure research that the importance of transmission electron diffraction patterns (TED) is: (i) establishing the crystallographic orientation correlations revealed during the practical observation of multiphase specimens and (ii) the knowledge of exact crystallographic orientation of a single crystal area in the specimen relating to image contrast interpretation.

On the other hand, it is well known that the spatial extension and geometrical form of the electron diffraction spots (see [1]) can lead to the appearance of some complex features in the experimentally registered TED. In [2] it is demonstrated that Ewald sphere curvatures can produce complicated reflection distributions when spikes are not simple in shape. Also, as a specimen is tilted, the reciprocal lattice (RL) spikes become inclined to the Ewald sphere surface and, though a spike may be near a low index zone, no reflections belonging to it will appear. The simplest distortions which could appear in an electron diffraction pattern are: (i) distortions of the spot-rows linearity and (ii) occurrence of some kinds of satellite spots.

To take into account these mentioned complex features, a program for computer simulation of complex ED patterns was written many years ago by R.A. Ploc and collaborators [3-5] - in Fortran, running on a CDC 6600 system and having as output a plotted TED pattern. The main characteristics of their mathematical algorithm (including graphics and for running on an IBM compatible PC, DOS or Windows) as direct screen display output are as follows:

(1) The possibility of the superposition of several "elementary" TED patterns, each being generated by a single crystalline phase having a supposed crystallographic orientation relative to the electron beam. In this way one may obtain as complex a simulated TED patterns as one may wish, by changing the input data to either the nature of the considered phase, or its crystallographic orientation relative to the electron beam, or both. This allows one to get patterns corresponding experimentally to: multiphase structures, epitaxially oriented structures, twin oriented phases, etc. All these patterns, simple and/or complex, are originating in the crystallographic model supposed to fit the actually observed TED in the microscope.

(2) The possibility of simulation of the "spiking" effect, i.e., to simulate those features occurring in the TED pattern which might be generated by the complex geometrical forms and the force extension of the "diffracting object", which in general is constituted of several crystalline grains under simultaneous direct observation in the microscope. Starting with the simplest model of a spike-rod originating in a platelette-like diffracting crystallite, with the same superposition method you can get more complex TED patterns corresponding to complex geometrical forms and orientations of all the observed grains.

(3) The possibility of simulation of a supposed tilt effect on a previously simulated TED pattern. The tilt axis can be chosen at ease and entered into calculation by input data. The rotated TED pattern can be compared with the experimental one, resulting after the same specimen tilt has actually been performed in the microscope. This could be a powerful method of verifying a supposed model conceived to describe the relative crystallographic orientations of the phases present in the observed specimen.

The geometrical parameters taken into account for performing the simulation are described in Figures 1 and 2. There are shown the two main kinds of geometrical orientations which have to be described mathematically in order to perform the simulation: (1) that of the crystalline phase under observation and (2) that of the TED pattern.

The detailed description of the geometrical model and of the mathemati-

cal algorithm on which is grounded the computer code can be seen in [3]. Here we give only a summarizing description of the input parameters in correlation with the mentioned figures.

Figure 1 shows the geometrical configuration of the 3 important elements: (i) the Ewald sphere, (ii) the electron beam and (iii) the rod-spike (considered as a vector - the \mathbf{g}_1 one) occurring at the ideal reciprocal lattice (RL) node (point P in Figure 1). Point \mathbf{P}^i belongs to the \mathbf{g}_1 vector and is its point of intersection with the Ewald sphere. The portion of the Ewald sphere accessible for direct observation in the microscope when using high energy electrons is considered, with a satisfactory approximation, as coincident within the photographic plane. The experimentally registered TED pattern is actually the pattern formed by all points of the \mathbf{P}^i kind, i.e., the points of intersection of the rod-spikes occurring at the actual RL nodes with the portion of the Ewald sphere visible on the screen. That is why the aim of the computer simulation is to calculate the geometrical coordinates of all the \mathbf{P}^i points which are expected to be registered on the photographic plate in well defined conditions. Finally, these intersection points are graphically displayed on the computer screen as the TED pattern and can be printed.

For the geometrical representation of the above mentioned \mathbf{P}^i points by their coordinates we have to take into account that:

(1) we need an orthogonal reference system in the photographic plane; that is the system defined by the unit vectors $(\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3)$ - (see Figures 1 and 2).

(2) the photographic plane coincides with a RL plane, designed by its $(\mathbf{U}, \mathbf{V}, \mathbf{W})$ Miller indices - (see Figures 1 and 2).

We can define the zone axis of the TED pattern to be simulated by entering as input data two RL vectors which have to belong to the $(\mathbf{U}, \mathbf{V}, \mathbf{W})$ plane we wish to see on the microscope screen: the \mathbf{g}_1 and \mathbf{g}_2 vectors (Figure 2). By entering input data values for the angles ψ_1 and ψ_2 , (from the same figure) we are in fact choosing the orientation of the simulated TED pattern relative to the orthogonal reference system already chosen: $(\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3)$. This can be linked also with the well known rotation occurring between the TED pattern and the contrast image, due to the rotation of the image plane by the lens coils. By entering an input data value for the angle Φ_x (Figure .2), we can define the orientation in the photographic plane [i.e., the $(\mathbf{U}, \mathbf{V}, \mathbf{W})$ RL plane, which is parallel to the specimen plane] of a rotation axis (designed as \mathbf{g}_r in Figure .2). \mathbf{g}_r is necessary for treating the case when we want to make a further simulation, aiming at getting the image of a rotated TED pattern. This will be the pattern originating in the new specimen position, reached after its tilting with the same angle value around the \mathbf{g}_r -axis. The variable δ is the one describing the rotation angle around this axis. The vector \mathbf{g}_r can be alternatively defined as a RL vector, i.e., by entering its (h, k, l) Miller indices. The occurrence of the second way of defining the rotation axis is flagged in a special way.

As can be seen in the Figures 1 and 3 for starting the calculation, we need to further define some more parameters:

(1) The orientation of the electron beam incident to the specimen, i.e., the orientation of the Ewald sphere. This can be defined in three different ways: (i) by means of entering values for the geometrical angles θ and Φ (see Figures 1 and 2), (ii) by defining the beam direction as an RL vector and (iii) by defining it as a direct lattice (DL) vector. The computer code can discriminate between these three ways of data input by means of the value entered for a specific flag variable.

(2) the orientation of the rod-spike, which can also be entered in three ways: (i) by entering values for the angles β^i and γ^i (see Figure 1), these angles being measured relative to the same $(\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3)$ orthogonal system of unit vectors, (ii) by defining the rod-spike as a RL vector and (iii) by defining it as a DL vector. The computer code can discriminate between these three ways of data input by means of the entered value for a specific flag variable. A supposed rod-spike length (equal to $|\mathbf{g}_s|$) is always entered along with each of these three ways of defining its orientation.

Besides these geometrical parameters we need to enter: (a) the crystallographic constants of the considered material phase: the lattice constants $\mathbf{a}, \mathbf{b}, \mathbf{c}$,

and α, β, γ , which describe the elementary cell; (b) the input values for the camera length, together with either the accelerating voltage (in eV) or the wavelength λ of the incident electrons (in Å).

The program can take into account a "spot invisibility" criterion after the calculation of all the values $|F_{gn}|^2$, where F_{gn} is the structure factor corresponding to the g_n ($n = 1, 2, \dots, m$) simulated spot. All these values are calculated on the ground of a series of input data describing: (i) the atomic species present in the elementary cell (a maximum number of 5 chemical species allowed) and (ii) their geometrical positions inside the cell, entered as fraction values of the a, b, c lattice constants (a maximum number of 20 atoms in the cell is allowed). The values of the atomic scattering factors f_g for each chemical element are taken from a table introduced in the program as a block data sequence. The "spot invisibility" criterion works either on the basis of a default value, or by taking into account a value entered by input data. In the default case, when no value is entered as a visibility limit, the program considers a TED spot as "invisible" (i.e., having too weak intensity to be registered on the photographic plate) when its $|F_{gn}|^2$ value is less than 1/20 of the highest value among all calculated $|F_{gn}|^2$ ($n=1, 2, \dots, m$) ones. An input value $\neq 0$ can be entered as a visibility limit, which overrules the default value mentioned above. The program can work even without any such criterion, in which case all the calculated TED spots are considered as "visible". The request to the program of taking into account or not such an "invisibility" criterion" is flagged by the presence of a specific input data line.

In summary, two main sets of input data lines have to be entered as successive Fortran formatted lines:

(1) In order to start the calculation (in the case when no invisibility criterion has to be taken into account) an initial set of 9 input data lines have to be entered in a rigorous succession. The meaning of this constraint is that the program needs at least one initialization of all the variables linked with the input parameters.

(2) If an invisibility criterion is to be taken into account, these first 9 lines are to be followed by a supplementary one containing the value linked with the invisibility criterion (which can be even = 0), followed by several other lines (in a number in accordance with the maximum allowed 5 atomic species and 20 atoms present in the elementary cell) containing input data which have to indicate: (a) the total number of atomic species, (b) their chemical symbols and (c) the unit cell positions of each of these atoms.

All of this input data is necessary for the initial calculation case.

In order to initiate new calculation cases any number of supplementary input data lines can be entered afterwards. They can contain new input values for any of the already initialized input parameters, for which a calculation has been already done. The succession in which the values of already defined variables are altered by means of new input data is arbitrary. In terms of the simulated TED pattern, the entering of a new input data line means to add to the list of the previously calculated spots a new set of spots to be drawn on the final pattern. This manner of entering the input calculation data is the way in which one can induce the simulation of several simple TED patterns which are to be superposed in order to get a final complex one.

The end of calculation input data, i.e., of the whole calculation, is flagged by a special input data line. ■

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Bibliography

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Note: The program can be run on a PC compatible with DOS, Windows 3.11 or Windows 95. Little RAM is needed, and it runs on a 386 with 8 MKB. What is important for the program is to "find" the fonts files for which it was compiled, but they can be delivered along with the *.EXE file.

One may request a copy of PATTERN.EXE, with examples, by Fax (011-40-423-1700) or by eMail (CSARBU@ALPHA1.INFIM.RO) - which will be sent by normal mail. We do not yet have a web site.

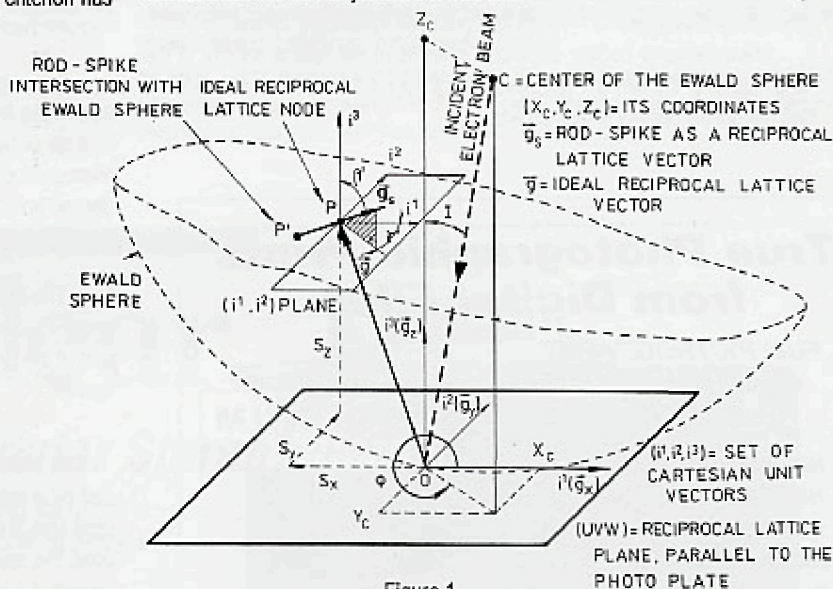


Figure 1

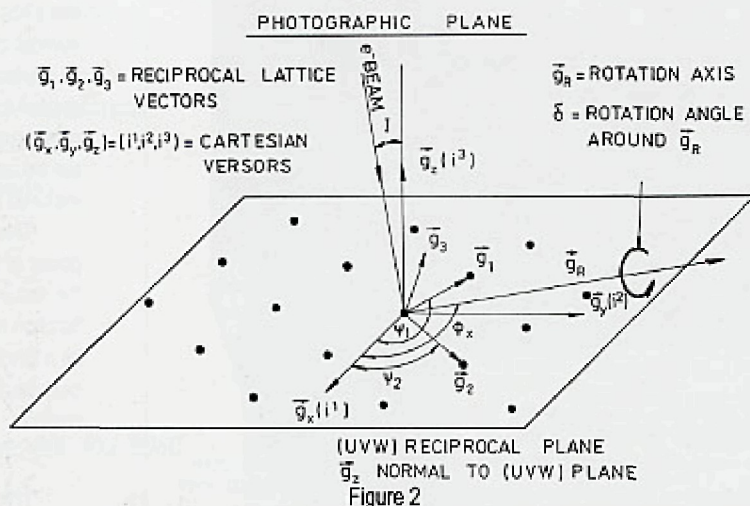


Figure 2