Developments in Computer Simulation of X-ray Diffraction Contrast Images of Stacking Faults

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Abstract

Computer-simulated X-ray section topograph images of a specimen containing a single large-area stacking fault are compared with the experimental image to illustrate useful improvements in simulation realism with regard to both image geometry and stacking-fault fringe contrast. The computer-program developments include exact treatment of the X-ray polarization factor so that anomalous transmission and the periodic fadings of fringe visibility occurring when unpolarized or partially polarized sources are used can be correctly computed. A procedure is described for photographing a cathode-ray-tube display to obtain records with acceptable resolution, contrast and freedom from distortion.

1. Introduction

The X-ray section topograph (Lang, 1957), in which both incident beam and Bragg-diffracted beam are transmitted through the specimen, is the simplest X-ray topographic technique for revealing lattice defects inside crystals by diffraction contrast, and it is also the best understood theoretically. When the specimen contains a stacking fault which is intersected by both the incident wave (K_o) and the diffracted wave (K_*) complicated fringe patterns are generated which were first explained by Kato, Usami & Katagawa (1967) in an application of the spherical-wave dynamical diffraction theory (Kato, 1961). Authier (1968) expanded the theory of Kato, Usami & Katagawa, casting it into a form readily applicable for computing diffracted intensities in the case of absorbing crystals. Since the mid-1970's, computer simulations of X-ray section topograph images have had instructive applications in studies of crystal-lattice defects. In the case of planar faults such as stacking faults a number of papers have shown computed diffraction contrast images, and comparisons with experiment have been discussed (Katagawa, Ishikawa & Kato, 1975; Authier & Patel, 1975; Wonsiewicz & Patel, 1976; Authier & Epelboin, 1977; Patel, 1979; Jiang & Lang, 1983). All but the first-mentioned of these works used computer programs based on the closed expressions given by Authier (1968) for the intensity of the K* wave at points on the X-ray exit face of the faulted specimen. Simulation programs based on the more general Takagi-Taupin equations of dynamical theory (Takagi, 1962; Taupin, 1964) applied to the stacking-fault problem have also been employed. An important consideration arising when computing images is how to display the calculated values of X-ray intensity. A wide range of computer peripherals has been employed to obtain simulated images of defects, ranging from an ordinary line printer to specially designed photoprocessing systems.

The work reported here has two aspects. The first involved development of a simulation program of wider scope than those previously available, to allow more options regarding diffraction parameters and image geometry, and to facilitate the extraction of particular intensity data. The second involved establishing a satisfactory but uncomplicated photographic procedure for producing hard copy from an advanced graphics terminal. To illustrate this work we show simulations exhibiting improved realism with respect to both geometrical parameters and the variation of fault-fringe visibility with fringe order. The experimental subject was a natural diamond containing a large-area stacking fault which has been studied by high-resolution X-ray section topographs (Jiang & Lang, 1983). The simulations were produced by a Ramtek graphics system connected to a DEC Vax 11/750 computer.

2. The simulation program GKSF

The computer procedure used to simulate the stacking-fault image consists of the two programs GKSF and IMAGE, written in standard Fortran. The first, the main program GKSF, calculates the intensity of the image and stores the data in the disk memory of the Vax computer. The second program, IMAGE, transfers the stored data into the file accepted by the Ramtek system and also allows the user to manipulate the image obtained, using the screen of the Ramtek...
display. The main program is based on the TOPEMP3 program devised by Dr Y. Epelboin, Laboratoire de Minéralogie–Cristallographie, Université Paris VI, and made available to us by Dr E. Pantos, SERC Daresbury Laboratory (Pantos, 1981). The GKSF program, like TOPEMP3, avails itself of the intensity expressions of Authier (1968) as a starting point. In the present work the TOPEMP3 program was substantially modified so as to introduce additional capabilities with regard to both input and output. These deal with a range of problems and can be categorized under four headings: (a) the properties of the X-ray source; (b) the separation of components in the expression for the total diffracted intensity; (c) the geometry of the image; and (d) extraction of specific intensity data. Brief explanations and examples for (a)–(d) are as follows.

(a) In this category the manner of handling of X-ray polarization by the computation is of major importance. The TOPEMP3 program assumes a mean value \( C = \frac{1}{2} (1 + \cos 2\varphi_q) \) for the X-ray polarization factor \( C = 1 \) and \( \xi \cos 2\varphi_q \) for the \( \sigma \)- and \( \pi \)-polarization modes, respectively, and the \( \sigma \)- and \( \pi \)-wave intensity patterns are amalgamated as a single pattern. The GKSF program calculates the intensity for the \( \sigma \) and \( \pi \) modes separately, and can superimpose them in any desired ratio. Thus it can simulate patterns corresponding to unpolarized X-rays, or to partially polarized X-rays as obtained with a monochromator crystal or, in the case of synchrotron sources, when the plane of incidence is neither parallel nor perpendicular to the orbit plane. The improvements afforded by exact treatment of the polarization factor are discussed below in §§ 3 and 4.

(b) The total diffracted intensity, \( I \), at a point in the section topograph image of a fault-containing crystal is given in Authier’s theory by

\[
I = I_1 + I_2 + I_3, \quad \text{where}
\]

\[
I_1 = I_p(1 - A \sin^2 \frac{1}{2} \alpha) \\
I_2 = B \sin^2 \frac{1}{2} \alpha \\
I_3 = C \sin^2 \frac{1}{2} \alpha + D \sin \alpha.
\]

In transmission through the faulted crystal, the \( K_p \) and \( K_q \) waves pass from crystal region I to crystal region II, across the stacking fault. The vector \( \mathbf{u} \) is defined as the translation of region II relative to region I, and this translation introduces the phase difference \( \alpha \) appearing in (1) and which is given by \( \alpha = 2\pi \varphi_q \mathbf{u}, \) where \( \mathbf{g} \) is the reciprocal of the interplanar spacing. In (1), \( I_1 \) is the intensity in the unfaulted-crystal pattern and \( I_2 \) is the intensity of the rays interbranch scattered at the fault surface separating regions I and II. \( I_2 \) is due to interference between \( I_1 \) and \( I_2 \) and contains the term \( D \sin \alpha \) from which the sign of \( \alpha \) can be determined when there is a major contribution of anomalous transmission (Borrmann effect) to the total transmitted intensity. [The quantities \( A, B, C, \) and \( D \) involve parameters such as specimen thickness, scattering factor and absorption, and are defined by Authier (1968).] The GKSF program allows \( I_1 \), \( I_2 \) and \( I_3 \) to be obtained separately as output data, so that their relative contributions at any point in the pattern can be determined.

(c) The diagrams of Kato et al. (1967) explain the geometrical shape of a stacking-fault image seen in the section topograph of a parallel-sided specimen oriented in the customary way with its faces normal to the plane of incidence of the X-rays. They show that when the fault plane is in general orientation with respect to the plane of incident and diffracted beams, and runs between X-ray entrance and exit surfaces of the specimen, the area on the topograph covered by the image of the fault is a trapezoid with one rectangular end. The rectangular end is located at that height on the section topograph where the fault plane intersects the ribbon-shaped incident X-ray beam at the X-ray entrance surface. The opposite oblique end of the fault fringe pattern corresponds to the trace of the fault plane at its outcrop on the X-ray exit face of the specimen. The TOPEMP3 program computes the section topograph image only within a rectangular area enclosing the above described trapezoid. Thus no image of the specimen section beyond the outcrop level of the fault on the X-ray entrance surface is displayed, i.e. no adjacent region of unfaulted crystal is imaged. Also, in the special fault-plane orientation known as the ‘symmetric case’, when the fault-plane outcrop on the X-ray exit surface of the specimen is parallel to the plane of incidence of the X-rays, and in consequence both ends of the stacking-fault-image area are rectangular, no unfaulted-crystal pattern appears adjacent to the image of the X-ray exit-surface outcrop of the fault. [This absence is evident in the TOPEMP3 simulations of a symmetric stacking fault shown by Jiang & Lang (1983).] In order to provide a realistic simulation of the experimental image it is desirable to include images of regions of faulted crystal both above and below the unfaulted region. These are particularly helpful in assessing whether the ‘first-fringe contrast’ is positive or negative (i.e. whether excess or deficiency of diffracted intensity relative to that from an unfaulted crystal appears in the fringe closest to the fault-surface outcrop at the specimen surface). It is from the sign of this contrast that the sign of the fault vector may be determined, via the term \( D \sin \alpha \) in \( I_2 \). The GKSF program allows the addition of images of segments of unfaulted-crystal pattern above and below the fault pattern, as needed. A further option allows simulations to be made which correspond to the image geometry applying when the stacking fault does not pass completely through the crystal. An application of these options is illustrated below.

(d) Two options provided in this category are, firstly, the display of one-dimensional scans along any chosen...
line parallel or normal to the plane of incidence, presenting in graphical form the variation of diffracted intensity with distance along that line and, secondly, the selection of any desired area out of the whole pattern for display. One application of the latter option arises when it is desired to view only that particular area of the image which is of concern for determining the sign of first-fringe contrast.

3. Application

Fig. 1 shows a section-topograph image that has been simulated by the GKSF program. It is one of a series of high-resolution section topographs of a stacking fault in an otherwise unusually perfect natural diamond which have been described by Jiang & Lang (1983). The stacking fault is in the symmetrical orientation. Hence the area of the image influenced by the stacking fault has horizontal bounds both above and below when (as in the orientation of all photographs reproduced here) the plane of incidence is horizontal. The micrograph, Fig. 1, includes short strips of unfaulted crystal above and below the stacking-fault image. The geometrical characteristics of Fig. 1 follow from the specimen and diffraction geometry which have been fully explained by Jiang & Lang (1983). The important parameters are summarized in Table 1. The

![Fig. 1. X-ray section topograph of stacking fault in a polished plate of natural diamond. Mo Kα radiation, 111 reflection, projection of the diffraction vector points to the left. Other parameters are given in Table 1. The image width is 470 μm. In the 'hour-glass' stacking-fault fringe pattern the intense blackening sloping from lower left to upper right corresponds to the intersection of the incident beam with the stacking fault. The lower-left limit of this blackening corresponds to the outcrop of the stacking fault at the X-ray entrance surface of the specimen, its upper-right limit corresponds to the termination of the fault within the crystal, close to the X-ray exit surface of the specimen.](image)

Table 1. Specimen and diffraction geometry of the section topograph, Fig. 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-ray entrance surface of specimen:</td>
<td>(001)</td>
</tr>
<tr>
<td>Specimen thickness:</td>
<td>101.3 μm</td>
</tr>
<tr>
<td>Plane of incidence of X-rays:</td>
<td>(110)</td>
</tr>
<tr>
<td>Orientation of stacking-fault plane:</td>
<td>(111)</td>
</tr>
<tr>
<td>Bragg diffracting plane:</td>
<td>(111)</td>
</tr>
<tr>
<td>Angle between fault plane and plane of incidence:</td>
<td>35°</td>
</tr>
<tr>
<td>Angle between Bragg plane and X-ray entrance surface:</td>
<td>54°</td>
</tr>
<tr>
<td>Radiation:</td>
<td>Mo Kα, 0.709 Å</td>
</tr>
<tr>
<td>Bragg angle:</td>
<td>9°91'</td>
</tr>
<tr>
<td>Extinction distance, δ polarization:</td>
<td>37.6 μm</td>
</tr>
<tr>
<td>Extinction distance, π polarization:</td>
<td>40.0 μm</td>
</tr>
<tr>
<td>Number of mean extinction distances in the polarization fade period:</td>
<td>16</td>
</tr>
</tbody>
</table>

The simulations, Figs. 2(a)–(e), are photographs of the output of a Ramtek graphic display system. This is a raster-scan system capable of driving industry-compatible cathode-ray-tube monitors. It is designed as a peripheral to the host computer and it performs a range of commands interactively, such as zooming, grey-scale changing etc. The raster has 1280 x 1024 pixels, and grey levels up to 256 in number are available. The CRT monitor, Ramtek model GM–859C, has a viewing area measuring 19 in (48 cm) diagonally across the face of the tube. It was photographed from a distance of about 1 m with a 35 mm camera equipped with a 40 to 80 mm focal-length zoom lens. With careful positioning of the camera and adjustment of vertical and horizontal deflection controls of the monitor, distortions of the photographic image could be kept below 1/2%. The photographic film used was Ilford Pan F, and it was processed with a standardized development of 4 min at 293 K in Ilford Microphen developer. Under these conditions the average contrast, G, is 0.55 when measured from a point at a density 0.1 above fog density to the point 1.5 log units higher on the photographic characteristic curve (i.e. the plot of photographic density versus logarithm of exposure).

The actual image width on the X-ray topograph is 470 μm. In the simulations 242 pixels were used to span this width. Hence the pixel area corresponded to a 1.9 μm square. This is adequately small, having regard to the resolution expected in topographs taken with Mo Kα radiation and the minimum fringe spacings actually resolved. [Jiang & Lang (1983) used a similar pixel size, 2.1 μm square, in their simulations.]

The number of grey levels used in the CRT display was 61, similar to the number, 65, provided by the Versatec
dot-matrix prints of Jiang & Lang. However, whereas the grey scale used in the TOPEMP3 program is logarithmic, of the form \( D = \gamma \log I + b \), where \( D \) = optical density, \( I \) = computed X-ray intensity and \( \gamma \) and \( b \) are constants, the grey scale employed here is linear. Equal steps of increase in X-ray intensity (i.e. of increase in blackness on the X-ray plates) are simulated by equal steps of decrease in screen brightness on the monitor. Thus film micrographs of the X-ray plates and film photographs of the monitor screen (or photographic prints made from such films) are directly comparable visually. A calibrating brightness step wedge can be photographed alongside the simulations when desired.

From Fig. 2(a) to Fig. 2(c), three stages of improvement in realism effected by the GKSF program are illustrated. These stages involve both geometry of the pattern and fringe contrast. Fig. 2(a) shows a major advance in fringe-contrast realism compared with the simulations of Jiang & Lang (1983) and earlier publications. It derives from exact treatment of the X-ray polarization factor. The most obvious benefit is correct portrayal of the 'polarization fades' in all of the \( I_1 \), \( I_2 \) and \( I_3 \) fringe systems. The fades in the \( I_2 \) and \( I_3 \) fringes are discussed by Jiang & Lang (1983) and only the essentials of the phenomenon need be recalled here. Fringe systems due to the \( \sigma \)- and \( \pi \)-polarization modes superimpose incoherently and their intensities should be added. Periodicities in the \( \sigma \) and \( \pi \) patterns are proportional to the respective extinction distances, \( \xi_{\sigma} \) and \( \xi_{\pi} \), with \( \xi_{\sigma} = \xi_{\pi}/(\cos 20_\mu) \). Provided \( \cos 20_\mu \) is not much less than unity, the fringe patterns can be expressed in terms of a mean extinction distance \( \xi_m \) given by \( (\xi_m)^{-1} = \frac{1}{2}((\xi_{\sigma})^{-1} + (\xi_{\pi})^{-1}) \). Periodic fadings of fringe visibility occur at separations of \( N \) fringes of period \( \xi_m \), where \( N = \frac{1}{2}(1 + C)/(1 - C) \), as shown by Hart & Lang (1965) and Hattori, Kuriyama & Kato (1965) in connection with the familiar Pendellosung fringe pattern in wedge-shaped crystals. In the present experiments \( N = 16 \). Stacking-fault diffraction theory shows that down the vertical median line of the image the depth period of the \( I_2 \) fringe system is \( \frac{1}{2} \xi_{\sigma} \), whereas that of the \( I_1 \) system is \( \xi_m \). Both \( \sigma \) and \( \pi \) components start in step at the outcrops of the stacking fault at the specimen X-ray entrance surface. Then, proceeding along the median line of the image i.e. towards increasing depth of the fault plane from the surface, the hyperbolic \( I_2 \)-system fringes fade first, and the first fade of the less sharply curved \( I_3 \)-system fringes occurs midway between the first and second

![Fig. 2(a)](image)

(a)

![Fig. 2(b)](image)

(b)

![Fig. 2(c)](image)

(c)

Fig. 2 (a) Simulation of stacking-fault contrast with the parameters given in Table 1, and representing the geometry when the stacking fault passes completely through the specimen from X-ray entrance surface (left-hand margin of section image) to X-ray exit surface (right-hand margin of section image). The parallel vertical fringes belong to the intensity component \( I_1 \) of equations (1). The fringes belonging to the \( I_2 \) intensity component are hyperbolae having the margins of the 'hour glass' as asymptotes. The \( I_2 \) fringes also lie within the 'hour glass' but are less curved than the \( I_3 \) fringes and tend towards horizontality at the top and bottom of the hour glass. By coincidence the specimen thickness is such as to contain just 4N mean fringes of the \( I_2 \) fringe pattern between top and bottom of the hour glass. This leads to accidental symmetry of positioning of polarization fades of the \( I_2 \) fringes relative to the waist of the hour glass. (b) Simulation of stacking-fault contrast with the fault-plane geometry of (a) but with the addition of images of fault-free regions above and below the stacking-fault image. (c) Simulation of image of faulted and unfaulted regions with fault-plane geometry corresponding to Fig. 1. i.e. fault plane terminating within the crystal close to the X-ray exit surface.
fades of the $I_2$ system. Matching of simulation with experiment is good.

While showing correctly the polarization fades Fig. 2(a) retains a limitation of previous simulations by excluding adjacent unfa ulted regions. This omission is rectified in Fig. 2(b). The addition of images of fault-free regions, correctly connecting with the stacking fault image, is an essential requirement for informative representation of 'first-fringe' contrast.

A special feature of the specimen of Fig. 1 is that the stacking fault does not run all the way between the (001) and (001) polished faces of the specimen. It cuts the (001) surface but terminates $94 \mu m$ short of the (001) surface in a bounding partial dislocation along $[1\overline{1}0]$, parallel to (001). For this reason the top of the 'hour-glass' pattern in Fig. 1 has less than the full width of the section topograph image. The simulation program can cope with this geometrical complication, as Fig. 2(c) shows.

4. Concluding remarks

The most significant difference between the experimental image and its simulations is the lack in the former of perfect focusing of interbranch-scattered rays at the waist of the 'hour-glass' pattern, and it has been concluded (Jiang & Lang, 1983) that an overall slight warping of the crystal due to change of lattice parameter as the crystal grew was the most likely cause. The calculations and simulations of Kato (1974) and Katagawa, Ishikawa & Kato (1975) are valuable for treating fault surfaces other than those associated with a pure translation fault. Their predictions for the case when the fault surface is a very-low-angle tilt boundary bear a general similarity to the pattern shown in Fig. 1, in so far as a pair of caustics replaces the ideal sharp focus at the waist of the pattern; but modelling of the defects in the crystal here investigated and computation of the consequent perturbation of the pure stacking-fault image fall beyond the scope of this report. However, verity in simulation of other characteristics of the experimental image, such as polarization fades, assists the identification of features not accounted for by the present diffraction theory. Two other differences merit comment. The first involves image texture. In the experimental image there is a high apparent granularity. This arises principally from statistical fluctuations in the number of X-ray photons absorbed in adjacent resolvable area elements and it is a fundamental resolution-limiting factor in practical X-ray topography with conventional sources and detectors (Lang, 1979). It is computationally possible to impose a granularity upon the simulation by introducing a random fluctuation in the intensity calculated for each pixel, but such a procedure could only detract from the information content in the simulation.

The second difference is the loss of resolution of the finely spaced vertical fringes of the $I_1$ system in Fig. 1 compared with the simulations. This is due to the finite width of the incident X-ray beam, effectively about $15 \mu m$ in Fig. 1. An equivalent blurring can be introduced into the simulations straightforwardly by adding together a series of similar images horizontally shifted with respect to each other. This can be done with the GKSF program and has provided advantageous realism in some cases. It was not included in the present computed images since it would have masked the polarization fades in the $I_1$ system fringes, which are instructively displayed in Figs. 2(a)–(c).

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