Simulation of Synchrotron White-Beam Topographs. An Algorithm for Parallel Processing: Application to the Study of Piezoelectric Devices

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Abstract

This paper presents a new algorithm for the integration of Takagi-Taupin equations taking into account the fact that X-ray diffraction is a parallel phenomenon. The diffraction equations show that the propagation of the waves is independent in each incidence plane. It is thus possible to compute in parallel the propagation of the waves in different planes. Two algorithms are presented: the first one for multiprocessor machines where the processors share a common memory, the second one for massively parallel computers. The program is written to achieve a high vectorization ratio and to make it as efficient as possible with modern superscalar and array processors. The simulation of the image of a defect has been divided into two independent parts. In the first one, one computes the derivatives of the deformation inside the crystal; in the second one, these results are used to simulate the image. This allows one rapidly to change the model for a defect, something that was not feasible in all previously written simulation programs since the computation of the deformation was part of the simulation. The study of stroboscopic images of the propagation of acoustic waves in piezoelectric devices is given as an example of the possibilities of this new program.

1. Introduction

Synchrotron white-beam topography is a powerful method to characterize nearly perfect crystals. New sources such as the European Synchrotron Radiation Facility (ESRF) have already demonstrated (Baruchel, Epelboin, Gastaldi, Härtwig, Kulda, Rejmankova, Schlenker & Zontone, 1994) that a wide range of experiments is feasible owing to the high energy of the ring and the intensity of the source.

In many cases computer simulation is useful to interpret the images and fully characterize the observed contrast. For instance, stroboscopic topography (Zarka, Capelle, Détaint & Schwartzel, 1987) allows one to study the propagation of ultrasonic waves in a piezoelectric device. Computer models have been applied to describe the deformation in a freely vibrating anisotropic elastic plate (Yong, Stewart, Détaint, Zarka, Capelle & Zheng 1992) but theoretical models cannot be checked against the experiment. Zheng, Zarka, Capelle, Détaint & Schwartzel (1989) have successfully compared a simple model with section topographs but this kind of experiment does not provide information in a large volume of the crystal. White-beam topography is a more efficient tool for characterization.

Carvalho & Epelboin (1990) have explained why the contrast of synchrotron white-beam topographs resembles, in most cases, translation topographs as recorded in the laboratory. The contrast may be explained as the superposition of the intensities produced by incoherent sources lying along the entrance surface of the crystal. This is due to the spectral width of the radiation and to the particle beam size and divergence in the storage ring. At the time Carvalho & Epelboin wrote this paper, it was not yet certain that this conclusion would be valid for low-emittance storage rings such as the ESRF. Baruchel et al. (1994) have shown that the simulated image of a dislocation, computed using this assumption, was in good agreement with the experiment.

However, up to now, the simulation of an image has required lengthy calculations and changing the model for the defect means fully rewriting the program, since deformation and diffraction calculations are intimately interlaced. It would be useful for the future users of the ESRF topography laboratory to be able to validate a theoretical model describing a defect in a material without having to rewrite the simulation program.

This paper describes a numerical algorithm that allows one to use the same program to simulate the images for any kind of defect. The user must separately compute the deformation for his or her own model, then use these data as input for the simulation program itself. A new algorithm has been established to vectorize the equations. This increases the speed of the calculation either on modern RISC superscalar workstations or on large supercomputers such as Cray computers. The diffraction phenomenon being parallel in its nature, this algorithm has been designed for the new generation of parallel
machines. The analysis of stroboscopic topographs using a simple model for the propagation of ultrasonic waves demonstrates the possibilities of this new program.

2. Theory

The simplest method to simulate a white-beam topograph is to add the contribution of individual point sources located along the entrance surface of the crystal (Fig. 1) as suggested by Epelboin & Soyer (1985). The distance between the sources must be chosen in agreement with the sampling of computed intensity nodes along the exit surface of the crystal. This sampling is very dense because it is linked to the distance between nodes in the network used for the integration of the Takagi-Taupin equations (the distance between nodes may be as small as 0.025 μm), which must be able to correctly describe the phase of the diffracted wave inside the crystal. The intensity is oversampled along the exit surface of the crystal and one must reduce the number of data to draw an image or a profile of intensity (Epelboin, 1981). Thus, the number of point sources between E and F (Fig. 1) along the entrance surface must be also oversampled to sum correctly all the contributions at point P. This increases tremendously the number of calculations and makes this method rather inefficient (Carvalho & Epelboin, 1993a).

The second method is to take advantage of the reciprocity theorem of optics (Carvalho & Epelboin, 1993b). The geometry of the experiment is reversed: a point source is located at point P along the exit surface at the position where one wants to compute the intensity in the topograph. The amplitude of the diffracted field is computed in a reverse geometry, both refracted and reflected directions $s_0$ and $s_h$ being exchanged with the $s_0$ and $s_h$ directions for the direct geometry of the experiment (Fig. 2). It may be shown (Takagi, 1969; Petrashen, Chukhovskii & Shulpina, 1980; Carvalho & Epelboin, 1993b) that the intensity, at point P in the experiment, is the sum of the intensities of all computed nodes between A and B along the exit surface in this reciprocal geometry. The distribution of the points P is no more linked to the network of integration, no oversampling is needed and the required resolution in the simulated image is chosen in agreement. This decreases the time of computing by one to two orders of magnitude.

Petrashen et al. (1980) have been the first to try to use the reciprocity theorem for the simulation of traverse topographs. Epelboin & Soyer (1985) have shown that the precision of the numerical algorithm is very critical. Conventional algorithms (Authier, Malgrange & Tournaire, 1968) or Petrashen (1976) did not permit one to apply this theorem and only the direct method could be used. Carvalho & Epelboin (1993a) have established an algorithm accurate enough to simulate the images using the reciprocity theorem.

The Takagi-Taupin equations (Takagi, 1969; Taupin, 1967), reduced to one second-order partial differential equation for the amplitude of the diffracted wave (Takagi, 1969; Carvalho & Epelboin, 1993a), may also be written in the reciprocal geometry (Carvalho & Epelboin, 1993b) as

$$\frac{\partial^2 \tilde{\Psi}}{\partial s_0 \partial s_h} + i 2 \pi \mathbf{h} \cdot \mathbf{u} \frac{\partial}{\partial s_0} \tilde{\Psi} + \left( \pi^2 k^2 C^2 \chi_h \chi_h + i 2 \pi \frac{\partial^2}{\partial s_0 \partial s_h} \mathbf{h} \cdot \mathbf{u} \right) \tilde{\Psi} = 0, \quad (1)$$

where $\tilde{\Psi}$ means the amplitude of the diffracted wave in this geometry, $\chi_h$ and $\chi_h$ are the $h$ and $h$ components of the dielectric susceptibility and $k = 1/\lambda$ is the wave number for the reflection $h$. $C$ is the polarization constant, which will be taken as 1 in the computation. $u$ means the local deformation at any point inside the crystal expressed in the reciprocal geometry axes (Fig. 2).

In the reciprocal geometry, the same type of transformation can be done as Carvalho & Epelboin, (1993a) used in the direct geometry:

$$\exp \left[ i 2 \pi \mathbf{h} \cdot \mathbf{u}(\tilde{s}_0, \tilde{s}_h) \right] \tilde{\Psi} = F \exp \left[ i 2 \pi \mathbf{h} \cdot \mathbf{u}(\tilde{s}_0, \tilde{s}_{hP}) \right] \Psi$$

and

$$\tilde{\Psi} = F \exp \left\{ -2 \pi \mathbf{h} \cdot \left[ \mathbf{u}(\tilde{s}_{0P}, \tilde{s}_h) - \mathbf{u}(\tilde{s}_{0P}, \tilde{s}_{hP}) \right] \right\} \Phi, \quad (3)$$

where $F$ is a constant of no interest in the present problem and the local deformation $\mathbf{u}$ is taken in the four points, inside the Borrmann fan, marked in Fig. 3:
M(\(\tilde{s}_0, \tilde{s}_h\)), M'(\(\tilde{s}_0, \tilde{s}_{hM}\)) and M''(\(\tilde{s}_0, \tilde{s}_h\)) on its edges and P(\(\tilde{s}_{0M}, \tilde{s}_{hM}\)) at its vertex. Then, (1) may be written either as

\[
\frac{\partial^2 \psi}{\partial s_0 \partial s_h} + W_\psi \frac{\partial \psi}{\partial s_0} + \pi^2 k^2 C^2 \chi_h \chi_h \psi = 0
\]  

(4)

or as

\[
\frac{\partial^2 \phi}{\partial s_0 \partial s_h} + W_\phi \frac{\partial \phi}{\partial s_0} + \left( \pi^2 k^2 C^2 \chi_h \chi_h \right) \phi = 0,
\]  

(5)

with

\[
W_\psi = -i2\pi \left[ \frac{\partial}{\partial s_0} \cdot \mathbf{h} \cdot \mathbf{u}(\tilde{s}_0, \tilde{s}_h) - \frac{\partial}{\partial s_h} \cdot \mathbf{h} \cdot \mathbf{u}(\tilde{s}_0, 0) \right]
\]  

(6)

\[
W_\phi = i2\pi \left[ \frac{\partial}{\partial s_h} \cdot \mathbf{h} \cdot \mathbf{u}(\tilde{s}_0, \tilde{s}_h) - \frac{\partial}{\partial s_h} \cdot \mathbf{h} \cdot \mathbf{u}(0, \tilde{s}_h) \right].
\]  

(7)

These equations are numerically integrated using a finite-elements method where nodes are located, inside the Borrmann fan, at the intersections of characteristic lines drawn parallel to the transmitted and reflected directions (Fig. 4). To achieve the required accuracy in the numerical integration, Carvalho & Epelboin (1993a) write the value of the diffracted wave at point 4 (Fig. 4) as a function of the values at points 1, 2 and 3. M is the point at mid-distance between 2 and 4. Equations (4) and (5) become

\[
\Psi_4 = [(Q_\psi - G)\Psi_3 - (Q_\psi + G)(\Psi_2 + \Psi_1) + 2\Psi_2] \times (Q_\phi + G)^{-1}
\]  

(8)

and

\[
\Phi_4[(Q_\phi - G)\Phi_2 - (Q_\phi + G)(\Phi_3 + \Phi_1)] - 2\Phi_1/(Q_\phi + G),
\]  

(9)

with

\[
G = (pq/4)\pi^2 k^2 C^2 \chi_h \chi_h
\]  

(10)

\[
Q_\psi = 1 - (p/2)W_\psi(\tilde{s}_{0M}, \tilde{s}_{hM})
\]  

(11)

\[
Q_\phi = 1 - (q/2)W_\phi(\tilde{s}_0, \tilde{s}_{hM})
\]  

(12)

\[
Q_\sigma = 1 + (q/2)W_\phi(\tilde{s}_0, \tilde{s}_{hM}).
\]  

(13)

p and q are the steps between 4 and 2 and between 4 and 3, respectively. \(\tilde{s}_{0M}\) and \(\tilde{s}_{hM}\) mean that the value is taken at point M (Fig. 4). \(Q_\phi^*\) and \(Q_\psi^*\) are the complex conjugates of \(Q_\phi\) and \(Q_\psi\), respectively.

Carvalho & Epelboin (1993a) have discussed the use of both (8) and (9). Owing to the form of its error term, which is of the third order, (9) converges more rapidly than (8), when the integration steps p and q are decreased, except in very deformed areas. Thus, (9) may be computed faster in most parts of the crystal. To compute the image of a dislocation, Carvalho & Epelboin (1993a) use (9) everywhere except near the core of the dislocation, where they switch to (8). The size of the core is estimated by computation of the size of the direct image of the dislocation (Authier, 1967). As we will explain in §3, our intention is to write a multipurpose program valid for any kind of deformation. It is difficult to establish a general criterion, without any prior knowledge of the structure of the defect, to switch between (8) and (9) without a lengthy computation time. Since this difficulty arises for some defects only and in a very limited area, we have chosen to use (9) everywhere. It means that the simulated images may become wrong in very deformed areas for some defects such as dislocations. Our experience is that this problem seldom arises because the direct image criterion is a very conservative one, (9) being still valid for rather large deformations. This problem does not exist in the present study.

3. Numerical algorithm

3.1. Vectorization of the Tagaki-Taupin equations

Steps p and q (Fig. 4) must be locally chosen to describe as well as possible the changes in the phase of the propagating diffracted wave. It would take too much time to determine them during the integration; thus, they

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Fig. 3. Notation used in the diffraction equations in the reciprocal geometry.

Fig. 4. Principle of the numerical integration. The value of the diffracted field at point 4 is computed from the knowledge of its values at points 2, 3 and 1. p and q are the elementary steps along \(\tilde{s}_0\) and \(\tilde{s}_h\), respectively.
are computed prior to the integration. Epelboin (1981) has suggested a method where they are computed from the knowledge of the analytical solution in the case of the perfect crystal. The amplitude $q$ is computed at nodes aligned along characteristic lines parallel to $\tilde{s}_0$ and $\tilde{s}_h$; one computes first the amplitudes for all nodes along 1, 2 then 3, 4. This choice has been made in the past because it does not require a large memory, since only two characteristic lines must be stored. However, it does not allow one to vectorize the calculation and thus it is less efficient when modern processors, especially array computers such as Cray ones, are used.

Let us introduce the following metrics: starting from point $P$ (Fig. 5), we call wavefront $n$ the line of nodes reached by a fixed number of $n$ translations, either $p$, $q$ or any combination of both. Nodes 2 and 3, for instance, belong to the wavefront numbered $n$ (in this figure $n = 5$). It must be noticed that the amplitude of the wave at node 4 (wavefront $n + 1$) depends on the amplitude at nodes 2 and 3 (wavefront $n$) and 1 (wavefront $n - 1$). The computation may be organized along these wavefronts. Let us call $V_n(a)$ the amplitude at a node $a$ belonging to wavefront $n$, $a$ being its index along this wavefront with index 0 for the node at the intersection of the wavefront with the $\tilde{s}_0$ direction. From Fig. 5, one may see that

$$V_n(a) = f[V_{n-1}(a-1), V_{n-1}(a), V_{n-2}(a-2)].$$

Equation (9) may be written as

$$V_n(a) = [[Q\Phi(n-a,a)-G(n-a,a)]V_{n-1}(a-1)$$

$$+ [Q\Phi(n-a-1,a)-G(n-a,a)]$$

$$\times [V_{n-1}(a)+V_{n-2}(a-1)]$$

$$- 2V_{n-2}(a-1)]/[Q\Phi(n-a,a)+G(n-a,a)].$$

Equation (10) becomes

$$V_n(a) = \frac{[R^*(a)-T(a)]V_{n-1}(a-1)}{[S(a)-T(a)][V_{n-1}(a)+V_{n-2}(a-1)]}$$

$$- 2V_{n-2}(a-1)]/[R(a)+T(a)].$$

Equation (17) is fully vectorized.

3.2. Computation of the deformation

Up to now, all simulation programs have calculated the deformation values at each node $M$ (Fig. 4) just when requested; it is part of the simulation itself. Changing the model for the defect means rewriting large sections of the program, which is always delicate and may take months. In the case of piezoelectric devices as well as in other studies, the simulation is intended to check various models that describe the propagation of the acoustic wave. We have thus decided to split the simulation into two independent programs. The first one computes the data for the deformation through all the crystal. Its results are stored on a disk then used as entry for the simulation program. To study another deformation model, it is just necessary to rewrite the first program and to run the same simulation program again. This may be done without any knowledge of the simulation program.

The values of the deformation appear in (15):

$$\frac{\partial}{\partial s_h}h \cdot u(M) = -\alpha_x h_1 \frac{\partial}{\partial x} u_1(M) + \gamma h_1 \frac{\partial}{\partial z} u_1(M)$$

$$- \alpha_y h_2 \frac{\partial}{\partial y} u_2(M) + \gamma h_2 \frac{\partial}{\partial z} u_2(M) + \gamma h_3 \frac{\partial}{\partial x} u_3(M).$$
where indices 1 and 3 denote the components along the \( x \) and \( z \) directions of \( u \) and \( h \) (Fig. 6). \( \alpha_h = \sin \Psi_h, \alpha_0 = \sin \Psi_0, \gamma_h = \cos \Psi_h \) and \( \gamma_0 = \cos \Psi_0 \).

In the symmetric case, \( \Psi_0 = -\Psi_h \) (18) is reduced to the first two terms, i.e.

\[
\frac{\partial}{\partial s_h} \mathbf{h} \cdot \mathbf{u}(M) = -\alpha_h h_1 \frac{\partial}{\partial x} u_1(M) + \gamma_h h_1 \frac{\partial}{\partial z} u_1(M). \tag{19}
\]

\( \partial[u_1(M)]/\partial x \) and \( \partial[u_1(M)]/\partial z \) are computed for each plane of incidence and stored in a large array. When (17) is computed, the value of the deformation at any node \( M \) is established by a simple interpolation between the previously calculated values at points \( C, D, A \) and \( B \) in this array (Fig. 7). The steps \( AB \) and \( AC \) must be small enough, so that the interpolation gives a correct value for the deformation at node \( M \). They depend on the defect and must be smaller if the deformation varies rapidly. Thus, the array that contains the values of \( \partial[u_1(M)]/\partial x \) and \( \partial[u_1(M)]/\partial z \) is very large. For instance, in the present study, with crystal 1000 \( \mu \text{m} \) thick and for an image 5000 \( \mu \text{m} \) large, it is of the order of 500 \( \times \) 1000. For each plane of incidence, it corresponds to a file of 2 Mbytes when written on the disk. The program samples the derivatives of the deformation in all the planes of incidence, which means 500 such files for an image that contains 500 lines. The total space needed to store these data is of the order of 1 Gbyte. This doubles in the asymmetric case. Such a space was not available in the past, which did not allow one to separate the computation of the deformation from the simulation itself.

It may be noticed that the interpolation coefficients needed to compute the deformation at any node in the integration network are the same for all equivalent nodes \( M \) in all Borrmann fans if each vertex is located on the deformation grid (Fig. 7): nodes \( M \) and \( M_1 \) are corresponding nodes for the calculations performed in the Borrmann fans of summit \( P \) and \( P_1 \), respectively. This allows one to speed up the second program, i.e. the simulation program: if one integrates (17) for all Borrmann fans, in a given plane of incidence, at the same time, it requires the calculation of the distances \( MA, MB, MC \) and \( MD \) only once for a series of equivalent nodes \( M \). This saves a large amount of computing time but requires the ability to store in the memory of the computer all the data needed for all the integrations in all these Borrmann fans. The space needed in the memory for the simulation program may be very large. It is proportional to the width of the image and the thickness of the crystal. For instance, it was 300 Mbytes with the data given previously. This was not available in the past. One could have organized the numerical routine to do the same thing but it requires many transfers between the processor and the storage device and, consequently, would make the program very inefficient.

3.3. Parallelization of the calculation

The diffraction phenomenon is naturally parallel: the equations say that the propagation of the waves is independent for each incidence plane. This means that each line of the image may be computed separately. One may give the computation of different lines to different processors when available. The technique depends on the hardware organization of the machine.

The simulation of an image may be described in the following steps (Fig. 8a):

(a) initialization, i.e. establishment of the network of integration and other data;

(b) for each plane of incidence, it is necessary to

(i) read the data of the previously calculated deformation for this plane and

(ii) compute the Tagaki-Taupin equations for each pixel \( P \) (Fig. 7);

(c) store the image.

We have found that all of the computation time is devoted to step (b). Step (a) takes a few seconds, while the computation of the intensity (step b) may take several hours. In a multiprocessor shared-memory computer such as a Cray C9x, one may easily parallelize loop (b), which may be distributed automatically among the available processors just by the addition of a few directives in the code. The overhead is only 1.5% when eight processors are used. This is much better than is usually expected from Amdahl’s law (Kleinrock & Huang, 1992). This arises from the independence between the calculations, which reduces the conflicts in accessing the

![Fig. 6. Axes used for the computation of the deformation.](image1)

![Fig. 7. Superposition of the grids of the network of integration (heavy lines) and for the sampling of the derivatives of the deformation (light lines). The value of the deformation at point \( M \) is interpolated from the values at points \( A, B, C \) and \( D \). The value at point \( M_1 \) in the other integration network uses the same interpolation coefficients.](image2)
common memory. However, it requires a large amount of private memory for each processor. For the larger images, using a Cray C98 where the total memory is 2 Gwords, we have not been able to use all eight processors. Thus, this parallelization is valid for small problems only.

The approach is different when a massively parallel computer is used. We have written a load-balancing algorithm that is explained in Fig. 8(b). We have chosen the PVM (parallel virtual machine) library (Sunderam, 1990), which is now a standard. It is portable on all platforms and also on a cluster of workstations. It is summarized as follows:

(a) Initializations:
   (i) start a master process and make the initialization as in Fig. 8a;
   (ii) spawn as many slave processes as the number of available processors;
   (iii) make the slaves wait for the master.

(b) Computation:
   (i) the master distributes the lines to be computed among the slaves.
   (ii) each slave:
      - receives a line number to be computed;
      - reads the corresponding deformation data;
      - computes this line of the image;
      - gives back the results to the master;
   (iii) the master stores each received line and gives a new line number to be computed to the slave.

This program was tested on an SP2 IBM with eight processors and we found that the speed-up is exactly proportional to the number of nodes being used. The communication between the processors is limited to a few kwords for each line of the image and this makes the parallelism very efficient.

4. Application

4.1. Stroboscopic topography of piezoelectric devices

As a test for the simulation program, we have studied the contrast of piezoelectric devices. Stroboscopic topography is very well adapted to such studies because the frequency of the vibrations in the crystal and the frequency of the pulsed beam are of the same order. Zarka, Capelle, Détaing & Schwarzel (1988) have built an experimental set-up at LURE and they have studied thickness shear modes in quartz resonators.

The experimental topographs have been recorded by Capelle, Détaing, Schwarzel & Zarka (1992). Zheng, Zarka, Capelle, Détaing & Schwarzel (1989) have explained their contrast in the case of section topographs. In the case of weakly excited resonators, they have used the theory for slightly deformed crystals (Kato, 1963) and, in the case of a more important excitation they have simulated the images as seen in a section topograph.

![Fig. 8. (a) Flowchart of the calculation for a multiprocessor machine. The loop is parallelized on all available processors. (b) Flowchart of the calculation for a massively parallel machine. The master process (left part) makes the initialization and creates as many slaves as available processors. A load-balancing scheme distributes the lines to be computed among them.](image-url)
The resonators were shaped in such a way that the (5, 0, 0) mode frequency is twice the pulsed synchrotron-radiation frequency, i.e. 3.16928 MHz. The electrical excitation of the resonator is derived from the radiation pulse signal. The shape of the resonator is designed so that it is forced to vibrate at this resonance frequency. The crystals were set with a Bragg angle of approximately 8° so that the selected incident X-ray wavelength for the 210 reflection is about 0.7 Å.

The devices are circular plates from a quartz AT-cut crystal. Their geometry is shown in Fig. 9. The upper surface is convex and the maximum thickness is chosen for the resonance frequency. It avoids a dispersion of the acoustic energy along the edges where the thickness of the resonator is smaller: it does not correspond to the resonance frequency and the crystal does not vibrate any more in these areas. For simplicity, we assume, in our calculation, that the slab has parallel faces, its thickness being the one in the center of the resonator. In the present experiment, the \( \text{Pendellösung} \) extinction distance \( \lambda \approx 101.6 \mu\text{m} \). Since the thickness variation in the real device is 160 \( \mu\text{m} \) from the centre to the edge, it means that we neglect approximately one thickness fringe.

We consider an ideal case where the acoustic vibration mode is a pure thickness-shear mode that can be approximated as (Tiersten & Smythe, 1979; Stevens & Tiersten, 1986):

\[
u = u_0 \exp\left(-\frac{(\alpha_x x^2 + \beta z^2)}{2}\right) \times \cos\left[n\pi z/r(x,y)\right] \exp\left(-i\omega t\right) \quad (20)
\]

\( \nu \) lies along the \( x \) axis, i.e. parallel to the diffraction vector \( h \) in the symmetric case. \( n = 5 \) in the present simulations. \( t = 1.3196 \) mm is the thickness of the device assumed as constant. \( \alpha_x = 0.445297 \) mm\(^{-2} \) and \( \beta_z = 0.509546 \) mm\(^{-2} \), which means that the vibration is reduced by a factor of about 2.810 \(^{-2} \) from the centre to the electrode edges. \( z \) is perpendicular to the surface. We have investigated an amplitude \( u_0 \) varying from 5 Å up to 100 Å but in real experiments (Zarka et al. 1987) it is never larger than 10 Å (Fig. 10).

In this model, the energy dissipation is neglected and \( u_0 \) becomes infinite at the resonance. More sophisticated models based on a development in Bessel functions are presently under investigation (Déaint, Carru, Schwartzel, Joly, Capelle, Zarka, Zheng & Philippot, 1992). A full model would require a finite-element calculation (Yong, Stewart, Déaint, Zarka, Capelle & Zheng, 1992). The computation of the derivatives \([19]\) is straightforward. We will study the simulations from the point of view of finding the accurate conditions for a good convergence of the calculation.

4.2. Integration of the Tagaki-Taupin equations

The steps of integration \( p \) and \( q \) \([10]\) must be chosen to obtain the convergence in the numerical integration \([17]\). As explained by Carvalho & Epelboin (1993a), the sampling of the nodes must follow as closely as possible the variations of the phase of the amplitude inside the crystal. Fig. 11 presents a profile of intensity along the central line of an image, i.e. along a line passing through the centre of the device. Fig. 11(a) is wrong: 10 fringes are visible, which is not in agreement with the experiment. The horizontal step, along the exit surface, varies from 0.2 up to 1.6 \( \mu\text{m} \), which is too large for an accurate convergence. Fig. 11(b) shows 13 fringes. The step varies from 0.1 up to 0.8 \( \mu\text{m} \). Fig. 11(c) shows 14 fringes, which is correct. The step varies between 0.025 and 0.2 \( \mu\text{m} \). However, the computation becomes very long: 90 times larger than in Fig. 11(a)! Fig. 11(d) is a good compromise: the number of fringes is correct as well as their intensity, except in the centre where it is slightly underestimated. The step varies from 0.025 up to 0.4 \( \mu\text{m} \) and the computation time is three times smaller than in Fig. 11(c). Choosing smaller steps than in Fig. 11(c) does not change the profile. Thus, for the following calculations, we will always use the conditions of Fig. 11(d). Other simulations using a more sophisticated deformation model have confirmed that these values are satisfactory for the study of piezoelectric devices.

One must firmly insist on the fact that such convergence study is absolutely necessary before starting the
study of a new deformation model, since there is no means to automatically find the convergence in the integration.

4.3. Sampling of the deformation

The sampling of the derivatives of the deformation must be dense enough to correctly interpolate the deformation at any node $M$ (Fig. 7). If it is too loose, the values of the derivatives are incorrect; if too dense, this means one must store on the disk a huge amount of data and increase the memory needed for the calculation. We found that the present deformation is correctly sampled with a step of 5 μm along the surface and 2 μm along $z$. The difference between the steps $x$ and $z$ may be easily explained: according to (20), the deformation and its derivatives vary much more rapidly inside the crystal along $z$ than along the surface. Such values must be checked before the study of any new model of deformation. We found that they are still correct for the study of the same resonator but with a vibration expressed as a development of Bessel functions. They are incorrect for drawing the profile of a dislocation previously studied by Carvalho & Epelboin (1993b).

One must emphasize the importance of a correct choice of this sampling. The simulation of the images shown in Fig. 12 is made computing 500 planes of incidence. In each plane, the deformation is sampled in a plane whose thickness represents 660 steps along the $z$ direction and up to 1500 steps along the $x$ direction. This represents $3.9 \times 10^8$ nodes, i.e. 3.1 Gbytes of storage for both derivatives for most computers and double for a Cray! This is not available at all sites.

Fig. 12 presents different simulations for various excitations. Owing to the symmetry of the device, the fringes appear as a set of concentric circles and we have computed a quarter of the image only. With the restriction of the convexity not being taken into account, the number of fringes is in agreement with the simulations. Changing the excitation from 5 to 10 Å, we found a variation of 2.5 fringes Å$^{-1}$, which is in agreement with the simulations made by Zheng et al. (1989). The total processor time needed to compute the image was 70 min on a Cray C908. The balance between the eight processors depends on the total load of the computer. In the best case, when all processors were equally available, the user time has been reduced to 10 min only. The time needed to compute the derivatives of the deformation was about 10 min, but this is meaningless. It varies according to the models of deformation.

5. Conclusions

Synchrotron white-beam topography is nowadays a powerful technique for the characterization of large crystals. The simulation of the image allows a full quantitative analysis of expensive experiments. We have built a versatile tool that permits one to simulate any model for the deformation without prior knowledge of the simulation technique for X-ray dynamical theory. Together with the use of modern multiprocessors or massively parallel machines, it makes the use of simulations possible for the analysis of the experiments done at modern synchrotron facilities.

Up to now, a new simulation program had to be written to study any new deformation model, and this took many months to do. It is much faster to just write a program to compute the deformation. The computation time is still long but becomes available everywhere. It is of the order of 10 to 20 h when only a modern workstation is used but may be reduced to less than 1 h when a Cray computer or the parallel version with a cluster or a massively parallel machine is used.

This means that it is now feasible to check rapidly any theoretical model. For instance, it is important for the telecommunication industry to design piezoelectric resonators with the minimum amount of dispersion of the acoustic energy. White-beam topography has already proved to be a powerful technique for the observation of this phenomenon. Theoreticians have built sophisticated models to explain the propagation of the acoustic waves. It is now possible to check this model by direct comparison between the simulation and the experiment. This work is in progress and will be presented in another paper.

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