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TITLE: SIMULATION OF BENT CRYSTAL SPECTROMETERS

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Simulation of Bent Crystal Spectrometers

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Abstract

In crystal spectrometers one traditionally labels each position in the dispersion/recording plane by a single wavelength value. A simple examination of the crystal spectrometers shows that different areas of the crystal contribute different wavelengths at the same position in the recording plane. Using collimators and apertures one may reduce these effects, as well as reduce the collected signal. Convolving the system response, in that case, may not allow simple analytic estimates of the sensitivity/responsivity of the system. A Monte-Carlo ray-trace program was written in order to study and simulate the real geometry including finite source size effects. The results of using the code will be presented, demonstrating the contributions to the resolution and absolute responsivity, for a particular parabolically bent crystal spectrometer.

I. INTRODUCTION

In designing crystal spectrometers, one may use standard optics programs for image formation and for studying the dispersion of the system. However, important questions regarding the resolution and throughput of the system require careful calculation of the transfer of the x ray intensity through the system. In what follows I will present the details of a program called CRYSTAL that attempts to include the reflectivity of the crystal and the sources' spatial and angular distribution in the estimate of the throughput. Section II will describe the geometry used, Section III will describe some of the details of the program, Section IV will apply the program to the specific case of a parabolically bent crystal spectrometer.

II. DESCRIPTION

A code CRYSTAL was written to analyze in 1-D the instrumental layout shown in Figure 1. The source emits x-rays in random directions, with random spatial distributions, (the distributions to be sampled can be specified by the user). The default distributions were uniform distributions. The rays reflect from the crystal which was placed with its vertex at the origin of coordinates. The axis of symmetry was the x axis. The reflectivity of the crystal follows the Bragg condition and the Rocking curve of the crystal. Aperture stops can be placed any place in the system. However, we specifically put an aperture at the focus of the system on the x-axis. The rays that make it then intercept an arbitrarily positioned receiving plane called the film plane. The output of the program are the statistics on the rays, e.g., number of rays that miss the crystal, number of rays that miss the aperture, number of rays

that miss the film, etc. Another most useful output is a plot of the intensity that made it to the film as a function of position on the film and as a function of the energy of the x-ray. The program allows for a quick study of the effect of varying parameters on the output on the film.

III. DETAILS

The program starts by choosing a ray on the surface of the source. The ray is chosen from a source angular and spatial distributions. A helpful feature of the code was the source spectral distribution function used. Delta function bins (see Fig. 2) distributed about a central energy bin were used. Their spacing increased geometrically with the difference between the bin number and the central bin number. This is analog, in energy space, to using a variably ruled pattern to test the spatial MTF of an optical system. The use of 11 energies was judged to be sufficient for the purpose of our studies. One can, of course, choose the intensity at each of these energy bins to replicate some line shape or spectral shapes at the source.

Reflection was assumed to follow Bragg's law. Thus for each energy and crystal spacing there is a central angle called the Bragg angle where the ray at that energy reflects with a peak reflectivity. At other incident angles the ray was reflected with a reflectivity that depended on the difference of the angle the ray makes with the surface and the Bragg angle. In the simulations the reflectivity function, also known as the rocking curve, was assumed to be a gaussian:

$$R = e^{-\left(\frac{\theta-\theta_B}{\sigma}\right)^2}$$

where sigma equals fwhm/1.6651. Of course, lorentzian, or other line shapes, could have been easily used by changing the appropriate subroutine AMPL in the code.

The detector plane was divided into 161 bins. The central bin was positioned at the intersection of the central ray and the film plane. The central ray was defined as that ray that started from the center of the source parallel to the x-axis. The bin width in micrometers is user chosen. The program keeps track of the contribution from each of the energy bins to a specific spatial bin.

IV. RESULTS

The program features will be demonstrated using a specific crystal spectrometer design. The particular geometry is shown in Fig. 3. A LiF crystal was parabolically bent to satisfy the equation $y = \sqrt{2\ p\ x}$, where $p = .375$. The vertex, of course, was on the origin of coordinates. The source was chosen to be equal in size to the crystal y projection, and centered on it. The particular geometry is not particularly advantageous for the use with a parabolical crystal, but simulates the effect of putting a finite input aperture a finite distance from the crystal. The best source distance is at infinity. The film plane resolution was set at 20 micrometers, to simulate the spatial resolution attributable to a combination of a fiberoptics faceplate with a layer of x-ray to visible fluor converter on the entrance of the faceplate. In all cases an aperture of diameter 100 micrometer was centered at the focus of the parabola and parallel to the x-axis. Two variations are shown in Figs. 4 and 5. In Fig. 4 the source cone angle

was varied from 10 to 3000 microradians, keeping the crystal rocking curve fwhm at 10 microradians. In Fig. 5 the source cone angle was fixed at 10 microradians, but the rocking curve fwhm was varied from 10 to 1000 microradians. For the case where fwhm = 10 then the plot actually gave the dispersion (1.1 eV/micrometer) on the film. The other cases show the effects of divergence. The increase in width of the pattern with source divergence is 5.7×10^{-4} (eV/microradian). The linewidth variation was 2.13×10^{-3} eV per microradian variation of the crystal fundamental rocking curve width. The plots show the contribution from each energy bin. The central energy bin is at 12000 eV, the other bins are separated by 50, 100, 200, 400 etc. eV, respectively. The present design thus allows for at least 50 eV resolution and at a contrast ratio of .5 allows a resolution of 20 eV for a source divergence of 3000 microradians and a crystal rocking curve full width at half maximum of 200 microradians.

V. SUMMARY

The program "CRYSTAL" has been written to analyze 1-d geometries of crystal bent spectrometers. The program allows for quick study of the variation of the output properties of the spectrometer with variation of spectrometer design. The program has been written in BASIC for the HP/80 and HP/200 series of computers and in FORTRAN/77. A typical case with one million starting rays take about 50,000 seconds on the HP87 and 16 seconds on the CRAY/1 using the CTSS operating system and the RCFT compiler.

FIGURE CAPTIONS

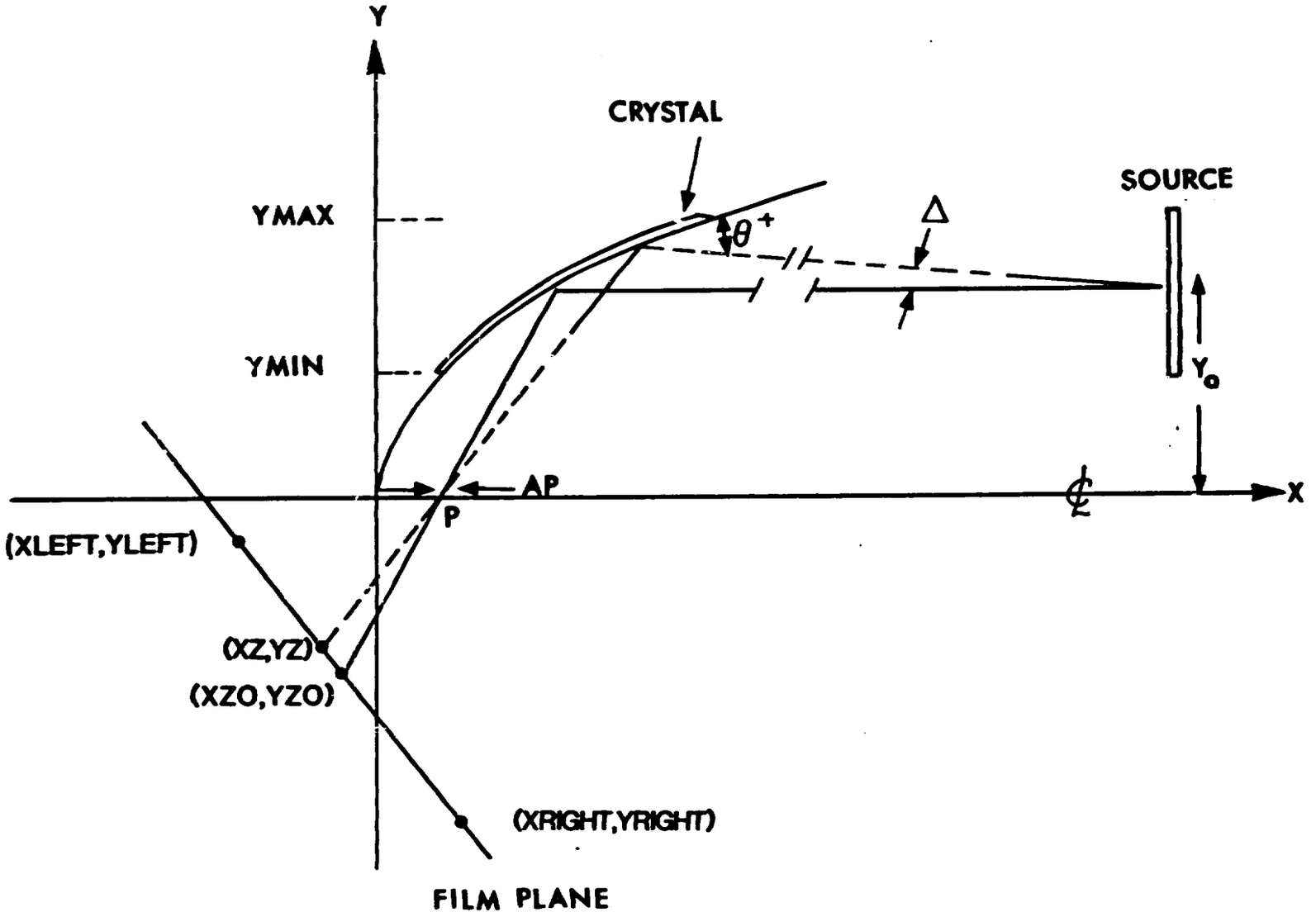
Figure 1. A schematic diagram of the geometry used in CRYSTAL. The central ray path is displayed by the continuous line. A general ray is displayed by the dashed line. The x-axis is an axis of revolution for the crystal. The source position, crystal surface equation, and film location and orientation are arbitrary. The crystal surface must pass through the origin, however, only the area between YMIN and YMAX are used.

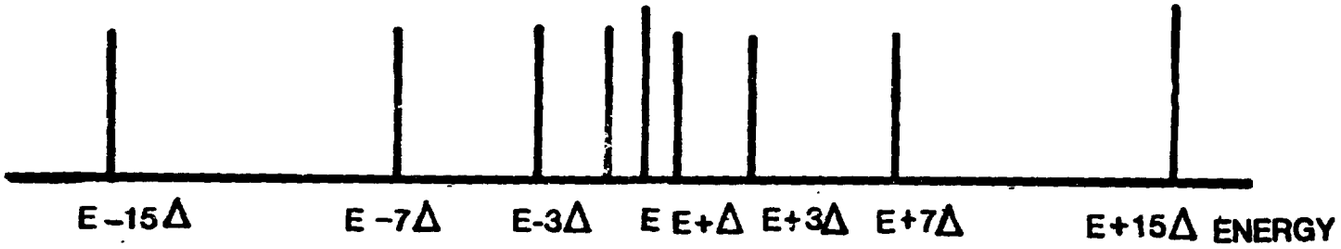
Figure 2. The default energy spectrum used in CRYSTAL. The energies are delta functions. The separation between successive peaks increased in geometric progression of powers of 2.

Figure 3. The Actual Geometry that was simulated in the presentation. The spectrometer consisted of a parabolically bent crystal, an aperture of diameter 100 micrometers centered at the focus of the parabola parallel to the x axis. The film plane had a resolution of 20 micrometers.

Figure 4. The variation of the line width with the divergence of the source. The divergence was varied from 100 to 3000 microradians. The crystal rocking curve FWHM was kept at 10 microradians for this figure. Ten million random numbers were used. The peak reflectivity was taken as unity.

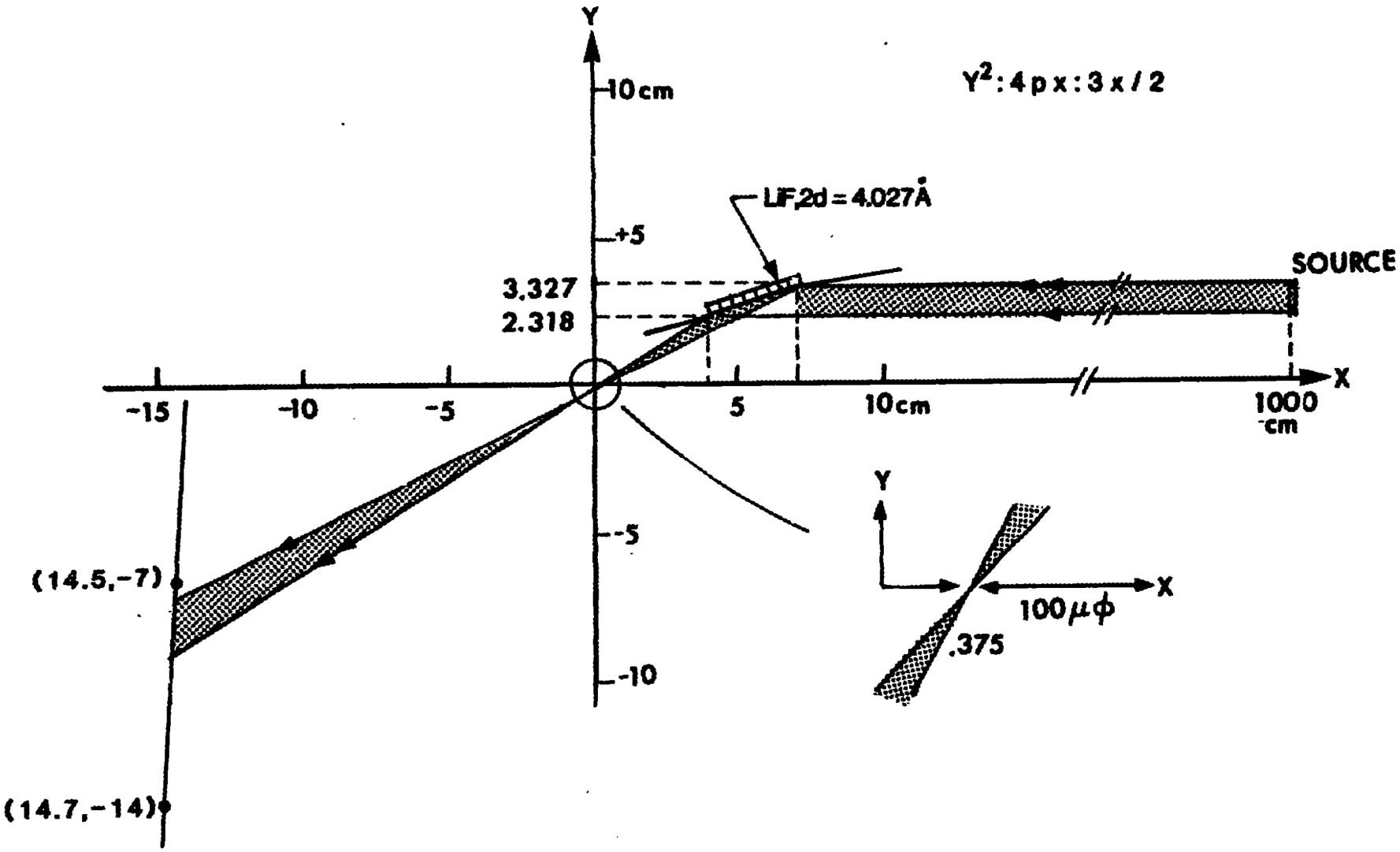
Figure 5. The variation of the line width with the FWHM of the rocking curve of the crystal. The source divergence was kept at 10 micrometers for this figure. FWHM was varied at 10, 100, 500, and 1000 microradians. Ten million random numbers were used, and the peak crystal reflectivity was taken as unity.

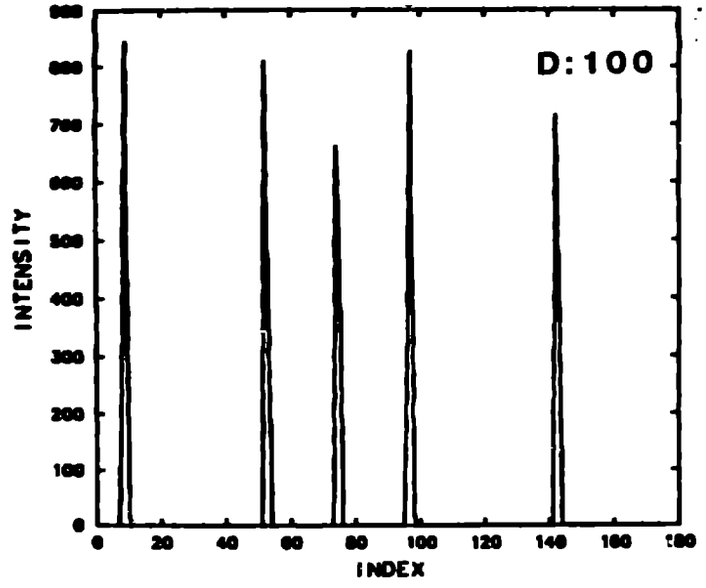

Y
CRYSTAL
SOURCE
YMAX
θ+
Δ
YMIN
Y0
AP
P
X
(XLEFT,YLEFT)
(XZ,YZ)
(XZO,YZO)
(XRIGHT,YRIGHT)
FILM PLANE



$$E(i) = E(i-1)+(i-6)\Delta \qquad i \neq 6$$
$$E(6) = E$$

ENERGY SPECTRUM


Y
10cm
$Y^2 : 4px : 3x/2$
LiF,2d = 4.027Å
+5
SOURCE
3.327
2.318
X
-15
-10
-5
5
10cm
1000 cm
-5
(14.5,-7)
-10
(14.7,-14)
Y
X
100μφ
.375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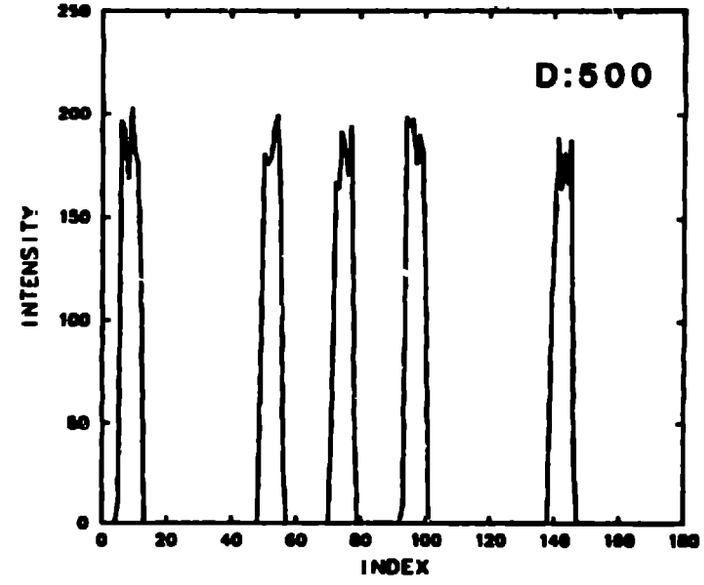
INDEX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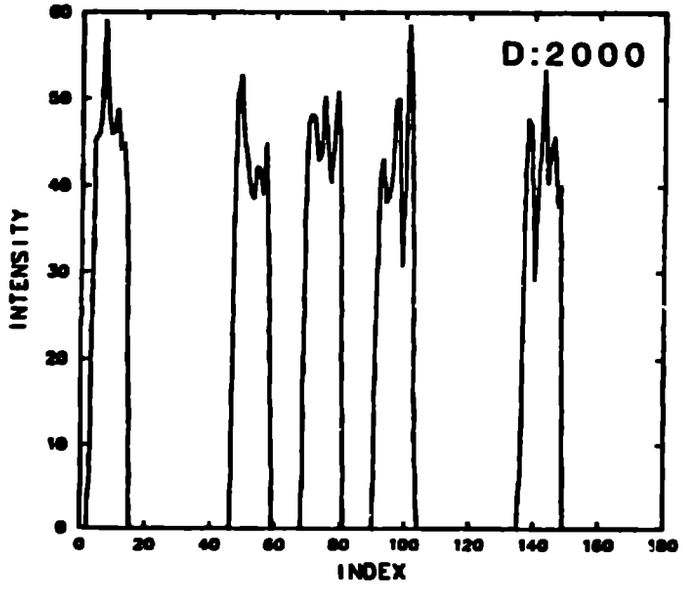
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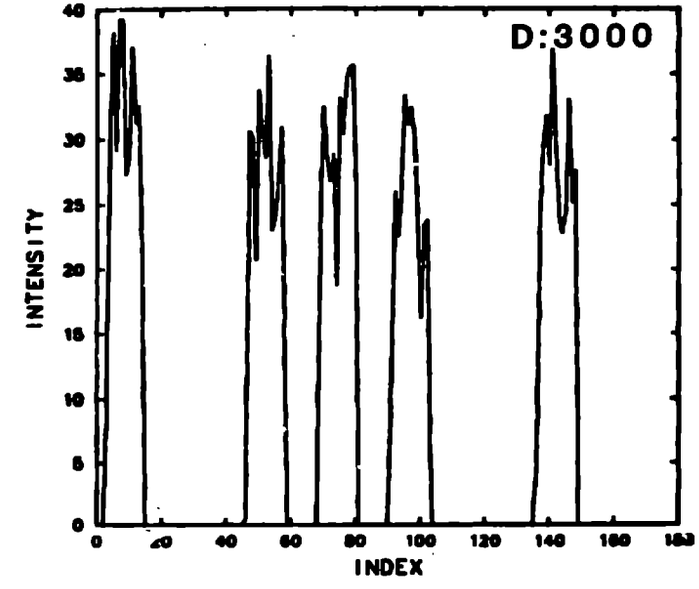
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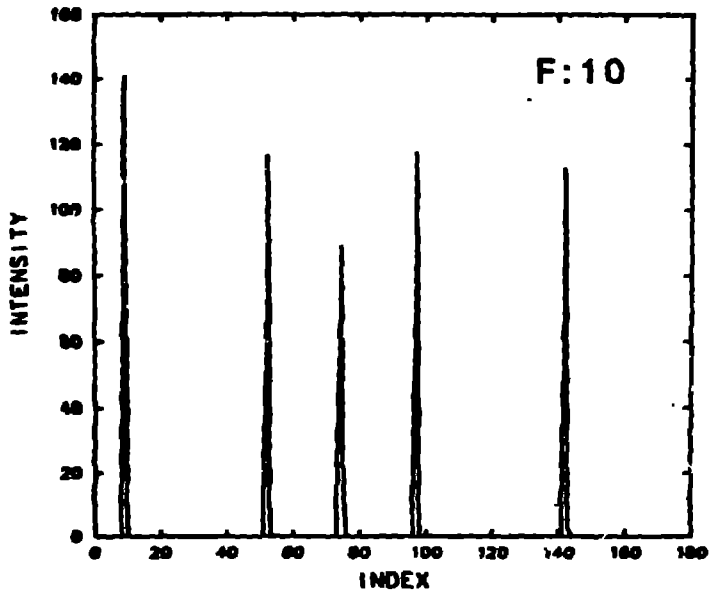
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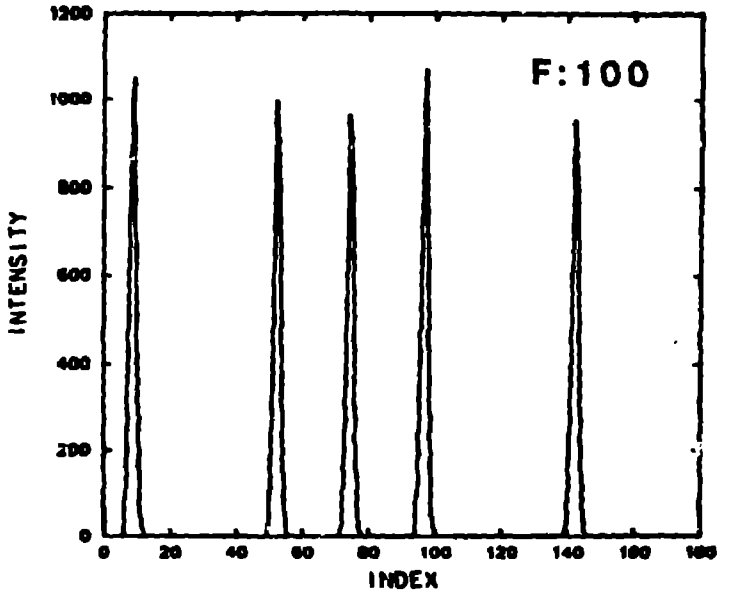
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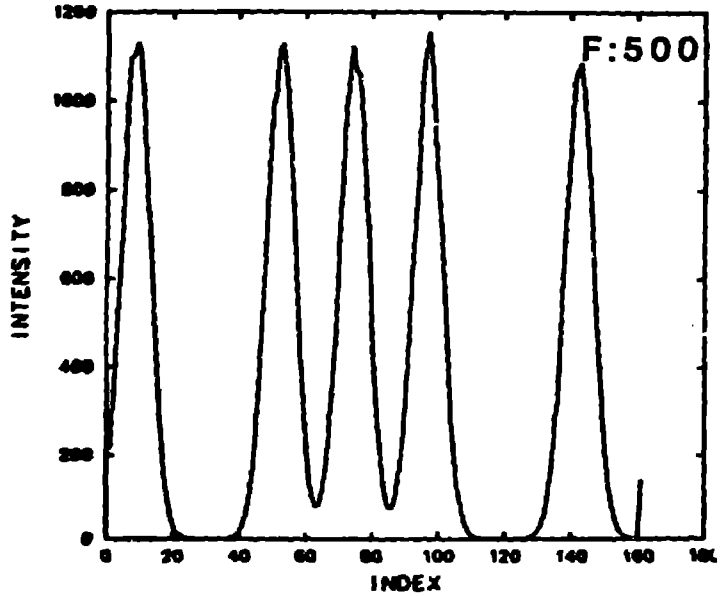
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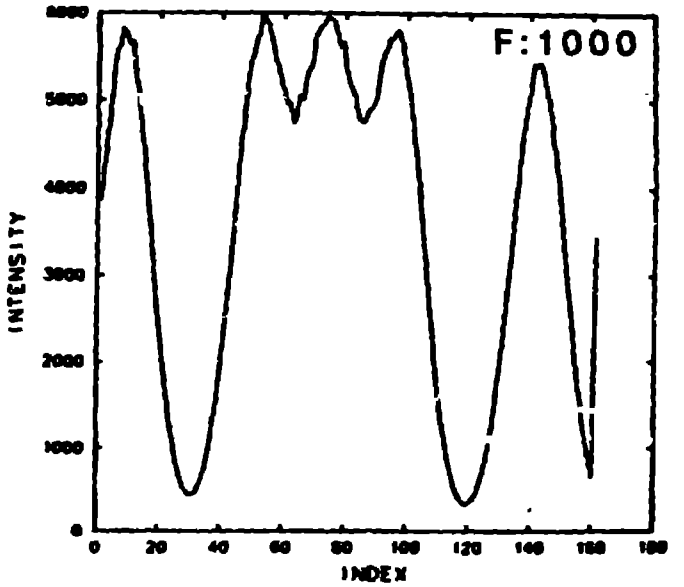
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