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Waviness effects in ray-tracing of "real" optical surfaces

M. Sánchez del Río* and A. Marcelli#

***European Synchrotron Radiation Facility, B.P. 220 38043 Grenoble-CEDEX, France**
#I.N.F.N. Laboratori Nazionali di Frascati, CP 13, 00044 Frascati, Italy

Abstract

Today ray-tracing calculations are playing an essential role in the design of synchrotron radiation beamlines. In particular, for the new generation of synchrotron radiation machines that will produce high brightness x-ray beams, the low emittance must be conserved along the beamline by choosing the best optical design. Quality of optical elements are limited by the technological manufacturing process, characterized by the values of roughness and waviness of the optical surfaces. Therefore a reliable description of an optical element is essential for having accurate results in ray-tracing simulations.
We present here a model for introducing the waviness effect of real optics surfaces in ray-tracing calculations and also show some examples of simulated surfaces in comparison with real measured surfaces.

1 Introduction

Ray-tracing calculations are an essential tool for any synchrotron radiation beamline design. SHADOW [1], in fact, is the most widespread ray-tracing code, which accepts different surface figures for simulating optical elements, such as mirrors, crystals or gratings and predicts the effects introduced by these optical surfaces on the image shape as well as on transmitted intensity, energy resolution, etc. The aberrations or distortions produced by an optical surface on the image point not only are caused by the geometry of the surface, but also are affected by the imperfections, defects and, in general, texture of the surface. Technological limits in the surface-manufacture process introduce different types of irregularities which determine the quality of a surface working at grazing incidence angle necessary in x-rays beamlines. A good characterization of the optical surfaces is accomplished using different types of profiling instruments, depending on the microscopic or macroscopic range of measurement.
It is certainly possible to use the measured profiles in ray-tracing calculations [2], and should give the best description of an optical surface. Unfortunately these profiles are rarely available and certainly never available before the design of beamlines and production of the optical element. Thus, the theoretical simulation under irradiation of a surface with the same characteristics and the same performance as the one to be produced is desired. Ray-tracing simulations are essential when comparing spherical and aspherical surfaces because, although spherical surfaces produce geometrical aberrations, superior figure accuracies can be achieved for spherical surfaces and, therefore, these surfaces may have better imaging properties than practically realizable aspherical surfaces. Ray-tracing of spherical and aspherical surfaces, including roughness and slope error values, is necessary to determine the best optical configuration.
We simulate the waviness of an optical surface by the superposition of a finite number of different frequencies in each surface profile; together, these give the realistic profile. Selecting appropriately the number of frequencies and their amplitudes enables us to reproduce the rms slope error and the power-spectral-density function, and investigate the optical performance of "real" surfaces which have the same characteristics.

2 Measurements and characterization of the surface texture.

The description of a surface is complicated and there is confusion concerning the definition of the surface imperfections and irregularities. Surface texture can be classify into three families: roughness, waviness and figure or geometry [3] (fig.1). The limits between them are unclear and it is necessary to specify the measuring procedure in addition to the spatial frequency range. Working with x-rays, we can consider intuitively that roughness produces diffraction of the photon beam (incoherent reflection) while waviness and figure errors determine a deflection of the reflected beam from the ideal path (coherent reflection).
Roughness is a random irregularity having an average period in the range of Å and which depends on the finishing processes and can be limited by the mechanical properties of the materials. Roughness increases the scattering of the photon beam, producing a blur of the image and intensity loss at the focal point.
Waviness or slope error is generally associated with the sinusoidal-like variations (or ripple) of the surface shape. The slope error spreads the image in the focal plane due to the

deflection of the incident beam at different angles. Moreover it produces a reduction in the transmitted intensity because of the shadowing effect of the ripples. The spatial period of wavy surfaces lies between tenths of micrometers and few millimeters, and is a function of the polishing process used in the final manufacture (diamond turning machines, mechanical polishing machines, etc.).
The figure or geometry is the macroscopic curvature of the surface. This gives the general surface shape (plane, spherical, ellipsoidal, etc.), and the deformations produced by form construction errors, thermal loads and the mechanical stress which can be induced by any mechanical device that clamps the optical element.
Profiles of real optical surfaces can be obtained from different types of devices [4], which use one of two phenomena: interference of a laser beam after reflection on the surface (non contact methods) and scanning of a test stylus instrument along the surface (contact methods). The selection of one of them depends on the surface spatial period to be measured and on the total length of the surface to be scanned. Once we have the measured or simulated profile $z_i \equiv z(y_i)$ we can define the following surface statistical parameters.
The micro-roughness is measured by means of root-mean-square roughness, defined as the square root of the mean value of the squares of the distances z_i of the points from the mean surface level [5]:

$$\sigma_{rms} = \sqrt{\frac{1}{N}\sum_{i=1}^{N} z_i^2} \qquad (1)$$

where N is the total number of measured points, i is the point index and z_i is the height of i-th point. Note that the definition of rms roughness is independent of the sampling along the scanning direction, but its value is dependent on the characteristics and set-up of the instruments used for the measurements.
The rms slope error is the parameter used for the characterization of the surface waviness. It is defined as the square root of the mean of the squares of the slopes:

$$\Delta_{rms} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\alpha_i - \bar{\alpha})^2} \qquad (2)$$

where

$$\alpha_i = atan\frac{z_{i+1} - z_i}{y_{i+1} - y_i} \qquad (3)$$

and

$$\bar{\alpha} = \frac{1}{N}\sum_{i=1}^{N}\alpha_i \qquad (4)$$

N is now the number of intervals in y direction and y_i are the coordinates of the measured points along the scanning direction.
This value of rms slope error depends on the step length considered in the sampling of the surface, the size of the averaging surface area in each data point and the amount of instrumental noise associated with each value of height z_i. This this single parameter is not enough to characterize a surface. In particular, for a sine wave of amplitude A and period P, when the sampling interval is much less than the period the formula (2) reduces to [4]

$$\Delta_{rms} = \frac{\sqrt{2}\pi A}{P} \qquad (5)$$

Now we show how the surface imperfections are a function of the characteristic lengths or periods. The figure, waviness and roughness frequencies included in the measured profile, are shown when calculating the Fourier Transform of the profile. They present a peak corresponding to each frequency. The power-spectral-density function (PSD) is the frequency spectrum of the surface profile measured in inverse length units and is basically proportional to the square modulus of the Fourier Transform. The PSD function can be calculated [6] by the relation

$$S(f_m) = \frac{2D}{N} \left| \sum_{n=1}^{N} e^{\frac{-2\pi i(m-1)(n-1)}{N}} W(y_n) z(y_n) \right|^2 \qquad (6)$$

where W is a weighting window (we used a Hanning window) to avoid border effects, and $D = y_n - y_{n-1}$ is the sample distance. The position of the peaks in the PSD function give the period of the oscillations included in the profile. The position of these peaks is independent of the sampling D of the profile. Thus determines the maximum frequency available ($f_{max} = (2D)^{-1}$, Nyquist frequency), while the minimum frequency is characterized by the total length L of the surface ($f_{min} = 1/L$). The PSD function can contain information of all figure waviness and roughness, depending on the range in which it is calculated and analyzed.

3 Analysis of waviness of measured surfaces. Simulation of "real" surfaces.

A real surface is characterized by the presence of many frequencies; only few of them are important to determinate the optical characteristics. This frequencies are determined by the measure of the PSD function (fig 2). The frequencies are characteristics of the surface considered and are almost the same for different profiles taken over the same surface. Low frequency signals are related to the length of the surface L which gives a fundamental frequency $(2L)^{-1}$ and its harmonics. Other low frequency signals present in the surface are due to the frequencies of the polishing and finishing processes of the surface. The important high frequencies correspond always to harmonics of the fundamental frequency. Our approach to "real" surface is based on the idea that any shape or profile can be simulated by a series of sine or cosine signals having frequencies which are multiples of the fundamental. In fact, selecting and modifying only few frequencies of the Fourier expansion of a flat signal of amplitude 1 in the interval $(-\pi/2, \pi/2)$

$$z(y) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n cos((2n+1)y)}{2n+1} \qquad (7)$$

will give us the desired profile. From (7), we rescale the length to the surface length, and taking only into account a limited number of harmonics n_{max} , fix the amplitude of each harmonic in function of the period and slope error selected, and shift the signal randomly a given fraction g of the surface length. This procedure gives:

$$z(y) = \sum_{n=0}^{n_{max}} A_n (-1)^n cos \frac{(2n+1)(y + y_n^0 + r g_n)}{L/\pi} \qquad (8)$$

where

$$A_n = \frac{C_n L \Delta_{rms}}{(0.5+n)\sqrt{2\pi}} \tag{9}$$

where C_n are weighting coefficients given by the user, y_n^0 are the initial shift values, r is a pseudo random number between 0 and 1 generated by the computer and g_n is a fraction of the total length L, which gives the maximum interval for the random shifting of each harmonic (we used $g_n = 0.1L$ for most of our calculations.
Now using this formula we can obtain a surface as shown in fig 3 and fig. 4 taking into account different profiles simulated by changing r in eq. (8).

4 Ray-tracing with simulated surfaces.

In ray-tracing calculations it is possible to investigate the effects of the geometry, the waviness and the roughness. In particular, SHADOW can accept independently, parameters of all these errors; this makes it possible to study the dependence of image distorsion on any one of them without changing the other values. Figure parameters come from the analytical equation of the optical surface together with mapping of the thermal and stress deformations which can be introduced after finite-element calculations. Roughness can be simulated in ray-tracing by considering the surface formed by overlapping gratings of different frequencies. As it is not possible to define mathematically the whole surface at submicroscopic level, the surface roughness characterization should be used via a probabilistic description. Monte Carlo simulations are often used in ray-tracing, not only for the description of the source, but also for the optical element characterization [7]. The grating frequencies for the roughness scattering can be probabilistically calculated looking at the PSD function of the surface. A model based on such an idea is already implemented in SHADOW [8] while an accurate model of waviness has not been implemented yet.
In the modeling of waviness, a single sinusoid with the selected rms slope error is usually adopted. We assume that the geometrical optics limit is valid: the x-rays wavelength is much smaller than the lengths characterizing the waviness. This means that the surface is locally plane, and each ray is reflected specularly from each tilted element of the optical surface. The single sinusoidal model or ripple is very naive, and results are not realistic, as figure 5 shows. Ray-tracing of a system with the waviness generated by our method can give more realistic results, comparable to those measured experimentally (see fig. 6). The comparison with the ray-tracing considering a single sine signal shows how the role played by the whole set of frequencies is essential to reproduce the spot size and shape of any beamline. As another example, figure 7 shows the effect of the waviness in the parabolical mirror of GILDA beamline [9]. This mirror is placed before the monochromator and the slope errors affect the energy resolution and the transmission due to the change of the divergence introduced in the photon beam.

5 Conclusions.

We have presented a method for the accurate simulation of waviness effects on optical surfaces such as mirrors, gratings and crystals. The performances of the surfaces produced by this method are very similar to those of real surfaces; therefore, this application, used together with SHADOW, can be very useful in the characterization of the performance of any grazing incidence x-ray beamline. Computer code for generating and analyzing the optical surfaces is available from the authors.

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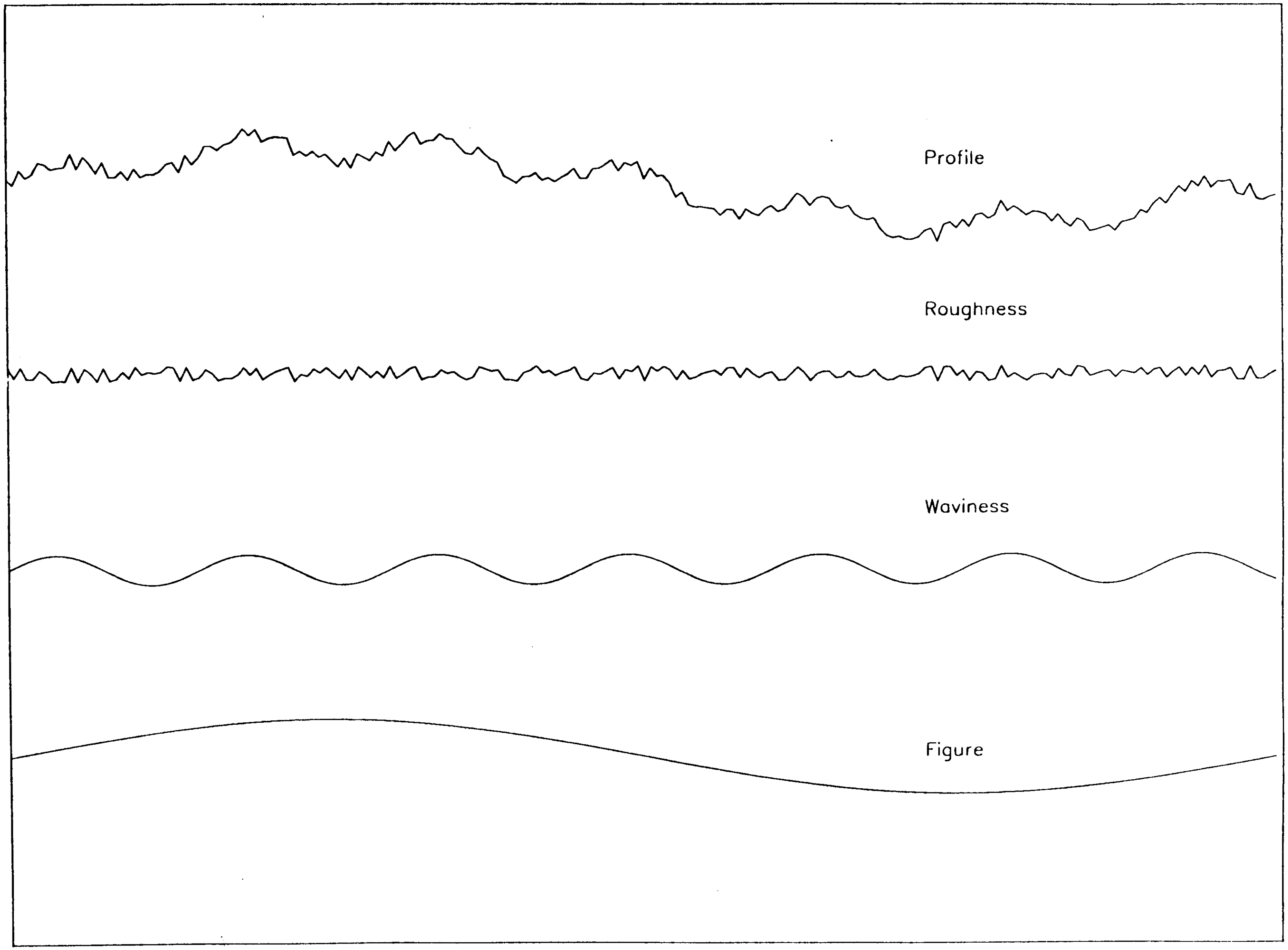
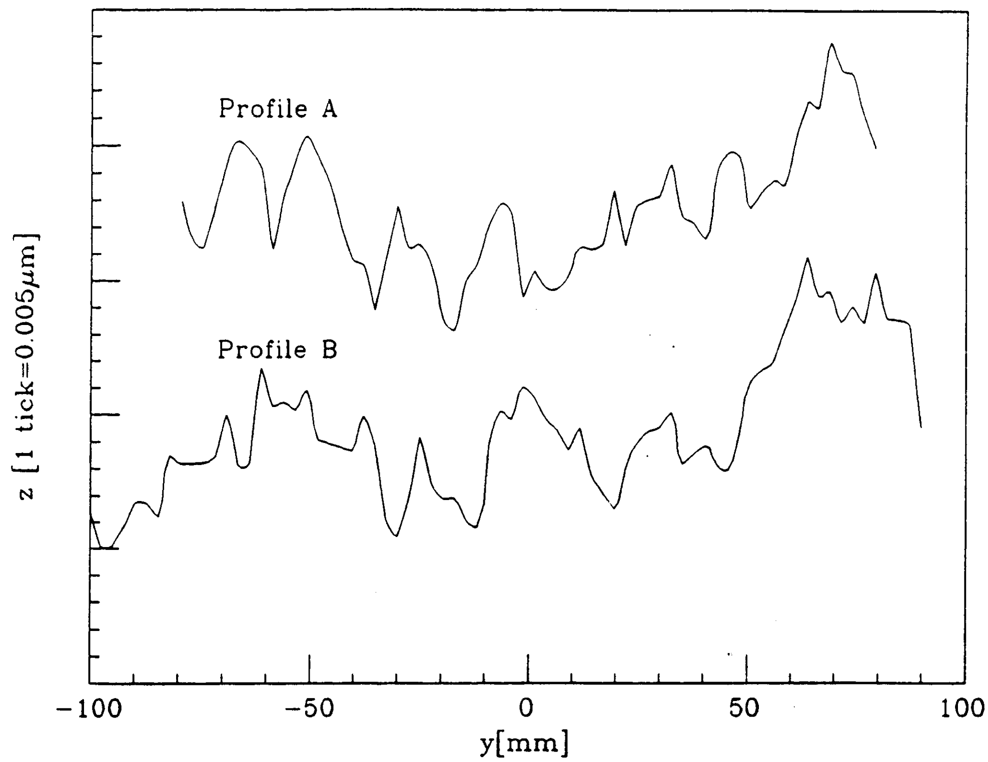


FIG. 1

A real surface can be described in terms of roughness, waviness and figure, depending of the irregularity sizes.



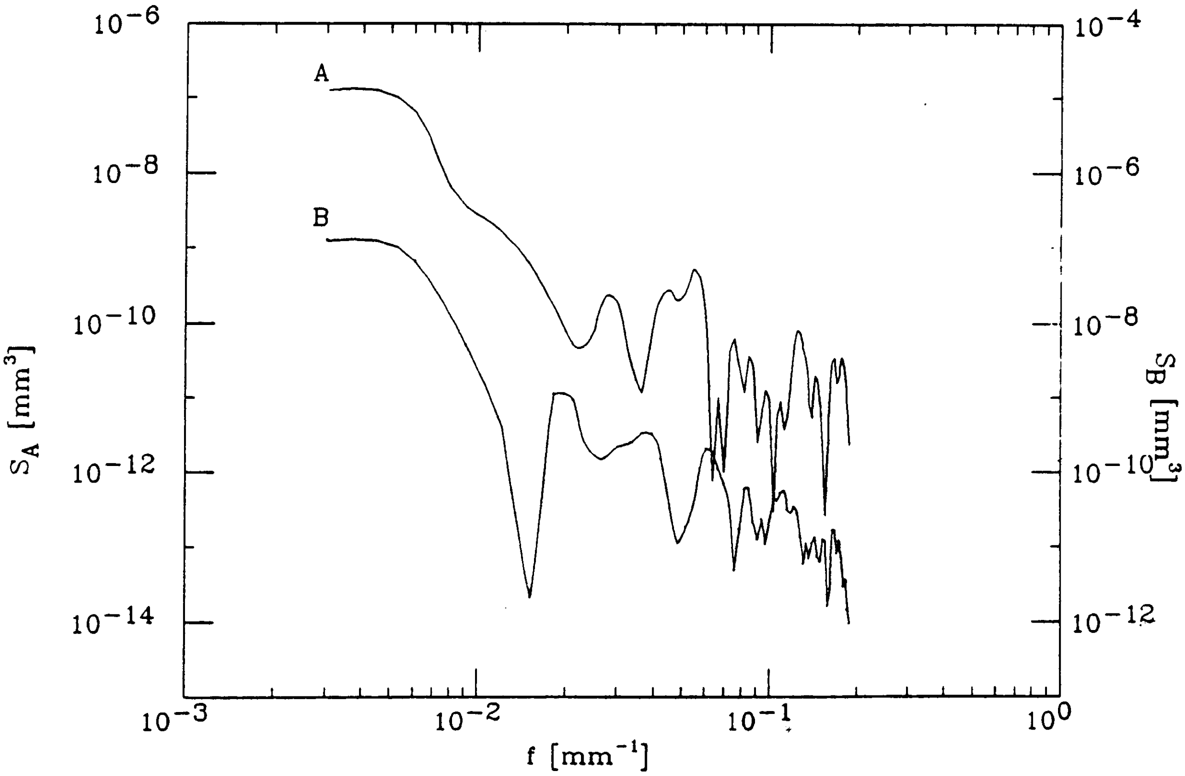


FIG. 2

Two waviness profiles of a real mirror (top) and their corresponding PSD function (bottom).

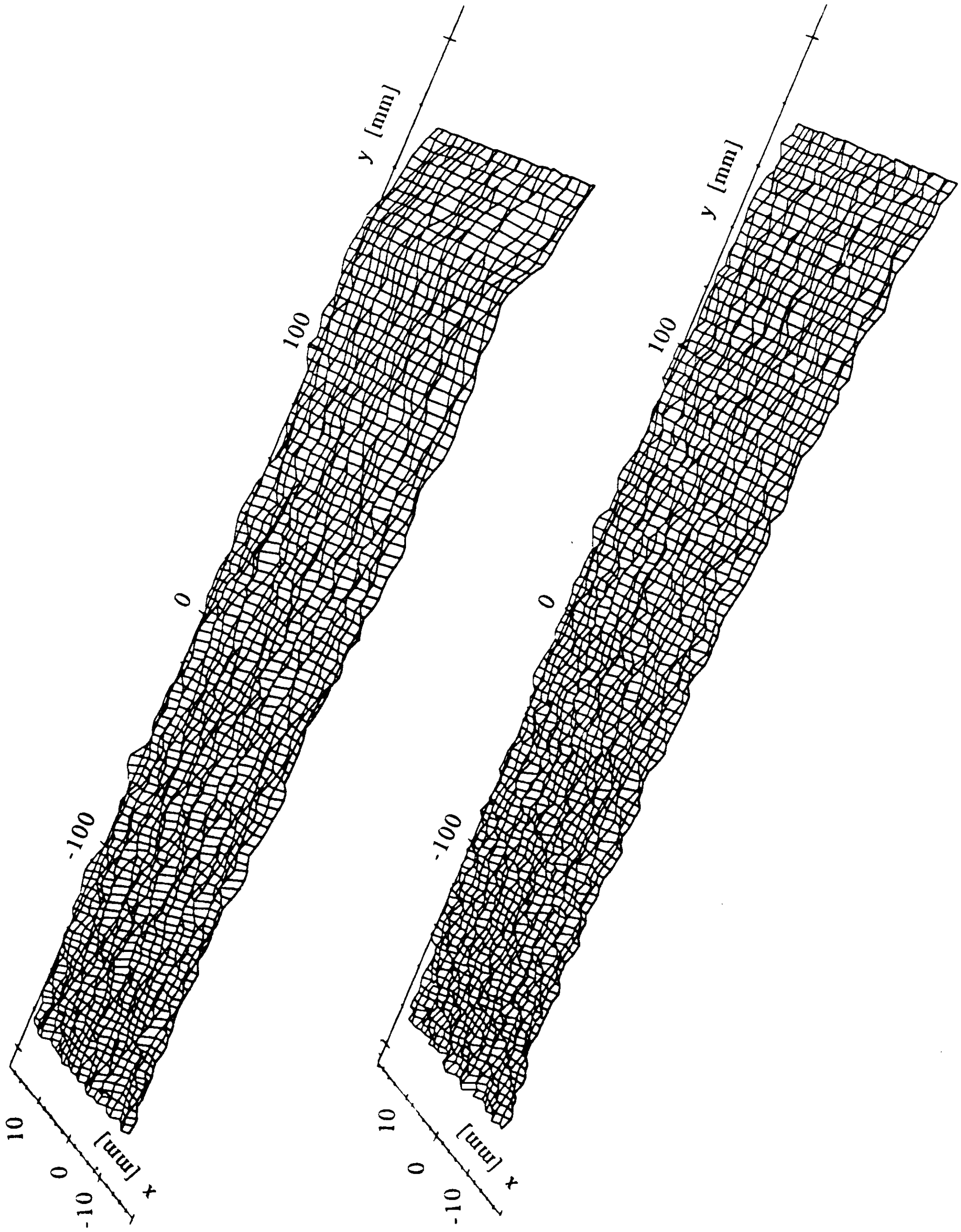


FIG. 3

Simulated waviness of optical surfaces with 0.4 arc sec slope error. The surface A has been generated considering $n_{max} = 32$, $C_n = 1, y_n^0 = 0$, and $f_n = 0.1, f_0 = f_1 = 0$. For surface B, $n_{max} = 56$ and the remaining parameters have been changed in a more complicated way. The total length of each surface is 350 mm and the width is 30 mm The vertical length is not scaled.

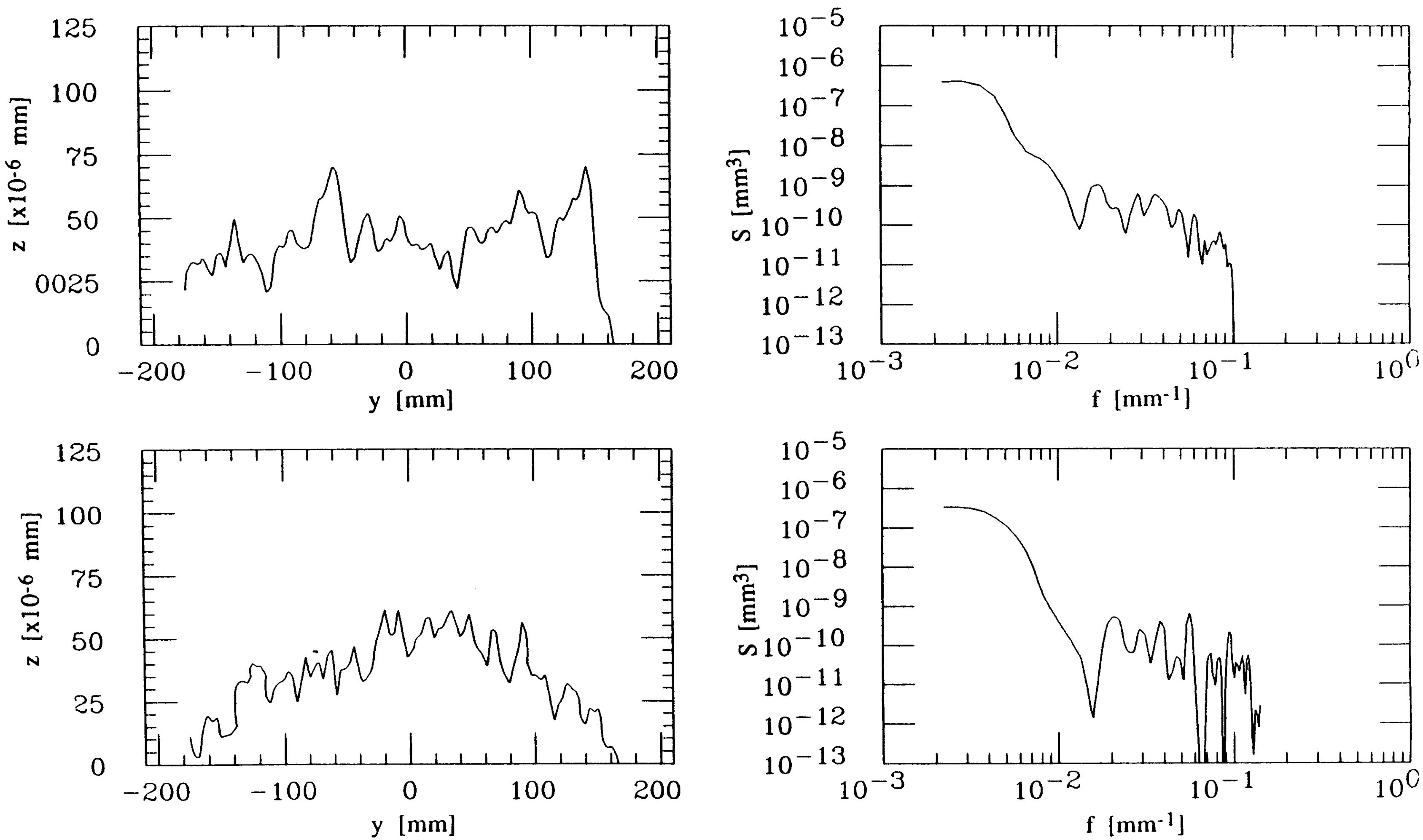


FIG. 4

A single profile of the surfaces A and B presented in fig.3. The corresponding PSD functions have been plotted on the right.

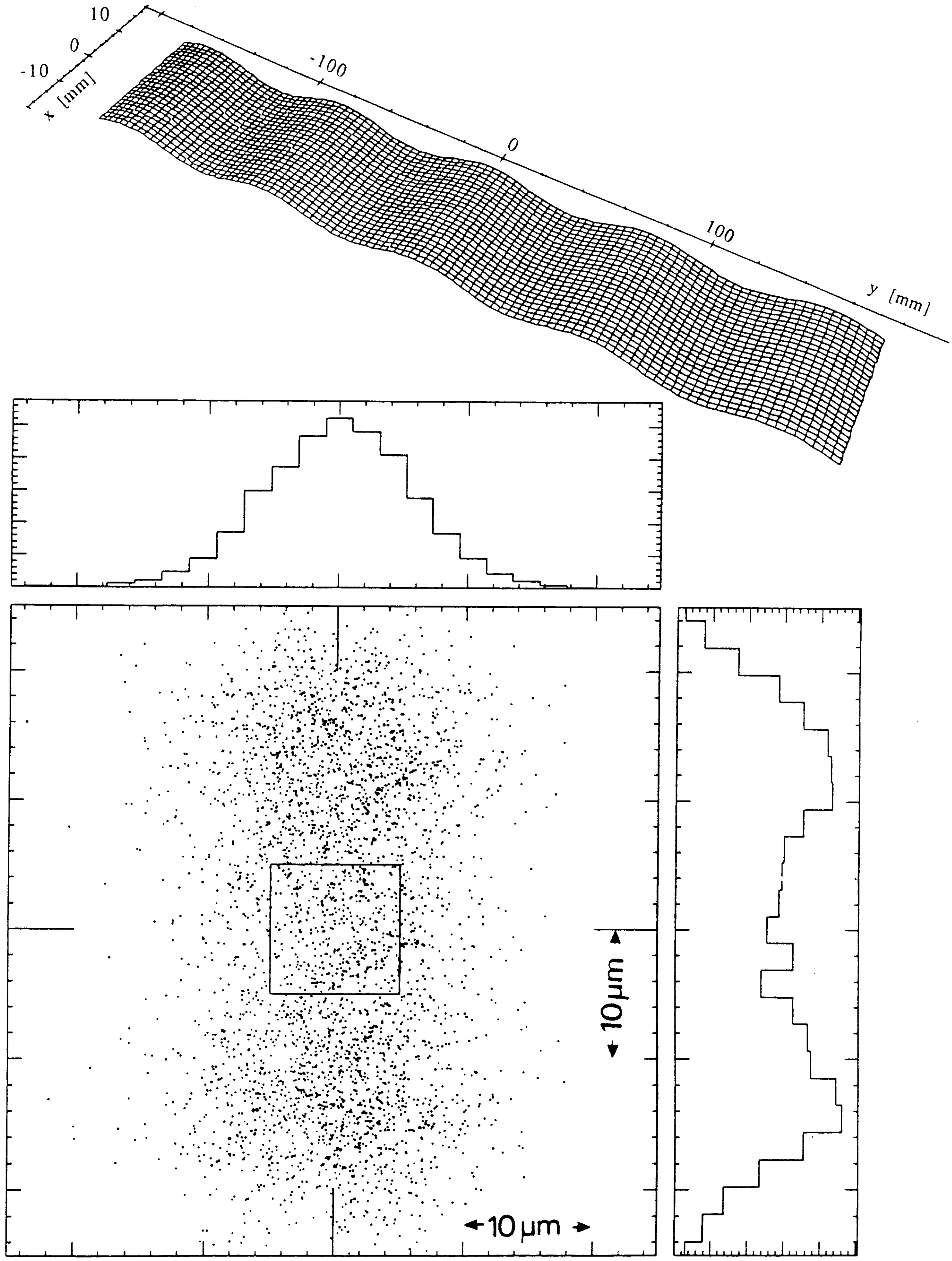


FIG. 5

Ray tracing image at sample plane of a microfocus beamline using an ellipsoidal mirror [2]. Sinusoidal model of waviness has been considered with $\Delta_{rms} = 0.4$ arc sec. Notice the non gaussian shape in the vertical plane produced by the single sine waviness model.

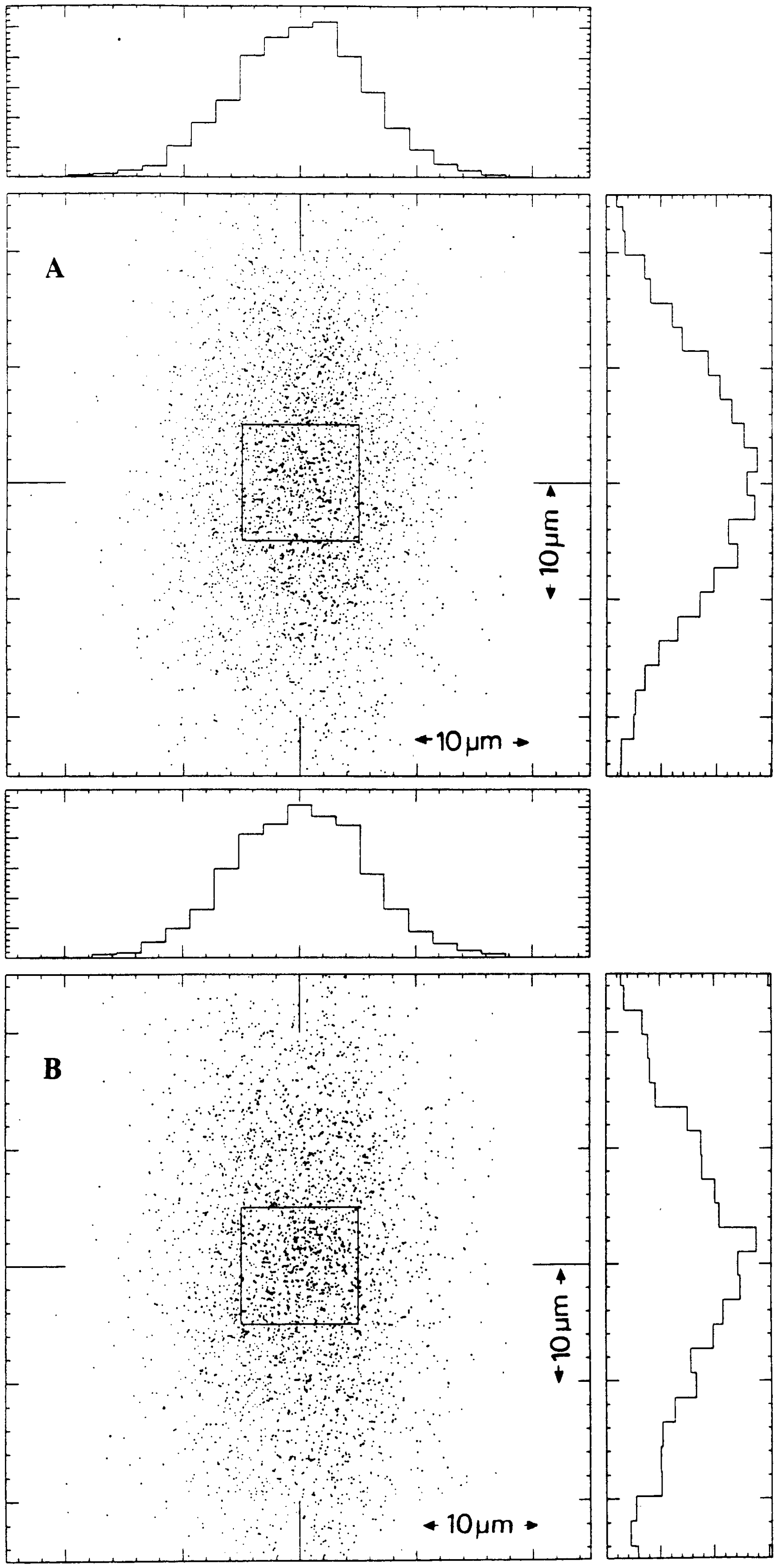


FIG. 6

Scattered images produced by ray-tracing of the same beamline as in fig. 5 except that different slope-error generators were used: A. The "actual" surface as measured was used. B. Simulated surface with the model presented here, parametrized with Δ_{rms} from experimental measurement.

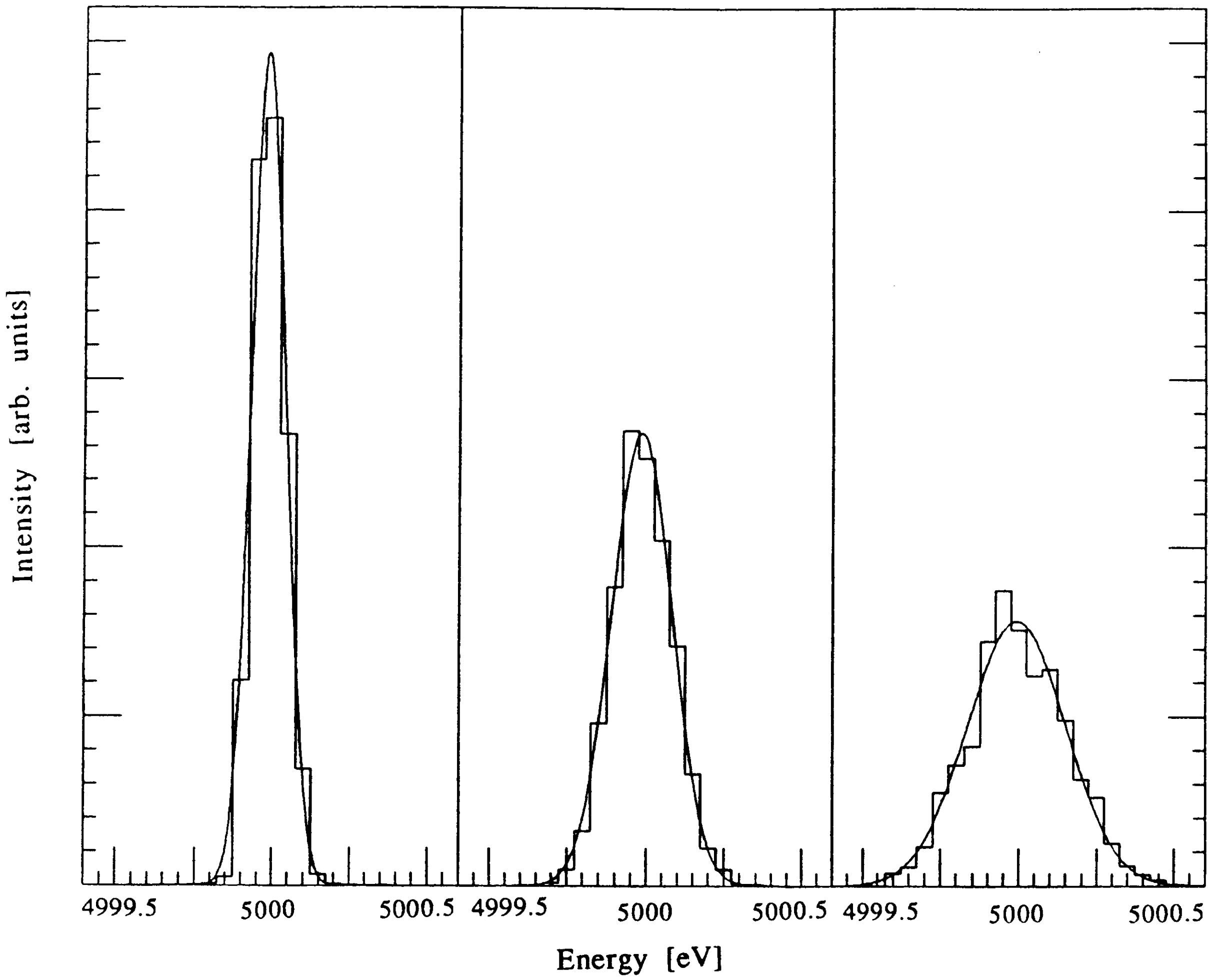


FIG. 7

Energy resolution calculations for the GILDA beamline [9] containing a parabolic mirror, for different values of slope error (no errors on the left, Δ_{rms}=2 arc sec on the middle and Δ_{rms}=4 arc sec on the right) at an energy of 5 KeV. The gaussian fits of the histograms give values of resolution of ΔE_{fwhm}=0.13 eV without errors, and 0.22 eV and 0.37 eV for 2 and 4 arc sec respectively. A silicon double crystal monochromator has been considered with (311) diffraction planes.