

## Computer training program on Fourier spectroscopy

Lidia A. Luizova, Marina E. Bagenova

Petrozavodsk State University, 185640 ,Petrozavodsk, Russia

### ABSTRACT

In addition to laboratory program on Fourier spectroscopy<sup>2</sup> a computer training program "Fourier-transform visible spectrometer" has been developed. The program main menu contains items: "Theoretical part", "Practical part" and "Exit". In the first part such topics as "Michelson interferometer", "Fourier spectroscopy advantages", "Fringe pattern scanning and recording", "Spectrum with interferogram connection" are discussed. Selecting one of these items students can see textbook pages with schemes and illustrations. Some pictures are animated. "Practical part" includes modeling of radiation spectra and interferograms. Students can simulate spectrum as sum of gaussian functions with arbitrary center position and width or as sum of monochromatic lines. Then interferogram with given full path difference and scanning step is calculated and corresponding spectrum is reconstructed. Comparing this spectrum with initial one students investigate the influence of scanning range and step on spectrometer resolution and available spectral range. There is also an opportunity to simulate some device imperfections: not exactly parallel mirrors, occasional mistakes of scanning step, noises, discretion and nonlinear respond of photo detector. The program has Russian and English versions. It is used as a part of laboratory training on physics and instead of lectures on Fourier spectroscopy for the Physics Electronic Department students. For advanced students we have also the program, which simulates Fourier-colorimeter.

**Keywords:** Fourier-transform, spectroscopy, interferometer, colorimeter, computer training, computer simulating.

### 1. INTRODUCTION

In the recent years Fourier transform spectrometers (FS)<sup>1</sup> play more and more significant role in fundamental and applied researches connected with spectrum studies. Therefore, it is necessary to introduce this device to the future engineers specialized in optics and spectroscopy. That encouraged us to include a Fourier-spectroscopy laboratory program in the study process<sup>2</sup>. Our experience on the subject revealed difficulties for students in understanding the principles and mastering in Fourier spectroscopy. Especially, this referred to the general properties of Fourier conversion which it is known are being widely used in many different fields of science - from the quantum mechanics to the holography and optical processors.

Taking into account the importance of this apparatus and an ability of easy-to grasp demonstration of its general features by introduction of the Fourier spectrometer we are considering the necessity of including this task to the general physics practicum for all students of Physics Department.

At the same time, we offer a computer training program to facilitate the acquaintance with Fourier spectroscopy concepts and specific features of a particular laboratory set-up. For the present this program is being used either jointly with a laboratory set-up or only for the introduction of the Fourier -spectroscopy method.

The work with the program assumes students to execute items of main menu and sub-menu step by step with a possibility to come back to any previous step. The main menu has two sections: "Theoretical part" and "Practical part", there is also an "Exit". The program is running on IBM PC/AT-compatible computer under MS DOS or Windows.

### 2. THEORETICAL PART

The items of the main menu "Fourier spectroscopy", "Michelson interferometer", "Interferogram, spectrum" and "Fringe pattern" give the students illustrated pages of the text book, where a history of development of the Fourier-spectroscopy method is given, principles of its work are explained and a circuit of Michelson interferometer is offered. Submenu "Theoretical part" is given in Fig. 1 on the left, on the right - one of the text-book pages.

The advantages of "Fourier spectroscopy" are revealed in section of "Advantage", namely:

1. In FS at each certain moment the information about all spectral compositions is received simultaneously, therefore, FS has a higher value of signal-to-noise ratio than grating and prism devices;
2. In FS one can use the large solid angle of a source and a detector and, as a consequence, get a higher signal level with the same resolution;
3. There is a possibility of studying spatially inhomogeneous objects, because Fourier spectrometer outlet in contrast to slit one maintains object image spatial structure. Using matrix photodetector and path difference scanning system we can receive a set of interferograms, corresponding to different spatial parts of an object. (This last advantage, as we know, is not being emphasized in literature usually. In our laboratory set-up a possibility of a simultaneous spectrum registration and a color identification (look below) of radiated or reflected object at three spatial points is implemented, although, in principle, their number is limited only to the resolution of the photoreceptor matrix and drawing optics<sup>3</sup>.

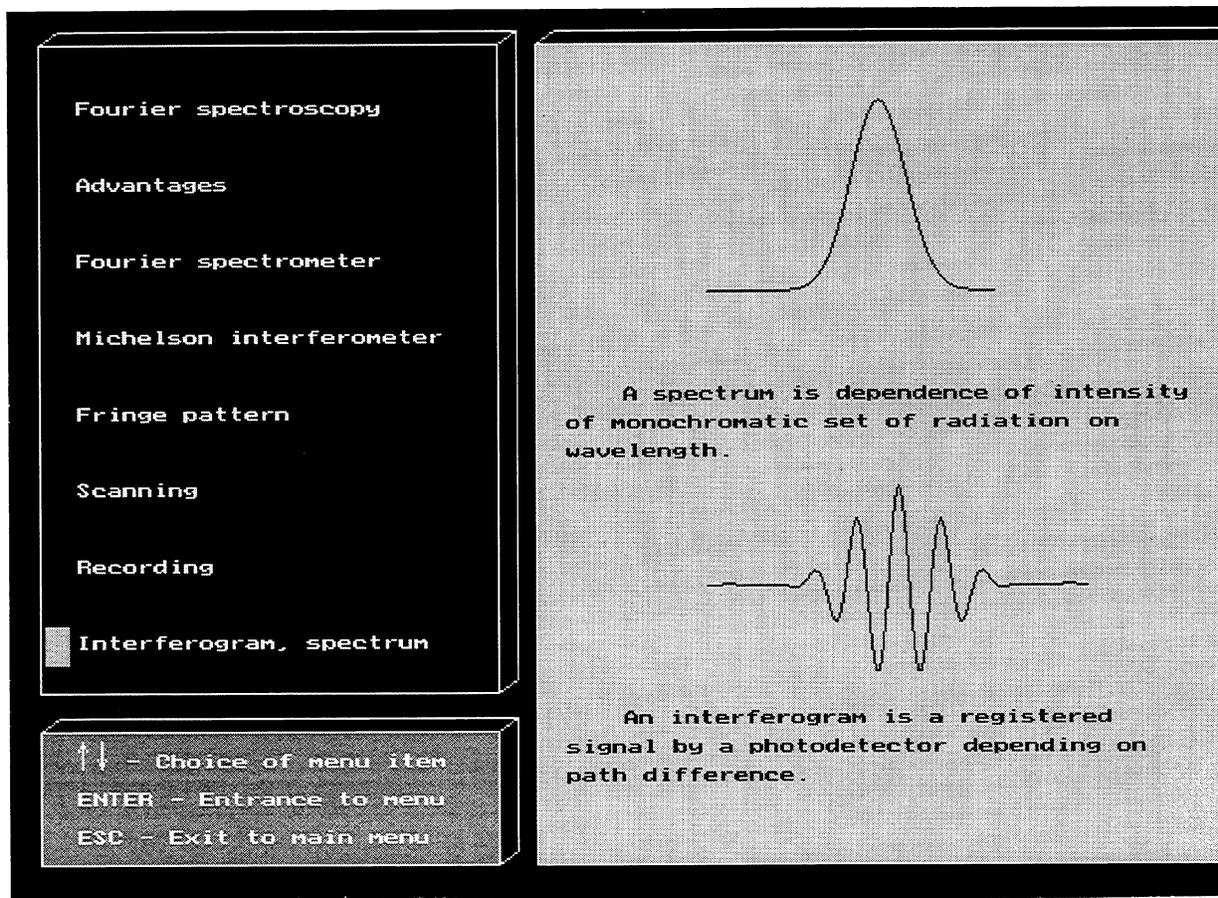


Fig.1. Submenu "Theoretical part" and example of the text-book page .

Submenu items "Fourier spectrometer", "Scanning" and "Recording" describe the real laboratory set-up. Our model differs from the most Fourier spectrometers presented in literature by its design to work in all visible spectrum range. For the training purposes such set-up has advantages of visibility (a student can observe the motion of the interference bands due to variation path difference), cheap cost and simplicity as far as for the path difference scanning not complicated mechanical assembly units are used, but a gas cell connected to a vacuum pump. The variation of the path difference occurs while an air leaks-in to the pumped out glass dish. Except for that, a possibility of constructing the Fourier colorimeter is demonstrated by this set-up. In the training program the scanning process on animated picture (Fig.2) is simulated, here the changing colors of interference fringes, gradual appearance on the computer display of interferogram and changing manometer indication are shown.

It's necessary to measure the readings of recording system with step of 380 nm for FS to operate on visible region of spectrum. This step is so small for FS that maintains the use on visible region (380-760 nm). To strive for this step is not a simple practical problem, probably this is the explanation of the fact that for a long time FS has been used on infrared region of spectrum only.

In the FS theory the step along the path difference is

$$h = \frac{1}{2(\sigma_{\max} - \sigma_{\min})}$$

where  $\sigma_{\max}, \sigma_{\min}$  - the bounds of spectral band in wavenumbers.

One can do the scanning of visible region by some methods. One of the simplest is the scanning by pressure. For this a glass dish is used that is filled in with a contiguous air flow through a capillary tube. The He-Ne laser radiation (the reference interferogram) is recorded simultaneously to tie a recorded signal with definite value of the path difference in interferogram.

ENTER - Exit to main menu

Fig 2. Illustration of the scanning and recording process in Fourier-transform visible spectrometer

### 3. PRACTICAL PART

There are two items in the menu: "Study" and "Modeling". The "Study" illustrates general features of the Fourier spectrometer, the submenu item "Resolution" includes main statements on spectrometer resolution theory and encourages the students to simulate the spectrum in the form of several monochromatic lines, then, to simulate the interferogram with a specified length and reconstruct the spectrum by this interferogram. Comparing this spectrum with the initial one students investigates the influence of the scanning range on the spectrometer resolution.

The second item "Step influence" explains the way of choosing a scanning gap  $h$  of path difference. Spectrum (as a function of wave number  $\sigma = 1/\lambda$ , where  $\lambda$  is wave length) reconstruction is performed by calculation of a discrete inverse transform. So, the spectrum recurs with the period of  $1/h$  and "reflects" from all points  $\sigma_k = k/h$  ( $k$ -any integer number). If the investigated interval of wave numbers is higher than this period, the spectrum overlap takes place and "odd" lines occur. At this point the student can simulate a spectrum in the form of several monochromatic signals and reconstruct it from the interferogram with a specified steps quantity ( $N$ ) and size ( $h$ ) (in nm). Here one can observe either an influence of interferogram full length ( $h*N$ ) on the resolution and the value of  $h$  on the spectrum "cleanness". In Fig. 3,4 an example of such work is shown. Simulated spectrum contains three lines (400,520 and 600 nm); in Fig 3. spectrum reconstructed from the interferogram with a step of 1000 nm is displayed, "odd" lines are marked; in Fig 4 the same spectrum reconstructed with low resolution is represented.

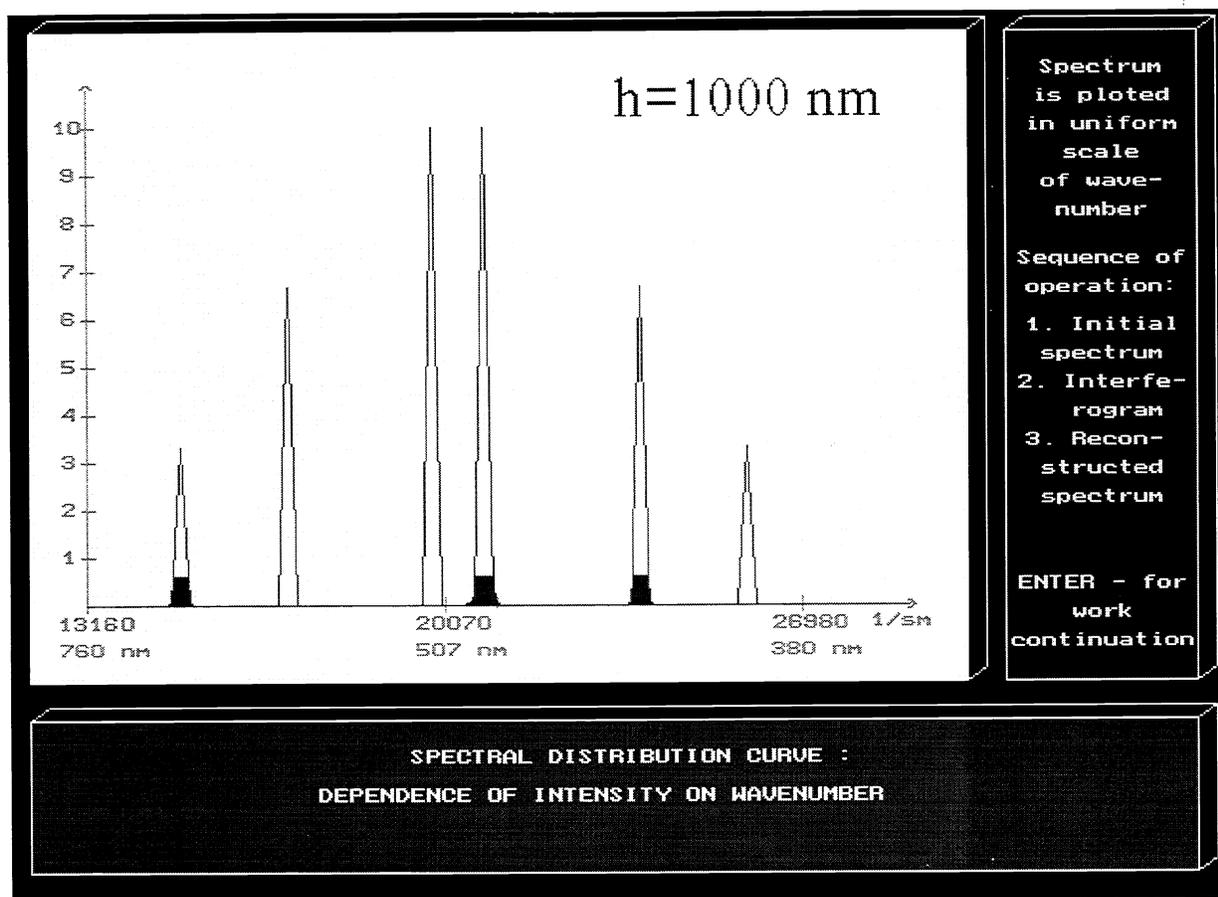


Fig 3. Appearance of “unreal” spectral lines when wrong step size is chosen.

From the item “Study” of section “Practical part” the student has to master the main feature of Fourier spectrometer that differs it from the slit (for instance, grating) monochromator. In the common spectrometer the scanning gap is concerned with a device resolution, and product of number of steps by a step size is a full width of the investigated spectrum. In the Fourier spectrometer it’s vice versa: the scanning step determines a full width of the accessible spectrum interval and a product of step number by a step size - the resolution of apparatus.

The next item “Modeling” enables to investigate the influence of device imperfection on the reconstructed spectrum. It has subitems “Modeling of spectrum”, “Modeling of interferogram” and “Spectrum reconstruction”. Simulating the spectrum in the form of several Gaussians of different width and intensity the student referring to the second subitem can simulate the interferogram of specified length with a specified step and can add to it distortions of the following type: not exactly parallel mirrors; occasional mistakes in scanning step, noises in photodetector response.

Coming to the third point of menu and reconstructing the spectrum one can study the influence of these distortions and, what is the most important, evaluate it’s acceptable limits for the specified type of the spectrum and device resolution. For example, the spectrum in Fig. 4. would not be appreciably distorted by step size relative mistake till 0.1. As to mirrors, one can see that computer simulated interferogram disappears when path difference from various parts of mirrors reaches a half of wave length (corresponding angle between mirrors planes is near  $10''$ ), but our real laboratory set-up runs satisfactory with this and even worse degree of mirror parallelism. It is good occasion for students to discuss problem of interference bands localization.

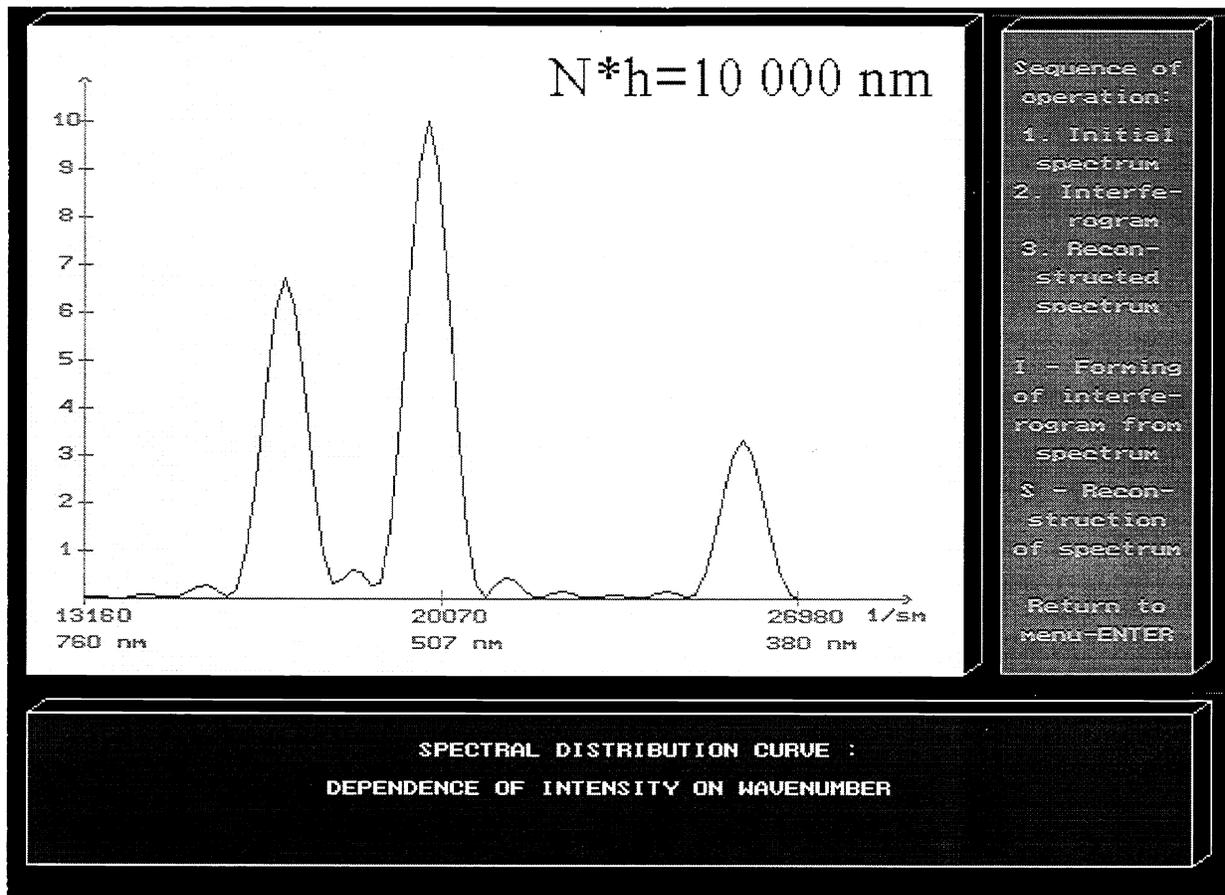


Fig.4. Three monochromatic lines, reconstructed from too short interferogram.

There are some variants of the program that let us simulate discretion and nonlinear response of photodetector and light source instability. Comparing the influence of imperfection of reading out system and a light source on the results of the spectrum study by the slit devices and by the Fourier spectroscopy students become convinced, that the sensitivity of devices to these distortions, generally speaking, depends on the spectrum type, but on the average is the same, excluding the influence of the source instability.

If the source is smoothly fading during the spectrum scanning, then in the slit spectrometer relation of line intensities, measured at the beginning and at the end of scanning, will be deeply distorted (and, therefore, the color of radiation will be determined incorrectly). At the same time the Fourier spectrometer transmit the intensity ratio from different parts of the spectrum practically without distortions (there can only be a minor decline of resolution). This result comes directly from the Fourier spectroscopy concepts and will be discussed more detailed in the next section.

#### 4.FOURIER COLORIMETER

One of the described program version and the program under which supervising our laboratory set-up is working illustrate the possibility to design a colorimeter based on the Fourier spectrometer<sup>3</sup>.

Color is integrated description of reflected or dissipated by object, passed through a transparent sample or emission radiation. Each color is to be specified by a triplet of numbers:

$$X = \sum_i S(\lambda_i) \cdot \bar{x}(\lambda_i); \quad Y = \sum_i S(\lambda_i) \cdot \bar{y}(\lambda_i); \quad Z = \sum_i S(\lambda_i) \cdot \bar{z}(\lambda_i), \quad (1)$$

or two chromaticity coordinates

$$x = X/(X+Y+Z); \quad y = Y/(X+Y+Z),$$

where  $S(\lambda_i)$ - radiation spectral power,  $\bar{x}$ ,  $\bar{y}$ ,  $\bar{z}$  are tabulated functions which correspond to visual response of "standard normal eye". Accurate X,Y,Z determination for any kind of spectral distribution  $S(\lambda_i)$  can be achieved only if visual spectrum is measured with spectrometer and then X,Y,Z will be estimated.

The colorimeter based on the Fourier spectrometer has the following advantages over slit (e.g. grating) one:

1. High sensitivity, which is important when faint radiation flows are to be measured<sup>1</sup>.
2. The opportunity of spatial inhomogeneous samples investigation<sup>3</sup>.

It is important to say that spectrum reconstruction is not obligatory, since X,Y,Z can be determined directly by interferograms<sup>3</sup>.

Using the Fourier transform property we can rewrite formulae (1) like this:

$$X = \sum_j \{F(\Delta_j) - F(0)/2\} Q(\Delta_j) \quad (2)$$

here  $\Delta_j$ -is path difference,

$F(\Delta_j)$ - interferogram reading in the point j,

$Q(\Delta_j)$  - the Fourier transform of functions  $f_1$  or  $f_2$ .

$$f_1 = \bar{x}(\sigma) / \sigma^2 / p(\sigma), \quad (3)$$

$f_1$  is used if we investigate self-emission sources.

$$f_2 = \bar{x}(\sigma) \cdot I(\sigma) / \sigma^2 / b(\sigma) / p(\sigma), \quad (4)$$

$f_2$  is used if we want to find chromaticity coordinates of samples illuminated by sources with spectrum  $I(\sigma)$ .

In (3,4) :  $p(\sigma)$ -photodetector spectral sensitivity,  $b(\sigma)$ -spectral distribution of any lamp we use in color measurements.  $Q$  is to be calculated before measurements and stored in computer memory.

Our simulating program allows to illustrate the concept of Fourier colorimeter and to investigate the influence of devices imperfection and source instability on chromaticity coordinates values.

The main difference between common (slit) and Fourier spectrocolorimeter is their "sensitivity" to light intensity variations. This fact is illustrated by Fig.5. Here a simulated spectrum is represented, in the left top corner one can see its interferogram, multiplied on monotonous decreased function. At the end of scanning the reading is equal to zero (this function describes source fading, or environment darkening, or detector sensitivity decreasing). The reconstructed spectrum in this case practically coincides with simulated one. Corresponding chromaticity coordinates are placed in right top corner. (The common spectrocolorimeter would give values:  $x=0.339$ ,  $y=0.194$ ).

Some results of simulating experiments with different spectra and different intensity variation functions are represented in Fig.6 and in Table 1. In Fig. 6 -curves C1-C4 simulate spectra  $S(\lambda)$ , A1-A3-different intensity variation functions  $J(t)$  (t-time, full scanning time T is assumed to be equal to 1, ordinates S, J- relative units). In Table 1 modules of chromaticity coordinates errors when one use two types of colorimeter are represented. One can see that only in the case of narrow single line common spectrocolorimeter has advantage, in all other cases presented here the Fourier spectrocolorimeter accuracy is higher.

But it is necessary to say that when intensity variation frequency increases this FS advantage will be lost, because Fourier transform interprets intensity oscillations as a spectral line presence. As to “white “ noise, our simulating experiments show that their influence on both colorimeters is nearly the same.

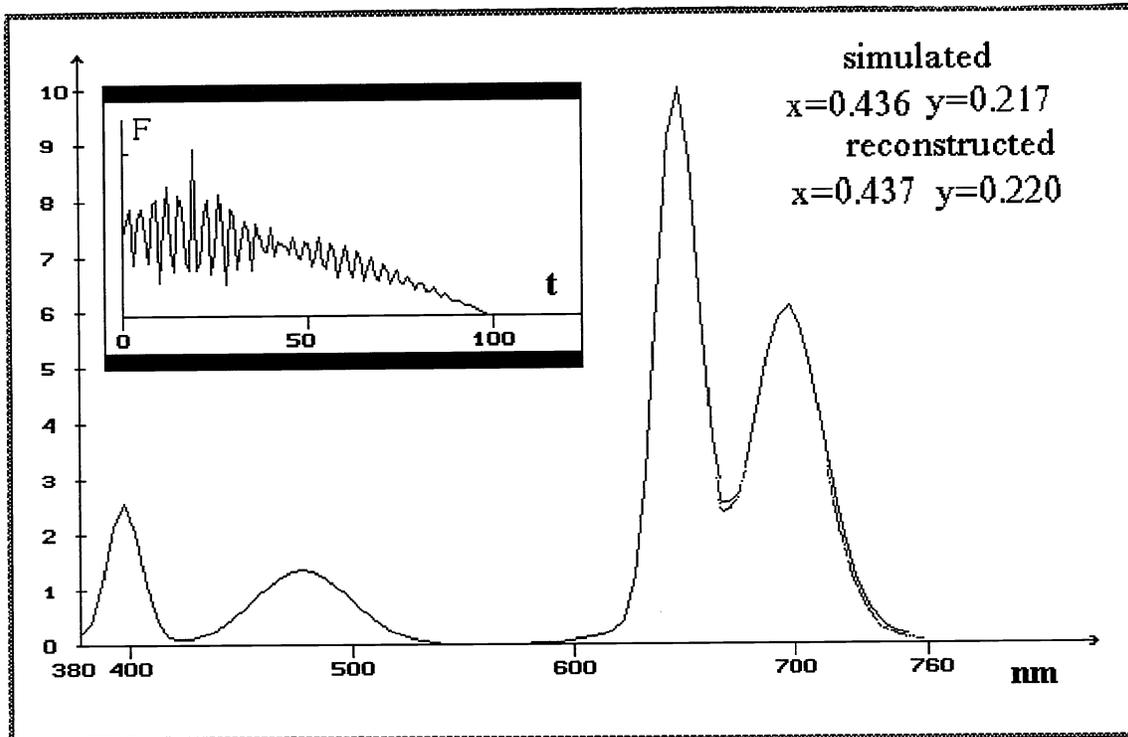


Fig.5. Simulated (lower curve) and reconstructed spectra , interferogram and chromaticity coordinates

Table 1. Modules of chromaticity coordinates errors  $|\Delta x|, |\Delta y|$  for different spectra S and different intensity variation function J (see Fig.6) with Fourier spectrophotometer (regular font) and common spectrophotometer (bold)

S	C1		C2		C3		C4	
	$ \Delta x $	$ \Delta y $	$ \Delta x $	$ \Delta y $	$ \Delta x $	$ \Delta y $	$ \Delta x $	$ \Delta y $
A1	0.005	0.006	0.003	0.000	0.010	0.009	0.000	0.001
	<b>0.000</b>	<b>0.001</b>	<b>0.022</b>	<b>0.023</b>	<b>0.063</b>	<b>0.035</b>	<b>0.064</b>	<b>0.032</b>
A2	0.013	0.018	0.001	0.001	0.009	0.001	0.000	0.004
	<b>0.001</b>	<b>0.001</b>	<b>0.019</b>	<b>0.023</b>	<b>0.046</b>	<b>0.028</b>	<b>0.041</b>	<b>0.024</b>
A3	0.040	0.100	0.001	0.001	0.010	0.003	0.001	0.004
	<b>0.001</b>	<b>0.001</b>	<b>0.025</b>	<b>0.015</b>	<b>0.052</b>	<b>0.028</b>	<b>0.058</b>	<b>0.017</b>

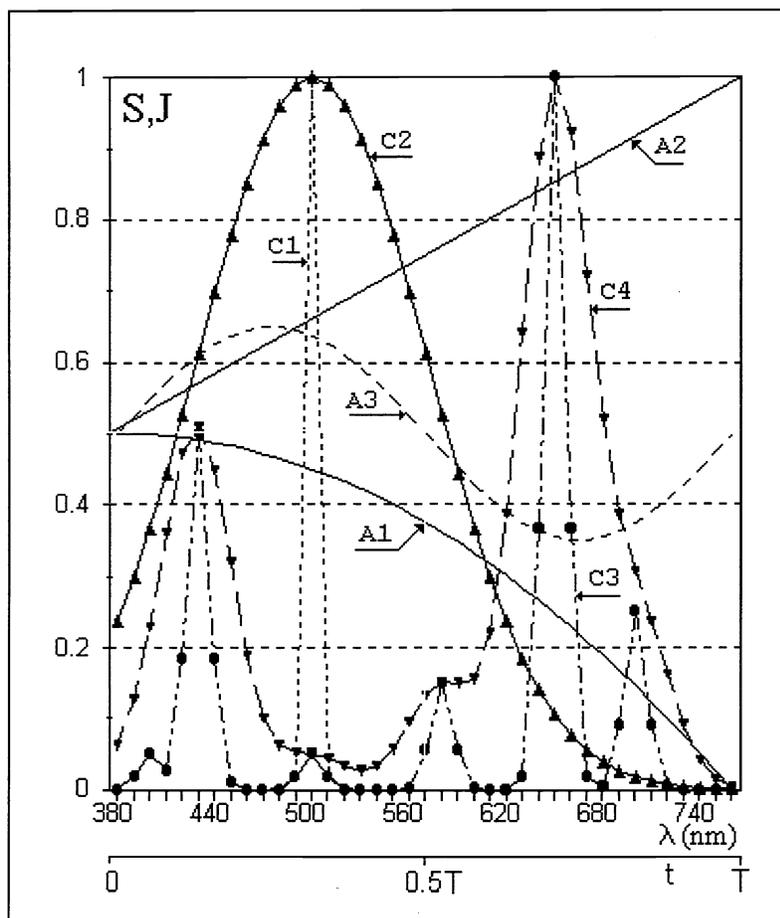


Fig. 6. Simulated spectra C1-C4 and intensity variation functions A1-A3.

$$A1: J(t)=J(0)\cdot(1-t^2/T)$$

$$A2: J(t)=J(0)\cdot(1+t/T)$$

$$A2: J(t)=J(0)\cdot[1+0.3\cdot\sin(2\pi t/T)]$$

## 5. CONCLUSION.

The experience of using the training program revealed that students work on it with an interest and delight and, as a result, they adopted (for some time at least) the Fourier spectroscopy concepts and begin not only understand, but feel the connection between the object and its Fourier-image. Those, who dealt with the Fourier colorimeter simulating receive additional knowledge on Fourier transform properties, spectroscopy and color measurement.

## 6. ACKNOWLEDGMENTS

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## 6. REFERENCES

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