

A NEW APPROACH TO CALCULATING X-RAY PATTERNS OF THE DIFFRACTOMETER FOR NANOSTRUCTURED COATINGS

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Abstract/Резюме: This work has focused on approach to calculating patterns of the diffractometer used for quality estimation of nanostructured coating. System of automated data registration and processing on the base of microcontroller is propoused. Some results of using new approach to calculating patterns of diffractometer as well a software for the comprehensive analysis of such data are reported.

KEYWORDS: NANOTECHNOLOGIES, NANOCOATINGS, ESTIMATION OF COATING QUALITY, DATA DIGITAL PROCESSING

1. Introduction/Введение

One of important directions of modern development of nanotechnologies is development of nanocoatings for tool materials. These coatings provide superhardness that rivals diamond in performance, improved wear resistance and toughness properties as well as meeting stringent regulatory and safety requirements[1].

Estimation of such coating quality may be performed with help of diffractometer, which signals measured in scanning are directly correlated to relevant structural properties of the coatings (Fig.1).

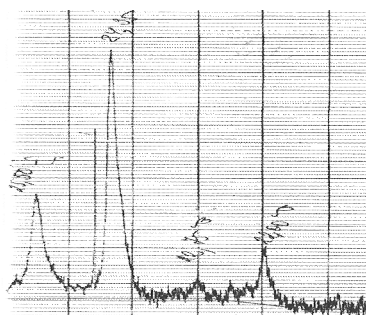


Fig. 1. Fragment of amplitude registration for X-ray diffractometer signals

To estimate of a coating quality it is required to perform at least two operations with test signals. There are fixing of peak-maximum angles at output plotter data, and estimating of peak-height (amplitude) output signals in relative terms, depending on the configuration of used equipment. Both operations are currently performed manually, which significantly increases the complexity of the processing of measurement results and does not guarantee an acceptable accuracy. In addition, significantly complicating the process of initial setup of equipment.

To eliminate these disadvantages it is necessary to add of measuring equipment with a system of automated data registration and processing (SADRP), performed on the base of analogue-to-digital converter (ADC) and personal computer (PC), as it is shown on Fig.2. Programmable graphic unit contains a set

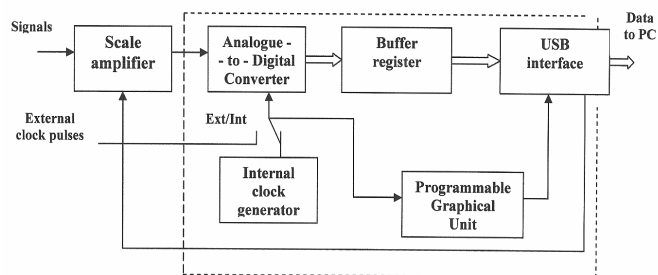


Fig. 2. Block diagram of SADRP

of graphics programs that provide representation of signal samples measuring equipment on the display PC in a form suitable for setting the measuring equipment and the subsequent processing of measurement results.

2. Problem solution/Решение проблемы

The microcontroller AT 90USB1287 includes embedded programmable ADC, generator, register and USB interface. If the microcontroller AT 90USB1287 is used as functional element of automated data registration and processing system it's software must:

- give the numerical value of signal to the PC via a USB interface;
- take a value of the sampling frequency of MS and to develop control signals for the internal trigger generator;
- take the value of the gain scaling amplifier, setting its transfer coefficient in accordance with the accepted values;
- provide self-health system is activated.

These functions are realized by the microcontroller main program, algorithm of which is presented on Fig.3.

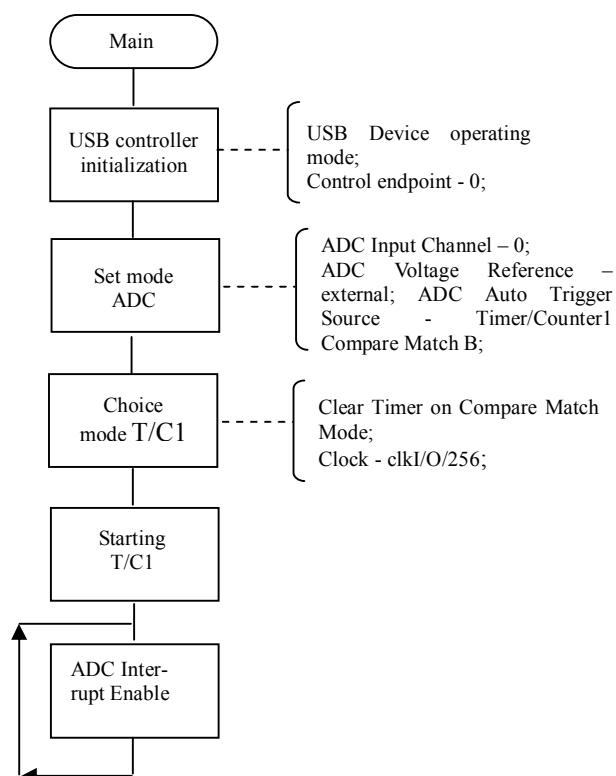


Fig. 3. The microcontroller main program algorithm

Algorithm of the microcontroller AT 90USB1287 interrupt program is shown on Fig.4.

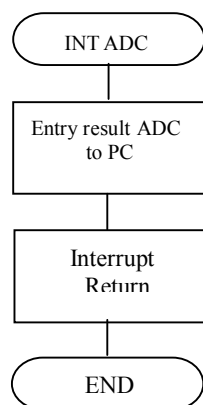


Fig. 4. The microcontroller interrupt program algorithm

The proposed algorithms of representation and signal processing is placed in the Programmable Graphical Unit.

3. Results and discussion/Результаты и дискуссия

3.1. PGU user interface. Block of graphical software is a standard application window with WinAPI interface written in a medium object-oriented programming Borland Delphi 7 using the compiler Object Pascal (Fig.5.).

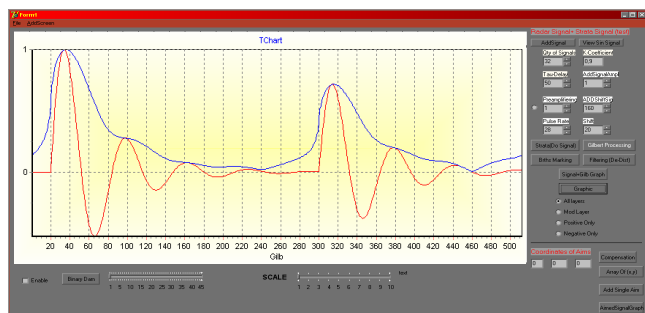


Fig. 5. Main window of the Programmable Graphical Unit.

The user interface (in right side from the Window) consist of several logically separated from each other groups of buttons and settings panels.

The Panel of Components TEdit (Fig.6.) is placed in the upper right corner. It intended to enter the parameters of entered signals .You can handle a number of signal realizations on the screen (**Qty of Signals**), signal delay (**Tau Delay**), the amplitudes of indicated signals (**Preamplifiering**), the number of samples in signal realization (**Pulse Rate**), damping signal coefficient (**K-Coefficient**), the amplitude of secondary pulse (**Add SignalAmpl**),

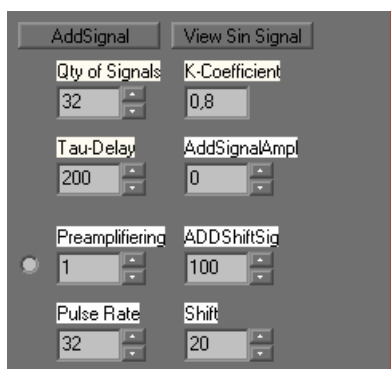


Fig. 6. Panel of Components

the location of the secondary pulse relative to the primary (**AddShiftSignal**), location of "the origin» (**ShiftZero**).

Under the Panel of Component control buttons are placed (Fig.7.), which intended to be used when submitting and processing



Fig. 7. Control buttons of programmable graphics

of measurement results:

- **Strata (Do Signal)** - synthesis signal;
- **BrthsMarking** - output color profile signal;
- **Gilbert Processing** - signal processing algorithm by the Hilbert transformation;
- **Filtering (De-Dist)**- signal filtering;
- **Graphic** - representation of input signals in the form of scan lines.

The choice of output signal levels (Fig.8.) carried

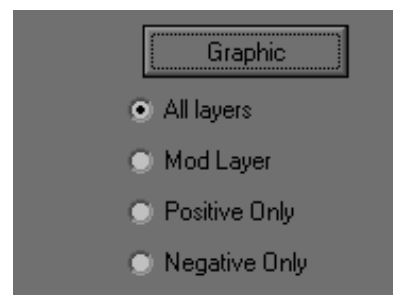


Fig. 8. Panel of signal choice

out by components:

- **AllLayers** - output signal for all levels;
- **Mod Layer** - module of output signals;
- **Positive Only** - registration for the positive components of output signals;
- **Negative Only** - registration for the negative components of output signals.

Under the main window Panel of signal level control with a button of binary filter - **Binary Dam** (Fig.9) and the Panel of scale control (Fig.9.) are situated.

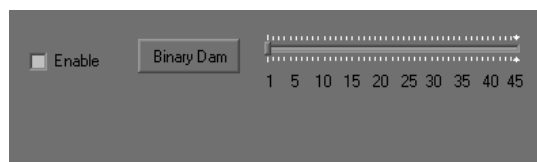


Fig. 9. Panel of signal level control

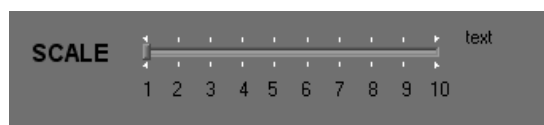


Fig. 10. Panel of scale control

Below we summarize the results of using of some algorithms for representation and signal processing of the Programmable Graphical Unit (PGU).

3.2. Amplitude representation of signals with using the scan-lines. Scan or temporary implementation of the signals with variable amplitude signal level, allow us to see the results of angular scanning of the sample for one or more test cycles (Fig. 11).

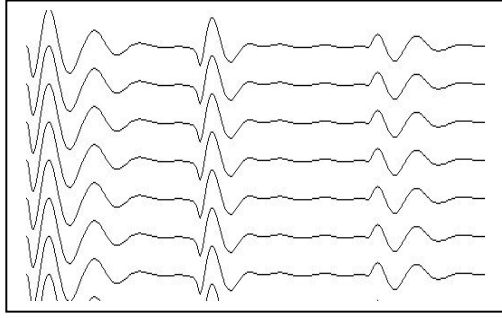


Fig. 11. Amplitude representation of signals

Data flow for algorithm of amplitude representation of signals (A-indication of signals) is shown in Fig.12.

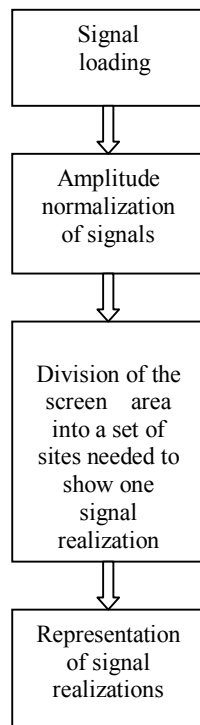


Fig. 12. Data flow of signal amplitude representation

3.3. Color representation of signals with variable number of colors. Color indication of levels recorded signals to visually divide the reference signal values on the level, color-coded to extremes and the place of decay. Separation of the signal level produced by two (in the case of a binary algorithm), or five colors, as it is shown in Fig.13.

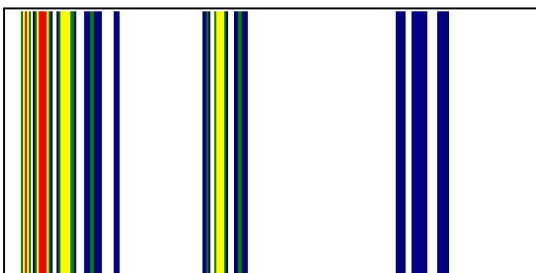


Fig. 13. Color representation of signals

Data flow for algorithm of color representation of signals is shown in Fig. 14.

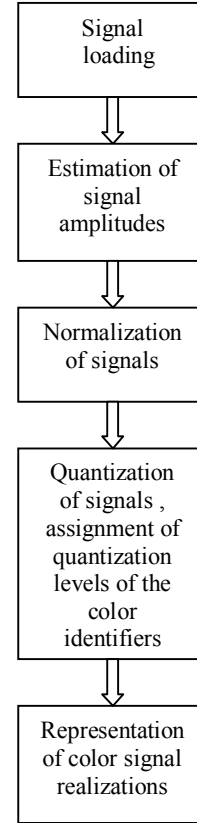


Fig. 14. Data flow of signal color representation

3.4. Amplitude representation of signals with using of the Hilbert transformation. As it known, Hilbert transformation is used for analytical signals [2] , which modulus (envelope)

$$O(t) = \sqrt{s^2(t) + s'^2(t)} \quad (1)$$

and phase:

$$\varphi(t) = \arctg[s'(t) / s(t)] \quad (2)$$

are depended from real $s(t)$ and imagine $s'(t)$ signal parts.

These signal parts are connected each with other by pair Hilbert transformations:

$$s(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{s'(\xi)}{t - \xi} d\xi, \quad (3)$$

$$s'(\xi) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{s(t)}{\xi - t} dt = \Gamma[s(t)], \quad (4)$$

where $\Gamma[.]$ is a denotation of the Hilbert transformation.

Modulus (1) for signal $s(t)$ of arbitrary shape - smooth positive function, which has only one maximum, as it shown in Fig.15.

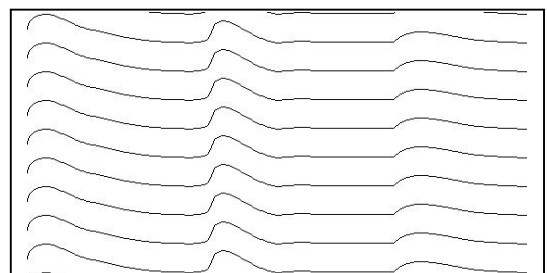


Fig. 15. Representation of signals after Hilbert processing

It must be mentioned there that direct calculation of the Hilbert transformation from equation (4) is impossible. Therefore the algorithm of Hilbert transformation calculations used here includes four main stages [3], namely:

- application of FFT (Fast Fourier Transform) for transition from the time domain to the frequency one;
- Hilbert transform in form of permutation of spectral real and imagine parts with inversion of a sign for imaginary part;
- inverse FFT for return to the time domain;
- normalization of signals accordance to (1) in form of computation of the square sum root of the initial $s(t)$ and Hilbert transformed $s'(t)$ signals.

Data for algorithm of amplitude representation of signals with using of the Hilbert transformation is shown in Fig.16..

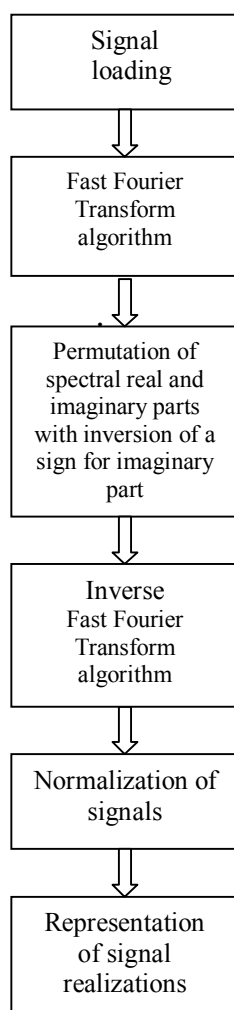


Fig.16. Data flow of signal amplitude representation of signals with using of the Hilbert transformation

It is evidence that signals after Hilbert processing may be represented in color form as it is shown in Fig.17.

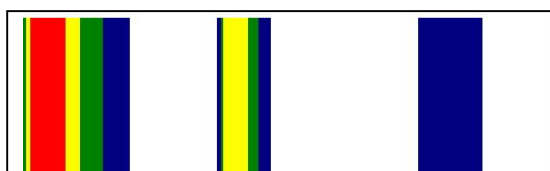


Fig.17. Color representation of signals after Hilbert processing

Signals represented in Fig.17 is the same as the signals which are shown in Fig.15.

Except reviewed main algorithms of digital signal processing there are many other ones in the proposed system of automated data registration and signal processing.

4. Conclusion/Заключение

For using with X-ray diffractometer the system of automated data registration and signal processing (SADRP) on base of microcontroller AT 90USB1287 is worked out.

The algorithms of the microcontroller main program as well as interrupt program are presented.

The Programmable Graphical Unit of SADRП has friendly user interface and wide possibility for representation and processing of diffractometer signals.

Three main algorithms of representation of signals. These are: amplitude representation of signals, color representation of signals, and representation of signals after Hilbert processing both in amplitude and color modes.

5. Литература/Литература

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