

## PARAMETERIZATION OF ATOMIC FORCE MICROSCOPY IMAGES OF SUPRAMOLECULAR ASSEMBLIES

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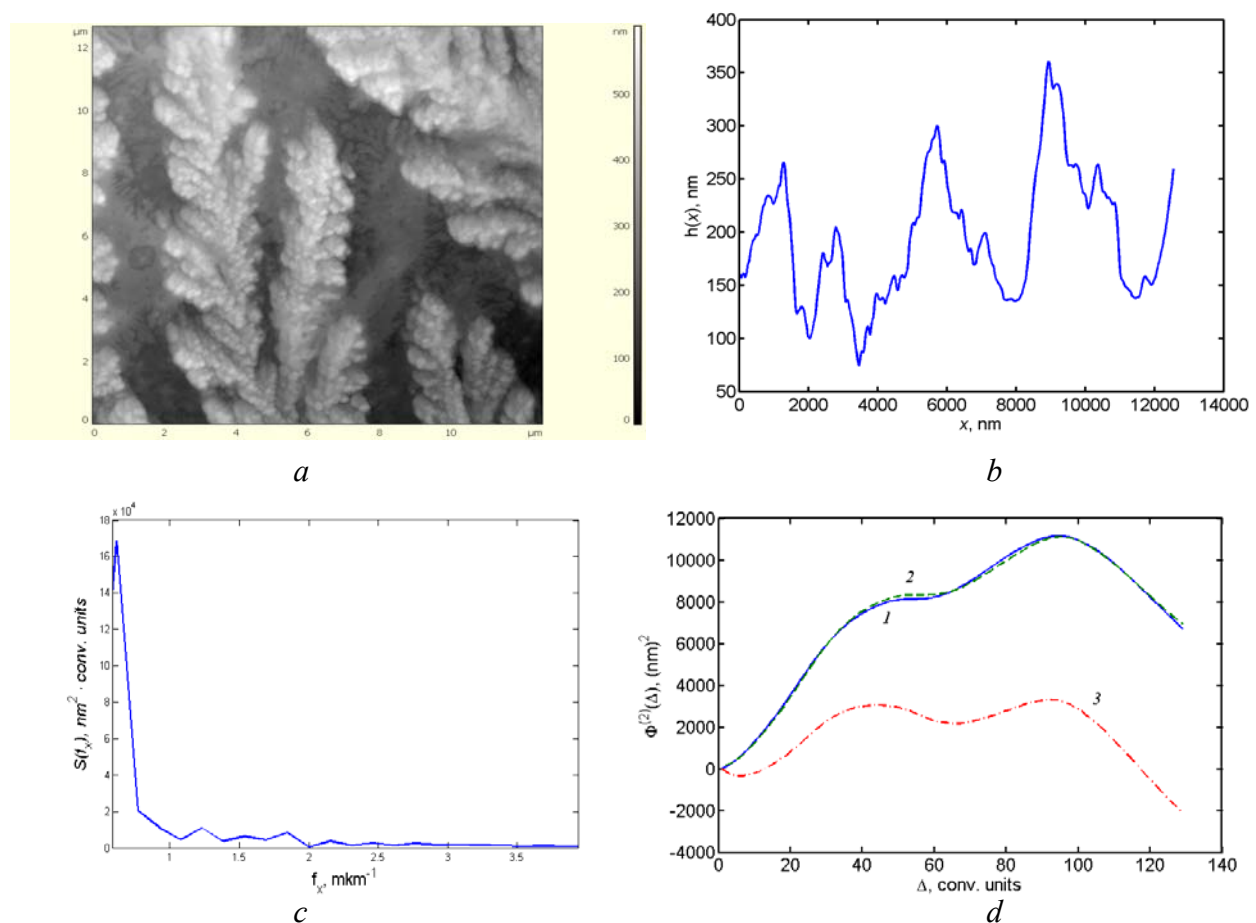
Atomic Force Microscopy (AFM) gives a possibility to study and control surface structure at submicron spatial scales. AFM images represent sampled surface “roughness profiles”  $h(x)$  along coordinate  $x$  in the interval of  $0 \leq x \leq L$  for a set of  $N$  parallel scans (usually  $N = 512, 1024$ ) within the visible image window. Our goal is to extract information from AFM profiles  $h(x)$ , which may generally be stochastic. Specific features of these profiles depend on the physicochemical characteristics of the specimen material, as well as on the conditions of surface formation, modification, operation, and the like. These dependencies are crucial in many engineering and scientific studies. The profiles contain regular (resonant) components as well as chaotic (“noisy”) components with “long memory”. The main questions are how to extract useful information about the chaotic surface structure and study the effect of various external factors on it by analyzing the spatial series  $h(x)$ , and separate out the information contents of chaotic and resonant components. These problems can be solved using Flicker-Noise Spectroscopy (FNS) [1-3]. According to FNS, the information hidden in chaotic surface profiles is represented by correlation links in sequences of different types of irregularities: spikes, jumps, and discontinuities in derivatives of different orders at all spatial hierarchical levels of the systems. In FNS, the tools to extract and analyze the information are “structural function”  $\Phi^{(2)}(\Delta)$  ( $\Delta$  is the space lag parameter) of the 2<sup>nd</sup> order and power spectrum  $S(f)$  ( $f$  – spatial frequency) of relief profile heights.

In order to determine FNS parameters based on the array of relief profile heights, all the profile  $h_i(x)$  scans forming the AFM image are split into  $M$  groups (usually  $M = 8-16$ ). For each group, the average profile is calculated and the FNS parameters are determined. The most informative parameters that show the differences in the surface structure are the mean  $\sigma$  square deviation of relief profile height relative to the basic profile (formed by the low-frequency resonant component determined from  $S(f)$ ), which is a measure of nano-relief jaggedness, and the measure  $S_{cs}(L_0^{-1})$  of surface sharpness, which is defined as the power spectrum corresponding to spike irregularities in the range of spatial frequency  $L_0^{-1} \sim 0.001-0.1 \text{ nm}^{-1}$ . In addition, the following parameters are introduced to characterize each averaged relief profile in the nanometer range:  $L_0$  and  $L_1$  – the correlation lengths of irregularities-spikes and irregularities-jumps respectively,  $H_1$  – the Hurst constant used to characterize the rate at which the memory (the information content of a dynamic variable) is lost over spatial intervals less than the correlation length ( $\Delta \ll L$ ),  $n$  – the flicker-noise parameter showing the loss of correlation links at spatial scales greater than  $L_0^{-1}$  for the sequences of irregularities-spikes in the averaged nano-relief. Examples of the FNS parameterization for highly heterogeneous surfaces, which were prepared by deposition of water-soluble supramolecular assemblies of bio-active substances on mica are demonstrated. Such layers for the AFM analysis were formed on the base of the high-molecular and low-molecular chitosan (HMCh

and LMCh correspondently), polyethylene-oxide and polypropylene-oxide copolymer (pluronic F127, PL) and porphyrin (dimegin, Dmg). The water solution of these substances is an effective medium for photooxidation of biological substrates (organic molecules, cells). The high efficiency of these processes was demonstrated in the photodynamic therapy of cancer cells and infected wounds [3]. Analysis of the AFM images of the obtained layers and the definition of the corresponding FNS parameter have demonstrated the formation of the LMCh-PL-Dmg nanoscale complexes which act as an effective photosensitizer.

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**Figure 1.** Example of AFM image parameterization with Flicker-Noise Spectroscopy. (a) – AFM image of a 13x13 mkm surface fragment of the LMCh + Plur deposited film on mica; (b) – typical averaged roughness profile  $h_4$  (the original AFM image was split into 8 equal stripes in the direction of cantilever movement; profile  $h_4$  was produced by averaging the scans of the 4<sup>th</sup> stripe, going from the top of the image); (c) – power spectrum  $S(f)$  for the low-frequency range of the roughness profile  $h_4$ ; (d) – structural functions  $\Phi^{(2)}(\Delta)$ : (1) – experimental curve; (2) – interpolated curve obtained as the sum of resonant interpolation  $\Phi_r^{(2)}(\Delta)$  (curve 3), obtained using the low frequency  $S(f)$  part (c), and chaotic interpolation  $\Phi_c^{(2)}(\Delta)$  for  $\sigma = 83.4$  nm,  $H_1 = 0.65$ ,  $L_1 = 1.5$  mcm. Other FNS parameters:  $S_{cS}(L_0^{-1}) = 320$   $(\text{nm})^2 \cdot \text{mcm}$ ,  $L_0 = 1.0$  mcm,  $n_0 = 2.0$