Neural network module for tuning an atomic force microscope in the study of photonic crystal films

E V Panfilova, A R Ibragimov, K V Mozer

1 Bauman Moscow State Technical University, 105005, Moscow, Russia

panfilova.e.v@bmstu.ru

Abstract. The article describes the use of neural network algorithms for setting the modes of investigation of photonic crystal films by tapping mode of atomic force microscopy. The photonic crystal thin films and monolayers obtained from colloidal suspensions by methods of sedimentation, centrifugation, vertical deposition, electrophoresis, and Langmuir-Blodgett are studied in this work. Study of films growth kinetics revealed that many factors were critical for reproducible deposition of the structure. To obtain high-quality images of samples, it is very important to get rid of artifacts and correctly configure the scanning parameters. To solve these problems it was proposed to use neural network algorithms. They allow to choose individual settings for each sample. We got acceptable results using a multilayer perceptron with one hidden layer.

1. Introduction

Photonic crystal colloidal films are promising for use in many fields of nanotechnology and nanoengineering [1,2]. Colloidal self-assembly has been investigated as a promising and practical approach for the fabrication of photonic nanostructures, including colloidal crystals, composite and inverse opals, and photonic glasses [3]. Unfortunately, many problems arise both in the formation of photonic crystal films and in their study. Firstly, self-assembly processes that occur during film deposition have been characterized by a large number of factors affecting the properties of the structure. Secondly, film irregularity, the presence of contaminants, the presence of electrostatic stresses, can significantly complicate samples research and distort its results. Atomic force microscopy is one of the most promising methods for studying nanoscale structures, including photonic crystals [4]. It includes a large number of different research modes, among which contact, semi-contact, and non-contact modes have proven to be reliable. All these modes are based on the analysis of viscous, elastic, and adhesive properties of the sample surface [5]. The contact scanning mode for colloidal films is destructive, therefore the studies were implemented by the amplitude modulation mode or tapping mode. A feature of this method is the difficulty of adjusting the scanning parameters and the high probability of artifacts in the image of samples. The following effects can be the reasons for the appearance of artifacts: uncontrolled transitions of the cantilever oscillation regime from the range of repulsive forces to the range of attraction forces; separation of the probe from the surface of the sample; excessive noise of the signal. It was found that when studying various bundles of the applied material, substrate, and the probe used, scanning parameters, such as the gain of the feedback circuit (gain), initial value of amplitude of a cantilever (set point), and the value of the scanning speed (rate) were required to be configured in a certain way. Therefore to obtain high-quality images, it is very important to correctly configure the scanning parameters.
To solve this problem it was proposed to use neural network algorithms. Developers of scanning probe microscopes offer similar solutions [6], but their products are universal and may not take into account the specific features of individual groups of samples. The neural network presented in this work is intended for use in studying same sized areas of similar samples of photonic crystal thin films and monolayers obtained from colloidal suspensions by self-assembly methods.

2. Methods description

Opal structures are obtained by deposition of colloidal microsphere particles. The process of deposition is simple and cheap because of self-assembly phenomenon of colloidal microsphere particles. Photonic crystal films are mostly fabricated by self-assembly methods: centrifugation, vertical deposition, gravitational sedimentation, electrophoresis and Langmuir-Blodgett methods [7]. In our laboratory we use all of them, but the first two demonstrate better reproducibility of sample properties. Therefore, in this work, they were used to obtain samples. Figure 1 shows the general schemes of these methods. We used polystyrene monodisperse latex (PS) and silicon dioxide microspheres of various diameters (200 nm...600 nm) and silicon, quartz, polycor, ceramic and lithium niobate substrates. In the process of obtaining films, we changed the parameters and modes of their deposition, such as the concentration of the colloidal suspension (1 %...10 %), the velocity of lifting the substrate from the colloidal suspension (0.1 mm/min...0.3 mm/min), the speed (1000 rpm…3000 rpm) and duration of rotation of the centrifuge.

![Figure 1.](image1.png)

The structure of the obtained films was monitored by Solver Next scanning probe microscope (NT-MDT, Russia) by the amplitude modulation mode of atomic force microscopy (AFM). In this mode, the probe “taps” on the surface of the sample, which is excited by an external piezoelectric element at the resonant frequency. With a sufficiently large amplitude, the cantilever breaks the established connection with the sample at each “tapping” period, thus, the influence of friction and capillary sticking is leveled. As variable scanning parameters, we used the gain of the feedback circuit (gain), the value of the parameter proportional to the force the probe is pressed against the sample (set point), and the scan speed (rate).

To configure these parameters, we used a neural network (NN) that took into account the characteristics of each sample. A NN is a computing model whose structure resembles the structure of neurons in the brain, with layers of several connected single processing neurons. The neurons are connected by weights, which are training over many examples. Training data is a specific number of observations, for each of which values of several variables are indicated. The NN will learn to find a match between the values of the input and known output variables. The algorithm was implemented on the basis of universal neural networks such as a multilayer perceptron (MLP) and a radial basis function network, both type of NN has 9 input neurons, one hidden layer and 3 output neurons. Figure 2 shows the scheme of NN.
Input variables corresponded to the above described parameters of the film deposition process and the materials. Output variables corresponded to the variable scanning parameters. All training data were determined directly from the results of the series of AFM research of colloidal films.

3. Results and discussion

The study of each sample was carried out in two stages. Initially, the image was obtained using the recommended standard settings of the gain, the set point and the rate. Then according to the picture observed on the screen of a personal computer, the parameters were adjusted by changing them in accordance with the improvement or deterioration of the observed picture. We attributed to applicable images in which the relative area without artifacts was at least 80 %.

Figure 3 shows the results of 600 nm PS particles diameter film scanning before and after adjusting the scanning parameters.

![AFM image of PS film on quartz: (a) standard settings: gain is 0.7, set point is 5.0, rate is 0.5, (b) adjusted settings: gain is 1.0, set point is 2.3, rate is 0.5.](image)

The training data file consisted of the research data about 200 samples. The most successful training algorithm turned out to be Back Propagation. The best NN was the MLP with 7 neurons in the hidden layer, logistic activation function in the hidden layer and linear activation function in the output one. When determining the number of neurons in the hidden layer, we took as a basis the half-sum of the input and output neurons. Due to the relatively small data set size more hidden neurons or the presence of a second hidden layer result in a higher total error. The resulting NN model allows you to take into account the influence of each factor, varying all three output parameters. For example, for 600 nm PS particles diameter film on policor substrate the following settings were defined: gain is 0.4,
set point is 0.6, rate is 0.3. However, for the same film on the ceramic substrate, they were significantly changed: gain is 1.1, set point is 2.5, rate is 0.5.

The list of input factors is adjusted now. For example, it can be supplemented with a variable responsible for the type of probe. When using probes such as NSG01, the atomic force microscope significantly distorted the spherical shape of particles, while producing a good quality image. When replaced with a probe of the NSG10 type, without detailed adjustment, the shape of the particles displayed as ellipses. And finally, when using a probe of the NSG10 type, with NN adjustment of the scanning parameters, the particles shape displayed as spheres and the image became closer to reality (Figure 4).

![AFM images of silica 300 nm particles diameter film on a quartz substrate](image)

Figure 4. AFM images of silica 300 nm particles diameter film on a quartz substrate (a) with a probe type NSG01 and standard scanning parameters (b) with a probe type NSG10 and standard scanning parameters (c) with a probe type NSG10 and configured scanning parameters.

To solve the curse of dimensionality we are currently working on expanding the training data set, data pre-processing and editing the neural networks.

4. Conclusion
The essence of the research conducted by the authors is to refine the technology for producing photonic crystal films. A feature of the statistics containing sample information is the presence of faulty samples, which are characterized by a variety of structural defects. Practice has shown that the use of a NN model significantly reduces the time spent on research. As a result it became possible to obtain high-quality images and reliable results.

References
[1] Gorelik V S & Friman A V 2013 Inorganic Materials 49(6) 577-80
[2] Baburin A S, Ivanov A I, Trofimov I V, Dobronosova A A, Melentiev P N, Balykin V I, ... & Rodionov I A 2018 In Nanophot VII 10672:106724D
[3] Gorelik V S, Kudryavtseva A D, Tareeva M V & Tcherniega N V 2014 Inorganic Materials 50(12) 1217-21
[4] Panfilova E V, Syritskii A B & Ibragimov A R 2019 In IOP Conf Series: Materials Science and Engineering Vol 699 No 1 (IOP Publishing) p 012034
[5] Pozdnyakova E D, Maslennikova E V, Komshin A S & Orlova S R 2019 In IOP Conf Series: Materials Science and Engineering Vol 489 No 1 (IOP Publishing) p 012008
[6] Take a shortcut to reliable AFM results with intelligent SCANT™ software Available at: https://www.ntmdt-si.ru/products/features/intelligent-scant-software (accessed 25 March 2020)
[7] Panfilova E V & Dyubanov V A 2019 In International Russian Automation Conf (Springer, Cham) pp 1044-52