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# Automation of Mathematical Modeling of Physical and Technological Processes in the Electronic Devices Manufacture

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**Abstract**—The variant of automation of the mathematical modeling process for forecasting the technological process parameters of manufacturing nano and microelectromechanical systems is proposed in the paper. For this task realization, a number of defects were identified and the causes of their occurrence were analyzed, as well as physical and technological transformations that occur in the substrates during technological processes. The software for automation of technological parameters forecasting process is developed and described.

**Keywords**—production, component, nanoelectromechanical systems, microelectromechanical systems, defect, silicon substrate, software.

## I. INTRODUCTION

One of the promising directions of research in electronic devices production technology is the development of nano and microelectromechanical systems (NEMS and MEMS). A special area of these systems use are telecommunications devices.

But there are contradictions between the need of further improve the quality of NEMS and MEMS components, the use of promising variants for the implementation of their production technological processes and operations and the limited known approaches to ensuring their quality and testing.

The work is aimed at solving the current scientific and applied problem of improving the quality of functional components of micro-optoelectronic systems by developing technological support for their individual production stages based on the study of physical and technological parameters and testing methods for micro-optical switches substrates.

As research object the functional components (FC) for optical signal switches of microoptoelectromechanical systems (MOEMS) were selected.

FC of MOEMS switches are usually silicon substrates with a thin film of metallization, or without it, which provides a high light beam reflectivity for redirecting it in the optical fibers [1-5]. One of the important characteristics of MOEMS FC is the defectiveness.

## II. ANALYSIS OF FC SUBSTRATES DEFECTIVENESS

Assume that the FC of MOEMS-switch is already fabricated and its parameters correspond to the specified in technical documentation. However, it should be noted that the practice of MOEMS switches operation indicates that the development of defects occurring during its manufacture (operation) is one of the main causes of failures and incorrect operation of the whole device.

Currently, there are a large number of methods and tools to detect manufacturing defects, but the capabilities of these methods are limited [2, 5-10]. The testing and checkout operations included in the modern technological processes (TP) structure cannot give a full guarantee of the defects absence in the production of such components. In this regard, there is an urgent problem of developing a model for predicting MOEMS FC defects, taking into account the physical and technological features of their production TP [11].

So the purpose of this research is to develop a method for predicting production defects for substrates of MOEMS FC on the basis of physical and technological models of TP of their manufacture.

If the substrate of the FC for MOEMS switch is considered directly at the stage of its fabrication TP, then the substrate structure can be divided into four main layers, in

which defects can be displaced. Such structures are characterized by the depth of the disturbed layer, roughness and various kinds of pollutions [5, 10].

Layer 1 is the outer relief, which characterized by chaotically placed protrusions, cracks and splinters. Layer 2 is disturbed layer that has separate punctures and microcracks, which tend to spread to the depth of other layers and grow. Layer 3 is deformed and characterized by accumulation of dislocations, continuation of microcracks and zones located around them that are the centers of mechanical stresses. And layer 4 is conditionally intact structure of the FC substrate.

The most important stage at which the manufacturing defects occur in the substrates is the first stage of the optical switch production TP. At this stage, it is possible to predict defects in the structures of substrates, their layers and sublayers, that allows at the next stages to build a TP which would provide for the opportunity minimize the variety, number and size of defects.

Defectiveness of FC at the production stage is laid on the basis of defects of three groups: 1) defects of a functional component substrate  $\Omega_s$ ; 2) defective spraying of thin films  $\Omega_c$ ; 3) defects of technological combination of structures  $\Omega_d$ .

In this view, it is possible to symbolize a generalized mathematical description of the MOEMS FC production defects set in the form (1):

$$\Omega_{md} = \Omega_s + \Omega_c + \Omega_d \quad (1)$$

If assume that a significant part of production defects occurs in particular because of the defect of the substrate plates or sublayers of MOEMS FC substrates, it was decided to consider the defects of MOEMS FC as the main and primary source of defects in the whole MOEMS-device.

The problem arises that at the stage of raw materials production, it seems unlikely to be able to track defects in structures and dependence of physical and technological parameters that directly affect the quality and compliance of initial characteristics to the required one. A special limitation on them is imposed by the kinetics of degradation processes in materials.

Based on the analysis of modern literature, physical and technological models of processes that take place in the manufacturing of MOEMS FC are developed. From the conducted research, we concluded that diffusion, corrosion and evaporation of materials are the main sources of defective structures.

The layers diffusion of the MOEMS FC substrate is expressed using Fick's second law: for one-dimensional diffusion (2) or diffusion through the film (3):

$$\frac{dV}{dt} = D \frac{d^2V}{dx^2}, \quad (2)$$

$$\frac{dV}{dt} = D \frac{\Delta V}{y}, \quad (3)$$

where  $D$  is the diffusion coefficient;  $V$  is concentration of the substance (component);  $y$  is the thickness of the FC substrate.

Thermal oxidation of silicon occurs due to the diffusion of components oxidation ( $O_2, H_2O$ ) through the oxide to the phase boundary  $Si-SiO_2$ , where the oxidation reaction takes place. The kinetics of the oxidation process is described by a model developed by Dilom and Gurov [5, 11-13]. Oxidation is a nonequilibrium process, the driving force of which is the deviation of oxygen concentration from equilibrium. The oxidant particles flow through the oxide for any point of the oxide  $V$ -layer is described by law (4, 5). Oxidation during the production of MOEMS FC substrates is a special case of diffusion:

$$\frac{dV}{dt} = V_0 e^{-\frac{E}{RT}}, \quad (4)$$

$$\frac{dV}{dt} = \frac{k_d k_p}{k_d + k_p h_0} V_0, \quad (5)$$

where  $E$  is the activation energy of the molecules involved in the reaction;  $k_p$  is chemical reaction rate constant;  $V_0$  is the reagent (e.g. oxygen) concentration on the outer surface at the boundary with the gas phase;  $h_0$  is coating thickness;  $k_d$  is diffusion coefficient in the process of corrosion.

If the substrate fabrication TP involves the use of electrical corrosion, the layer of corroded material can be expressed as (6) [5]:

$$V_E = \gamma_{(-)} Q, \quad (6)$$

where  $\gamma_{(-)}$  is erosion coefficient;  $Q$  is electric current.

The wear depth for the substrate layer of MOEMS FC can be determined as (7):

$$h = \frac{\gamma_{(-)} Q}{\rho S_0} = \frac{\gamma_{(-)}}{\rho S_0} \int_0^t idt = \frac{\gamma_{(-)}}{\rho S_0} I_{CP} t, \quad (7)$$

where  $\rho$  is specific density;  $S_0$  is the area of the worn surface part;  $I_{CP}$  is average value of current strength;  $t$  is the time of current action.

If in the TP of the FC substrate production there is electro-chemical corrosion, (8) express the amount of current-transferred substance and (9) express the wear depth for the FC substrate layer:

$$V = \eta Q = \eta \int_0^t idt = \eta I_{CP} t, \quad (8)$$

$$h = \frac{\eta}{\rho S_0} I_{CP} t. \quad (9)$$

In TP there are not uncommon cases of violation of the dependence between the rate of solvents evaporation and their boiling points due to the fact that the liquid molecules are conjugated at normal temperature. This causes a decrease of the substance pressure for a given temperature range [5].

First of all, it should be noted that the rate of solvent evaporation from the film is not the main physical characteristic, it is only a technological parameter that reflects the influence of a number of basic physical properties such as pressure, evaporation and solvent vapor density. To obtain practical data on the evaporation rate it should be measured under certain conditions: temperature, relative humidity.

Increasing the evaporator concentration reduces the rate of solvent evaporation and thus promotes the formation of a dense, so-called active (selective) layer on the FC surface. Regulation of FC porosity can be carried out by changing the concentration and conditions of solutions evaporation, as well as the introduction of special substances in this process [2, 5, 10-14].

The evaporation rate of the substrate material or sublayers of MOEMS FC can be expressed as (10):

$$V' = \frac{k_p}{\sqrt{2\pi R}} \cdot p \sqrt{\frac{M}{T}}, \quad (10)$$

where  $M$  is the molecular weight of the evaporated material;  $p$  is pressure;  $R$  is gas constant;  $T$  is absolute temperature.

An important indicator of each physical and technological process is speed. Diffusion and chemical reactions can serve as a basis for determining the rate and, therefore, the description of the kinetics of the processes under consideration. Physics makes it possible to explain the kinetics of the medium thermodynamic parameters on the basis of the behavior of the particles set of which this medium consists.

The microscopic state of a particles set is completely given by the canonical variables ( $X$ ). From the macroscopic point of view, the state of matter is determined by a rather limited number of parameters sufficient for the macroscopic characteristics of the environment. Macroscopic parameters, including the volume of the substance that reacted, are functions of the canonical variables:  $V_k(X)$ , and  $k = 1, 2, \dots, n$ , where  $n \ll N$ .

Thus, the macroscopic system is represented by setting the density of variables probability  $\omega(X, t)$ . This phase probability density is called the phase probability distribution, or simply the phase distribution.

Knowing  $\omega(X, t)$ , the statistical mean value you can be calculates using (11), as well as the root-mean-square deviation, which show itself as a fluctuation of the disturbed layers observation area (12):

$$V = \int V(X) \omega(X, t) dX, \quad (11)$$

$$\Delta V = \sqrt{(V - \bar{V})^2}. \quad (12)$$

Using the basic provisions of Gibbs's theory [5, 12], it is possible to calculate the average levels and fluctuations of any physical values that are functions of coordinates, if the dependence of the these values average levels on external constant forces acting on them is known. It is not possible to estimate these forces for specific objects. It is possible to conclude the hierarchical nature of fluctuations given by different order of relaxation time for microscopic and macroscopic parameters.

The occurrence of defects in any structure (regardless of the object physical state or the impact nature) is a random variable whose behavior can be described using fluctuation theories. That is, it is a random deviation of any value from the random variable average level that characterizes a system with a large number of chaotically interacting particles.

To display fluctuations, taking into account the impossibility of full use of the statistical physics results caused by lack of necessary quantitative information about the Hamiltonian set of interacting particles, it is possible to use methods of statistical analysis of observations results to determine and predict defects in the FC substrates for MOEMS switches.

### III. SOFTWARE DEVELOPMENT

Based on obtaining mathematical models of physical and technological parameters for TP of MOEMS FC substrates production, the next step is to calculate data sets to select the optimal variant of TP for different parameters, such as minimizing defects in the structures of substrates.

In order to reduce the complexity of solving the data analysis problem, it is proposed to introduce processes visualization in the TP of the substrates production for MOEMS FC, using the developed software, the interface of which is shown in Fig.1.

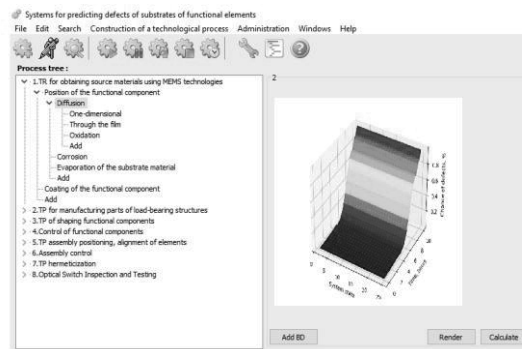


Fig. 1. The interface of the developed software

With the developed software help, it is possible to reduce labor costs of solving the problem of forecasting production defects in the substrates of MOEMS FC, to increase the accuracy and reliability of the information obtained in the development of manufacturing TP of such objects as a whole.

Using a number of initial parameters for MOEMS FC substrates, focusing on the requirements of their defects

minimizing and using data from previous experimental studies of a particular perform variant, the developer can make decision about the optimal TP use and its parameters.

At this stage of research, the base of TP input parameters was formed for the manufacture of MOEMS FC substrates made of silicon.

The software makes it possible to store material parameters, values of constant coefficients and variables, equipment parameters.

The program has the choice functions of standard equipment for the enterprise, the ability to adjust the parameters of the manufacturing TP, such tabs can be up to 50.

New projects can be created, saved and the parameters can be changed, due to adjustments, there is the possibility of changing each parameter separately or adjusting the parameters of the manufacturing TP to predict defectiveness and choose the equipment for production. The operator himself decides on the use of the existing TP, or the development of a new one, on the obtained technical conditions basis.

In this case, the basis for making such a decision can be a physical and technological model for predicting the parameters of defect formation in the substrates of MOEMS FC, proposed in this research.

According to the available theoretical and experimental data, the person who makes the final decision on the TP variant for the product manufacture can also analyze the behavior of the system for the time interval that goes beyond the experimental or calculated results, but allows analyze the product condition at its subsequent operation stage.

#### IV. CONCLUSIONS

On the basis of the conducted complex research of possible mechanisms of failures occurrence types of defects were systematized and the reasons of their occurrence and also the physical and technological transformations taking place in substrates during technological processes of their manufacturing were analyzed.

As a result, variables were selected for the physical and technological base formation of the defect prediction mathematical model.

Specified physicochemical processes can serve as a basis for determining the speed and, consequently, the description of the kinetics of the processes under consideration.

To reduce labor costs and ease of the obtained information analysis, according to the proposed mathematical models, the numbering of each TP is performed to embody the possibility of graphical visualization the simulation results using the developed software.

The decision maker, i.e. the technologist, can analyze the behavior of the technological system, i.e. to predict the technological process parameters, which can cause

production defects of the functional components substrates, as well as adjust the technological processes of their manufacture.

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