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Defect Engineering: Application in Automation System Components Production Technological Processes

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Abstract

Defect engineering is a field of scientific development that finds application in various fields. At the same time, the goals of using its approaches may differ radically. This article provides an overview of common applications of this concept. The authors propose to use the capabilities of defect engineering in the production of MEMS and MOEMS to predict failures, as well as to make possible changes and adjustments to the technological process.

Key words: Defect engineering, Automation system, MEMS, MOEMS, Silicon structures

Introduction

At present, more than twenty technological methods and directions for manufacturing MEMS and MOEMS products based on silicon structures are known [1]-[8].

Silicon is the main semiconductor material that has become the most widely used due to the high electrophysical characteristics of devices based on it [9].

Silicon is the basis for substrates of electronic products, functional components of MEMS and MOEMS. MEMS and MOEMS are usually the main components of sensors and actuators for automation systems.

Control and testing operations included in the structure of modern technological processes cannot provide a full guarantee of the absence of defects in the production of this components type and their behavior over time, taking into account the operating conditions [9]-[12].

Most of the defects arise precisely because of defects and (or) the presence of impurities in the raw materials of substrates or substrates sublayers of MOEMS functional components and during the technological process of their manufacture [12]-[16].

Therefore, it was decided to consider the defects of the substrates of the layers and sublayers of the MOEMS functional component, as the main and primary source of the MOEMS component defect as a whole.

To do this, the work provides a brief analysis of related works.

Related works

Defect engineering is a rather interesting direction in the development of science, which is largely based on the properties of specific materials. Many authors suggest using it for various purposes. Let's look at at least some of them.

At first note, that defect engineering is regarded as one of the efficient approaches to modulating the physical and chemical properties of materials for energy-related applications [17].

Kimoto, T., & Watanabe in their review [18] introduce the advantages and present status of SiC devices and then defect engineering in SiC power devices is presented.

In [19] scientists write, that recent studies have highlighted the potential of defect engineering for boosting the light-harvesting, charge separation, and adsorption characteristics of

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semiconductor photocatalysts in reductive processes such as water splitting and CO2 reduction. And they explore the potential of defect engineering to similarly enhance photocatalytic N2 fixation in this paper.

Authors [20] note, that defect engineering is an effective strategy to enhance the performance of photocatalysts and photoelectrodes. But the widely reported benefits of defects in the photocatalytic system may not necessarily cancel out the negative spillover effect of charge recombination. To inspire innovative defect engineering for further improving the STH conversion efficiency, they provide the perspectives from their point of view.

Shi, Z. and co-authors [21] write that defect engineering allows for the effective exposure of active sites and optimization of electronic structure. It has emerged expeditiously as an essential strategy to enhance polysulfide modulation, and hence expedite Li–S chemistry.

In their work [22] Yan, X., Zhuang, L., Zhu, Z., & Yao, X. note, that defect engineering provides a feasible and efficient approach to improve the intrinsic activities and increase the number of active sites in electrocatalysts. Here they observe recent investigations on defect engineering of a wide range of electrocatalysts. And different defect creation strategies are desribed.

Researchers in [23] systematically summarized recent advances regarding defect engineering in electrode materials for rechargeable batteries. They say, that the defects can not only effectively promote ion diffusion and charge transfer but also provide more storage/adsorption/active sites for guest ions and intermediate species, thus improving the performance of batteries.

In [24] it is noted that increasing attention is being devoted to modulating the surface/interface electronic structure of electrocatalysts and optimizing the adsorption energy of intermediate species by defect engineering to enhance their catalytic performance.

Article [25] presents leverage a defect engineering strategy to develop a simple yet efficient redox nanozyme by constructing enzyme-mimicking active centers and investigated its formation and catalysis mechanism thoroughly.

In [26] the challenges and opportunities of silanol defect engineering in tuning the properties of zeolites to meet the requirements for specific applications are presented.

Zhu, J., & Mu, S. [27] draw our attention to the fact that the inevitable defect sites in architectures greatly affect physicochemical properties of carbon nanomaterials, thus defect engineering has recently become a vital research orientation of carbon-based electrocatalysts.

Thus, we see that defect engineering is being widely used. Further in the article we will consider defect formation as the basis for defect engineering in MEMS and MOEMS.

Defect engineering in the production of automation system components

The main problem arises in the fact that at the stage of raw materials production, it is unlikely that it will be possible to track the defectiveness of structures and the dependence of physical and technological parameters that directly affect the quality and compliance of the initial characteristics of MOEMS components, a special limitation is imposed by the factor of kinetics of degradation processes in materials during and operating conditions of the product.

However, the main reason for the limitation of the resource characteristics of the functional components of MOEMS are manufacturing defects that develop over time during the operation of the MEMS.

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In this regard, there is an "open" scientific and practical task of predicting and managing the defect formation of layers and sublayers of MOEMS functional components, which is solved by controlling operating parameters, the development of defects embedded during production, which in turn do not always worsen the parameters of microsystems [28]-[31], but on the contrary, they can improve over time, even with the right approaches and certain operating conditions [20]-[33]. Technological defects prediction and control in the manufacture of silicon structures is a rather promising direction in technological processes development for the manufacture of MEMS and MOEMS.

The control possibility became the basis for the development of a promising scientific direction in the production technologies of semiconductors, materials and devices of electronic equipment - defect engineering [33], [34], which is based on the defect formation processes prediction and control.

Microelectromechanical systems are formed by combining mechanical elements, sensors, and electronics on a common silicon substrate using micro- and nanofabrication technologies [3]. The methods used in the manufacturing processes of MEMS can be attributed to one of the following classes:

– three-dimensional processing with a high aspect ratio;
- surface treatment;
– mixed technology using the first two;
– hybrid technology with assembly of mechanical and electronic parts at the level of atomic-molecular splicing;
– others (fiber, micromechanical processing, bulk polymer);
– multilayer film structures [3].

We can distinguish three types of the most common defects formed on silicon:

- surface: formed due to various types of mechanical processing, such as laser cutting, grinding, polishing, the main method of elimination is the etching of the surface layer of the silicon substrate;
- angular: due to anisotropic etching, which causes the seeds of cracks - the main method of elimination is the use of isotropic etching, with the help of which the edges of the substrate are rounded, which practically eliminates (minimizes) corner defects;
- volumetric: arise due to heat treatment and lead to the emergence of internal stresses, which, in combination with edge, surface and volume imperfections of the structure, can lead to the concentration of stresses and the subsequent splitting of the substrate along the plane.

If we consider the defect formation of such components through the prism of physico-chemical transformations and reactions, it is possible to single out several main mechanisms of the occurrence of production defects of MOEMS functional components, the development of which is associated with the transformation of the micro- and macrostructure of the starting materials that occur during the production and operation of MOEMS functional components .

1. Diffusion of layers and sublayers of MOEMS functional components can be represented using Fick's second law: for one-dimensional diffusion (1) or diffusion through a film (2):

$$\frac{dV}{dt} = D\frac{d^2V}{dx^2}, \quad (1)$$

$$\frac{dV}{dt} = D\frac{\Delta V}{y}, \qquad (2)$$

where $D -$ diffusion coefficient;
$V -$ concentration of the diffusion component;
$y -$ film thickness.

2. Chemical corrosion of layers and sublayers of MOEMS functional components can be represented in the form (3), and in the presence of protective films (4):

$$\frac{dV}{dt} = V_0 e^{-\frac{E}{RT}}, \qquad (3)$$

$$\frac{dV}{dt} = \frac{k_d k_p}{k_d + k_p h_0} V_0, \qquad (4)$$

where E – activation energy of molecules participating in the reaction;
$k_p -$ chemical reaction rate constant;
$V_0 -$ reagent concentration on the outer surface at the boundary with the gas phase;
$h_0 -$ coating thickness;
$k_d -$ diffusion coefficient during corrosion.

3. Electrical corrosion can be expressed as the amount of material worn (5) and the depth of wear (6):

$$V_E = \gamma_{(-)} Q, \qquad (5)$$

$$h = \frac{\gamma_{(-)}}{\rho}\frac{Q}{s_0} = \frac{\gamma_{(-)}}{\rho s_0}\int_0^t i\,dt = \frac{\gamma_{(-)}}{\rho s_0} I_{CP} t. \qquad (6)$$

where $\gamma_{(-)} -$ erosion coefficient;
$Q -$ amount of electricity;
ρ – specific weight;
$s_0 -$ the area of the surfaceworn part;
$I_{CP} -$ the average value of the current;
$t -$ current action time.

4. Evaporation of the material (speed of the process) can be expressed as (7):

$$V' = \frac{k_p}{\sqrt{2\pi R}} \Big/ p\sqrt{\frac{M}{T}}, \qquad (7)$$

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where $M-$ the molecular weight of the material being vaporized;

$p-$ pressure;

$R-$ gas constant;

$T-$ absolute temperature [35]-[41].

On the basis of the given differential equations of the physical and technological processes of defect formation, during the production of MEMS and MOEMS functional components, it is necessary to develop a mathematical model that would make it possible to predict the occurrence of certain defects and explain the degree of their influence on the parameters and probability of component failures.

Thus, during the implementation of technological processes, the defects that have arisen further develop in accordance with the objective patterns of changes in the micro- and macrostructure of the materials that make up the elements and devices of MEMS and MOEMS.

Considering various materials and processes of production defects development, analyzing and generalizing the process mechanism, it is possible to conclude that there are three main types of the above changes: diffusion of components, corrosion (chemical, electrical, electrochemical) and evaporation.

Analysis of the capabilities of defect detection tools and data on the causes of MEMS and MOEMS failures shows that a significant part of defects may not be detected. Therefore, it is necessary pay attention to the prediction of parametric failures in the process of production tests and maintenance, as a result, they make decisions about the technical condition and technologies of the production of devices [33]-[37].

Modern prediction methods are based on functional analysis, theory of series, theory of extrapolation and interpolation, theory of probabilities and mathematical statistics, theory of random functions and random processes, correlation and spectral analysis, and theory of pattern recognition [38]-[41].

When displaying the time dependence of parameters, linear and quadratic models are used [40]. Work [39] shows that increasing the order of the model above the second does not lead to a significant increase in the accuracy of the forecast, but significantly complicates the calculation procedures.

Within the framework of prediction using the recognition theory [39], it is used to identify areas in n-dimensional space that correspond to certain degrees of efficiency of MEMS and MOEMS, and to determine the limit of the permissible level of efficiency.

Much attention is paid to the prediction quality [30]-[43], i.e., a set of such prediction characteristics, which together make it effective and useful in management, ensure obtaining a reliable description of the object for a certain perspective and the possibility of reliable use of prediction results for the control procedure.

Prediction results are always related to certain management procedures, and prediction quality can be evaluated from the point of view of the needs of control itself, its sensitivity to possible prediction errors.

The main directions for a justified determination of prediction quality should be sought in the assessment of uncertainty, which carries one or another description of the object.

Prediction quality, first of all, depends on the completeness and quality of the description of the object itself, the prediction procedure carries a specific component - "time" and therefore descriptive topological characteristics are supplemented by dynamic ones.

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VOLUME-3, ISSUE-3

The assessment of prediction results must be carried out based on the accounting of internal processes and external influences on MEMS. Obtaining predictive results under the influence of variable external factors increases prediction effectiveness, makes it an effective tool for control the production of MEMS and MOEMS.

Currently existing verification methods in the vast majority operate only with statistical procedures [37], [39], which are reduced to the estimation of confidence intervals for the considered results.

At the same time, two types of errors are assumed: errors that are determined by the information or description of the object, and errors directly in the prediction method.

Errors of the first kind are quite easily formalized and can be calculated by statistical methods.

The analysis of the source information involves the identification of a set of statistical indicators, including the determination of the type of distribution. Many statistical calculations and criteria are valid only for the normal law of distribution, otherwise the estimates are ineffective.

The methods of improving efficiency are: detection of anomalous observations, selection of non-periodic components, determination of jump-like changes to the trend of the investigated process, determination of variations of the investigated process, determination of variations of the investigated indicator, its periodicity [33].

When making prediction calculations, you should always evaluate and find the optimal match between the information and the method used to obtain the presiction.

There is a need to develop methods for improving the prediction quality, based on the description of objects and operating with some new concepts for prediction: stability, inertia, connectivity, complexity, appearance and functional integrity of the object, accuracy and completeness of the description, decision-making risk.

Thus, the concept of inertia characterizes the object's resistance to changes in its own trajectory over time under the influence of the external environment; sustainability implies a certain priority of development directions in time, the choice of any certain trajectories by the object, both in the space of the considered indicators and in time.

For adequate assessment, forecasting, prediction and management of MEMS and MOEMS defects, it is necessary to thoroughly study the physico-chemical processes underlying their production, the various possible conditions of their operation, and on the basis of the obtained information, after careful analysis, develop mathematical models that would give representation and explanation of the occurrence and development of production defects over time.

Conclusion

This article discusses defect engineering and its areas of application. To reduce the number of defects in the production of MEMS and MOEMS, we propose to use defect engineering approaches. The article analyzes the main defects that occur on silicon. Thus, modeling and mapping the processes of the development of production defects for predicting parametric failures, changing and correcting the technological processes of MEMS and MOEMS production is an actual scientific and practical task that can be tried to be solved on the basis of defect engineering.

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VOLUME-3, ISSUE-3

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