Modelling nanoscale objects in order to conduct an empirical research into their properties as part of an engineering system designed

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Abstract. We have conducted a research into the major, in terms of their future application, properties of nanoscale objects, based on modelling these objects as free-standing physical elements beyond the structure of an engineering system designed for their integration as well as a part of a system that operates under the influence of the external environment. For the empirical research suggested within the scope of this work, we have chosen a nanoscale electronic element intended to be used while designing information processing systems with the parallel architecture – a memristor. The target function of the research was to provide the maximum fault-tolerance index of a memristor-based system when affected by all possible impacts of the internal destabilizing factors and external environment. The research results have enabled us to receive and classify all the factors predetermining the fault-tolerance index of the hardware implementation of a computing system based on the nanoscale electronic element base.

1. Introduction

Designing up-to-date technical objects of various applications suggests obtaining a full set of knowledge about the properties of systems designed and the dynamics of their change in the future operation when affected by the external environment. This is the only way to provide the main indices of operation reliability and quality for any facility. At the moment, computer modelling is considered to be the main tool for solving this problem [1].

From the viewpoint of the system theory and system analysis, individual physical properties of elements and their interrelationship appear to be important constituents of the system’s quantitative and qualitative characteristics. In the systems, which use the components whose sizes lie within the nanoscale range, the goal of empirical analysis of their properties is much more difficult than in the macroscopic world.

In particular, an analytical review of the research in the field of modelling, digital design and practical analysis of nanoscale objects [2-4] did not reveal any instances of efficient applications of the methodologies which determine overall influence of nanoscale elements’ properties on the system they comprise in the field of development of trainable information processing systems with a parallel architecture.
The proposed herein way of enhancing the study of nanoscale objects by applying extra research on a system when affected by external and internal destabilizing factors helps achieve maximum operation quality indices for any engineering system including the one based on nanoscale elements.

The key advantage of such an approach is that it makes it possible to develop efficient methods of engineering solution of the problems caused by imperfection of the existing nanoscale materials and influences of the external environment before new and non-negative qualities arise. It makes the research topic and its prime objective relevant and important for the development of nanoscale engineering.

Thus, the prime objective of this work is an empirical research on the major, in terms of their future application, properties of objects in the nanoscale range, based on modelling such objects as free-standing physical elements beyond the structure of a future system as well as constituents of a system running under the influence.

2. Methods

Within the scope of this research, we have taken a nanoscale element intended to be used when designing information processing systems with the parallel architecture – a memristor (Figures 1 and 2). The theory of reliability of memristors as elements of electric circuits still lacks an intensive and detailed study [5].

![Figure 1](image1)

**Figure 1.** Two terminal structures based on a memristor. The resistance of a switching medium determines the state of the device.

![Figure 2](image2)

**Figure 2.** The type of resistance switching in memristor.

A memristor [6] is a passive element in microelectronics; its resistance depends on a charge that has passed through it. When a voltage in the circuit is turned off, a memristor does not change its state and it registers the last resistance value. The following equations describe the voltage-current characteristic (1) and resistance (2) and others important properties of a memristor (3), (4):

\[
v(t) = \frac{R_{on} \cdot w(t)}{D} + R_{off} \left(1 - \frac{w(t)}{D}\right) \cdot I(t)
\]

\[R = \rho \cdot \frac{d}{S}
\]

\[w(t) = \mu \frac{R_{on}}{D} \cdot I(t)
\]

\[M(q) = R_{off} \left(1 - \frac{\mu \cdot R_{on}}{D^2} \cdot q(t)\right)
\]
where \(v(t)\) – voltage, \(I(t)\) – current, \(w(t)\) – thickness of memristor’s doped region, \(D\) – total thickness of a memristor, \(Ron\) – minimum resistance value of a memristor, \(Roff\) – maximum resistance value of a memristor, \(R\) – resistance, \(\rho\) – resistivity of the material, \(d\) – thickness of the active layer, \(S\) – contact surface, \(M(q)\) – ionic mobility.

The research, conducted earlier [7-9], shows that as a rule the reliability indices of memristors are exposed to a negative impact caused by the decomposition effect of the resistance values when reading its logical state. To read the data stored in a memristor in the form of the value of its resistance, we apply a voltage able to make the current flow through the memristor, but not able to impact considerably the resistance in order to re-write the data. However, an extremely small variation of the resistance takes place anyway due to the physical properties of the material – hysteresis (Figure 3), and the effect itself has a cumulative nature and after a number of read operations there is a possibility of losing the data stored in the memristor.

\[
\begin{align*}
M(q) &= \int_{-\infty}^{\infty} M(x) \, dx \\
I(x) &= \frac{d}{dx} M(x) \\
V(x) &= \int_{-\infty}^{x} I(t) \, dt \\
WVR &= \text{write voltage region} \\
RVR &= \text{read voltage region} \\
DVR &= \text{diode voltage region}
\end{align*}
\]

Figure 3. The typical I-V characteristic of a memristor with different voltage regions: WVR – write voltage region, RVR – read voltage region, DVR – diode voltage region.

It is obvious that the dependency described above is not the only reason for a possible data loss. To reveal all possible external and internal destabilizing impacts on each element individually and as a part of the system let us conduct an empirical research on it according to the following plan:

- modelling an individual element of the system;
- choosing the experiment target function;
- modelling the dynamic processes in the element under the influence of internal and external destabilizing impacts;
- identifying the factors impacting the target function;
- integrating element’s model into system’s model;
- modelling the dynamic processes in the system under the influence of internal and external destabilizing impacts;
- identifying the factors impacting the target function.

3. Results and Discussion

As for an environment for the experiment, we chose a tool for modelling and simulating physical objects – the «Simscape» application software package that is controlled by the «Matlab». We synthesized simscape memristor models (Figure 4) [10]. The target function is used for evaluating the acceptability of influence of each impact on the element and the system, appearing at the stage of building and operation of the engineering system designed.

At the first stage, we studied the variations in the weighing coefficients of the synapses connected with the physical properties of these objects. Such properties included a variation of resistance of the
memristor (2) used as a synapse related to degradation of the nanoscale material caused by the repeated current flow going through it due to frequent reference to the data stored in the element.

The experiment results, presented in table 1, demonstrate that the fault-tolerance index of each individual memristor outside the system depends on the physical properties of the material and the accuracy degree of the recorded information which can be caused by distortions of information upon its transfer or storage.

![Figure 4. A memristor based on equations (3), (4) and (5): the model in Simscape/Matlab and electric parameters (v(t), i(t) and M(q)) of the electrical circuit.](image)

At the next stage, we synthesized a model of the architecture of an artificial neural network which serves the approximation function of a differential equation containing memristors in the capacity of synaptic links among neurons (Figure 5). We also simulated a training process of the system in question carried out at the stage of creating suchlike engineering systems. Training is a process of adjusting the weighing coefficients of synaptic links and threshold shifts of each neuron. After each iteration of the training process, we analyzed the variation of the target function. Then programmatically, we simulated the operation process for the trained system by submitting the input information (both with and without information distortion) for its processing. Like in the first instance, we considered the degree of involvement of these variations in the operation process of the entire system, expressed via the target function, as the experiment results.
At the end of the second stage of simulating experiments, we have achieved the results reflecting the picture of the dynamic variations (Table 1). These results prove that all the simulated processes impact the target function.

**Table 1.** The factors influencing the fault tolerance of the modelled system.

| Factors                        | The period of influence (iterations) | The maximal change of resistance of the memristor (%) | The change of accuracy of system functioning (SSE criterion) |
|-------------------------------|-------------------------------------|-------------------------------------------------------|-----------------------------------------------------------|
| The degradation of the memristor | 1 000 000 iterations of reading information | 17                                                   | 0.107                                                    |
| The training process          | 50 000 iterations of tuning of weight coefficients | 8.9                                                  | 0.008                                                    |
| The distortion of input data  | 30 000 the distorted values of input datas | 47                                                   | 0.11                                                     |

All presented factors in the table can be divided into internal and external. The internal factors are those that are specified by the system’s structure: a qualitative and quantitative set of elements as well as interrelation between them. The external factors are those that are related to the teaching process (insufficient generalizing performance) and destabilizing factors (distortion of input data). Various distortions of an information signal, deliberate physical impacts on the system and others can serve as such factors. For the purpose of making a complete classification, all these factors can also be separated into the ones which have informational (caused when some informational processes or a person interfere in the system’s information status) nature and those with material origins (physical properties of the material used for making the system’s elements).

4. Conclusion
The major conclusion, which has to be drawn on the basis of the proposed research, is that despite the reason causing distortion or full failure of a system’s element, it results in a variation of the parameter’s number value of this element. For this reason, it is advisable to consider only the variation
value and not to pay attention to the factor that has caused this variation. This approach will make it possible to develop multi-purpose methods for providing the specified reliability indexes by engineering facilities. Such methods will introduce a common practice of engineering information processing facilities and make it possible to reduce the existing dependence on the development of new nanoscale materials designed to make electronic elements with the best reliability performance.

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