Predictor of reliability indicators for nanoelectronic heterostructure devices with transverse current transfer under conditions of limited experimental information based on Bayesian inversion

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Abstract. Predictor of the reliability indicators of resonant tunneling diodes with a generalization of the methodology for nanoelectronic heterostructure devices with quantum confinement and transverse current transfer has been developed. The advantage of the developed software is the possibility of interactive input of additional experimental information for further calculation of point and interval estimates of the reliability indicators of semiconductor devices using Bayesian inversion, which allows predicting these indicators under conditions of limited experimental information.

1. Introduction
The rapid development of micro- and nanoelectronics has led to the creation of promising devices, in which semiconductor heterostructures act as a low-dimensional channel [1-7]. Due to the small size of the channel of such devices, difficulties arise in ensuring their reliability due to the significant influence of degradation processes during their operation and even during their manufacture. Modern computational models make it possible to predict the reliability indicators of such devices at the stage of their design [8-11]. The validation of computational models is a mandatory procedure, which requires the availability of appropriate experimental information obtained during the tests [12]. In accordance with the established standards and regulatory documents [13-15] for the statistical evaluation of reliability indicators of the required level of confidence and accuracy, a regulated number of experimental samples is required (for example, to obtain point and interval estimates of reliability indicators with a confidence level of 90% and with a relative error of 5%, at least 500 objects are required for the accelerated test plan [NUN] when the exponential law of reliability is valid [13]). Due to the high cost and complexity of the manufacturing process, it is not always possible to provide the required number of test objects.

Thus, the actual task is to develop a methodology for the statistical evaluation of the reliability indicators of nanoelectronic heterostructure devices with quantum confinement and transverse current transfer under conditions of limited experimental information.

2. Algorithm for statistical evaluation of reliability indicators of nanoelectronic devices based on Bayesian inversion
The established standards and normative documents [13-15] make it possible to determine the relative error and confidence level of the statistical evaluation of the reliability indicators of nanoelectronic devices based on experimental information of a fixed volume. This means that in the case of a limited number of experimental samples with a given reliability, it is possible to carry out a statistical evaluation with a significantly lower value of accuracy. In conditions of limited maximum number of experimental samples, as well as in the case of the possibility of replenishing the database with
additional experimental information, it is preferable to carry out an evaluation taking into account a priori information (an evaluation in the presence of basic and additional information). It is proposed to carry out such a calculation using Bayesian inversion, which allows correcting a priori estimates as additional information becomes available to narrow the a priori confidence interval, and hence increase the accuracy. Based on this, an algorithm for the statistical evaluation of the reliability indicators of nanoelectronic devices under conditions of limited experimental information using Bayesian inversion is proposed (Figure 1).

![Algorithm for statistical evaluation of reliability indicators of nanoelectronic devices in conditions of limited experimental information.](image)

**Figure 1.** Algorithm for statistical evaluation of reliability indicators of nanoelectronic devices in conditions of limited experimental information.

The developed algorithm assumes that the experimental data for statistical evaluation were obtained as a result of testing nanoelectronic devices, the manufacturing process of which is in a state of statistical controllability and acceptable reproducibility. The main advantage of the developed algorithm is the ability to enter additional information for the subsequent refinement of statistical estimates of the reliability indicators of semiconductor devices, which will provide an increase in accuracy due to the application of the Bayesian approach at a given confidence level under conditions of a small number of experimental objects.

### 3. General logic framework of Bayesian approach in statistical estimation

As the basis of the algorithm for the statistical evaluation of the reliability indicators of nanoelectronic devices in conditions of limited experimental information, consider the Bayesian approach [16-17]. Bayesian statistical methods apply Bayes’ theorem to calculate and refine probabilities after new experimental data are obtained. Bayes’ theorem describes the conditional probability of an event based on both additional experimental data and a priori information.

The construction of Bayesian point and interval estimates of the parameter $\theta$ with known additional experimental information $x_1 \ldots x_n$ is based on the use of knowledge of the posterior distribution $f(\theta | x_1, \ldots, x_n)$, which is defined as
\[
f(\theta | x_1, \ldots, x_n) = \frac{f(\theta)f_L(x_1, \ldots, x_n | \theta)}{\int f_L(x_1, \ldots, x_n | \theta)f(\theta)d\theta}.
\]

(1)

Here \(f(\theta)\) is the prior distribution, \(f_L(x_1, \ldots, x_n | \theta)\) is the likelihood function. Then the mean value of the posterior distribution

\[
\hat{\theta}^B = E(f(\theta | x_1, \ldots, x_n)) = \int \theta f(\theta | x_1, \ldots, x_n)d\theta
\]

(2)

or the modal value of the posterior distribution

\[
\hat{\theta}^B = \arg \max_{\theta} f(\theta | x_1, \ldots, x_n)
\]

(3)

is used as Bayesian point estimates.

Thus, the problem of determining Bayesian estimates of the parameters of the distribution of operational indicators of nanoelectronic devices is reduced to determining the prior distribution and calculating the likelihood function with known additional experimental information. The formation of the a priori base is carried out by conducting point and interval estimates of distribution parameters using maximum likelihood methods and central statistics methods on the basic experimental information with low accuracy at a fixed confidence level in the case of a small sample size (Figure 1, Block A). Regardless of the size of the main and additional sample the using of the Bayesian approach makes it possible to reduce the value of the a priori confidence interval, which means that the accuracy of the interval estimation increases at a given level of confidence.

4. Results

On the basis of the presented algorithm and the general logic framework of Bayesian approach, a methodology for evaluation the reliability indicators of nanoelectronic devices using Bayesian inversion was developed. According to this methodology, software was developed that allows to determine the value of reliability function of resonant tunneling diodes (RTD) at the corresponding operating time and the gamma-percentile operating time to failure at a given probability \(\gamma\) under conditions of limited experimental data, as well as to make point and interval estimates of operational device parameters (Figure 1, Block C). The value of the current and the differential resistance at the operating point is considered as the operational parameters of the RTD. The interface of the developed software is shown in Figure 2.

The interface of the developed software contains 5 areas (Figure 2):

1 - research object area: display of the research object with its operational parameters with the ability to change the operational limits for each parameter, as well as with the ability to select a parameter for detailed consideration of the change in its point and interval estimates on the specified operating time.

2 - area of interactive input of information: input of a time point (Figure 1, Block B); specifying the path to the file and marker for cells with basic and additional data; changing the default values of confidence and probability \(\gamma\).

3 - area for initiating software actions: starting the process of recording data at the specified time point (Figure 1, Block B); updating graphic information (area 4 and 5) after changing the data in areas 1 and 2 or entering additional or basic information into the database at a time point; displays detailed information on the operating parameter selected in area 1.

4 - area for graphical display of the results of estimation the reliability indicators of the research object.

5 - area for graphical display of point and interval estimates of the operational parameters of the research object on the specified operating time.
Figure 2. Interface for predictor of RTD reliability indicators in conditions of limited experimental information based on Bayesian inversion.

The advantage of the developed software is the ability to load the main sample with the formation of an a priori base at a new time point (Figure 1, Block B, logical link "no") or to load an additional sample in the presence of a priori information at the corresponding value of the operating time in the database with further calculation to improve the accuracy of the a priori estimate (Figure 1, Block B, logical link "yes"). In the case of user input of the main sample, the a priori base is formed by conducting point and interval estimates of operational parameters using the maximum likelihood method and central statistics method, while in the case of entering an additional sample, the distribution parameters are recalculated using Bayesian inversion in accordance with relation (1).

The reliability function of the RTD at the corresponding operating time is calculated by integrating the multivariate distribution function f of the operating parameters of the device within the established operating limits. The graphic interpretation of the calculation is shown in Figure 3, where f(X) and P_x are the distribution function of the current at the operating point and the probability of finding this parameter in the established operational limit of 2 ... 4 mA, f(Y) and P_y are the distribution function of the differential resistance in operating point and the probability of finding this parameter in the established operational limit of 200 ... 500 Ohm, f(X, Y) and P_{X,Y} are the multivariate distribution function of the entered operational parameters and the value of reliability function of RTD at the corresponding operating time.

The calculation presented in Figure 3 was carried out using the developed software based on real experimental data obtained as a result of accelerated tests of RTDs, the two-barrier quantum system of which includes AlAs barriers and a GaAs well with a thickness of 2.9 and 4.9 nm, respectively. The top and bottom spacers are homogeneous undoped GaAs layers with a thickness of 2.1 nm. Accelerated tests were carried out in a mode with a constant temperature exposure of 200 °C. As a result of the statistical evaluation of the experimental data, the gamma-percentage operating time to failure of the RTD is 53.33 hours at a given probability of 95%.
Figure 3. Graphical interpretation of the calculation of the RTD reliability function value on the corresponding operating time.

5. Conclusion

Thus, a methodology was developed for evaluation the reliability indicators of nanoelectronic heterostructure devices with quantum confinement and transverse current transfer using Bayesian inversion, which makes it possible to predict these indicators under conditions of limited experimental information. As a result of statistical processing of experimental data obtained during accelerated tests of RTDs (at a temperature exposure of 200 °C) the following reliability indicators were determined using the developed predictor of reliability indicators for nanoelectronic devices: the RTD reliability function value 92.77% at the operating time of 72 hours, the gamma-percentile operating time to failure 53.33 hours at a given probability of 95%.

In accordance with the methodology, a predictor of reliability indicators for RTD has been developed. The main advantage of this predictor is the possibility of a step-by-step refinement of the statistical estimates of these indicators while collecting additional experimental information obtained not only during accelerated tests, but also during the operation of these devices.

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