A priori probabilistic model for the reliability of an "organised structure"

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Abstract. The basic possibility to create information model of the certain product (a semiconductor electronic device, or its element: *p-n* junction, quantum well, etc.) has been considered. Each product may be represented uniquely as a certain sequence of the Numbers set by technical requirements, drawings and process charts. The set Number may be realised only with a certain probability, therefore, the Number (N) in the initial engineering data is set with a maximum deviation from a mean value, i.e., the tolerance $\pm\Delta N$. During operation or storage, such processes as wear or ageing destroy the product deforming the tolerance of the set sequence of numbers, what is accompanied by inevitable increase of entropy. Hence, each product is endowed with the information negentropy, which may be calculated and may serve as initial value when solving an adequate equation of production of the thermodynamic entropy. As a particular example, the simplified model has been considered: a semiconductor plate covered on each side with insulator, which degrades during storage. The equality of a square of the tolerance and the real Number dispersion determined by the probability with which the Number realises with the set tolerance was taken as the base approximation.

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1. Introduction

For solving the reliability problem of a organised structure (OS), two kinds of information are basically used [1]: *a priori* formalised on the basis of priori assumed probability distribution for realisation of those or other OS properties, and *a posteriori*, based on the empirical data received as a result of tests.

Any OS, i.e. a certain product, or a semiconductor electronic device in a case in which we are interested, or its element may be represented uniquely with a certain sequence of Numbers set by technical requirements, OS drawings and process charts, i.e. a sequence of technological operations (TO) of its production [2].

At that, each Number may be realised only with a certain probability, therefore, the Number is set in the initial engineering data as its mean value (⟨Number⟩) with a tolerance deviation ±ΔNumber.

It is presumed that produced OS is endowed with information negative entropy – negentropy [3]. During operation or storage, such processes as wear or ageing destroy the OS with deforming, first of all, a tolerance of the set sequence of numbers, what is accompanied by inevitable increase of entropy.

Before to begin creation of offered model for the *a priori* reliability estimation, we want to define a point of issue in terms of the theory of probability. Let us agree that we do not reconstruct existing developed methods of *a priori* reliability estimation (APR) or *a posteriori* reliability estimation (APO) [1, 2].

The idea of the offered method is based on the following probabilistic hypothesis [3]. If all geometrical, physical and chemical, qualitative, *etc.* digital OS characteristics determined by Numbers with indication of tolerance $\pm\Delta N$ on drawings or documents are mixed in a random manner, we shall receive an unorganised system with the maximum information entropy. By making inverse procedure and returning all numerical characteristics to their places on the drawing in a random manner, we shall receive an OS featuring the negentropy. The latter may be calculated, if we postulate the following positions:

1) A strictly defined sequence of numbers set by drawings and process charts is an information OS model

endowed with the appropriate negentropy as we said above.

2) Each Number from the sequence is set with the maximum deviation from its mean value $\langle N\rangle$, i.e. the tolerance $\pm\Delta N$. During OS production, the Number and the tolerance are realised with a certain probability $P(J)$.

3) The dispersion of each Number equal to $\langle[\Delta(N)]^2\rangle$ may be expressed through the tolerance determined by a designer and implemented by a technologist. The basic assumption is as follows: the tolerance is set as $\pm\Delta N$ and, hence, it may be expressed approximately (at least, formally) through dispersion of Number as:

$$\langle[\Delta(\text{Number})]^2\rangle^{1/2} = \pm\Delta N. \qquad (1.1)$$

4) Technological operation is defined by a set of conditions R [1, 4] on the realisation of which an event A occurs, i.e. realization of $\langle N\rangle$ within of the tolerance $\pm\Delta N$. There exists a probability distribution for realisation of each allowable deviation, i.e. the tolerance established for the given technological operation.

5) The complete probability that the OS will be produced according to the deviations from their mean value given on drawings ($\pm\Delta N$) can be calculated by the Bayes a priori estimation method [1]. The full Bayes conditional probability determines the probabilistic space where the characteristics set by the design exist under the accepted OS production technique.

In order to calculate negentropy, we shall use a known Bayes formula [4] for the conditional probability $P(A / B)$ of an event A (the next TO, the probability $P(A)$) under the condition that an event B occurred (the previous TO, the probability $P(B)$):

$$P(A/B) = \frac{P(AB)}{P(B)}. \qquad (1.2)$$

$P(AB) = P(A)\,P(B)$ is the probability that two independent events realize, i.e. TOs which are independent on each other in themselves. The operation B can be considered as an event which may be realised, and only with one of n incompatible events (TO_i) A_1, A_2, ..., A_i, ..., A_n. In such case, the formula for full probability TO B will be

$$P(B) = \sum_{i=1}^{n} P(A_i)\cdot P(B/A_i). \qquad (1.3)$$

In our case, the complete conditional probability of realisation TO A_i, i.e.

$$P(A_i/B) = \frac{P(A_i)\cdot P(B/A_i)}{\sum\limits_{i=1}^{n} P(A_i)\cdot P(B/A_i)}, \qquad (1.4)$$

allows to estimate quantitatively the negentropy TO A_i, which is “expend” in operation process, returning the OS to a chaotic “initial” condition (deterioration).

The negentropy value corresponding to the probability (1.4) may be used as an initial condition for quantitative solution of the entropy production equation [5] which reflects the evolution of separate OS characteristics due to OS operation or during its storage (that is, in practice, ageing).

2. Thermodynamic entropy and its balance equation

For a case of semiconductor technologies (growth, doping, *p-n* junction formation, structures, *etc.*), is necessary to use the thermodynamic approach to determination of the entropy and its production (for example, ageing).

The entropy production in the thermodynamics [5-7] is associated with the presence of spatial heterogeneity in the distribution of temperature, partial chemical potentials μ_i and convective speed U_0. In this case, the spatial heterogeneity of the chemical potential is caused by spatial heterogeneity for the concentration of components C_i and/or temperature.

In the most common form, the equation of the entropy balance **S** may be written through the density of the entropy flow J_S, entropy production per a unit of volume σ_S and the sum of mass density of a component system $\rho = \sum n_i$ as

$$\frac{\partial(\rho\cdot \mathrm{S})}{\partial \mathrm{t}} = -\mathrm{div}J_\mathrm{S} + \sigma_\mathrm{S}. \qquad (2.1)$$

As $J = \rho U_0$ is a convective flow, the full entropy flow J_S develops from the convective entropy flow $\rho\cdot s\cdot U_0$ and an additional flow having another physical origin $J_S' = J_S - sJ$. From (2.1), in view of that $\frac{\partial\rho}{\partial t} = -\mathrm{div}J$, we get:

$$\rho\cdot\frac{\partial S}{\partial t} = -\mathrm{div}J_\mathrm{s}' + \sigma_\mathrm{S}. \qquad (2.2)$$

This equation is applicable to a case of diffusion in gases: local violation of chaos (equilibrium state), for example, due to the increase of density of particles and change of their speeds, will become gradually more homogeneous both in a configuration space and space of speeds. It is also applicable for consideration of ageing of local formations in semiconductor structures.

For solving a specific problem, it is necessary to develop mathematical (probabilistic) model for generation process of OS defects caused by tests/operation, i.e. the specific mechanism of the entropy production. Such specific mechanism can be simulated using the same Bayes methods of statistical evaluation [1].

The complex OS model demands to determine weak parts in practice. Theoretical estimations should be carried out for these weak parts with subsequent "summation" of such estimations by a principle of simple model. *E.g.*, for the analysis of Eq. (2.2) under the conditions of local (we mean a part of the OS) quasi-equilibrium, it is possible to use thermodynamic correlations. For example, it is valid for a homogeneous system:

$$Tds = d\varepsilon + Pdv ,$$

where s, ε, v are specific values for the entropy, energy and volume, respectively, referred to a mass unit of the system. Of course, the time variant of this equation will be simply

$$T\frac{ds}{dt} = \frac{d\varepsilon}{dt} + P\frac{dv}{dt} . \qquad (2.3)$$

In order to put Eq. (2.2) to a form comparable with (2.3), we will use a known identity [7]

$$\frac{d}{dt} = \frac{\partial}{dt} + U_0 \cdot \mathrm{grad} .$$

Then, for any physical value F, we will receive [7]:

$$\rho\frac{dF}{dt} = \frac{\partial(\rho \cdot F)}{\partial t} + \mathrm{div}(\rho \cdot F \cdot U_0). \qquad (2.4)$$

At this stage, we receive a general scheme for theoretical estimations of OS characteristic stability under a known initial negentropy value.

By similar further specifications (in particular, by designating the relative density of a component system as $C_i = \rho_1 / \rho$), we shall generate the equation for entropy production in an n-component system

$$\rho \cdot \frac{\partial S}{\partial t} = \frac{1}{T} \cdot \rho \cdot \frac{\partial \varepsilon}{\partial t} + \frac{P}{T} \cdot \rho \cdot \frac{\partial v}{\partial t} - \\ - \sum_{i=1}^{n} \frac{\mu_i}{T} \cdot \rho \cdot \frac{\partial C_i}{\partial t} . \qquad (2.5)$$

The basic initial phenomenological equations are written above. The latter also supposes a solution under a known initial entropy value, negentropy S_0 in our case, approaches to finding of which are schematically stated in equations (2.1) − (2.5).

3. Elementary model

The considered elementary model is as follows: plate is cut off from the semiconductor, two planes covered with an insulating layer. The form and parameters of the model are shown in Fig. 1.

TO$_1$: The plate is cut out the semiconductor. We suppose that the probability to obtain the thickness x within the tolerance $\pm\Delta x$ is determined by a Gaussian distribution $P(x)$; we also accept that the thickness dispersion $\langle(\Delta x)^2\rangle \approx (\pm\Delta x)^2$. Then, if the mean value of the plate thickness is $\langle x\rangle$, we will get for $P(x)$:

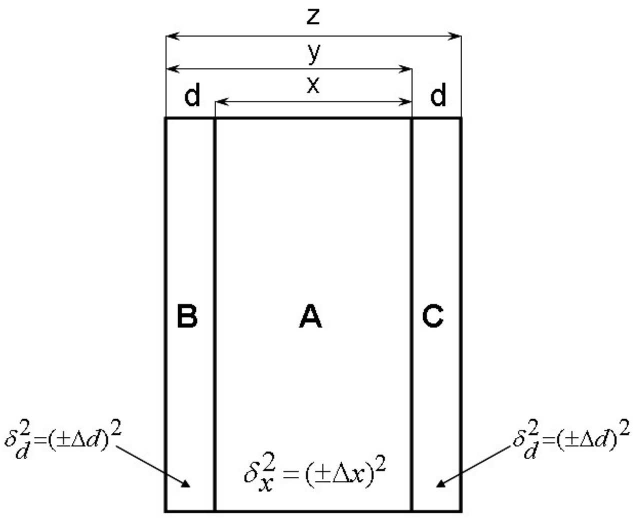

Fig. 1. The form and parameters of the model.

$$P(x) = \frac{1}{\sqrt{2\pi \cdot (\pm\Delta x)^2}} \cdot \exp\left[-\frac{(x - \langle x\rangle)^2}{2 \cdot (\pm\Delta x)^2}\right]. \qquad (3.1)$$

TO$_2$: One side of the plate is covered with an insulating layer (below, an index 2 refers to the TO's number). The mean thickness of the insulating layer is $\langle d\rangle$, and the dispersion is $\langle(\Delta d)^2\rangle$, that is, it is equal to square of the tolerance. The total thickness of two layers $y = d + x$ with a dispersion $\langle(\Delta y)^2\rangle$ is defined by the conditional probability that TO$_1$ having the probability (3.1) is made within the tolerance $\pm\Delta x$, and TO$_2$ is made within the tolerance $\pm\Delta d$. Then

$$P(y / x) = \frac{1}{\sqrt{2\pi \cdot (\pm\Delta d)^2}} \times \\ \times \exp\left[-\frac{(y - x - \langle d\rangle)^2}{2 \cdot (\pm\Delta d)^2}\right]. \qquad (3.2)$$

From (3.1), (3.2), the full conditional probability $P(y)$ for realisation of "plate A + layer B" may be written as

$$P(y) = \int_{-\infty}^{+\infty} P(x) \cdot P(y / x) \cdot dx = \\ = \frac{1}{\sqrt{2\pi \cdot \left[(\pm\Delta x)^2 + (\pm\Delta y)^2\right]}} \times \\ \times \exp\left[-\frac{(y - \langle x\rangle - \langle d\rangle)^2}{2 \cdot (\pm\Delta x)^2 + 2 \cdot (\pm\Delta y)^2}\right]. \qquad (3.3)$$

TO$_3$: The plate is covered with an insulating layer from an opposite side (index 3). The mean thickness of the insulating layer is $\langle d\rangle$, and the dispersion is $\langle(\Delta d)^2\rangle = (\pm\Delta d_2)^2$. The total thickness of the plate and two layers $z = x + d + d$ with the dispersion

$\langle(\Delta z)^2\rangle = (\pm\Delta x)^2 + 2(\Delta d)^2$ is defined by the conditional probability (i.e., under condition that the concrete value $x = x + d$ according to (3.3) realises)

$$P(z/y) = \frac{1}{\sqrt{2\pi\cdot(\pm\Delta d)^2}}\times \times\exp\left[-\frac{(z-(x+d)-\langle d\rangle)^2}{2\cdot(\pm\Delta d)^2}\right] \quad (3.4)$$

of the event that TO_1 is made within the tolerance $\pm\Delta x$ and TO_2 within the tolerance $\pm\Delta d_2$, has the same probability distribution as TO_1.

By analogy to (3.1), the full probability $P(z)$ considering (3.3) and (3.4) is equal to

$$P(z) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} P(x,y,z)\cdot dx\cdot dy = \int_{-\infty}^{+\infty} P(y,z)\cdot dy = \int_{-\infty}^{+\infty} P(y)\cdot P(z/y)\cdot dy = \frac{1}{\sqrt{2\pi\cdot\left[(\pm\Delta x)^2 + 2(\pm\Delta y)^2\right]}}\times \times\exp\left[-\frac{(z-\langle x\rangle - 2\langle d\rangle)^2}{2\cdot\left[(\pm\Delta x)^2 + 2(\pm\Delta y)^2\right]}\right]. \quad (3.5)$$

So, at presence of distribution function for a random variable $P(X)$, it is possible to define the ensemble entropy (negentropy) of random variables as [3]

$$S = -\int_{-\infty}^{+\infty} P(X)\cdot\ln P(X)\cdot dX .$$

In particular, under the Gaussian distribution (3.1)

$$S = -\int_{-\infty}^{+\infty}\frac{1}{\sqrt{2\pi\cdot\langle\Delta x^2\rangle}}\cdot\exp\left[-\frac{(X-\langle X\rangle)^2}{2\cdot\langle\Delta x^2\rangle}\right]\times \times\left(\ln\frac{1}{\sqrt{2\pi\cdot\langle\Delta x^2\rangle}} - \frac{(X-\langle X\rangle)^2}{2\cdot\langle\Delta x^2\rangle}\right)dX = = \ln\sqrt{2\pi\cdot e} + \ln\left[\langle\Delta x^2\rangle^{1/2}\right] = \ln\sqrt{2\pi\cdot e} + + \ln\left[(\pm\Delta x)^2\right]^{1/2} = S_{const} + S_{\pm\Delta x}$$

Here, we received an example of the scheme for definition of the initial negentropy value $S_0 = S_{\mathrm{const}} + S_{\pm\Delta x}$ under the Gaussian distribution for the probability that an event consisting in realisation of size $\langle x\rangle \pm \Delta x$ occurs considering that $\langle(\Delta x)^2\rangle \approx (\pm\Delta x)^2$.

4. The entropy of ensemble as a whole. Degradation.

As a result of manufacturing of the plate and covering of both sides with a dielectric, we received a structure of total thickness $z = x + 2d$ with the probability distribution defined as (3.5). The entropy of this ensemble is

$$S = -\int_{-\infty}^{+\infty} P(z)\cdot\ln P(z)\cdot dz = = \ln\sqrt{2\pi\cdot e}\cdot\sqrt{(\pm\Delta x)^2 + 2\cdot(\pm\Delta d)^2}\,. \quad (4.1)$$

Let's assume now that the characteristic $d_0 = d_2 + d_3 = 2d$ degrades, for example, decreases with time according to the law $d(t) = \frac{d_0}{f(t)}$, where $f(t)$ is a growing function of time, and $f(0) = 1$. The mean value of the ensemble degrades in the same way.

Considering (3.1), the probability distribution for the realisation of the thickness x within the tolerance $\pm\Delta$, i.e. $P(d(t))$, will also change as

$$P(d(t)) = \frac{1}{\sqrt{2\pi\cdot(\pm\Delta d)^2}}\times \times\exp\left[-\frac{(d_0-\langle d_0\rangle)^2}{2\cdot\sigma_t^2}\right]; \quad \sigma_t^2 = (\pm\Delta d)^2\cdot f^2(t). \quad (4.2)$$

According to the above, the entropy of ensemble changes in time

$$S = S_0 + \ln\sigma_t = S_0 + \ln\sigma_0 + + \ln f(t) = S_0 + S(0) + \ln f(t).$$

In this case, $S(0)$ is a required initial entropy value for a part of the whole ensemble (only for dielectric layers).

For the whole ($z = x + 2d$) ensemble, the entropy is equal to:

$$S = S_0 + \ln\sqrt{(\pm\Delta x)^2 + (\pm\Delta d)^2\cdot f(t)}.$$

Let's accept now that allowable (critical) values for thickness of dielectric layers are equal to d_{cr}. Then, with change in time of $d(t)$, distribution of probabilities changes, of course, with the entropy; in such case, failure of the whole ensemble is possible.

Graphically, this situation is depicted in Fig. 2 where distributions of probability $P[d(t)]$ are shown when the film of the set thickness d_0 degrades under the exponential law up to the critical value of d_{cr}.

There also exists the possibility to estimate the number of failures of the above structure in a time interval from t up to $t + \Delta t$. The number of working structures at the moment t is: $\int\limits_{d_{cr}}^{\infty} p(d(t))\cdot\partial d$, and at the moment $t+\Delta t$ their number is $\int\limits_{d_{cr}}^{\infty} p(d(t+\partial t))\cdot\partial d$.

The difference between these values is a number of failures $\gamma(t)$ within the interval $t \div t+\Delta t$:

$$\gamma(t)=\left[\int\limits_{d_{cr}}^{\infty} p(d(t))\cdot\partial d-\int\limits_{d_{cr}}^{\infty} p(d(t+\partial t))\cdot\partial d\right]\cdot\frac{1}{\Delta t}=$$

$$=p(d_{cr})\cdot d_{cr}\cdot\left.\frac{\partial f(t)/\partial t}{f(t)}\right|_{t=t_{cr}}.$$

Let's illustrate this, as above, with an example of the degradation law exponential in time $f(t)=\exp(\alpha t)$. Then

$$\frac{\partial f(t)/\partial t}{f(t)}=\alpha;\quad d_{cr}=d_0\cdot\exp(-\alpha t_{cr});$$

$$t_{cr}=\frac{1}{\alpha}\cdot\ln\frac{d_0}{d_{cr}};$$

hence,

$$\gamma(t)=p(d_{cr})\cdot d_{cr}\cdot\alpha=$$

$$=\frac{d_{cr}\cdot\alpha}{\sqrt{2\pi\cdot\sigma^2(t_{cr})}}\cdot\exp\left(-\frac{d_{cr}-\langle d_0\rangle}{2\cdot\sigma^2(t_{cr})}\right)$$

where

$$\sigma^2(t_{cr})=\sigma_o^2\cdot\exp(2\alpha t_{cr})=$$

$$=[\sigma_0\cdot\exp(\alpha t_{cr})]^2=\left[\sigma_0\cdot\frac{d_0}{d_{cr}}\right]^2.$$

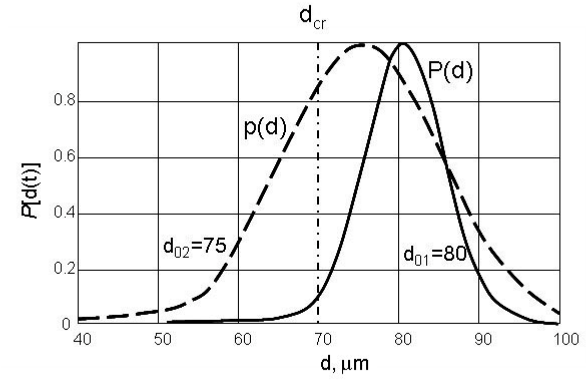

Fig. 2. Probability distribution $P[d(t)]$ for a case: film of the set thickness d_{01} = 8 μm with the dispersion of 5 μm (curve d_{01}) degrades under the exponential law $\langle d(t)\rangle=\frac{d_0}{\exp(\alpha\cdot t)}$, reaching the value of d_{02} = 75 μm with the dispersion of 10 μm (curve d_{02}). The critical value of thickness of the film: d_{cr} = 70 μm.

Simple transformations result in:

$$\gamma(t)=\frac{d_{kp}\cdot\alpha}{\sigma_0\cdot\frac{d_0}{d_{cr}}\cdot\sqrt{2\cdot\pi}}\cdot\exp\left(-\frac{(d_{cr}-\langle d_0\rangle)^2}{2\cdot\sigma_0^2\left(\frac{\langle d_0\rangle}{d_{cr}}\right)^2}\right)=$$

$$=\frac{\frac{d_{cr}^2}{d_0}\cdot\alpha}{\sqrt{2\pi\cdot\sigma_0^2}}\cdot\exp\left(-\frac{(d_{cr}-\langle d_0\rangle)^2}{2\cdot\sigma_0^2}\cdot\left(\frac{d_{cr}}{d_0}\right)^2\right).$$

The probability of non-failure operation is expressed by $\gamma(t)$ as

$$F(t)=\exp(-\gamma(t))=\exp\left(-\alpha t\cdot\frac{d_{cr}^2}{\langle d_0\rangle\cdot\sqrt{2\pi\cdot\sigma_0^2}}\times\right.$$

$$\left.\times\exp\left(-\frac{(d_{cr}-\langle d_0\rangle)^2}{2\cdot\sigma_0^2}\cdot\left(\frac{d_{cr}}{\langle d_0\rangle}\right)^2\right)\right).$$

5. Conclusions

1. If real tolerances lose, during storage or operation, connection with the set tolerances, the OS may not meet to the technical requirements of reliability.
2. We consider indisputable that the OS (semiconductor device) may be represented uniquely with a certain sequence of the Numbers which includes specific characteristics of this OS. The elaborated produced OS should be endowed with a certain information negative entropy.
3. If tolerances of the Numbers determining the design and technological OS contents may be connected, to some approximation, with the dispersions of appropriate probabilistic distributions as $(\text{dispersion})^{1/2}\cong\pm(\text{tolerance})$, it is natural to use the Bayes formula to determine the full conditional probability that the OS is made according to the requirements to its initial characteristics.
4. Hence, it is also possible to calculate the initial value of the information entropy in order to solve the negentropy production equation on a basis of the physical, chemical and other data on the properties of various OS parts (structures).
5. Critical negentropy values which changes in time may be reasonably included into the technical requirements list as the data for calculation of *a priori* quantitative reliability characteristics of the device.

An extremely simplified model considered above demands very complex calculations. The real device is even more complex, but this circumstance may not discredit the approach itself to the solution of the *a priori* reliability forecasting problem on the basis of tolerances.

It is known from practice that the standard failure of the device of any complexity is caused by failure of the so-called weak parts, but not failure the device as a whole. In this connection, the method offered here may be applied to weak parts, essentially facilitating data processing with the use of the appropriate PC programs.

In summary, we want to emphasise the main thesis prompting to develop the proposed approach to APR: if APR and APO results are close for the given OS, the further improvement of this OS has to be charged to designers, not technologists.

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