

# Monte Carlo method used for a prognosis of selected technological parameters

Małgorzata Langer

**Abstract**—In this paper a smart modeling approach for realistic simulation of selected technological parameters is presented. The technology of making contacts with plasma vapor deposition (PVD) method has been chosen for this purpose. The analysis is based on the Monte Carlo (MC) method and uses the Excel worksheet – the simplest tool, easily accessible to anyone. The statistic parameters are calculated and discussed as we introduce this experiment to demonstrate the advantages of design for six sigma (DFSS).

**Keywords**—DFSS, MC method, PVD, contacts, Excel randomizing.

## 1. Design for six sigma

Design for six sigma (DFSS) [1] and its metric – the probability of non-compliance [2] make it possible to consider different sources of variation when applied in manufacturing. The philosophy of this approach is that variation exists in all systems, components, and procedures. The probabilistic analysis is to be run when analysing and optimising all the successive phases of the design and its implementation (Fig. 1a). DFSS approach may also be applied in research, such as experiments, simulations, result analysis, etc. (Fig. 1b). In this paper a methodology presented in Fig. 1b is proposed.

Using DFSS one analyses the whole statistical distribution of input values or parameters over their possible range, instead of estimating the influence of extreme (therefore rare) values on the operation or the condition of the object. Thus instead of calculating the limits of the result range, one calculates the probability of the distribution of possible results. And the distribution of probability is the basic metric for DFSS.

When an output response represents the total influence of independent input values and parameters, the output distribution tends to be normal as a result of the central limit theorem [3]. The significance of this is that there is no precondition for probability distributions of the input design parameters (they do not have to be normal) to obtain a normal output response. The majority of physical phenomena and variables are represented by the normal distribution.

The Tchebychev inequality known in statistics [3], states that at least  $1 - (1/k^2)$  per cent of any distribution is within the product:  $(\pm k \times \text{deviation} \times \text{mean})$ .

Table 1

The per cent of normal distribution covered by the range calculated with Tchebychev inequality

$k$ [--]	1	1.415	2	3	4	5	6
[%]	68.3	84.3	95.5	99.7	99.99	99.99994	99.9999998

In the case of normal distribution the percentage in this range is known exactly (Table 1).

## 2. Monte Carlo method

Monte Carlo (MC) methods were used already in 1947 to simulate the neutron transport in the research on the hydrogen bomb [4]. Since their first presentation (at a conference in Los Alamos in 1949), they have been used to predict “almost everything”, from a simple bingo game, through weather forecasts to atomic fusion.

The goal of the MC method is to simulate an existing object (an equation, a model, a process, etc.) by randomly sampling the input ranges (input distributions) and then calculating the output response. The flow chart is shown in Fig. 2.

The fundamental problem of using MC to perform a probabilistic analysis is that it requires a large number of trials to obtain a sufficient confidence in the results. With the development of PCs many techniques have been developed to generate random numbers; with many of them still requiring huge time and memory resources. MC methods can be applied to extremely complex finite element models, fluid dynamics, etc., but every trial may last long hours and the computer grids (parallel processing) are the only solution to meet these demands. They are beyond the scope of this paper, as we propose to use Excel RAND() function, that is adequate for application in a great number of cases.

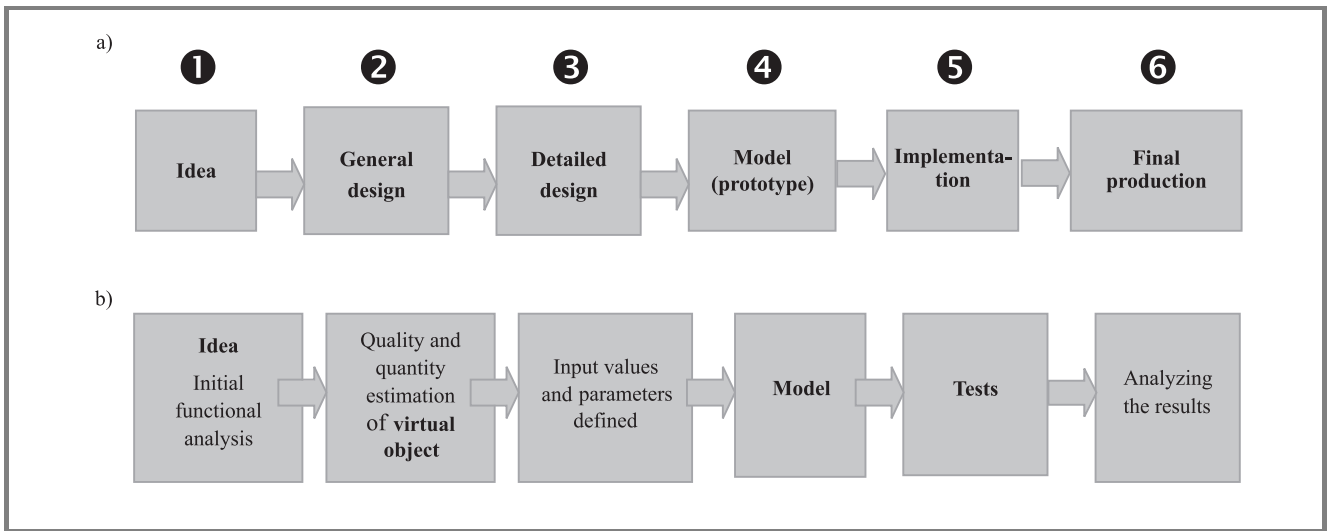


Fig. 1. Phases of considering the variations (a) in the production; (b) in testing the model.

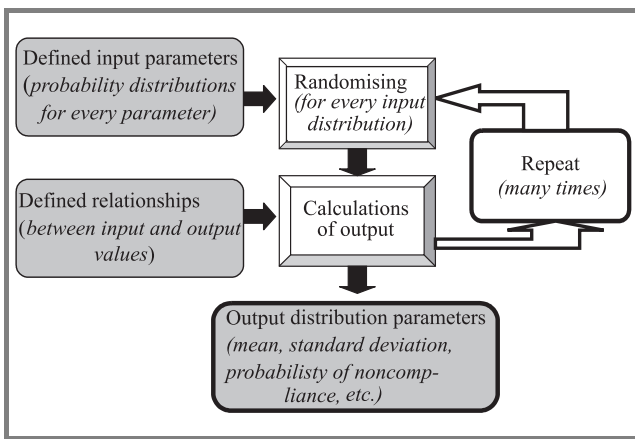


Fig. 2. Monte Carlo method. Flow chart.

### 3. Distributions prepared in Excel

A standard uniform random number (any number between 0 and 1; denoted as  $RU$ ) is required to generate a random value from any probability density function. In Microsoft Excel the  $RAND()$  function returns  $RU$ . Some experts claim that the algorithm applied in Excel does not meet the rigorous standard required for cryptography, but it is absolutely sufficient for simulations in engineering. Random numbers for a standard normal distribution (denoted as  $RN$ ; both mean and standard deviation are equal to zero) can be computed with Box-Muller method, known since 1958 [4]:

$$RN = \sqrt{-2 \ln(RU1)} \cdot \cos(2\pi \cdot (RU2)), \quad (1)$$

where  $RU1$  and  $RU2$  are uniform random numbers.

The Excel function is:

$$RN = \text{SQRT}(-2 * \text{LN}(\text{RAND}())) * \text{COS}(2 * \text{PI}() * \text{RAND}()).$$

Having  $RU$  and  $RN$  numbers one may generate a common distribution (e.g., uniform, normal, log-normal, exponential, etc.) using the appropriate formulae with the desired values of mean and standard deviation. For a uniform distribution between the minimum (min) and maximum (max) values the random value (denoted as  $RV$ ) is calculated as:

$$RV = (\max - \min)RU + \min \quad (2)$$

and for a normal distribution:

$$RV = \text{mean} + \text{deviation} \cdot RN. \quad (3)$$

The more random numbers we generate, the closer the mean and the standard deviation are to specified values. If one generated an infinite number of  $RNs$  – the calculated mean and deviation would be equal exactly to the specified ones.

As it was mentioned before, Microsoft Excel may be used to generate random numbers. The maximum number of MC trials is limited by the maximum number of rows in the worksheet (65,536 trials in Excel 2002). It is assumed that one thousand trials already meet the requirements, with a limited confidence. The author checked tens randomised normal distributions (ND) with one thousand runs, assuming the mean of 10 and the calculated means equalled to 9.8–10.2 so the error was not greater than 2 per cent. A screen capture with typical results is shown in Fig. 3. In the simulated experiment described later 5000 trials were used.

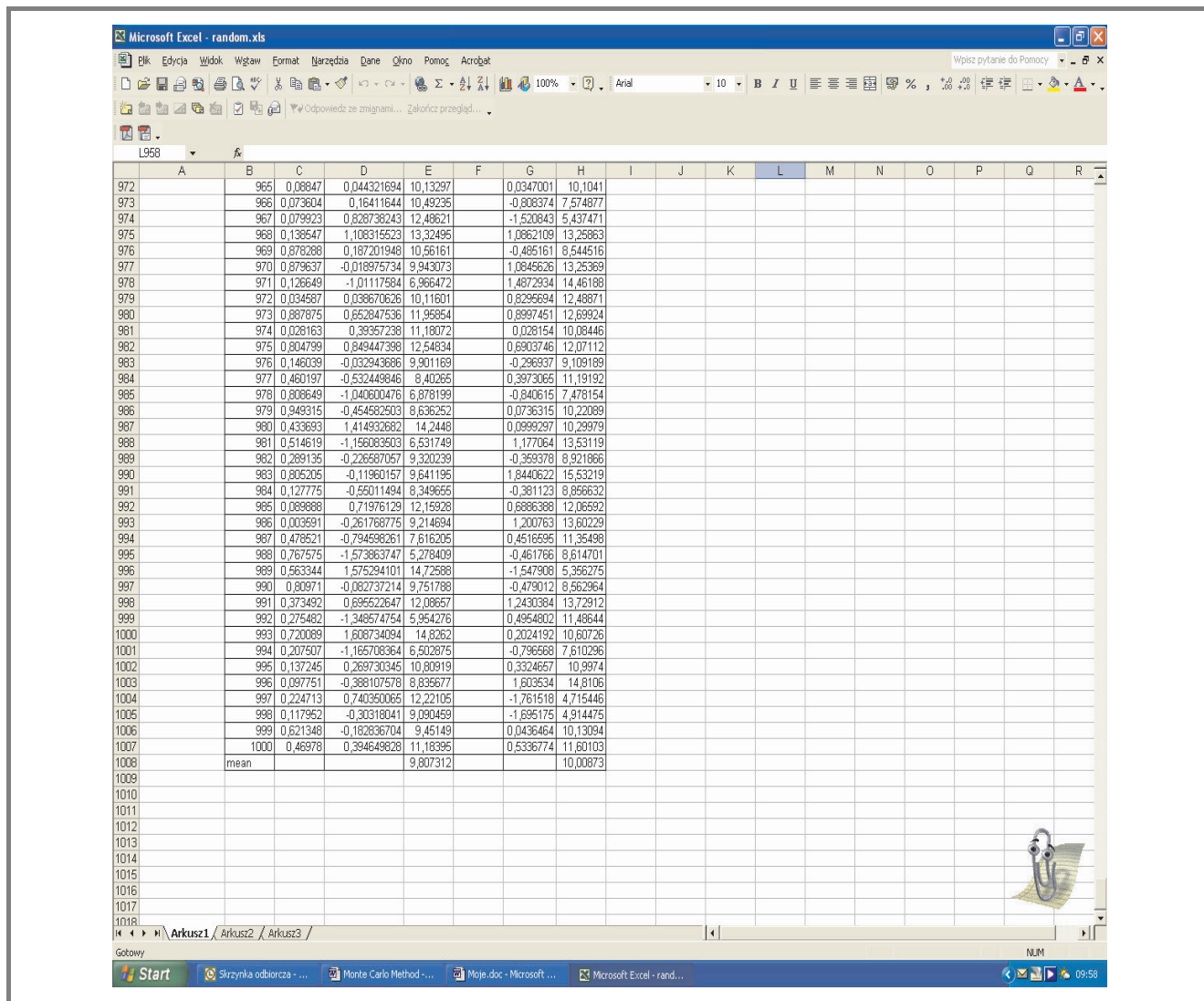


Fig. 3. The part of the spreadsheet to check the error at one thousand trials.

### 4. The experiment

The MC method was used to simulate plasma vapor deposition (PVD) metallization from a resistive source (Fig. 4) intended to form aluminium contacts. A detailed description of this process may be found, e.g., in [5, 6]. The technique is used in the Technical University of Łódź, Institute of Electronics (TUL IE) during studies to improve the quality of contacts to such materials as SiC. The process takes place in a vacuum chamber (Fig. 5). The goal of the virtual experiment is to anticipate the solution of the Langmuir formula [5] for the evaporation rate:

$$v = 77.8 \sqrt{\frac{M}{T}} \cdot p_s \quad [\text{g/cm}^2\text{s}], \quad (4)$$

where:  $M$  – molecular weigh [g/mole],  $T$  – material temperature [K],  $p_s$  – vapor pressure at the temperature  $T$  [Pa].

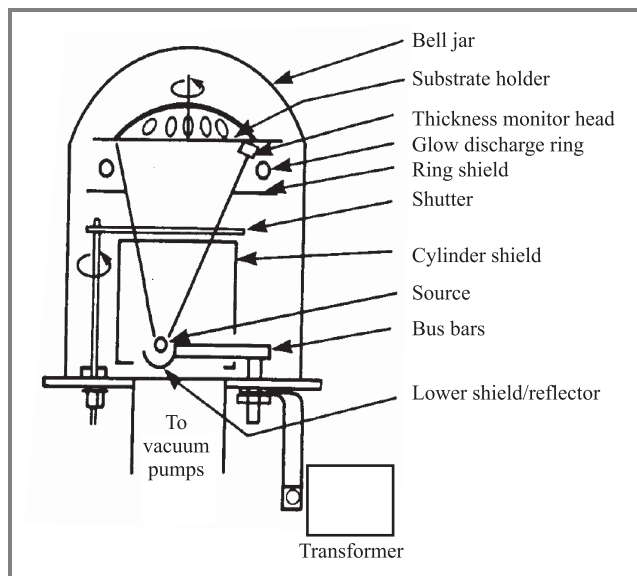


Fig. 4. The typical system for PVD from the resistive source [from student manual, TUL IE].

Table 2  
Range and distribution of input parameters

Parameters	Experiment I		Experiment II	
	Range	Distribution	Range	Distribution
Purity of aluminium	±0.5%	uniform	±0.5%	uniform
Temperature	±1% (~12 degrees)	Gaussian (deviation = 0.66)	±2%	Gaussian (deviation = 1.3)
Pressure	±10% (changes logarithmically)	Gaussian (deviation = 1)	±20%	Gaussian (deviation = 2)

The formula (4) is true when the pressure of residual gases is lower than  $1.33 \cdot 10^{-4}$  Pa. It takes 30–40 min to deposit a layer with the typical thickness of 1–1.2  $\mu\text{m}$  at substrates heated to ~475 K. Process duration increases to 40–60 min at temperatures of 572–625 K [7]. The pumping, heating and cooling rate strongly affects the quality of the layers.

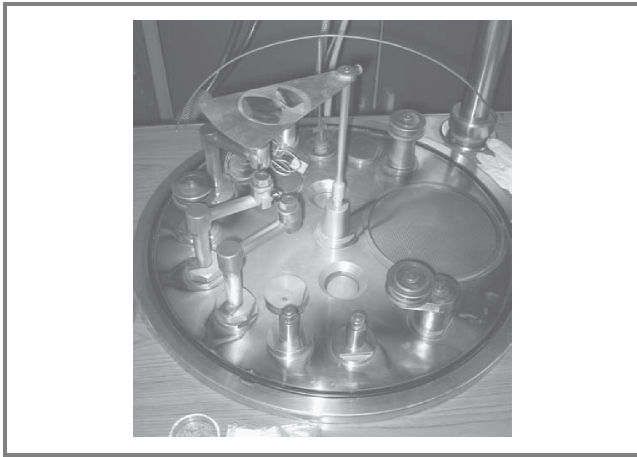


Fig. 5. The interior of the chamber in TUL IE.

The melting point of pure aluminium is 932 K and its evaporation takes place at 1421 K. The optimum evaporation rate is  $0.85 \cdot 10^{-4}$  g/cm<sup>2</sup>s [5]. Temperature stability is very important here since its increase by approximately 10–15 per cent may elevate the pressure as much as ten times, and the evaporation rate depends on the diffusion of the outer layers of the cloud of vaporised aluminium.

### 5. The MC simulation

The optimum values of input (purity of aluminium  $M$ , temperature  $T$  and vapor pressure  $p_s$ ) and output (evaporation rate) parameters are assumed to be 100 per cent. The goal of the simulation is to study the variation of evaporation rate with the variation of input parameters (strongly depending on the conditions in the lab).

The range and distribution of input parameters are listed in Table 2. Every experiment covers 5000 trials.

The obtained distribution of evaporation rate is presented in Fig. 6 for experiments I (Fig. 6a) and II (Fig. 6b).

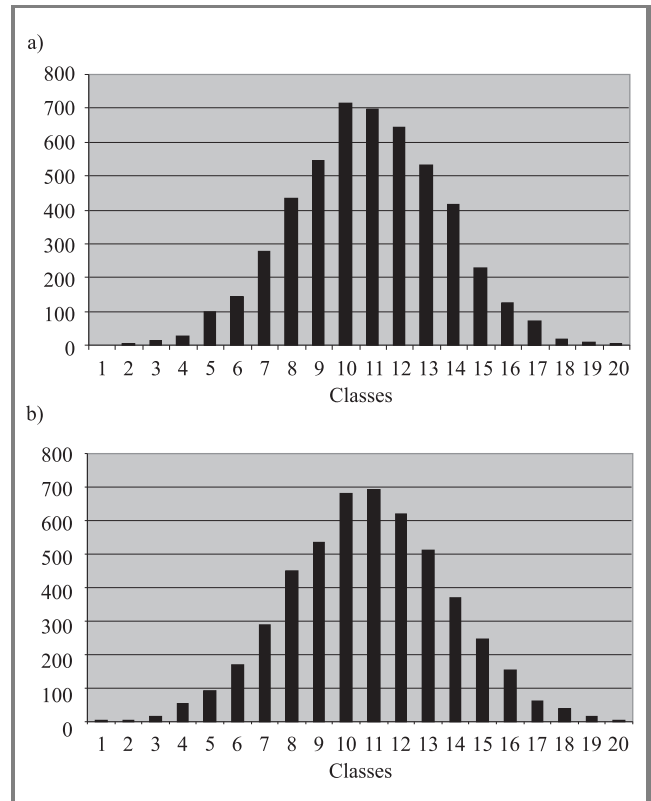


Fig. 6. The distribution of results – quantity of events in the classes: (a) experiment I; (b) experiment II.

The whole range of rates (maximum rate – minimum rate) was divided into 20 equal sub-ranges (we have established 20 classes). Quantities in classes are listed in Table 3, which contains also basic statistical parameters. The accepted limit value may be chosen arbitrarily. The last row in Table 3 means that the assumed maximum allowed change of the output (i.e., evaporation rate) is 5 per cent for our experiments. It may be seen that more

than 30 per cent of output values will not meet this requirement in experiment II and less than 5% in experiment I.

Table 3  
Simulation results

Classes	Quantity in classes	
	Experiment I	Experiment II
1	1	2
2	5	3
3	12	16
4	29	52
5	98	94
6	144	168
7	275	289
8	433	450
9	547	533
10	717	681
11	698	694
12	644	619
13	532	511
14	417	369
15	226	245
16	125	154
17	71	63
18	16	37
19	7	15
20	3	5
Parameters	Values	
Mean [%]	100.022	99.99087
Deviation	1.066626	2.110416
Min value [%]	96.00374	92.44879
Max value [%]	103.7724	107.0591
Median [%]	100.0243	100.0857
Within the range of coarse values: 98–102	95.5% of events	68.3% of events

These are our probability of non-compliance (PNC) results for the assumed parameters.

## 6. Conclusions

The example given in this paper focused on math and statistics, but MC method may be used in numerous considerations. When the distribution type for a population is determined, one can simulate any object for which an appropriate model exists. One can calculate characteristic parameters for the investigated distributions; determine what

the tolerance limits or the range should be (based on expected behavior); estimate how great is PNC for a given case and assumptions. The presented example shows how helpful Excel may be in this research. In the investigated case the time to make a population and to calculate the statistic parameters was very short (a few seconds). Thus it has been demonstrated that Excel is sufficient as a DFSS tool.

## References

- [1] K. Simon, "What is DFSS?", *Isixsigma Mag*, 2004, <http://www.isixsigma.com/library>
- [2] C. Frangkais, D. Rubin, and X. Zhou, "Clustered encouragement designs with individual noncompliance: Bayesian inference with randomization, and application to advance directive forms", *Biostatistics*, no. 3, pp. 147–164, 2001.
- [3] C. W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry and The Natural Sciences*. Berlin [etc.]: Springer, 2004.
- [4] "Innovative stochastic algorithms", <http://members.shaw.ca>
- [5] *Cienkie warstwy metaliczne*. Warsaw-Wrocław: PWN, 1974 (in Polish).
- [6] V. Shashkin *et al.*, "Microstructure and properties of aluminum contacts formed on GaAs (100) by low pressure CVD with dimethylethylamine alane source", *J. Electron. Mater.*, vol. 30, no. 8, pp. 980–987, 2001.
- [7] *Procesy technologiczne w elektronice półprzewodnikowej*. Warsaw: WNT, 1980 (in Polish).



**Małgorzata Langer** graduated from the Faculty of Electrical Eng., Technical University of Łódź (TUL), Poland, in 1978. She received her Ph.D. degree in electronics, in 1999. After several years in international marketing she joined TUL in 1988, first in The Institute of Materials Science and then The Institute of Electronics (since

2004 as Associate Director on Science). Her science and research interests are in thermal management and semiconductor devices modeling, advanced technologies in microelectronics, theory of experiments, etc. She is the author and the co-author of over 50 publications, also quoted, and has been involved in several international, domestic, and university research and teaching programs.

e-mail: [malgorzata.langer@p.lodz.pl](mailto:malgorzata.langer@p.lodz.pl)

Institute of Electronics

Technical University of Łódź

Wólczańska st 211/215

90-924 Łódź, Poland