

Modelling and detection of failure in medical electrodes

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Original scientific paper

In this paper we have studied the failures in medical electrodes such as electroencephalogram electrodes (EEG) being used for collecting brain signals. As those electrodes have to guarantee high level of reliability it is important to explore and predict the possible occurrence of failures in their structure. The electrode tip (needle) made of stainless steel is covered with thin oxide film acting as a dielectric and determining the total electrode resistance. In fact, studying the fluctuations of that resistance gives the insight into defects of the whole structure. The electrical properties of the oxide layer are characterized by charge hopping mechanism and the total resistance could be modeled by implementing random resistance network (RRN) methodology.

The applied computational algorithm is based on Monte Carlo simulation procedure with direct and iteration methods. The obtained simulation results show non-gaussian Bramwell-Holdsworth-Pinton (BHP) distribution of the total resistance fluctuations, and they verified by the experiments.

Key words: Cold solder, oxide layer, failure detection, biased percolation, RRN simulation

Modeliranje i detekcija kvara u medicinskim elektrodama. U ovom je radu razvijen model za simulaciju predviđanja defekata u posebnim elektrodama koje se koriste pri mjerenju i prikupljanju signala mozga. Ključni dio elektrode je njen čelični vrh prekriven tankim oksidnim slojem koji ujedno djeluje kao dielektrik. Upravo fluktuacije vrijednosti otpora dielektrika odnosno njihovo rasipanje od normalne do BHP raspodjele, korištene su kao osnova predloženog modela. Pritom je primjenjena metodologija mreže nasumičnih otpora (RRN), algoritam temeljen na Monte-Carlo simulacijama kao i teorija usmjerene perkolacije. Definiran je i poseban parametar kao indeks intervala valjanosti za svaku elektrodu. Simulacije su potvrđene mjerenjem u laboratorijskim uvjetima na komercijalnim EEG elektrodama.

Ključne riječi: Hladni spoj, oksidni sloj, detekcija kvara, usmjerena perkolacija, mreža nasumičnih otpornika

1 INTRODUCTION

Modern technological tendency of miniaturization can cause circuit failure and significantly affect the reliability and lifetime of wide range of electrical devices. In certain devices such as medical electrodes, failure is unacceptable and it is important to explore and predict its possible occurrence. Manufacturing procedure of medical electrodes carries a risk of failure which significantly affects the impedance of the electrode and consequently the collected signals. Currently known methods for failure detection are based on measuring the resistance (impedance) as the only parameter for the electrode validity [1,2]. Unfortunately that is not sufficient to predict the failure. Therefore, this work has been focused on improving and developing more sophisticated methods for electrode testing.

In electronic devices, failure is primarily caused by the degradation (being caused by electromigration and oxidation) of metallic interconnects and solder joints which lose their conduction properties. The nature of electromi-

gration in solder joints is currently not understood in full, and is expected to be different from that in metal interconnect lines. Many electromigration studies have been performed on Al and Cu line interconnects [3] while two experimental studies have been reported on the electromigration behaviour of solder joints [4] and [5]. On the other hand, oxide layer on the used stainless steel tip acts as a dielectric and determines total electrode resistance.

The properties of this layer have an important influence on the solder joint conductivity and behaviour of the electrode in general. In EEG electrodes current is not sufficient to activate electromigration process. The mechanism responsible for occurrence of failure is electrical breakdown in metal-insulator structure. The aim of presented work is to explore the nature of cold solder joint in medical electrodes by performing detailed numerical MC simulations and developing appropriate algorithm for predicting and detecting the breakdown effect. Biased percolation theory and RRN are used to model the two-phase joint struc-

ture [6]. This approach also allows us to model the metal-insulator structure as a two dimensional network, where the conductive paths are represented by regular resistors (small resistance) while the insulating (oxide) parts represent defects (high resistance).

2 SOLDER JUNCTION STRUCTURE

The Corkscrew electrode consists of a needle (0,6 mm in diameter) and lead wire (1 m long). In the manufacturing process these parts are connected by soft soldering procedure which is responsible for the behaviour and quality of electrode in general. The electrode tip (needle) is made of stainless steel AISI 304 which has a thin oxide film that circumfuses the needle surface. In general, oxide films can be passively or thermally grown; they are composed of two layers: outer iron oxide layer and inner mixed iron-chromium oxide layer [7]. According to the same study the film thickness varies from 8 nm at 50° C to 30 nm at 450° C, mainly occurring in outer iron oxide layer. In the same temperature range, the thickness of outer layer is increased by a factor of four, while the thickness of the internal layer is not significantly affected. Figure 1 gives a schematic representation of the oxide structure and transport processes of thermally grown oxide film. In this case, for thermally grown oxide it is assumed that the inner layer consists of a mixed iron-chromium spinel oxide ($Fe_{2-x}^{3+}Cr_x^{3+}Fe^{2+}O_4^{2-}$) with $0 \leq x \leq 2$ [8].

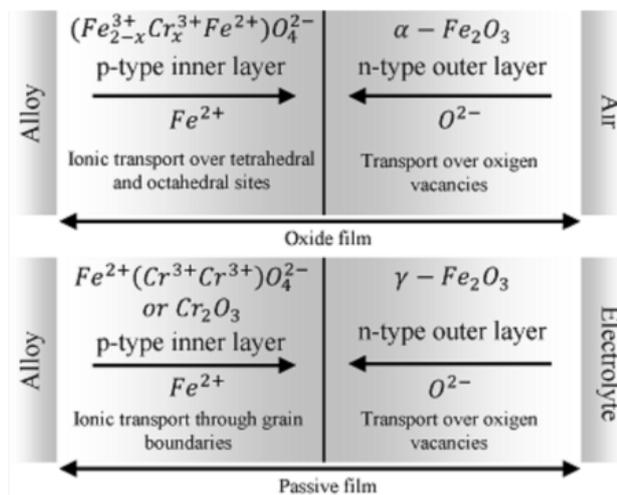


Fig. 1. Schematic representation of the diffusion processes through the individual layers of thermally grown oxides and passive films [7]

The transport of iron ions in the inner layer competes with that of oxygen ions in the outer Fe_2O_3 layer. Hence, conductivity of the inner layer, σ , is determined by hopping between Fe_{2+} and Fe_{3+} in the octahedral sites of the spinel

present in the inner region of the film and is given by [9]:

$$\sigma = (\sigma_0/T) [Fe_{oct}^{2+}] [Fe_{oct}^{3+}] \exp\left(\frac{-E_H}{K_B T}\right) \quad (1)$$

where $[Fe_{oct}]$ denotes the concentration of Fe cations in the octahedral sites, E_H is the hopping activation energy and σ_0 is a constant.

As the manufacturing process of EEG electrodes includes soft soldering procedure which uses temperature in the range from 300° C to 350° C it is reasonable to assume that thermally grown oxide layer dominates at the tip surface over the passive oxide layer. According to this assumption, we investigate properties of structure consisting of two conductors (lead wire and stainless steel tip) and oxide layer between represented as two plate strip sandwich structure shown in Fig. 2. Proposed structure acts as a dielectric between two outer contacts such as in a MOS structure and electrical properties are defined by hopping conductivity of the oxide film. Considering the percolation nature of hopping mechanism, percolation based simulation model is proposed. Detailed description of simulation model and applied numerical methods are given in the following section.

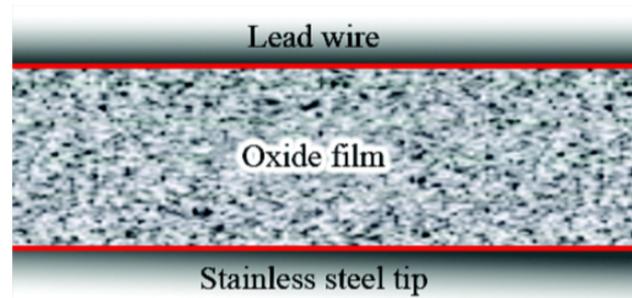


Fig. 2. Schematic representation of solder joint microstructure

3 MODEL DESCRIPTION

3.1 Percolation theory

Electrical conductivity of disordered materials cannot be explained only by fundamental mechanisms such as tunnelling or hopping. That's why in the model has been included also the bond percolation theory [10]. The oxide film that forms between stainless steel and lead can be represented by a 2D network of randomly placed conducting elements (vertices) and it can be modelled using (bond) directed percolation theory (DP). DP is a mathematical model of directed connectivity in disordered systems dependent on the number of conducting elements as well as their placement. For a given number of conducting

elements there is a finite probability p for which the system will conduct. Percolation in such random network is a directed process and model has to be built to achieve the best possible directionality (Markov - process). Since the voltage difference between the bottom of network (stainless steel interface) and the top (lead interface) is not negligible, directionality is achieved by a biased percolation model [3,11]. Current distribution in this network is modelled using directed bond percolation as well. Each vertex potential can be calculated considering network bottom/top potential and conductance of each neighbouring bond, using Laplace's equation with finite difference method (Kirchhoff's current law).

3.2 Random resistance network

In order to describe microstructure deformations as a consequence of fluctuations we propose a resistor network for modelling resistance behaviour of solder junction. Proposed microstructure can be considered a two-dimensional RRN network made of two types of resistors: oxide is represented as resistors with high resistance, while low resistance resistors represent conductive paths through the oxide layer. Initially, the microstructure is fully ordered and represented as ideal resistor network which contain only low resistance resistors. We have described a solder junction with disorder structure as a two-dimensional rectangular network made of regular resistors r_{reg} disposed on a square lattice. If outermost contacts are treated as terminals made of highly conductive material, terminal resistance can be neglected and total number of resistors N_{tot} is determined by $2LN + N - L$ where N and respectively are the vertical and the horizontal size of the network (see Fig. 3). The external bias, constant voltage V or constant current I , is applied to the outermost contacts located on the opposite sides of network. The local temperatures for each resistor T_n are calculated by taking into account Joule's heating and thermal distribution between neighbouring resistors [11]. The resistance for n -th resistor ($r_{reg,n}$) is taken as a linear function of the local temperature T_n , by using temperature coefficient of the resistance α . In the presence of external bias, breakdown is simulated by replacing regular resistors with high resistance ones ($r_{reg} \rightarrow r_{hr}$ where $r_{hr} = 10^9 r_0$) where high resistance resistors are associated with non-conductive oxide inside the microstructure. In the analysed microstructure breaking resistor process is caused by disappearance of hopping mechanism. In this case, defect generation is defined as thermally activated process with probability given by:

$$W_{D,n} = \exp\left(-\frac{E_D}{K_B T_n}\right), \quad (2)$$

where E_D is the activation energy characteristic for high resistor generation, T_n is the local temperature and K_B is

Boltzmann's constant. On the other hand, recovery process which allows returning of breaking resistors to the initial state and reestablishment of hopping conductivity is given by:

$$W_{R,n} = \exp\left(-\frac{E_R}{K_B T_n}\right), \quad (3)$$

where E_R is the activation energy characteristic for defect recovery process.

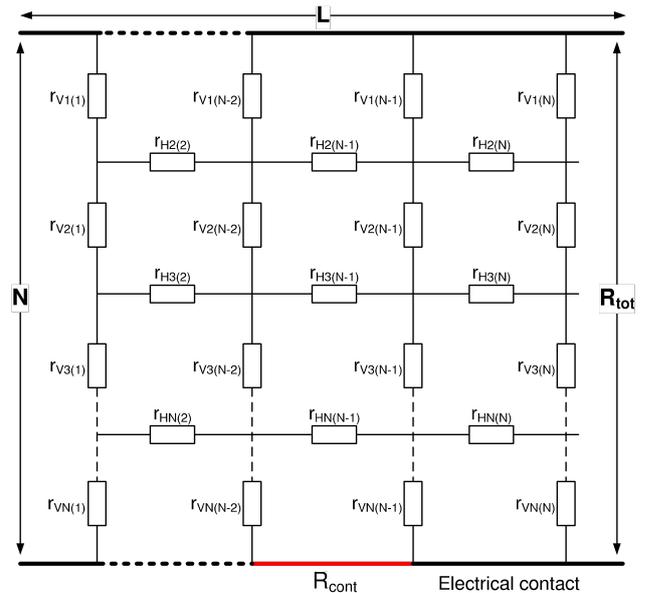


Fig. 3. RRN model used in the simulation. The length of the grid is denoted by L and width by N .

The resistance of outermost contacts R_{cont} is considered low enough to be neglected. As the most important parameter, total grid resistance R_{tot} is calculated.

3.3 Simulation procedure

MC simulation procedure starts from ideal resistor network composed of low resistance resistors and calculates local currents through the elementary resistors. Knowing the currents it is possible to calculate power dissipation, temperature and defect probabilities. Following the derived probabilities, defects are generated or recovered and new network configuration is defined. In the next step all "global" and "local" values are recalculated. Overall MC simulation procedure is implemented through the following algorithm steps:

1. Initialize RRN.
2. For each k calculate: conductance matrix, node voltages, elementary resistors currents, power dissipation and temperature.

3. Compute defect probability and generate defects accordingly.
4. Redefine conductance matrix and node voltages.
5. Calculate total resistance; if total resistance is greater than critical resistance, break.
6. Recalculate elementary resistors current, power dissipation and temperature.
7. Compute defect recovery probability, generate defects accordingly.
8. Average total resistance.
9. Repeat until k equal to number of iterations.

The main parameter of the random resistance network is the total resistance, which can be calculated using several different methods or by direct application of Kirchhoff's laws. For thin film modelling transfer-matrix formulation based on consecutive enlargement of the network in one direction by adding horizontal and vertical segments is especially suitable. According to this formulation, network of size $N \times L$ is described by the transfer matrix AL and expanded by increasing its length to $L + 1$, i.e. by adding one column of horizontal and vertical segments. Then, transfer matrix A_{L+1} in the next step can be calculated using recursive relation [10]:

$$A_{L+1} = V + A_L (I + HA_L)^{-1} \quad (4)$$

Added segments are represented by their respective vectors h_i and v_i and forming $V[N \times N]$ and $H[N \times N]$ tri-diagonal matrices calculated according to [12]. The conductance of the total network is defined as the first element of inverse transfer matrix [13]. Analogously, total resistance R_{tot} is given as:

$$R_{tot} = [A_L^{-1} (1, 1)]^{-1} \quad (5)$$

When calculation is based on iterative method, the matrix condition number grows in each calculation step. Accuracy does not significantly affect the total resistance, error on the 8th digit could cause the opposite current direction and out of range voltage. Hence, this method is not reliable for calculation of "internal" values. Internal values can be calculated by methods based on matrix of conductivity which could be formed by finite difference (node) or finite element (resistor) formulation. Although both approaches give identical matrix of conductivity as result, based on bond-resistor similarity in bias percolation system, finite element formulation is preferred [15]. After calculation of defect probabilities and defining new network configuration, transfer-matrix method is employed in

order to determine total resistance R_{tot} in the next step of MC. Combining direct and iteration methods MC simulation procedure allows sufficient accuracy and effective computational algorithm to minimize computational time and memory requirements. For larger dimensions of RRN simulation model, parallel computing is more suitable.

3.4 Simulation results

Simulation results are obtained by the previously defined MC simulation procedure where each iteration step is associated with an elementary time step at appropriate time scale. Then, simulation results for the network evolution could be represented either in time or frequency domain [16,17]. In the simulation procedure, the network evolution indicates two possible cases; breakdown when percolation threshold is reached and steady-state. Although both cases are important, in order to analyse fluctuations before breakdown occurrence we focused on the steady-state.

The simulations are performed with parameters: $N = 20$, $L = 100$, $r_0 = 3\Omega$, $\alpha = 10^{-3}\text{K}^{-1}$, $A = 5 \times 10^7 \text{K/W}$, $E_R = 0.02 \text{eV}$, $T_0 = 300 \text{K}$ and constant current bias of $100\mu\text{A}$. The bias current is approximate to typical EEG signal amplitude. To verify proposed model at different levels of disorder in RRN, activation energy of defect generation in the range of 0.04eV to 0.15eV is used as input parameter. The level of disorder in the model represents the oxide layer contribution to the conductivity of the entire solder joint. Low level of disorder is equivalent to high conductivity while high level of disorder represents pre-breakdown regime characterized by lower conductivity. Normalized fraction of defects as a measure of disorder of the RRN exhibits exponential dependence on E_D activation energy as shown in Fig. 4.

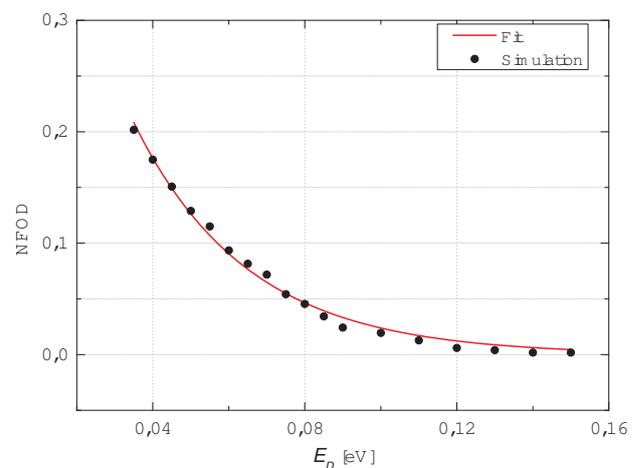


Fig. 4. Normalized fraction of defects for different values of E_D .

Simulation results are fitted to the exponential function as follows:

$$NDOF(E_D) = k_1 e^{-k_2 E_D}, \quad (6)$$

where k_1 and k_2 are coefficients of the fitted function.

Simulated results and fitted functions for the range of defect activation energy (E_D) are shown in Fig. 4.

A typical evolution of a 20×100 network in steady-state, composed of $r_0 = 3\Omega$ resistors and characterized by E_D in the range of interest from 0.04 eV to 0.15 eV, is shown in Fig. 5. A small reduction of the activation energy causes exponential increase in the fraction of defects and in the level of disorder. The higher disorder manifests itself through the formation of clusters of defects (missing bonds-resistors) characteristic for bias percolation systems. For this choice of the input parameters the fraction of defects is far from percolation threshold and steady-state is reached.

Perpendicular orientation of the defect clusters to the direction of applied bias (current) is also evident. In comparison with other bias percolation systems in this case hot-spot effect is not present due to applied low bias current which significantly reduces possibility of thermally activated defect generation process.

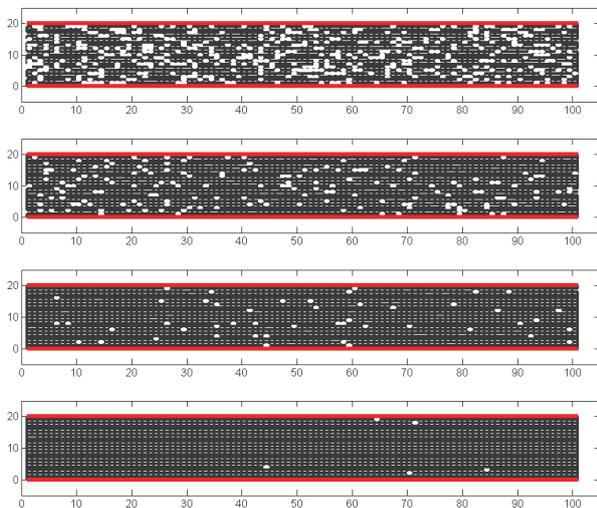


Fig. 5. Evolution of 20×100 RRN for different values of E_D which ranges from 0.04 eV to 0.15 eV from top to bottom.

Total resistance evolution of a 20×100 RRN with the same parameters used to obtain Fig. 5 are reported in the Fig. 6. All presented curves correspond to steady states or linear regime of the network with negligible probability of breakdown. A greater difference between E_D and E_R

means a lower value of the activation energy characteristic for the defect recovery process and thus a greater probability of defect recovery. This process acts contrary to defect generation process and it reduces the fraction of defects in the network, keeping the network in steady state. For each steady state curve, the resistance fluctuates around a different average value and amplitude of fluctuations is determined by the fraction of defects and the difference $E_D - E_R$. The resistance average value and the amplitude of fluctuations increase with the level disorder in the network. Although the total resistance evolution in time domain provides certain information about RRN regime, the analysis of the distribution function of resistance fluctuations is more suitable for insight into the structure of the network.

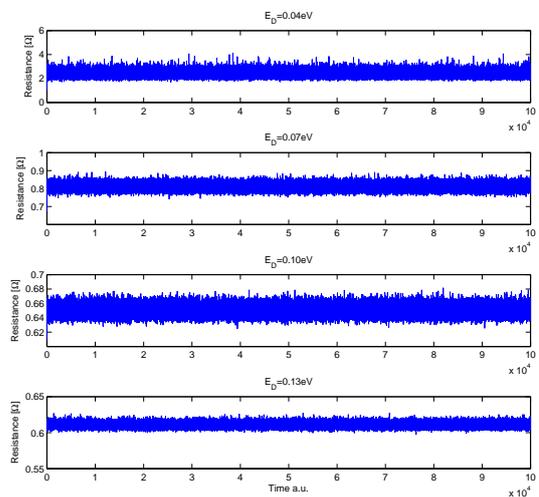


Fig. 6. Resistance evolutions for different values of E_D difference which ranges from 0.04 eV to 0.15 eV from top to bottom.

Figure 6 shows distribution functions for different values of activation energies and same input parameters used for steady state curves in Fig. 6. For low level disorder of the network ($E_D = 0.15$ eV) resistance fluctuations have a minimum amplitude and fluctuation distribution function is close to Gaussian distribution. By contrast, increasing level disorder of network causes higher values and non-Gaussian fluctuations of resistance with enhancement of probability for negative fluctuations with respect to Gaussian distribution. This non-Gaussian behaviour of fluctuation amplitudes increases with increasing fraction of defects in RRN which can be generated by bias, temperature or other degradation process. Therefore, distribution function of resistance fluctuations can be used to estimate the formation of clusters in RRN structure while non-Gaussian

behaviour may signal pre-breakdown regime and can be considered a relevant precursor of failure.

According to the input parameters, bias current and substrate temperature is not sufficient to increase defect generation probability which implies that only degradation can cause high level of disorder and finally breakdown. This scenario corresponds to behaviour of EEG electrodes where cold solder may occurs during the lifetime.

In Fig. 7 (a) simulation results for the probability density function (PDF) of resistance fluctuations are given and qualitatively compared with theoretical distributions; Gaussian and Bramwell-Holdsworth-Pinton (BHP) distribution [18]. It is evident that for higher activation energy E_D , PDF shows Gaussian-like behavior. Reducing the difference between activation energies ($E_D - E_R$) increases the probability of negative fluctuations (distribution tail) and simulated PDF converges towards the theoretical BHP distribution.

In Fig. 7 (b) the PDF of resistance fluctuations for a narrow range of activation energies (E_D) is given. It is clearly shown the transition from Gaussian to BHP distribution. The transition curves related to the distribution tail region are denoted by elliptic area.

The distribution tail is primarily controlled by the fraction of defects and can be quantified by using left asymptote of the BHP distribution:

$$\Pi(x) \propto |x| \exp\left(-\frac{\pi}{2}bx\right), \quad (7)$$

where b is the BHP distribution parameter and x is the normalized fluctuation signal.

In this sense, the functional dependency of the parameter b on the activation energy E_D is computed and the results are shown in Fig. 8. Simulation results are fitted to the exponential function as follows:

$$b(E_D) = k_3 + k_4 e^{-k_5 E_D}, \quad (8)$$

where $k_3 - k_5$ are coefficients of the fitted function.

For activation energy under the value of 0.05 eV the BHP parameter b abruptly increases and the RRN network approaches the pre-breakdown region.

Thus, the analysis of the distribution functions shows that the level of disorder in RRN can be estimated from the resistance fluctuations. This fact is the main advantage of this model, which provides the possibility of getting an insight into the order of the structure based on the behaviour of macroscopic quantities. Therefore, it is reasonable to propose RRN model as breakdown or failure prediction tool in disordered structures with two phase conductivity behaviour.

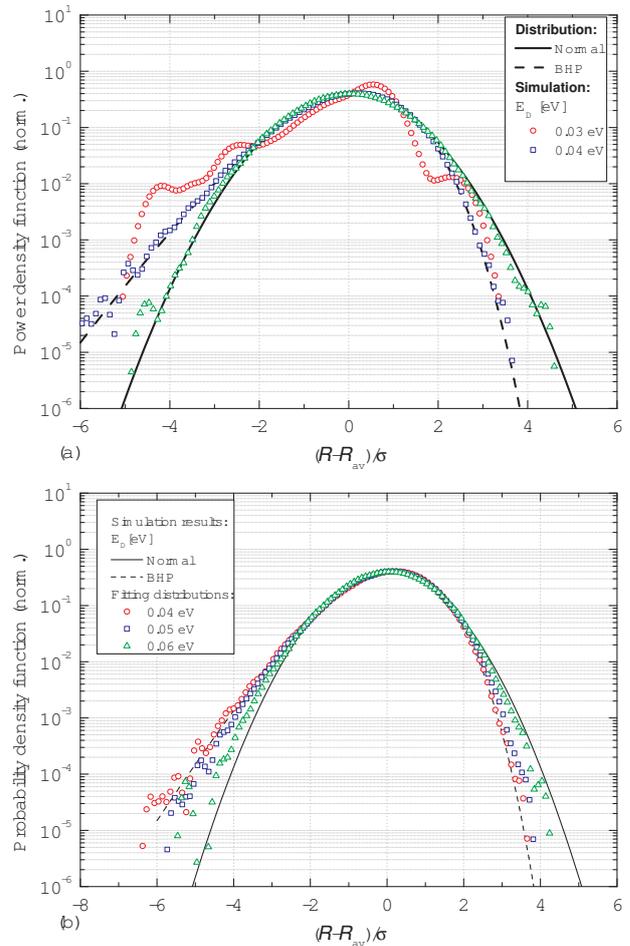


Fig. 7. Distribution functions of the resistance fluctuations for different values of E_D in the range: (a) from 0.03 to 0.09 eV; (b) from 0.04 to 0.06 eV.

4 MEASUREMENT RESULTS AND DISCUSSION

In order to verify proposed model and algorithm as failure prediction tool, measurements on several commercial EEG electrodes under laboratory test conditions are performed. Building upon simulation results from previous section that show non-Gaussian behaviour of resistance fluctuations and discontinuous distribution of energy over time in pre-breakdown regime, we investigate the resistance fluctuations of commercial EEG electrodes by focusing on the same type of behaviour. Resistance fluctuation measurements are performed on Corkscrew electrodes previously tested by the manufacturer with the label of validity, while obtained experimental results are analysed in order to compare them with simulation results presented in previous section. According to the behaviors given in Fig. 9 and Fig. 10 the experimental results show the Gaussian behaviour for valid electrodes and the non-Gaussian

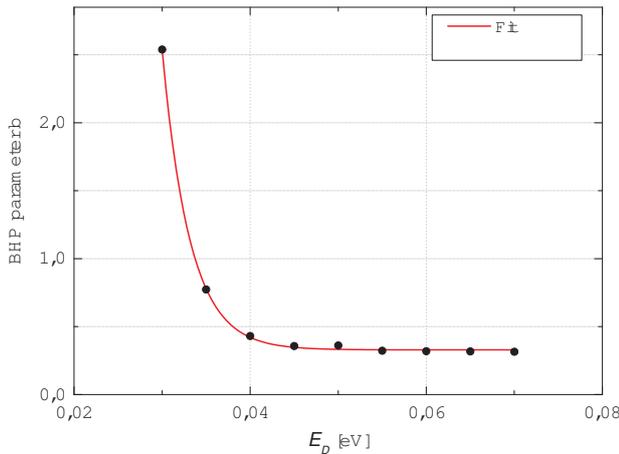


Fig. 8. BHP parameter b as a function of different values of E_D .

behaviour for faulty ones.

In a first step of model verification, two electrodes labeled as valid are taken as references and compared with simulation results. Reference electrodes have identical Gaussian behaviour of resistance fluctuations as a RRN network with low level of disorder. A condition associated with a high hopping probability and good conductivity of the oxide layer in the solder joint, equivalent to ideal RRN.

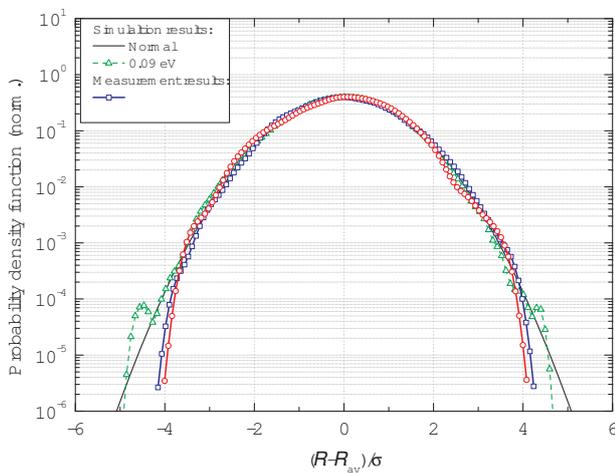


Fig. 9. Distribution functions of the resistance fluctuations for the reference (valid) electrode and low disorder RRN.

In the next step, the identical measurements are applied to two faulty electrodes and compared to simulation results obtained for a network with high disorder level. The experimental results reported in Fig. 10 (a) and (b) show enhancement of probability for negative fluctuations ("distribution tail"). They are identical to simulation results for

high disordered networks characterized by high E_D activation energy. Non-Gaussian behaviour shown as "distribution tail" indicates high fraction of defects in the oxide layer and evolution toward percolation threshold or breakdown. Hence, the deviations of the Gaussian distribution could be indicator of the pre-breakdown regime and possible failure in the EEG electrodes.

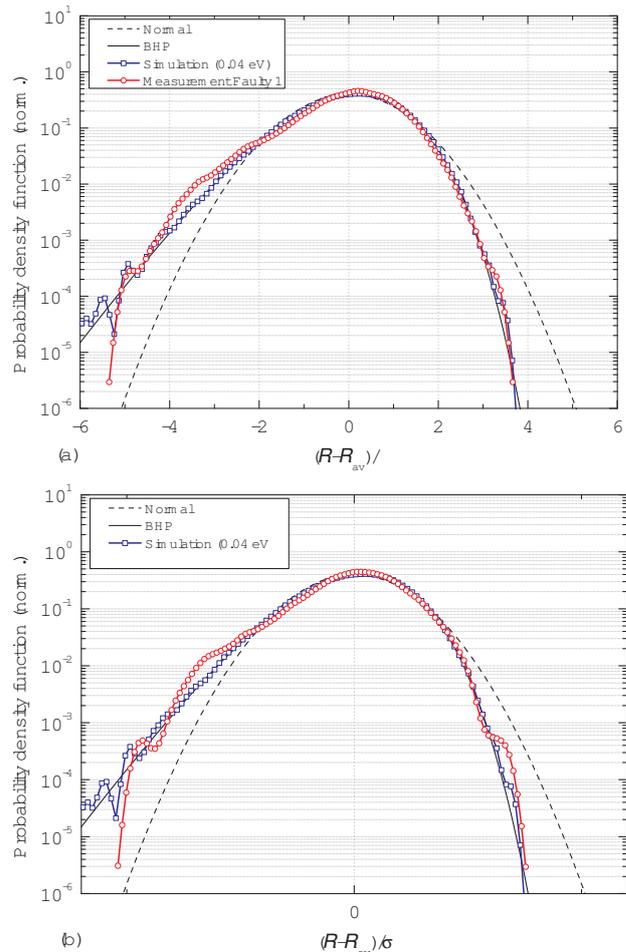


Fig. 10. Distribution functions of the resistance fluctuations for the valid electrode taken as the reference electrode 0.045 eV.

The values for parameter b given in Table 1. are derived from the graphs shown in Fig. 10. The value of b for fault electrodes is in pre-breakdown region, Fig. 8.

Table 1. BHP parameter b extracted from measurements data of EEG electrodes

Electrode sample	BHP parameter b
Faulty 1	0.6061
Faulty 2	0.4164

5 CONCLUSION

In this paper we presented a simulation model and an algorithm for possible use in medical EEG electrodes failure prediction. Here we investigated the possibility of modelling cold solder joint with focus on the prediction of failure in order to avoid faulty electrodes emerging on the market. The proposed simulation model is based on the grid resistors vertically and horizontally aligned which is known as random resistance network (RRN) model and in particular on the biased percolation model [3,6,11]. Computational algorithm is implemented through the Monte-Carlo simulation procedure by combining direct and iteration method for the total resistance calculation.

In simulation results we primarily focused on the resistance fluctuations over the time for wide range of the defect fraction which defines the level of disorder in the network. Obtained results indicate that both the total average resistance and the resistance fluctuations increase with the level of disorder in the network and that this disorder clearly manifests itself in the non-Gaussian behaviour of the fluctuation distribution. This emergence of non-Gaussian behaviour in the pre-breakdown can be considered a relevant precursor of failure. Similarly, non-Gaussian behaviour is found in the experimental results where the oxide layer presence in the solder joint causes enhancements of the negative resistance fluctuations.

The distribution of the resistance fluctuations in low level disorder RRN and valid electrodes is close to Gaussian behaviour, with identical amplitude and other distribution parameters. Energy distribution of the resistance fluctuations in time-frequency domain is also analysed with partial correspondence in simulation and experimental results. It was concluded that the behavior of the fluctuations distribution can be considered a measure of the fraction of defects in the researched structure and an indicator of the pre-breakdown regime, with possibility of the failure in the future.

From the resistance fluctuations distribution shape it has been derived the special parameter (quality index) allowing us to assess whether the EEG electrodes within the interval of tolerance have been acceptable or not. By the proposed method it is possible to predict both the failure and long-term stability of the electrode.

Furthermore, the obtained results could be used as a good starting point in failure prediction for many electronic devices having the oxide layer in the structure.

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