MODEL OF ELECTRIC CONDUCTIVITY OF THICK-FILM RESISTORS
II. SIMPLE COMPUTER MODEL

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The paper deals with a simple computer model of the quasihomogeneous structure of thick-film resistors (TFR). The results of computer experiments were used to quantify some parameters describing the geometry of this structure. A comparison with experimental data obtained by measuring the real films showed a satisfactory agreement with respect to the meandrine character of the backbone and with that to the effective angle introduced in the first part of the present paper.

1. INTRODUCTION

From the standpoint of macrostructure, thick-film resistors (TFR) are composites comprising a fine-grained conductive component at volume concentration v (in most cases some oxidic compound of ruthenium such as Ru_2O, $Bi_2Ru_2O_7$, $Pb_2Ru_2O_6$) dispersed in a glassy matrix. The actual structure of the films, i.e. the distribution topology of the conductive particles, depends primarily on the firing temperature and the parameters of the glass employed [1]. In principle, it is possible to distinquish two limit cases of the film structure. One is the so-called segregated structure with the conductive particles distributed over the surface of substantially larger glass particles [2], the other being the so-called quasihomogeneous structure in which the distribution of conductive particles is close to a homogeneous one, more precisely to a statistically random dispersion in the glass which takes place in the course of firing [3] . The conditions under which these structures are formed were described in [1] and their properties, studied from the standpoint of the percolation theory, in [5 ,6]. In the present study, we shall only be concerned with the quasihomogeneous structure. The random distribution of conductive particles in the film has the result that the local directions of electric field contain an angle, Θ_i (Fig. 1). Within the framework of the model, attention will be paid to some geometrical properites of the backbone of the conductive cluster. The backbone is undesrtood to mean the first conductive path which, at increasing concentration of the conductive phase in the film, will connect (in the direction of the external electric field) the two opposite sides of the model (specimen). The critical volume concentration of the conductive component at which the conductive backbone is formed, is designated v_c in the percolation theory. A concentration growth over the $v > v_c$ region results in the formation of additional conductive paths acting parallel with the backbone or its sections. According to our concept of the mechanism of conductivity in TFR [6, 7, 8], the backbone becomes electrically conductive once its longest section (distance between neighbouring conductive particles) is smaller than a certain critical distance l_c, while l_c is larger than the sum of the radii of the neighbouring particles.

2. THE MODEL

The model was realized on a PC-AT computer. Using a generator of pseudorandom numbers, N points with coordinates $(x_k,\ y_k,\ z_k)$, representing the centres of conductive particles, were placed in a chosen volume $1\times1\times d$, where d is the thickness. The particles are assumed to have a spherical shape with a constant diameter. In such a structure of random-dispersed points, a backbone of the conductive cluster, composed of m sections l_i in length was seeked, namely connecting lines between neigbouring points in the backbone, having the coordinates $(x_{i-1},\ y_{i-1},\ z_{i-1})$ and $(x_i,\ y_i,\ x_i)$. The voltage applied shall have the direction of coordinate x, which means that the respective backbone will connect the model sides with $x = 0$ and $x = 1$. The backbone is defined as follows: For all $x_k > x_{i-1}$

1. $l = x_1 = \min(x_k),\ x_0 = 0$
2. for $1 < i < m-1$,
$$l_i = \min\left[(x_k - x_{i-1})^2 + (y_k - y_{i-1})^2 + (z_k - z_{i-1})^2\right]^{1/2},$$
3. $l_m = 1 - x_{m-l}$, when
$$1 - x_{m-1} < \min\left[(x_k - x_{m-1})^2 + (y_k - y_{m-1})^2 + (z_k - z_{m-1})^2\right]^{1/2}$$

The total backbone length is $l = \sum l_i$. Similarly to the study [8], let us introduce the "meandrine factor" of the backbone as the ratio of its length to that of the model (specimen). To eliminate errors due to the first and last sections, with smaller numbers m of sections, as the former are parallel with coordinate x, the

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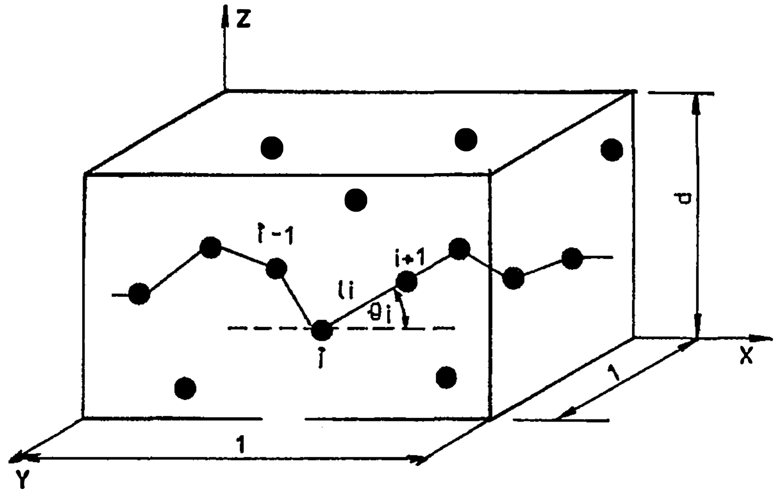

Fig. 1. Introduction of angle Θ_i into the model employed.

meandrine factor M is calculated from the equation

$$M = \left(\sum_{i=2}^{m-1} l_i\right) / (1 - l_1 - l_m) \, . \quad (1)$$

Then there is the mean distance between the points in the backbone:

$$\langle l_i \rangle = m^{-1} \sum_{i=1}^{m} l_i \, , \quad (2)$$

which, as has already been shown, in the case of dimensional effects plays a role similar to the mean free path of charge carriers in homogeneous conductors. Finally, calculations were made of effective angle Θ_{ef}, introduced in Part I of the present study, within the framework of the piezoresistivity theory, as a certain mean value of angles contained between the directions of local electric currents and the vector of the external electric field:

$$\Theta_{ef} = \arccos \left[(m-2)^{-1} \sum_{i=2}^{m-1} \cos^2 \Theta_1\right]^{1/2} \, . \quad (3)$$

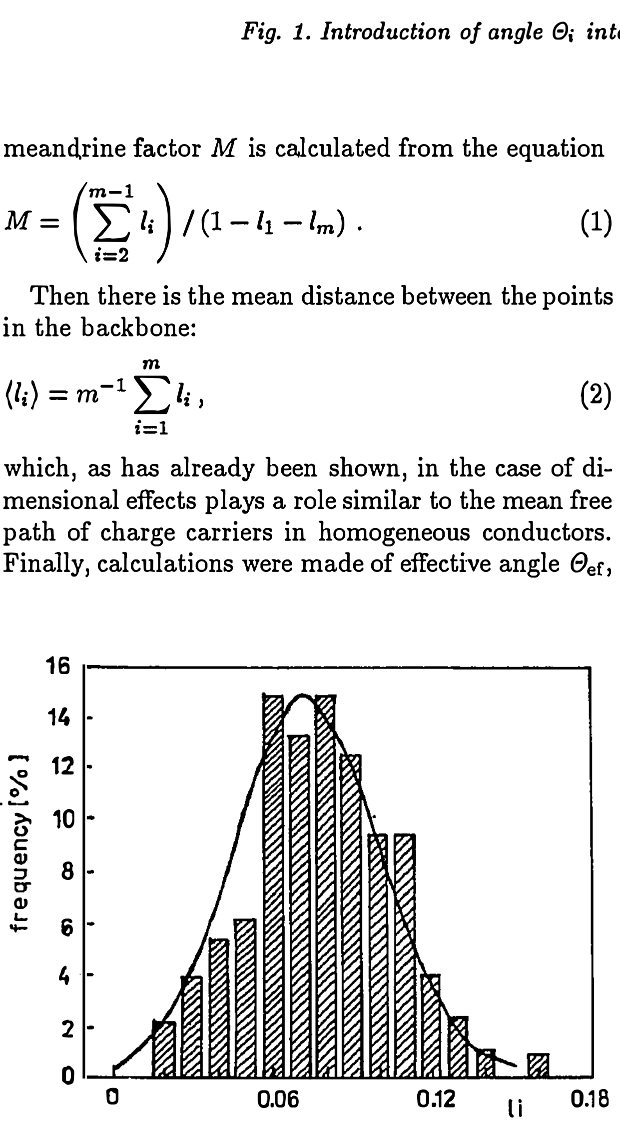

Fig. 2. An example of probability density of standard distribution obtained from the mean value of $\langle l_i \rangle$ and dispersion σ for a five-times repeated model with $n = 1000$, in comparison with a histogram of actual distribution.

3. RESULTS

The first stage was concerned with models of cube form ($d = 1$) which contained various numbers of points from the $N \in \langle 100, 16000 \rangle$ interval. It was found that the lengths, l_i, of the individual backbone sections are subject to standard distribution (Fig. 2) with parameters ($\langle l_i \rangle$, σ) and variation coefficient $\sigma / \langle l_i \rangle = 0.36 \pm 0.02$, independent of the number of points N. The effect of volume V of the cube-shaped model was verified at the same time (with a wall length other than unity). As logically expected, the concentration of points $n = N/V$ and not their number proved to be the characteristic quantity for describing the model. The mean value of the distance between two points in the backbone is well described by the equation

$$\langle l_i \rangle = (0.74 \pm 0.03) \, n^{-1/3} \, . \quad (4)$$

Similarly, there is the relationship between the number of points m in the backbone and concentration n:

$$m = 2.5 n^{1/3} \, ,$$

which, including its dispersion, is plotted in Fig. 3. Independently of concentration n and the dimension of

54.9 found by modelling; in both instances the effective angle was defined by equation (3). The term meandrine factor of conductive paths in TFR was used by the authors of [8] who obtained $M \in \langle 1.66, 1.92\rangle$ or $\langle 1.78, 2.04\rangle$ (according to the chosen value of the Poisson film modulus) by applying their piezoresistivity theory on the results of measuring films prepared from commercial pastes. The agreement with the value established by modelling, $M = 1.86$, can be considered very satisfactory. The fact that according to the results published in [8], the meandrine factor, unlike the modelling results, depends on planar resistivity of layers and the concentration of the conductive phase, can be explained so that these concentrations in the commercial pastes employed differ substantially from v_c.

5. CONCLUSION

The simple computer model of a quasihomogeneous structure of TFR allows the topology of the skeleton of the conductive cluster to be precisioned, particularly with respect to its backbone. The comparisons of values of M and Θ_{ef} parameters obtained by modelling exhibit a very satisfactory agreement with the results of experiments carried out on actual resistor films. The parameters obtained, in particular Θ_{ef} and M, as well as the distribution of l_i and the relationship between $\langle l_i\rangle$ and the concentration of conductive particles n, appear to be highly promising for utilization in further theoretical investigations.

References

[1] Kubový, A., Havlas I.: Silikáty *32*, 109 (1988).
[2] Bigers J.V., McKelvy J.R., Schulze W.A.: J. Amer. Cer. Soc. *65*, 13 (1982).
Inokuma T., Taketa Y., Haradome M.: IEEE Trans. Comp. Hybrids and Manufact. Technol. CHMT-7, 166 (1984).
[3] Nordstrom T.V., Hills C.R. in: Proc. Inst. Microel. Symp. Los Angeles 1979, p.40.
[4] Kirkpatrick S.: Rev. Mod. Phys. *45*, 574 (1973).
[5] Kubový A.: J. Phys. D: Appl. Phys. *19*, 2171 (1986).
[6] Kubový A.: Silikáty *32*, 289 (1988).
[7] Kubový A., Stefan O.: Thin Solid Films *135*, L9 (1986).
[8] Winkler E.M., Steenvoorden G.K.: Thin Solid Films *152*, 487 (1987).

MODEL ELEKTRICKÉ VODIVOSTI TLUSTOVRSTVÝCH RESISTORŮ

II. Jednoduchý počítačový model

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Jednoduchý počítačový model je založený na generaci N bodů (reprezentujících vodivé částice) do zvoleného objemu s pomocí generátoru pseudonáhodných čísel. Ve vytvořené struktuře je hledána páteř vodivého klasteru (perkolační struktury). Jednotlivé modely jsou chrakterizovány koncentracemi bodů. Pro páteř byla počítána střední hodnota $\langle l_i\rangle$ vzdálenosti sousedních bodů podle vztahu (2), meandrovitost M definovaná vztahem (1), počet bodů m a efektivní úhel zavedený v první části této práce [9] rovnicí (3). Výsledkem počítačových experimentů jsou vztahy (4) a (5) mezi střední vzdáleností $\langle l_i\rangle$ a koncentrací n, hodnoty efektivních úhlů $\Theta_{ef}(3D) = 54.9 \pm 1.3$ deg a $\Theta_{ef}(2D) = 42.0 \pm 0.4$ deg, meandrovitosti $M(3D) = 1.86 \pm 0.03$ a $M(2D) = 1.48 \pm 0.02$. Z výsledků studia rozměrových jevů (obr. 4) a odhadu $\langle l_i\rangle$ pro reálné vrstvy s tloušťkami kolem 15 μm bylo zjištěno, že se běžné vrstvy TFR chovají jako 3D struktury. Uvedené porovnání s experimentálními hodnotami Θ_{ef} z první části této práce a M [8], získanými měřením reálných vrstev, ukazuje na dobrý souhlas a to opravňuje k přesvědčení, že výsledky počítačových experimentů jsou použitelné v různých teoretických odhadech.

Obr. 1. Způsob zavedení úhlu Θ_i v použitém modelu.

Obr. 2. Příklad hustoty pravděpodobnosti normálního rozdělení získané ze střední hodnoty $\langle l_i\rangle$ a rozptylu σ pro 5× opakovaný model s $n = 1000$ v porovnání s histogramem skutečného rozdělení.

Obr. 3. Závislost počtu bodů m v páteři na jejich koncentraci n v 3D struktuře.

Obr. 4. Rozměrové jevy nalezené pro meandrovitost M a efektivní úhel Θ_{ef}.