NUMERICAL MODELLING OF ELECTRIC CONDUCTANCE OF A THIN SHEET

M. Kollár, J. Franek

*Slovak University of Technology, Faculty of Electrical Engineering and Information technology,
Department of Electromagnetic Theory*
e-mail: mojmir.kollar@stuba.sk, jaroslav.franek@stuba.sk

Summary In this paper the numeric modelling of total resistance of a thin sheet, with local conductivity in randomly distributed grains higher then is that of the basic matrix, is presented. The 2D model is formed by a structure of longitudinal and transversal conductors interconnected in nodes of a square net. In all nodes, using iteration procedure, the potential is determined from which the conductance of sheet is computed between two touching electrodes. The described model can be used to imitate the behaviour of heterogeneous thin conducting sheets prepared by different techniques. The model was verified in some cases where the net resistance is well known from the theory.

1. INTRODUCTION

During the preparation of thin conducting sheet (for instance magnetic or other) samples, beside other parameters also their total conductance is often monitored. The results of such measurement are of primary interest namely if the samples are not electrically homogenous. Even though in the sheet a material with known conductivity may be dominant, during its preparation, there may appear (due to phase transition) more or less randomly distributed grains with different conductivity, see Fig. 1, [1]. One may expect that with the growth of the volume part having different conductivity then has the ambient material, the total conductance of the sheet (measured between two touching electrodes) will be an important characteristic of the whole process. However there is certain evidence of somewhat irregular nature during the growth of the grains with a higher conductivity [2]. The thickness of these sheets is typically around hundreds or less nm.

From a standpoint of the electric conductance (resistance) as measurement on area, excited by that purpose, with the cross dimensions of several mm – in the presented contribution we are engaged with (computer) modelling of a 2D square-network. Between each pair of neighbouring nodes a local conductor (resistor) is defined. The edge points of this net (in contrast to internal ones, each having 4 neighbours) have only three, and the four corner-points only two neighbours. At two distinguished locations in the net (connection of the measuring electrodes) there are sets of points with known potential. After the potential of all remaining nodes is evaluated it is simple to determine the current flowing to or from each of the electrodes, and consequently, the total resistance (conductance) that would be measured between them. The properties of such a model are to a substantial extent determined by the rules which govern the distribution of grains with lower/higher conductivity (their location and dimensions) on an area with otherwise homogeneous (and higer/lower) conductivity.

2. THEORY AND MODEL

The aim of numeric modelling is to determine the electric conductance (resistance) between two electrodes (sets of selected nodes) on a square area. Evaluation of the potential in individual nodes of the net, indexed by rows and columns as i, j (*ie* matrix $I \times J$) is based on so-to-say, algorithm for the electric circuit solution by the well commonly known node voltage method [3].
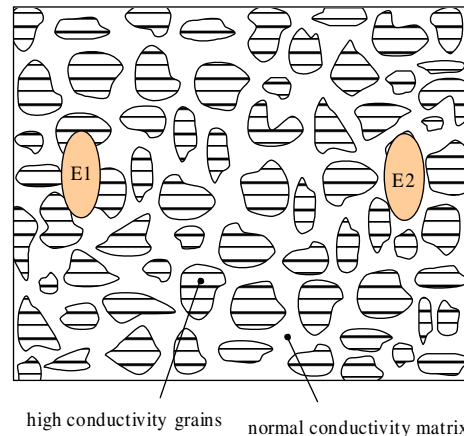

Fig. 1. Figuring the "conductivity" structure of a thin sheet and placement of two electrodes E_1 and E_2, used to measure the resistance or conductance in-between.

The potential of any internal node having four neighbours (excluding those under the electrodes), is given by expression

$$\varphi_{i,j} = \frac{\varphi_{i+1,j} GT_{i,j} + \varphi_{i-1,j} GT_{i-1,j} + \varphi_{i,j-1} GL_{i,j-1} + \varphi_{i,j+1} GL_{i,j}}{GT_{i,j} + GL_{i-1,j} + GL_{i,j-1} + GL_{i,j}}$$
(1)

and the potential of nodes at the upper edge ($i = 1$) each having three neighbours, respectively of the left upper corner ($i = 1$, $j = 1$) node which has only two neighbours is

$$\varphi_{1,j} = \frac{\varphi_{2,j} GT_{1,j} + \varphi_{1,j-1} GL_{1,j-1} + \varphi_{1,j+1} GL_{1,j}}{GT_{1,j} + GL_{1,j-1} + GL_{1,j}}$$
(2)

$$\varphi_{1,1} = \frac{\varphi_{2,1} GT_{1,1} + \varphi_{1,2} GL_{1,1}}{GT_{1,1} + GL_{1,1}} \qquad (3)$$

where $GT_{i,j}$ a $GL_{i,j}$ are the local conductivities in transversal and longitudinal directions (relative to the electrode position, compare Fig. 2). For other edge and corner nods similar expressions are easily obtained. The mesh (of resistors) is organized in such a way that matrix GT is I-1$\times J$ while matrix GL is $I \times J$-1.

In the case of isotropic conductivity there would be no difference between GT and GL elements, of course unless their values are not (random) position dependent from some other reason. In general formulae (1) to (3) are consistent with electrically isotropic and non-homogeneous sheets; and in a special case: with homogeneous but anisotropic (all the $GT_{i,j}$ are same, all $GL_{i,j}$ are same, but $GT_{i,j} \neq GL_{i,j}$), or homogeneous and isotropic (all of $GT_{i,j} = GL_{i,j}$). In the last case the formulae (1) to (3) will change to

$$\varphi_{i,j} = \frac{\varphi_{i+1,j} + \varphi_{i-1,j} + \varphi_{i,j-1} + \varphi_{i,j+1}}{4},$$

$$\varphi_{1,j} = \frac{\varphi_{2,j} + \varphi_{1,j-1} + \varphi_{1,j+1}}{3} \text{ and } \varphi_{1,1} = \frac{\varphi_{2,1} + \varphi_{1,2}}{2},$$

what are terms well known as the numerical solution of Laplace equation $\Delta \varphi = 0$, in an homogeneous, isotropic 2D surrounding. Let us note, that terms (2) and (3) are in fact reflecting the so called Neuman boundary condition (anticipation that only tangential component of current at the edge of conducting area exists) and are thus given by extrapolation in the vicinity of the border, where the required invariant normal component of the potential is essential. By other words, if in (1) for $i = 1$, (*ie* on the upper border) we shall introduce an „mirror assumption" according to which in the outside points behind this border (in an extended matrix index $i = 0$ would be appropriate), it will hold $\varphi_{0,j} = \varphi_{1,j}$, and also $GT_{0,j} = GT_{1,j}$ and we get (2) directly from (1). Similarly one can attain (3).
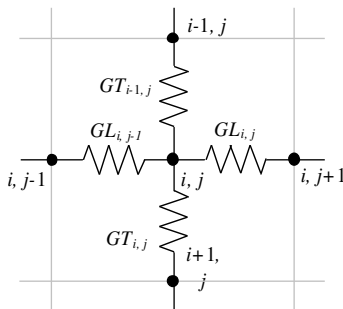

Fig. 2. A cell simulating local conductivity structure

To solve linear set of equations (1) to (3) one can advantageously use an iteration (relaxation) method. After creating initial matrix of the potential values (could be of zero, or randomly distributed, or similar) a new matrix is calculated, meanwhile in the

procedure it must be taken into account if the actual element of matrix is not that of the node under the electrode or the edge or corner node or eventually if it belongs to an internal node. After a sufficient number of the steps, when the matrix elements (node potentials) are changing only slightly, the procedure is finished. However, for solving the above set of equations we have used two different procedures. One of them (A) allowed arbitrary placement of the electrodes (in interior of the sheet) second (B) allows only to put them on the sheet edges. The first method (A), in which the iterations were performed left to right and then down in the matrix as a whole, usually needed more iterations and, in some cases gave somewhat different values of the total sheet conductance when computed from the "currents" of the first or the second electrode respectively. The second (B), uses rather a sophisticated way in which the iterations along the border and in interior of the sheet are performed as two separate procedures and not always node repeated one directly after another. Using the latter treatment, after the same number of iteration cycles as in the previous one, the results received at both electrodes were much closer to each other, unless the length of individual electrodes was markedly different. These differences faded away in both methods when a finer mesh was introduced, nevertheless on account of inconvenient computing time consumption. The results presented in this paper were obtained in the MathCad [4] environment. Typical were $J = 61$, $I = 41$, and several hundreds of iteration steps. To approve the refinement of the mesh we have used in some instances as high values as $J = 601$, $I = 401$, and sometime also extended iterations up to several thousand of cycles.
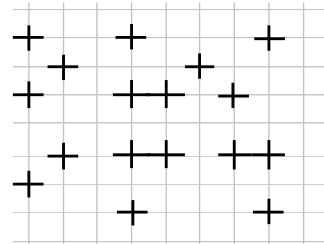

Fig. 3. Depicting random distribution of grains with a higher conductivity (represented by cells from Fig. 2) as the scattered crosses in the original matrix background.

An important feature of the model is the way how we inject the grains with a higher conductivity into original homogeneous sheet, and how this will be reflected by the magnitude of the conductances (resistors) in the mesh. One of the used modes (in Variant 1) prescribed the inclusion of a quaternion (4 resistors from Fig. 2) with a higher longitudinal and transversal conductivity to every k–th cell counting in transversal direction, and inclusion of the same into every m–th cell, counting in longitudinal direction. If $k = m$ the cells with a

higher conductivity form a square mesh, which is (in comparison with the basic grid) the more sparse, the greater are the numbers (k, m). If $k, m = 1$, all the resistors (local conductances) in mesh are of the high values and the „background" with a lower conductivity disappears. Normally one would of course rely rather on a random distribution.
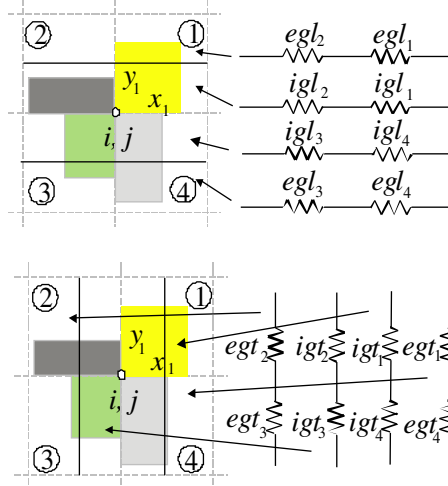

Fig. 4. To modelling of random distribution of grains with higher longitudinal conductivity (up), and higher transversal conductivity (down), in all four quadrants of a cell.

Another way (Variant 2) for alternative use may be explained as follows. In Fig. 4 there are shown four quadrants of an area to be represented by one cell of (four) resistors. The dimensions of the suppositional grain in each quadrant (1 to 4) are generated as

$$x_v = L + (1-L) \cdot rnd(l)$$
$$x_v = T + (1-T) \cdot rnd(t). \tag{4}$$

Parameters L, l and T, t determine to what extent these are random or regular. When the random number generation is suppressed ($l = 0$, $t = 0$) the "reduced" dimensions $L, T \leq 1$ are deterministic. If only random "growth" is desired ($L= 0$, $T= 0$) values of $l, t \in (0,1)$ are the appropriate seed. Note that each quadrant is large 1×1. Now, according to scheme in Fig. 4 we have

$$egl_v \leftarrow if\left(y_v > \frac{1}{2}, 1-y+\frac{y-1/2}{1-kx}, \frac{1}{2} \right)$$

$$igl_v \leftarrow if\left(y_v > \frac{1}{2}, \frac{1/2}{1-kx_v}, \frac{1}{2}-y_v+\frac{y_v}{1-kx_v} \right)$$

$$egt_v \leftarrow if\left(x_v > \frac{1}{2}, 1-x_v+\frac{x_v-1/2}{1-ky_v}, \frac{1}{2} \right) \tag{5}$$

$$egl_v \leftarrow if\left(y_v > \frac{1}{2}, \frac{1/2}{1-ky_v}, \frac{1}{2}-x_v+\frac{x_v}{1-ky_v} \right)$$

providing that individual resistors are proportional to areas depicted in Fig. 4, and combined in series and/or in parallel accordingly. Parameter $k = 1- \varepsilon$ where the ratio $\varepsilon = low\_conductivity / high\_conductivity$

stands for the material properties. To get from (5) only four resistors describing one cell (like in Fig. 2), we add the interior (igl, igt) conductances in each (i, j) cell individually, whilst the edge (egl, egt) elements are composed from the adjacent areas with centres at: i, j and $i+1, j$ and $i-1, j$ and $i, j+1$ and $i, j-1$, taking a special care of those belonging to the edge or corner areas. An example of GL and GT matrix for $I = 5$ and $J = 7$ is given below for $T = L = t = l = 0.5$

$$GL = \begin{pmatrix} 0.513 & 0.579 & 0.521 & 0.526 & 0.549 & 0.575 \\ 1.437 & 1.521 & 1.531 & 1.525 & 1.522 & 1.404 \\ 1.08 & 1.131 & 1.141 & 1.189 & 1.08 & 1.177 \\ 1.535 & 1.391 & 1.428 & 1.431 & 1.466 & 1.509 \\ 0.569 & 0.549 & 0.528 & 0.514 & 0.528 & 0.513 \end{pmatrix}$$

$$GT = \begin{pmatrix} 0.513 & 1.437 & 1.138 & 1.373 & 1.134 & 1.492 & 0.517 \\ 0.575 & 1.402 & 1.162 & 1.457 & 1.199 & 1.51 & 0.565 \\ 0.57 & 1.486 & 1.158 & 1.551 & 1.094 & 1.408 & 0.6 \\ 0.595 & 1.464 & 1.014 & 1.386 & 1.103 & 1.37 & 0.55 \end{pmatrix}$$

the same, in case $T = L = t = l = 0$ corresponds to matrices with original conductances (with no newly created grains)

$$GL = \begin{pmatrix} 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 0.5 & 0.5 & 0.5 & 0.5 & 0.5 & 0.5 \end{pmatrix}$$

$$GT = \begin{pmatrix} 0.5 & 1 & 1 & 1 & 1 & 1 & 0.5 \\ 0.5 & 1 & 1 & 1 & 1 & 1 & 0.5 \\ 0.5 & 1 & 1 & 1 & 1 & 1 & 0.5 \\ 0.5 & 1 & 1 & 1 & 1 & 1 & 0.5 \end{pmatrix}$$

while in case of $T = L = 1$ and $t = l = 0$, the whole sheet has been changed to a homogenous one grain state with a higher conductance. In these examples $\varepsilon = 1/2$.

$$GL = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \quad GT = \begin{pmatrix} 1 & 2 & 2 & 2 & 2 & 2 & 1 \\ 1 & 2 & 2 & 2 & 2 & 2 & 1 \\ 1 & 2 & 2 & 2 & 2 & 2 & 1 \\ 1 & 2 & 2 & 2 & 2 & 2 & 1 \end{pmatrix}$$

In the cases, with even distribution, the edge elements are one half of those in interior as they appropriately pertain to the occupied areas, compare Fig. 4.

3. TESTING THE MODEL

The reliability and exactness of the used numeric procedure (the mesh density, number of iterations *etc*) was tested by comparing the numerical solution with several cases of known potential distributions. Two of them are given below, both described by equal and unit GL and GT matrices.

• In the first case we considered two electrodes on the opposite edges of a rectangular area with 2:3 side ratio. After about hundred of iterations the numerical result in method A (in matrix 61×41) agreed with the theoretical value to six decimal places. Using method B, gave somewhat worst results (matching to 2 digits in a matrix 61×41 and to 3 digits in a matrix 601×401).

• The second test was in determining the resistance between two adjacent points of an infinite square mesh with equal resistors R (possible only in method A). Theory gives a simple result $R/2$, and after around 600 iterations in a mesh of 61×41 elements the result was as close as 0.99953 of this value.

4.   EXAMPLES OF SIMULATION RESULTS

Variant 1 — To explain what a behaviour one can expect with a random distribution as depicted in Fig. 3. It is essential to check a situation with even distributions of type: k/m = 1/1,1/2, 2/1, *etc* as given in table   below. The values given in table are conductances G_{E1}/G_{E2} as determined from the "currents" of first and second electrode respectively (should be equal) after 100 and 1000 iterations. Small numbers k, m mean higher density of the high conductivity cells.

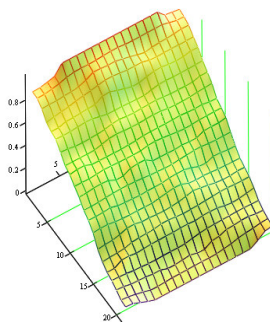| k/m	100 steps	1000 Steps
1/1	39.87/39.87	
1/2	20.45/20.74	
2/1	2.35/1.53	2.151/1.742
2/2	2.13/1.49	1.944/1.663
2/3	1.84/1.37	1.683/1.494
3/2	1.61/1.63	
3/3	1.48/1.47	

Fig. 5. Distorted potential distribution with grains developed most in longitudinal direction.

As expected, a sparse distribution of the higher conductivity cells leads to a lesser net conductance. However, distributions 1/2 and 2/1 which are of "equal surface density" result in markedly different net conductance due to formation of the current conducting paths in case 1/2, in contrast to case 2/1, when these paths are perpendicular to the main current stream. The difference at 2/3 and 3/2 is of course not so pronounced. Even in a case of random distributions under certain circumstances, particular-

ly at the beginning of grain creation this may be an useful indicator.

Variant 2 — With parameters $L = 0.9$, $T = 0.1$ and $l = 1$, $t = 1$ we get G_{E1}=2.859, G_{E2}=2.582 after 1000 of steps in 21×21 matrix (Fig. 5) while in 201×201 matrix with the same parameters G_{E1}= 3.026 and G_{E2}=3.033 after 100 steps (other random instance).
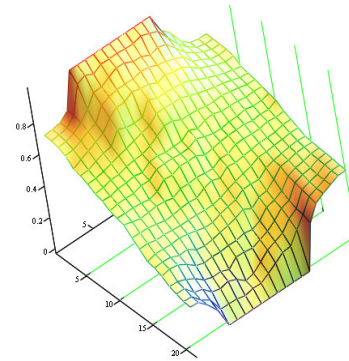

Fig. 6. Distorted potential distribution with grains developed most in transversal direction.

With parameters $L = 0.1$, $T = 0.9$ and $l = 1$, $t = 1$ we get G_{E1}=5.792, G_{E2}= 5.169, after 1000 of steps in 21×21 matrix (Fig. 6) while in 201×201 matrix with the same parameters G_{E1}=7.936 and G_{E2}= 7.928 after 100 steps (again, a new random distribution instance). For comparison if $L = 0.5$, T =0.5 and $l = 1$, $t = 1$ G_{E1}= 3.821 and G_{E2}= 3.943 while with no random distribution G_{E1}= G_{E2} = 1.47293 with a negligible mismatch of 10^{-12}. The shown data were computed at ε =1/40, perhaps a seldom value in practice while ε = 1/2 is more realistic one.

5.   CONCLUSION

It is believed that the conductance measurements may give a useful piece of information about the grain growth despite that changes are expected be much less that shown here, to clarify the principles. At least, one can well expect to measure different conductance dependences in the course of the phase transition in thin sheets during their preparation. A better understanding of the effects, the distribution of the newly creating phase - with a different conductivity than has the original matrix - may have on the net conductance (resistance) of the samples is thus of primary importance.

REFERENCES

[1] D. Muller, P. Švec: Nucleation effects during crystalli-zation in disordered metastable metallic systems, J. Ele. Eng., **55**, no. 10/S (2004), p. 28-30

[2] P. Švec: Private communication

[3] David E. Johnson: Basic Electric Circuit Analysis, 5th Edition, Wiley, January 1995

[4] www. mathsoft.com