Fast field solver programs for thermal and electrostatic analysis of microsystem elements

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Abstract

To solve the problem of fast thermal and electrostatic simulation of microsystem elements two different field solver tools have been developed at TUB. The μS-THERMANAL program is capable for the fast steady state and dynamic simulation of suspended multi-layered microsystem structures, while the 2D-SUNRED program is the first version of a general field solver program, based on an original method, the Successive Network Reduction. This program offers a very fast and accurate substitute of FEM programs for the solution of the Poisson equation, e.g. solving a 32000 grid problem in about 6 minutes on a 586 PC. Application examples show the usability of the tools.

1. Introduction

Thermal effects play fundamental role in the operation of many microsystem elements, as infrared sensors, rms meters, etc. Even if the thermal effect is not the base of the operation like in the previous examples, exact calculation of the always present thermal effects is required in many cases during the design of microsystem elements. Electrostatic fields have to be calculated during microsystem design e.g. in the case of capacitive displacement sensors and during the analysis of actuators based on the electrostatic force. All these problems require fast and reliable field solver programs capable to solve the Laplace or Poisson equations.

FEM methods can always be used for this purpose, but the drawbacks are well known, the huge amount of time required to define the problem and for the calculation, and the difficulty of modifying the once already analyzed structure.

There exist well established methods and tools for the thermal simulation of integrated circuits and other layer-structured systems, but the integrated microsystems raise new problems in the thermal simulation, since the frequently used suspended structures, such as cantilevers, membranes, bridges etc. have different boundary conditions from those of the simple silicon cubes of conventional integrated circuits. The μS-THERMANAL program has been developed for the thermal simulation of suspended microsystem elements, based on the THERMANAL program, which has been used for the steady state and frequency domain thermal simulation of multi-layered semiconductor structures for more than 18 years. In this paper after a short presentation of the THERMANAL program we present those features of the μS-THERMANAL program that were developed especially for the simulation of dedicated microsystem elements.

During our work in the thermal simulation of 3D SOI structures we encountered the problem, that the accuracy of the applied FEM simulation tool had to be limited down to an unacceptable value if we wanted to have the simulation results in a reasonable time (in days, in this case). To overcome this problem we have developed a new dedicated field solver program, which works currently in two dimensions, but it is expandable to 3D, it is very fast, accurate and very easy to use. The applied method is a finite difference method, the algorithm is successive node reduction, leading finally to the thermal impedance matrix of the boundary nodes. The temporary name of the program is 2D-SUNRED, coming from SUccessive Node REDuction. In the second part of our paper we present this program with application examples.

2. The μS-THERMANAL program

Overview of the features

The ancestor of this program, the THERMANAL program was an early realization of the well known algorithm of Kokkas [1], with the extension for unlimited number of layers [2]. In the model of Kokkas the structure consists of equally shaped rectangular layers stacked on an ideal heat sink. The dissipating elements are on the surface of the uppermost layer only, and the heat is removed via the bottom surface, the side walls are adiabatic. Heat transfer is assumed only by conduction. The differential equation of the heat flow (the Laplace equation) is written up for each layer, and the solutions are matched on the layer interfaces.

In the algorithm of [1] the solution of the differential equation is constructed in the form of two-dimensional Fourier-cosine series. In our program this series is calculated by Fast Fourier Transformation (FFT) method – resulting in a quick solution method in most cases.

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We have extended this model by the consideration of free convection cooling, the detailed description can be found in [4]. This extension is very important in the case of microsystems, where the presence and cooling effect of the surrounding air can not be neglected in most of the cases.

The assumption that the dissipation occurs only on the surface is rather rough, even in the case of ICs. This is why we modified the original algorithm also towards considering dissipators in several different layers. The mathematical description of the algorithm can be found in [5].

Simulation of membranes

The above discussed algorithm relatively easily can be extended to calculate the temperature distribution on multi-layer structured membranes as well, where the dissipation pattern and the structure of the membrane are given. In this case the boundary conditions are different from the usual IC structure: the top and the bottom surface of a membrane are adiabatic, while the side walls are isothermal, considering the bulk silicon nearly ideal heat sink.

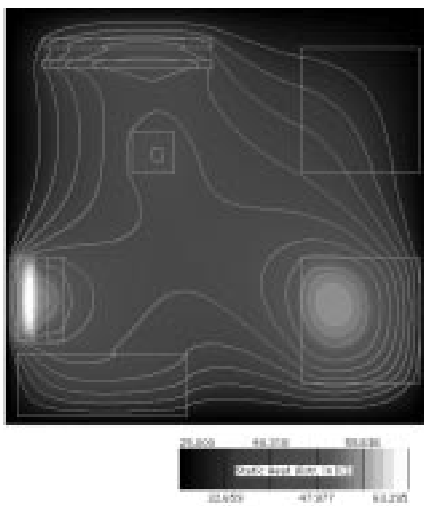

Fig.1. Steady-state temperature distribution on a membrane surface. The rectangular shapes are the dissipating elements.

These boundary conditions are fulfilled by using Fourier-sine expansion instead of Fourier-cosine [4]. Simulation results of a membrane structure are presented in Fig.1.

Simulation of bridge structures

On the top and bottom surface of the bridges the boundary condition for the temperature is adiabatic, like in the case of membranes. The side wall conditions are different now for the neighbor sides, the two isothermal sides (the fixings of the bridge) are between the two adiabatic sides. These boundary conditions are fulfilled using Fourier-sine expansion in x_1 direction and Fourier-cosine expansion in x_2 direction [4]. µS-THERMANAL simulation results of a multi-layer bridge structure are presented in Fig.2. Fulfilling of the side wall conditions are easily observable, the effect of the presence of air under the surface is considered appropriately. The structure and the dissipation pattern is the same as in Fig.1, but the difference in the temperature distribution because of the different side wall conditions is considerable.

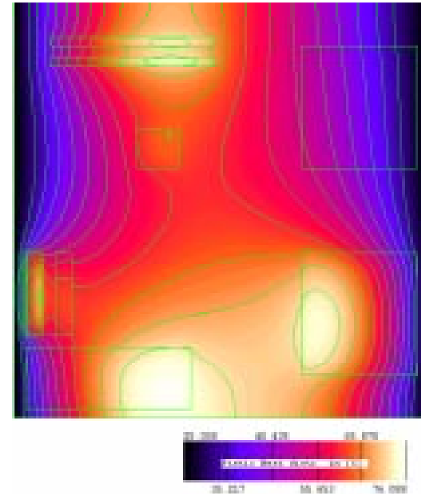

Fig.2. Steady-state temperature distribution on the surface of a multi-layer bridge structure. The left and right sides are the fixings of the bridge.

Simulation of cantilevers

A cantilever is fixed only by one side wall, consequently it can be always considered as a half bridge with special symmetry conditions. This is how cantilever problems are solved in the µS-THERMANAL. The cantilever is mirrored to form a symmetric bridge, and the bridge problem is solved with the previously discussed boundary conditions. This way the symmetry axis of the bridge, which is the free end of the cantilever, automatically fulfills also the adiabatic boundary condition.

Extension for heat transfer via beam leads

From heat transfer point of view a special class of microsystem elements are the parts suspended on thin and narrow strips. H shaped membranes and cantilevers with a narrow neck belong to this class, just like the ball grid array attachment of conventional IC chips. In these structures the leads act as heat sinking elements. In the µS-THERMANAL program we consider them as dissipating elements with negative dissipation. [3].

The analysis of a membrane structure suspended at two opposite sides by two narrow necks is shown in Fig.3. This example is also appropriate for the comparison of the µS-THERMANAL simulations with FEM simulations. The good agreement in the simulation results of the two programs is clearly visible in Fig.3, but the µS-THERMANAL program needed 500 times

less CPU time for the calculation than the SYSTHERM [6] program. About 9 minute was required to prepare the µS-THERMANAL task in contrast with the 1 hour preparation time required for the SYSTHERM task preparation for someone who uses SYSTHERM every day.

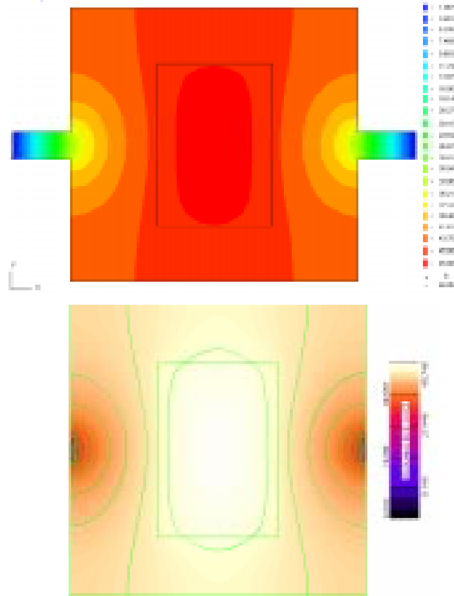

Fig.3. Comparison of narrow-neck suspended membrane simulations. Top: SYSTHERM simulation, bottom: µS-THERMANAL simulation

3. SUNRED: a 2D thermal and electrostatic simulator

This tool is designed especially for the fast calculation of the thermal behavior of arbitrary shape integrated microstructures. A special requirement was to calculate on a grid that is fine enough to obtain not only the temperature distribution but the accurate streamlines of the heat-flow as well.

An interesting feature of this simulator is that characteristic methods of three disjunct disciplines are combined in it. These fields are

- the electromagnetic field theory,
- the linear network theory and
- image processing.

Combination of these methods resulted in a very useful tool.

The model

The current 2D version of the program treats the linear heat conduction problems in two dimensions. Anisotropy can be taken into account. The equation being solved is

$$\partial_i \lambda_{ij} \partial_j T(x_i) = p(x_i) \qquad {}_{i,j=1...2} \qquad (1)$$

where λ_{ij} is the heat conductivity, $T(x_i)$ is the thermal field and $p(x_i)$ is the incoming heat flux density. This is the well-known Poisson equation, the mathematical description of many physical phenomenon. Electrical current-stream fields and electrostatic potential fields can be described by the same equation, which means that the program is capable to solve such problems as well.

The investigated area is a rectangle. A dense equidistant grid is spawned to this area defining a cell matrix. The suggested grid size is either 128×128 or 256×256 (for a PC, higher resolution can be used on workstations). A material type is assigned to each cell. This assignment is performed by constructing an image – in the sense of the digital image handling methods. Each pixel of this digital image corresponds to a grid-cell whereas the material type constituting the cell is coded by the color of the pixel. Thus, in order to enter a problem two files have to prepared:

- the “problem-image” which can be in any usual image format (the suggested format is the BMP),
- the “material-table” assigning different material parameters to each color.

This method of problem definition provides a very easy and fast input of arbitrary shaped complex geometrical arrangements (using any general picture editing tools). Limitation is coming only from the finite resolution of the digital image. Real images, e.g. a microscopic image of some IC structure may also be used as geometry input.

On the edges of the investigated area either forced temperature or zero heat-flow can be prescribed – individually, for any grid points of the boundary. Excitations can be defined inside the area as well, forcing a given temperature or a given heat-flux to any cell, only a new “color” should be introduced for each excitation value in the problem image.

The solution of Eq.(1) is accomplished using the method of *finite differences* . The cells of the field are squares (or rectangles) described by an electrical model, with a node in their center (Fig.4a.). Heat flux can be forced into them – this corresponds to the current flowing into this node. Forced temperature means the forced voltage value of the cell node.

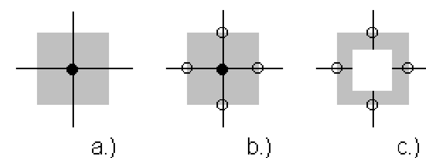

Fig.4. Cell, center node and terminal nodes

The boundary between different materials is lying always on the cell edges. In other words: each cell is "filled" by a single material. Each cell has four terminals in the direction of its four neighbors (Fig.4b.). On the terminals each cell can be described by a 4×4 matrix. This way the center node is hidden, but knowing the terminal temperatures the temperature of the center node can be back-calculated. Fig.4c. presents that the cell shows four terminals to the outside and the inner node is hidden.

The model of the cell is shown in Fig.5. In the present steady state version it contains four thermal conductances. The value of these depend on the thermal conductivity of the material filling the cell and on the geometry. This basic cell can be described by an admittance matrix of 4×4 size.

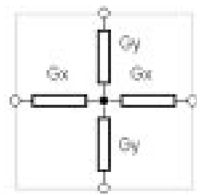

Fig.5. Circuit model of a single cell

The solution algorithm

The solution of the problem is done by the electrical solution of the whole model network. This raises serious problems because of the size of this network. Using a grid of 128×128 lines the model network consists of 32768 nodes. For a 256×256 grid arrangement this number is 131072. Although the corresponding circuit matrix is extremely sparse the solution of such a big network is a hard problem.

We have not considered iterative solutions – only direct methods have been investigated. A successive procedure has been developed for the network reduction – the essential features of which are briefly presented in the following.

Four basic cells can be assembled to form a block or macrocell as shown in Fig.6a. In other words: a *1st order cell* has been built from four *zero-order cells*. The four inner connecting terminals of the cells can be eliminated; they should not appear in the outside-directed description (Fig.6b.). The size of the Y matrix of the 1st level cell is 8x8 containing 64 values (which is equal to the 4x16 elements of the four zero-level cells).

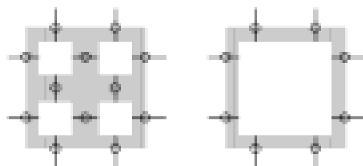

Fig.6. Four basic cells will constitute a 1st level cell

Using four 1st level cells we can assemble a 2nd level cell as shown in Fig.7. The inner terminals can be eliminated again.

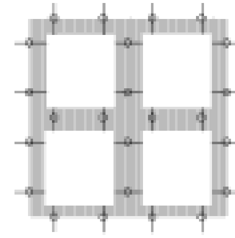

Fig.7. Building a 2nd level cell

Continuing this successive building of higher and higher level cells we obtain finally the matrix of a single cell – the terminals of which are lying on the four edges of the investigated rectangular field. Matching with the boundary conditions means the solution of this matrix for the U or I constraints, given individually for the terminals lying on the boundaries of the investigated field. The voltages of all the inside nodes can then be calculated by a successive back-substitution.

The advantage of the presented solution algorithm lies in the fact that most of the grid nodes are eliminated before the final solution of the system equation. Supposing e.g. a problem field of 128×128 grid points we have 32768 inner nodes but we should solve an equation of only 4×128=512 unknowns.

The hierarchical network reduction requires $\log_2(128)=7$ successive steps for the 128×128 grid, 8 steps for the grid-size of 256 and so on. The detailed analysis of the T total computing time gives

$$T = 63.5\, N^{3/2}\, (T_{*+}) \qquad (2)$$

where N is the node number for the whole model network and (T_{*+}) is the time of one multiplication and one addition. This time should be compared to the $Ordo(N^3)$ time requirement of a "brutal force" Gauss elimination. For a 32768 node problem the solution time is only 6 minutes on a 586 PC, thanks to the efficiency of the successive network reduction algorithm.

It should be emphasized that the network reduction step has to be executed only once for a structure. Changes in the excitations or in the boundary conditions require to repeat the back-substitution only – which requires much less time than the reduction itself.

In the present phase of the development the algorithm handles the steady-state case only. The implementation of the frequency and time-domain solutions does not hold any difficulties however, we are currently working on these extensions.

Presentation of the results

The results of the simulation are treated as images again. The temperature (or potential) fields which are

essentially 2D scalar functions can be considered as black-and-white images. The brightness of the image points is proportional to the temperature (or potential) of each point. The program provides the results in form of digital images, in the standard BMP image format. Such a potential image is shown in Fig.8.

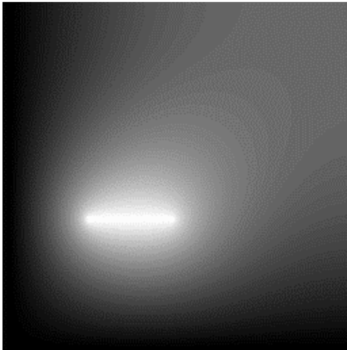

Fig.8. Grayscale image of a potential field (a horizontal electrode in a conducting corner)

Although this image gives a good qualitative view of the potential field, the potential values can not be read from this picture. A basic procedure of image processing can help to overcome this problem. This procedure is the intensity transformation: an arbitrary $b_{tr}=f(b)$ function is used to map the original b pixel intensities into the b_{tr} brightness values. A set of appropriately chosen functions offer a rich variety of presentations for the same temperature (potential) field, and provides the good quantitative evaluation at the same time. Fig.9a. is an example for the intensity mapping functions, the corresponding image is shown

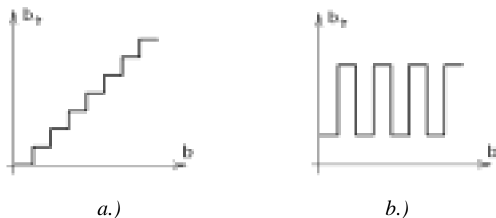

Fig.9. Brightness mapping functions

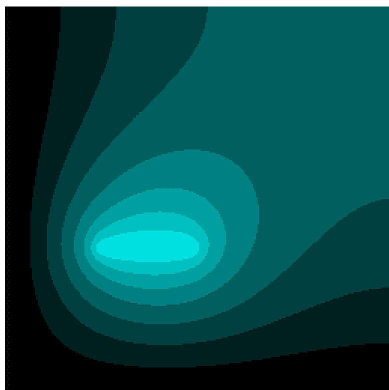

Fig.10. The stepped brightness mapping function and the resulting image

in Fig.10. The stepped character of the *f(b)* function results in abrupt intensity changes in the image, and the boundary between the different intensities traces an equipotential line. The telegraph-signal-like intensity mapping of Fig.9b. produces an even more explicit drawing of the equipotential lines (see Fig.11.) Using color displays intensity-color mappings are possible as well providing striking, rainbow-like pictures.

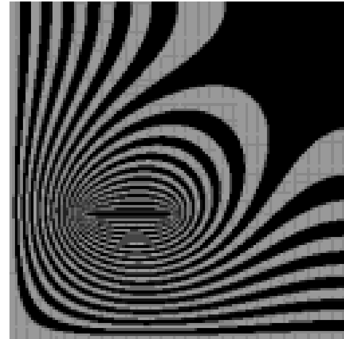

Fig.11. Potential or temperature field using the telegraph signal like intensity mapping.

The temperature field or potential image is usually not enough to visualize thermal, electrostatic or streaming fields. Tracing of the heat-stream lines (or electrical field lines) is an often encountered requirement. Especially in the case of temperature fields the streamlines provide an easy way to “discover” how and where the heat flux is streaming.

To obtain streamline pictures further image processing steps are required. The simulator provides the J_x, J_y components of the $\boldsymbol{J}$ current density vector in form of two intensity images. These vectors have to be turned by 90°. This can be made simply by interchanging the two images and negating one of them:

$$G_x = J_y \qquad (3)$$
$$G_y = - J_x$$

It can be easily proven that the *P(x,y)* potential function of this ***G*** field is suitable to trace the streamlines. The equipotential lines of this *P pseudo potential* are the streamlines of the original field. Visualization of these lines can be proceeded in the same way as in case of the real potential field.

For the sake of the mathematical correctness it should be mentioned that this pseudo potential can be constructed if and only if there is no divergence in the ***J****(x,y)* vector-field. This means that the procedure can be applied only on the divergence-free regions of the field.

Examples

In the first example the thermal field of a micromachined bridge is calculated. In order to demonstrate the capability of the program an irregularly shaped bridge has been analyzed. A single dissipating

shape is defined on the bridge. The calculated temperature distribution of the structure is shown in Fig.12. It is not so easy to see from this plot where the most important part of the heat stream is flowing. The streamline calculation helps us to have an image. In Fig.13. the streamlines are plotted. These streamlines are suitable to examine the division of the heat flux between the two possible paths.

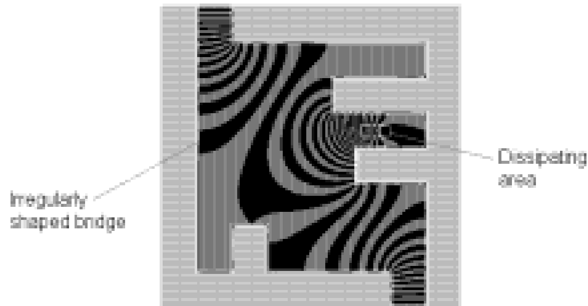

Fig.12. Isothermal lines on the bridge

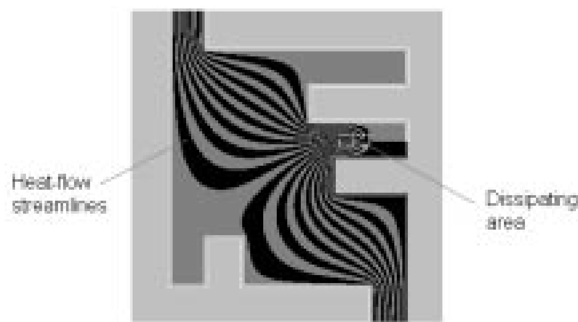

Fig. 13. Streamlines of the heat-flow

In the second example a 3D stacked submicron CMOS SOI structure [8] is investigated. The heat is generated in the upper transistor. The results of the simulation are shown in Fig.14. The highly different thermal conductivity of the silicon and the SiO_2 leads to the surprising fact that the heat stream makes a detour (see the white arrows) around the SiO_2 region.

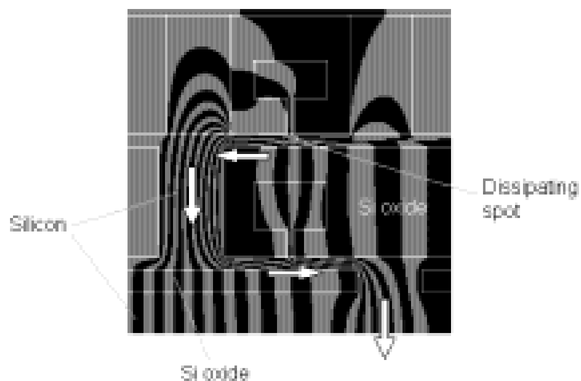

Fig.14. Heat-flow in a stacked SOI structure

4. Conclusions

Two new, fast and easy-to-use simulation tools have been developed for the accurate thermal and electrostatic simulation of dedicated microsystem elements and special 3D structures.

With the help of the novel 2D-SUNRED program arbitrarily shaped structures can be analyzed with very high accuracy in minutes in a PC – enabling also the visualization of the accurate heat flow paths in the material, that we could not obtain with usual FEM programs. The program calculates currently in two dimensions. The development of the dynamic and the 3D version of the program is in progress, they can be hopefully presented already at the conference.

Using the μS-THERMANAL simulator as the field solver of electro-thermal simulators, like the SISSI program [7], even the accurate dynamic electro-thermal simulation of electronic circuits realized on microsystem elements becomes possible.

Acknowledgments

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