# Heat Transfer Simulations in the Frequency Domain with the Application of Thermal Influence Coefficients Method

Katarzyna Gnidzińska, Grzegorz Jabłoński, Andrzej Napieralski, and Gilbert De Mey

***Abstract*—In this paper an extension of thermal influence coefficients method to frequency domain has been presented. The method allowed the steady-state analysis of three-dimensional heat flow in multilayered structures. The presented modelling is based on Fourier and Hankel transforms, two-port network theory and correction coefficients for close-area distances, allowing emulation of finite heat sources by infinitesimal ones.**

***Index Terms*—thermal modelling, thermal simulation, AC**

## I. Introduction

THE traditional approach to heat transfer is confined to steady-state and time-domain. It may be deemed sufficient for a variety of purposes, however it does not suffice for all the phenomena. The exploration of frequency-domain ceases to be negligible when structures become relatively small, e.g. the microelectronic structures. In this case, the cut-off frequency becomes considerably high, the high frequencies penetrate the structure and the penetration no longer can be perceived as depth-less. The periodic heat sources can e.g. result from some unwanted thermal coupling within a circuit or energy waves deliberately applied to the surface in order to carry out the non-destructive testing (NDT) i.e. lock-in thermography [8].

The nomenclature for AC thermal modelling is derived from the terminology in the electric domain as it implies the existence of the periodic sources. The numerical simulations performed in AC are not entirely realistic, as the genuine sinusoidal heat sources are of no existence. The method assumes that the sinusoidal components are superimposed on DC background.

The semi-analytic solution for a 3-D heat flow in microelectronic multilayered structures has been derived on the basis of thermal influence coefficients method extended to frequency (AC) domain.

## II. Thermal Influence Coefficients Method

The thermal influence coefficients method of thermal analysis has been developed for steady-state approach [2]. The method was intended for three-dimensional heat flow in multilayered structures. The heat sources can be of an arbitrary shape and are located at the upper surface of the structure. At the bottom layer, the constant heat exchange is assumed (e.g. large heat sink or forced convection). It is also assumed that the only mechanism of heat transfer that takes place, is conduction. The convection and radiation are negligible, which is a reasonable assumption for most of the cases. Hence, the lateral planes of a structure are adiabatic. Furthermore, the layers are homogeneous and isotropic (can be described by a constant thermal conductivity $k\,[Wm^{-1}K^{-1}]$ and (volumetric) heat capacity $C_v\,[Jm^{-3}K^{-1}]$). To introduce the lateral boundary conditions method of images has been employed. The thermal conductivity of the interface between layers is expressed by $g_i[Wm^{-2}K^{-1}]$, i.e. interface thermal conductance.

The proposed extension exploits the idea of employing frequency domain to thermal analysis.

## III. Multilayer Structure

A multilayer structure is a structure consisted of several ($n \geq 1$) layers of different materials ($k_i$ and $C_{vi}$), having finite thickness ($t_i$). The set of layers is supposed to have the same lateral dimensions (Fig.1). However, at the beginning the semi-infinite structure is considered. The lateral dimensions are introduced later by using image method.

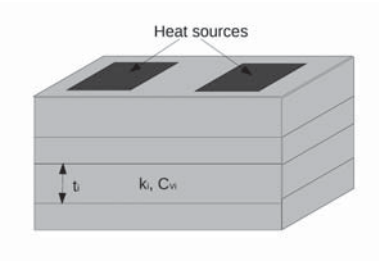


Fig. 1. Multilayer structure with heat sources at the upper surface

The distribution of heat in a given space over time can be described by Fourier equation:

$$\frac{\delta T}{\delta t} - \alpha \nabla^2 T = 0 \tag{1}$$

where $\alpha$ is thermal diffusivity $[m^2 s^{-1}]$ and $\alpha = k/C_v$.

The analysed problem is axially symmetric therefore can be expressed with cylindrical coordinates $(r, \varphi, z)$ leaving out the azimuth. Hence, the temperature distribution is merely the function of radial distance and height ($T = f(r, z)$).

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To provide explicitly the frequency domain to the equation, the phasor notation is introduced. The relation between a signal $x(t)$ and its corresponding phasor $X$ is defined as:

$$x(t) = Re[Xexp(j\omega t)] \tag{2}$$

The heat equation in phasor notation (AC heat equation) is formed:

$$\nabla^2 T(r,z) - \frac{j\omega}{\alpha} T(r,z) = 0 \tag{3}$$

In order to significantly simplify the solution and eliminate the $r$ coordinate, Hankel transform [3], [6] can be used. Thanks to the transformation, the AC heat equation changes to a differential equation depending only on $z$, with frequency $\omega$ and Hankel variable $p$ as parameters:

$$\frac{d^2\bar{T_i}}{dz^2} - {m_i}^2\bar{T_i} = 0 \tag{4}$$

where:

$$m_i = \sqrt{p^2 + \frac{j\omega C_v}{k}} \tag{5}$$

and $\bar{T}$ denotes the Hankel transform of $T(z)$.

The problem formulated by the equation 4, represents a one-dimensional heat flow. Using $\bar{T_{iI}}$, $\bar{T_{iO}}$, $\bar{\phi_{iI}}$ and $\bar{\phi_{iO}}$ as the transformed distributions of temperature and heat flux at each layer's "input" and "output", we can use the two-port network theory to express the dependencies between them [4]:

$$\begin{bmatrix} \bar{T_{iI}} \\ \bar{\phi_{iI}} \end{bmatrix} = [A_i(m_i)] \begin{bmatrix} \bar{T_{iO}} \\ \bar{\phi_{iO}} \end{bmatrix} \tag{6}$$

where:

$$[A_i(m_i)] = \begin{bmatrix} cosh(m_i t_i) & \frac{sinh(m_i t_i)}{m_i k_i} + \frac{cosh(m_i t_i)}{g_i} \\ m_i k_i sinh(m_i t_i) & \frac{m_i k_i}{g_i} sinh(m_i t_i) + cosh(m_i t_i) \end{bmatrix} \tag{7}$$

The parameter describing thermal contact between layers is the interface thermal conductance. In practice it may depend severely on the quality of the physical interface. However, in all of the simulations presented in the paper, the perfect contacts have been assumed ($g \to \infty$).

The $A_i(m_i)$ matrix fully characterises thermal parameters of a layer and the interface with the next one, as well as geometry (thickness) of the material.

For the whole $n$-layer structure, the subsequent transformations of the equation 6 lead to:

$$\begin{bmatrix} \bar{T_{1I}} \\ \bar{\phi_{1I}} \end{bmatrix} = [A(m)] \begin{bmatrix} \bar{T_{nO}} \\ \bar{\phi_{nO}} \end{bmatrix} \tag{8}$$

where $[A(m)] = [A_1(m_1)][A_2(m_2)]...[A_n(m_n)]$. According to the initial assumptions $\bar{\phi_{1I}}$ and $\bar{T_{nO}}$ are known (power dissipation at the upper surface and reference temperature at the bottom), and $\bar{\phi_{nO}}$ and $\bar{T_{1I}}$ are given by:

$$\bar{T_{1I}} = \frac{1}{A_{22}} \bar{T_{nO}} + \frac{A_{12}}{A_{22}} \bar{\phi_{1I}} \tag{9}$$

$$\bar{\phi_{nO}} = \frac{1}{A_{22}} \bar{\phi_{1I}} - \frac{A_{12}}{A_{22}} \bar{T_{nO}} \tag{10}$$

As an example let us consider an infinitesimal heat source with the total power of $P$. The Hankel transform of power distribution generated by the circular source with the radius $r$ is given by:

$$\mathcal{H}(\phi_1) = \mathcal{H}(\frac{P}{\pi a^2} H(a-r)) = \int_0^\infty \frac{P}{\pi a^2} H(a-r) J_0(pr) r dr = \frac{P J_1(ap)}{\pi a p} \tag{11}$$

For $a \to 0$ the equation assumes the form:

$$\bar{\phi_1} = \frac{P}{2\pi} \tag{12}$$

Assuming a single-layer substrate with a thickness of $t$, the reference temperature at the bottom equal to zero and infinite thermal conductivity of the contact, the expression 9 yields:

$$\bar{T_{1I}} = \frac{\tanh(mt)}{mk} \frac{P}{2\pi} \tag{13}$$

Thus:

$$T_{inf}(r) = T_{1I}(r) = \frac{P}{2\pi k} \int_0^\infty \frac{\tanh(mt)}{\sqrt{p^2 + j\omega \frac{C_v}{k}}} J_0(pr) p dp \tag{14}$$

where $T_{inf}$ denotes the temperature contribution from the infinitesimal heat source.

## IV. Highly Oscillatory Integrand

The chosen modelling method, including Hankel transformation, on one hand allows some very advantageous simplification of the problem, but on the other it has its drawbacks. The transformed distributions are relatively easy to be obtained (as the three dimensional heat flow has been reduced to one dimension), however the computation of the inverse transform is complicated on its own. The integrals involving Bessel functions are of highly oscillatory nature. Provided that the integral of the form:

$$I(p) = \int_0^\infty f(x) J_0(\rho x) dx \tag{15}$$

has a $f(x)$ that goes to zero slowly as $x \to \infty$, the integration is performed over many oscillations of $J_0(x)$. In such case, the traditional numerical techniques become inefficient.

### A. Straightforward approach

None of the built-in Octave (high-level interpreted language for numerical computations) integrating functions could handle the problem of infinite oscillations. The easiest solution is to iteratively carry out integration dividing the infinite interval into subsequent steps.

The idea is to divide the integration into two steps. First, to deal with the arbitrarily long (parametrised) beginning of

the integrand, therefore at first reducing the problem to a finite integral. Then, the rest of the integrand is the oscillating Bessel-function tail, that can be treated period by period, until the subsequent integrals will have negligible (quantitatively described) influence on the result. Zeros of the Bessel tail can be easily found using cosine approximation (22). After the first step, the first positive-derivative zero is found to make sure second step takes into account only full periods (Fig.2). Otherwise, the results from subsequent periods would cause the integral to oscillate and highly reduce the accuracy.

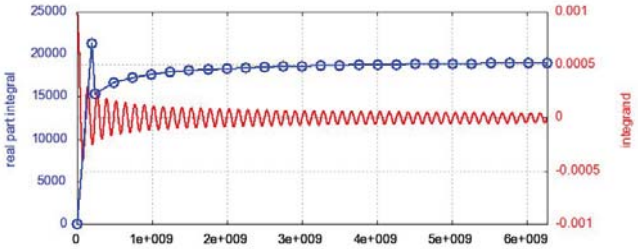


Fig. 2. Numerical integration of inverse Hankel transform

The main problem of the described approach is to determine at which point the remaining Bessel-function tail has negligible influence on the result. A parameter has been chosen, to compare the current integral (over last period) to the previously computed overall result. When the subsequent step makes the result to change by less than the set accuracy, the integration stops.

Depending on the set accuracy, the method can give results with less then $< 1\%$ error, however for high accuracies the computation time gets unacceptable and there is a need to accelerate integration.

### B. Convergence acceleration

To accelerate integration, the Euler's transformation can be used [3]. The method allows convergence acceleration when integrating between the zeros of $J_0(p)$ (the only order of Bessel function considered here is $n = 0$, however the method works for higher orders as well). The considered integral can be represented as a series (16) provided that the absolute value of each $I_i$ integral is taken.

$$I(r) = \int_0^\infty J_0(pr) f(p) dp = \sum_{k=1}^{\infty} (-1)^{k+1} I_k \tag{16}$$

Using aforementioned Euler's transform we get:

$$I(r) = \frac{1}{2} I_1 - \frac{1}{4} \Delta I_1 + \frac{1}{8} \Delta^2 I_1 - ... \tag{17}$$

where $\Delta$ is the forward difference operator:

$$\Delta^n a_0 = \sum_{k=0}^{n} (-1)^k \binom{n}{k} a_{n-k} \tag{18}$$

It appears that not only the integration can be vastly accelerated (Table IV-B), but also the method of convergence acceleration tends to give much more accurate results (Fig. 3). The highlighted cells indicate that for a given accuracy the integration error is less than $0.5\%$.

TABLE I
COMPARISON OF METHODS - NORMALISED TIME CONSUMPTION

| | normalised computation time | |
|---|---|---|
| set accuracy | straightforward | accelerated |
| 1e-2 | 0.003 | 0.002 |
| 1e-3 | 0.011 | 0.004 |
| 1e-4 | 0.050 | 0.006 |
| 1e-5 | 0.218 | 0.009 |
| 1e-6 | 1.000 | 0.013 |

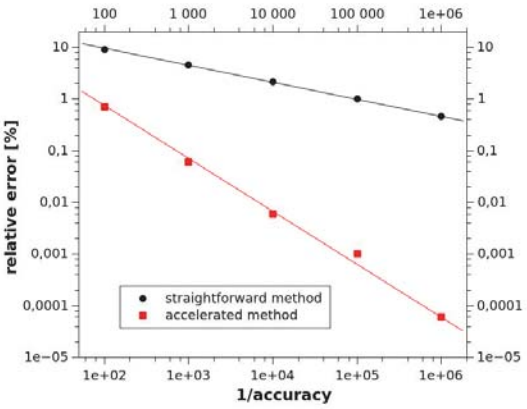


Fig. 3. Numerical integration - errors of the simple and the accelerated method

However, it is important to notice that the method works well when infinitesimal sources are considered. Otherwise, if the size is finite, i.e. it is circle-shaped, it introduces another Bessel function to the integrand (Eq.19 - 21) and the formula Eq.(16) no longer describes it.

The circle shaped heat flux is given by:

$$\phi = \frac{P}{\pi r^2} H(a - r) \tag{19}$$

where $a$ is the radius of the circle and $H(\cdot)$ is the Heaviside step function. Hence, the corresponding Hankel transformed heat flux is expressed by:

$$\bar{\phi} = \frac{P J_1(ap)}{\pi a p} \tag{20}$$

and the integral takes form:

$$T_{1I} = \frac{P}{\pi a k} \int_0^\infty \frac{1}{p} J_0(pr) J_1(ap) dp \tag{21}$$

The integrand is a product of two Bessel functions with different periods. The term period can be used as these functions can be approximated by cosine [7]:

$$J_0^\star(x) = \sqrt{\frac{2}{\pi}} \sqrt{\frac{1}{x}} \cos(\frac{\pi}{4} - x) \tag{22}$$

for $x \geq 1$. A product of two Bessel functions does not exhibit a regular pattern and its integral can no longer be perceived as an alternating series of integrals computed between function's zeros. Thus, the method of convergence acceleration by using Euler's transformation 16 is in this case of no use.

## V. Heat Sources and Distance Corrections

To effectively simulate a heat source of an arbitrary shape and size, the discretization grid is used. The upper surface of the structure can be thus divided into $n_x \times n_y$ squares of the same size ($A \times A$), where the size of a square can be treated as a parameter. In this way, the physical heat source can be represented as a set of square-shaped sources.

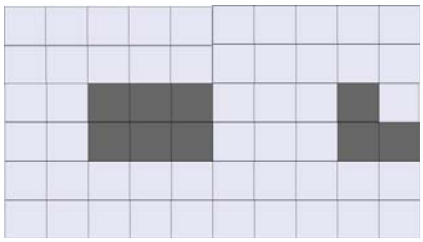

Fig. 4. Discretization grid allows representing heat sources as a set of squares

A problem arises when it comes to the computational complexity of introducing square heat sources versus infinitesimal ones. For a punctual source over a single layer of solid with thickness $t$, temperature distribution is given by (14). For a square source, it is necessary to use the superposition principle and integrate (14) over the entire source area, which results in longer computation times:

$$T_{square}(r) = \int_{-\frac{A}{2}}^{\frac{A}{2}} \int_{-\frac{A}{2}}^{\frac{A}{2}} T_{inf}(r)dr \qquad r = \sqrt{(x-x_0)^2 + (y-y_0)^2} \tag{23}$$

However, as it can be easily observed, for further distances from the source, its geometry does no longer have influence on the temperature distribution and a finite size source can be approximated by the infinite one (Fig.5).

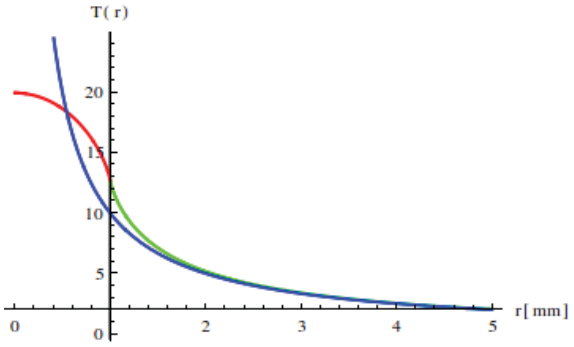


Fig. 5. Comparison between $T(r)$ of an infinite and finite size circular heat sources with radius $r = 1$mm

### A. Distance corrections

The emulation of the square shaped source by an infinitely small one is possible only for further distances (for the chosen accuracy - above $3A$). For closer areas, it is necessary either to take into account the geometry of the square source by integration over its entire area, or to find some means allowing us to use the results obtained for the punctual source.

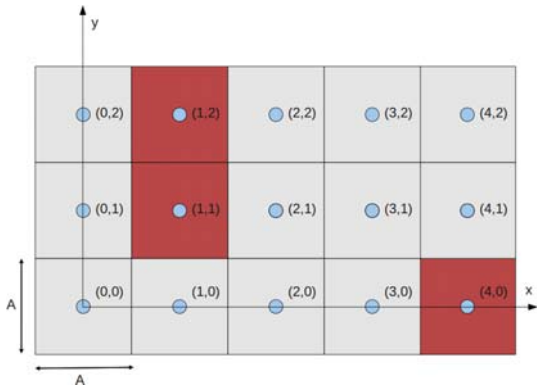


Fig. 6. Temperature computation at point (0,0)

For the steady-state approach, it is possible to determine the equivalent distances ($\xi$) at which the temperature resulting from an infinitesimal heat source is equal to the temperature resulting from a square shaped source at the specific distance and orientation [1]. For example, in figure 6, we want to compute the temperature in point (0,0) resulting from contributions of square heat sources with centres (1,2), (1,1) and (4,0):

$$T((0,0)) = T_{inf}(\xi_{(1,1)}A) + T_{inf}(\xi_{(1,2)}A) + T_{inf}(4A) \tag{24}$$

For sources located at (1,1) and (1,2) an application of equivalent distance is essential to obtain an accuracy above $0,5\%$. The source (4,0) is far enough to be approximated by infinitesimal source.

For AC approach, the problem is slightly more complicated. It turns out, it is impossible to determine one value for each discrete distance. It appears that $\xi$ depends on the product of the frequency and the square of grid size divided by the thermal diffusivity of the upper layer, denoted as $\zeta$:

$$\zeta = \frac{\omega A^2}{\alpha} \tag{25}$$

The dependency between $\zeta$ and equivalent distance can be computed numerically for an infinite thickness of the structure. For each grid point within the considered area, the temperature is calculated for a square shaped source:

$$T(r) = \frac{P}{2\pi kA} \times \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{1}{\sqrt{x^2+y^2}} \exp\left(-\sqrt{\frac{j\omega A^2}{\alpha}}\sqrt{x^2+y^2}\right) dxdy \tag{26}$$

The result is compared with the results achieved for a punctual heat source. The dependency for a set of $\zeta$ values is tabulated in a form of a lookup table and later equivalent distance for any requested distance can be interpolated.

It is worth noting that carried out computations show there is a need to consider amplitude and phase separately. In Fig. 7, there is an example comparison between those two. "Cell(0,0)" means that the grid point under consideration is the heat source itself.

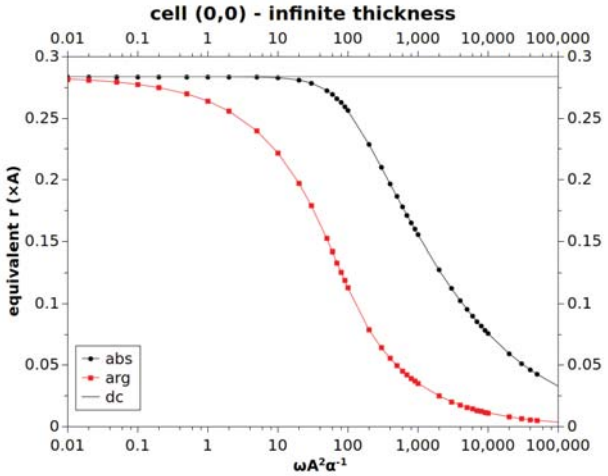


Fig. 7. $\xi$ vs $\zeta$ for an example grid cell - amplitude and phase

Having systematized all the close-area equivalent distances for the semi-infinite substrate (later referred to as reference equivalent distance) does not guarantee that the same distance can be used for finite thickness. The accuracy of this approach has been verified numerically for various values of the $t/A$ ratio. The simulations have shown, that for thickness smaller than the quintuple of grid size $A$, the error caused by applying those reference equivalent distances rises significantly. For thicker substrates the approximation is very accurate (Fig.8). Therefore for most of the cases, the thickness does not exclude the lookup tables to be of use. For larger sources, they have to be divided using smaller grid.

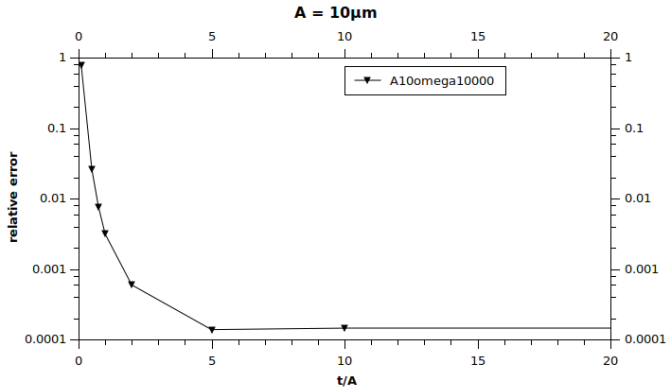


Fig. 8. Relative temperature magnitude error resulting from using reference equivalent distance for finite thickness substrates

## VI. Image Method

To introduce lateral dimensions to the structure, method of images is applied [9]. It superimposes the plane sources and sinks (denoted by plus and minus signs respectively) onto the existing infinite body. In case of the one dimensional, insulated BCs case, the location of the sources is as follows:

$$\begin{array}{ll} 2nL + x - x' & n = ..., -2, -1, 0, 1, 2, ... \\ 2nL + x + x' & n = ..., -2, -1, 0, 1, 2, ... \end{array} \quad (27)$$

## VII. Verification

The method has been verified and it gives accurate results. The achieved simulation results were compared with other methods that give solutions for three dimensional heat conduction (Fig.10,12). The error in the worst case is below $1\%$.

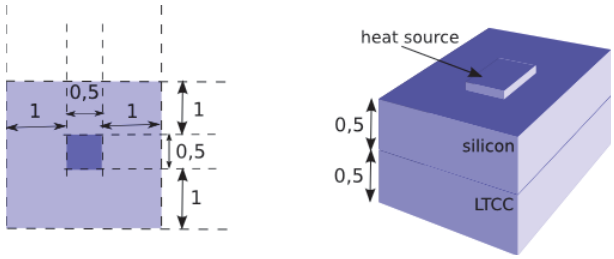


Fig. 9. Double layered structure with rectangular heat source: top view and three dimensional view (all dimensions in [mm])

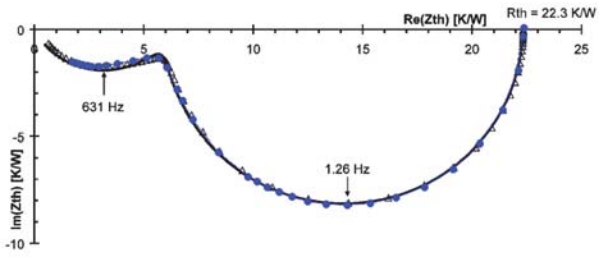


Fig. 10. Comparison between simulation results and theoretical ones for the structure presented in Fig.9

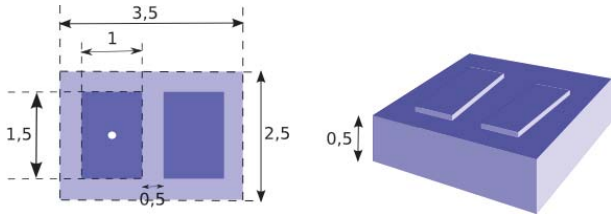


Fig. 11. Single layered silicon structure with two rectangular heat sources: top view and three dimensional view (all dimensions in [mm]). The thermal impedance plot is calculated for the centre of the left-hand source.

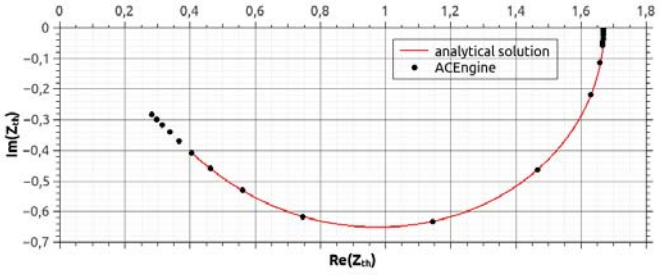


Fig. 12. Comparison between simulation results and theoretical ones for the structure presented in Fig.11

## VIII. Conclusion

The extension of the thermal influence coefficients method to frequency domain has been presented. The idea behind introducing the frequency domain to thermal analysis, is that for distances encountered in the microelectronic structures, the penetration depth for higher frequencies is no longer negligible. The three dimensional heat flow has been transformed to one dimensional problem, and thanks to that simplification the two port network theory could be employed. The accuracy of the computations depends significantly on the ability of effective inversion of Hankel transform. The highly oscillatory integrand caused by the Bessel function can be neatly converged using Euler's transformation. The solution not only allows the significant speed up of the computations, but also results in higher accuracy achieved within much shorter time. The heat sources at the upper surface of the structure has been modelled as a set of square shaped sources. Those were emulated by infinitesimal ones. For the close area, the equivalent distances for both amplitude and phase have been determined and expressed in the form of lookup tables giving the ability for later interpolation. The equivalent distance was proved to be dependent on frequency, grid size and thermal diffusivity. It was shown that for the use of lookup table thickness of a structure must be taken into account only when it is smaller than a grid size.

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**Gilbert De Mey** received the M.S. and Ph.D. degrees from Ghent University, Gent, Belgium, in 1970 and 1975, respectively. Since 1991, he has been a full time Professor with the Faculty of Engineering at Ghent University. He has published more than 250 technical papers in the international literature and has regularly chaired or co-chaired conferences on microelectronics and thermal management. His research and teaching activities include the wide range of physical electronics, with particular interest to heat transfer in electronic devices.