# 9. Finite Element Method (FEM) for Thermal Analysis

## 9.1. Introduction

Thermal analysis is a very important part of simulation-based design. Namely, if an electromagnetic field exists in a certain material, power losses are inevitable. They appear in dielectric materials due to dielectric imperfections, i.e. due to their extremely small but finite conductivity. Magnetic material is usually electrically conductive and the time-derivation of the magnetic field in it induces electric currents and consequently power losses. Thus, the power loss in any electromagnetic device manifests by heating up the structure. If the produced heat is significant and the reached temperature too high, the device should contain a cooling system to maintain the desired operating temperature. Therefore thermal analysis plays an important role in our simulations. In this chapter we will present the basic equations of thermal analysis and aspects of their FEM discretization. At the end of the chapter we will apply this knowledge and perform a thermal analysis of a micro AC/DC thermo-converter.

## 9.2. Fundamental Laws of Heat Transfer

Thermal analysis studies the heat transfer between material bodies due to their temperature difference [1]. According to the modern physical understanding of heat transfer phenomena there are three different mechanisms of heat transfer [2]:

1. conduction,
2. convection,
3. radiation.

*Heat conduction* is based on the exchange of energy between either molecules or free electrons in the material. Therefore, it depends on the material properties and occurs in solids, liquids and gasses if there is a temperature difference. The fundamental equation of heat conduction is known as Fourier's[1] law which, in the 1D case, can be expressed as follows [1, 2]:

$$q_x = -k\frac{dT}{dx} \tag{9.1}$$

where $q_x$ is the heat flux in the x-direction (in $W/m^2$), $k$ is the thermal conductivity (in $W/(mK)$) and $dT/dx$ is the temperature gradient.

*Heat convection* is related to the macroscopic motion of the molecules of liquids and gasses. Namely, those molecules have freedom of motion and therefore the ability to move from a hot to a cold region carrying energy with them. The term convection is also often used to describe the heat transfer between a surface and an adjacent fluid. The basic equation of heat convection is called Newton's[2] law of cooling [1, 2]:

$$q = h(T_w - T_a) \tag{9.2}$$

[1] Jean Baptiste Joseph Fourier (1768 - 1830), French mathematician and physicist.
[2] Sir Isaac Newton (1643 – 1727), English physicist, mathematician, astronomer, alchemist, and natural philosopher.

where $q$ is the convective heat flux (in $W/m^2$), $T_w$ - $T_a$ is the temperature difference between the wall and the fluid and $h$ is the convective heat transfer coefficient or the so-called film coefficient (in $W/(m^2K)$).

*Heat radiation* is related to the well known physical properties of the material bodies. Namely, all bodies at any temperature emit thermal radiation in the form of electromagnetic waves. These waves propagate in the surrounding space and strike other bodies. The surface of a nearby body partially absorbs the incoming thermal radiation. The remaining part of the radiation is reflected back into the surrounding space. The heat radiation for a general surface is described by Stefan-Boltzmann's law [1, 2]:

$$q = \varepsilon \sigma T_w^{\ 4} \tag{9.3}$$

where $q$ is the radiative heat flux ($W/m^2$); $\sigma = 5.669 \cdot 10^{-8}\, W/\left(m^2 K^4\right)$ is the Stefan–Boltzmann constant, $T_w$ is the surface temperature at the heat emitting body ($K$), and $\varepsilon$ is the emissivity of the surface describing its radiative properties (a black surface has the maximum emissivity $\varepsilon = 1$).

In general all of these three ways of heat transfer are present at the same time and have to be taken into account in thermal simulations. However, as we will see later, depending on the properties of the involved materials, geometry, character of the surfaces of bodies and expected temperature level some of them are dominant and some can be neglected.

## 9.3. Heat Transfer Equation

The partial differential equation that describes heat transfer can be elegantly derived using the energy conservation law. Namely, let us consider the elemental volume shown in Figure 9.1.

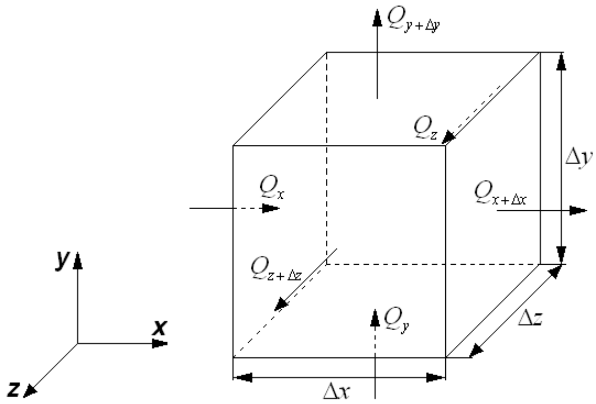


Figure 9.1. An elemental volume in the Cartesian coordinate system used for the derivation of heat transfer equation is depicted.

For this elemental volume the incoming and outgoing thermal energy per unit time (power) can easily be calculated because its surfaces are perpendicular to the coordinate axes. Thus we will define the following three incoming thermal powers with respect to each coordinate axes:

$$Q_x = q_x \, \Delta y \, \Delta z \tag{9.4}$$

$$Q_y = q_y \, \Delta x \, \Delta z \tag{9.5}$$

$$Q_z = q_z \, \Delta x \, \Delta y \tag{9.6}$$

where $q_x$, $q_y$ and $q_z$ are thermal fluxes in all three coordinate directions given in ($W/m^2$). Using a Taylor series expansion, the corresponding thermal powers leaving our volume element can be written as follows:

$$Q_{x+\Delta x} \approx Q_x + \frac{\partial Q_x}{\partial x}\Delta x \tag{9.7}$$

$$Q_{y+\Delta y} \approx Q_y + \frac{\partial Q_y}{\partial y}\Delta y \tag{9.8}$$

$$Q_{z+\Delta z} \approx Q_z + \frac{\partial Q_z}{\partial z}\Delta z \tag{9.9}$$

It is important to mention that all higher order terms in the expansions (9.7-9.9) were neglected. Having equations (9.7-9.9) it is now possible to continue our analysis and to apply the following energy conservation law on the elemental volume:

Incoming Power + Generated Power = Stored Power + Outgoing Power (9.10)

or in an exact mathematical form:

$$Q_x + Q_y + Q_z + G\ \Delta x\ \Delta y\ \Delta z = \rho\ \Delta x\ \Delta y\ \Delta z\ c_p\ \frac{\partial T}{\partial t} + Q_{x+\Delta x} + Q_{y+\Delta y} + Q_{z+\Delta z} \tag{9.11}$$

where $G$ is the generated thermal power per unit volume (*W/m*$^3$), $\rho$ is the density of the material (*kg/m*$^3$), $c_p$ is the specific thermal capacity under a constant pressure (*J/(kgK)*), $T$ is the temperature (*K*) and $t$ is the time (s).
By introducing equations (9.7-9.9) into (9.11) we obtain:

$$-\frac{\partial Q_x}{\partial x}\Delta x - \frac{\partial Q_y}{\partial y}\Delta y - \frac{\partial Q_z}{\partial z}\Delta z + G\ \Delta x\ \Delta y\ \Delta z = \rho\ \Delta x\ \Delta y\ \Delta z\ c_p\ \frac{\partial T}{\partial t} \tag{9.12}$$

Using equation (9.4) and Fourier's law, the first term on the left-hand side of (9.12) can be transformed into the following:

$$\frac{\partial Q_x}{\partial x}\Delta x \overset{(9.4)}{=} \frac{\partial q_x}{\partial x}\Delta x \Delta y \Delta z \overset{(9.1)}{=} -\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right)\Delta x \Delta y \Delta z \tag{9.13}$$

In the same way the two remaining terms can be written as:

$$\frac{\partial Q_y}{\partial y}\Delta y \overset{(9.1,\,9.4)}{=} -\frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)\Delta x \Delta y \Delta z \tag{9.14}$$

$$\frac{\partial Q_z}{\partial z}\Delta z \overset{(9.1,\,9.4)}{=} -\frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right)\Delta x \Delta y \Delta z \tag{9.15}$$

By inserting (9.13-9.15) into equation (9.12) and by dividing it by the volume of the element $\Delta V = \Delta x \Delta y \Delta z$ we obtain:

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right)+G=\rho\, c_p \frac{\partial T}{\partial t} \tag{9.16}$$

Equation (9.16) is the transient heat conduction equation. The stationary equation or the so-called steady-state equation can be easily obtained by setting the time derivative in (9.16) to zero:

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right)+G=0 \tag{9.17}$$

## 9.4. Heat Transfer Boundary Value Problem (BVP)

As we have seen before, in addition to the partial differential equation describing the problem we always have to define corresponding boundary conditions. If we speak about the transient analysis one has to be careful about the initial condition, as well. The heat transfer BVP reads:

$$\frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right)+G=\rho\, c_p \frac{\partial T}{\partial t} \text{ in } \Omega \subseteq R^3 \tag{9.18}$$

$$T=T_p \text{ over } \partial_D\Omega \text{ (prescribed temperature)} \tag{9.19}$$

$$q_p=-k\frac{\partial T}{\partial n} \text{ over } \partial_{N1}\Omega \text{ (prescribed heat flux)} \tag{9.20}$$

$$-k\frac{\partial T}{\partial n}=h\left(T_w-T_a\right) \text{ over } \partial_{N2}\Omega \text{ (convection)} \tag{9.21}$$

$$T=T_0 \text{ in } \Omega \subseteq R^3 \text{ at } t=t_0 \text{ (initial condition)} \tag{9.22}$$

Boundary condition (BC) (9.19) belongs to Dirichlet's class of BCs because it is the prescribed temperature over a certain surface. BCs (9.20) and (9.21) are the so-called Neumann's BCs because they determine the normal derivative of the unknown function. The initial condition (9.22) prescribe the values of the unknown function over the entire domain at the initial moment of time $t_0$.

As one can see, in the heat transfer BVP (9.18-9.22) only the heat conduction and convection are represented. The radiation is in general very complicated and requires much more effort for the mathematical description of implementation. However, from the micro- and nano-structures point of view the operating temperatures are not that high and radiation is usually not significant. The dominant components of heat transfer are the conduction and convection which are already included in our BVP.

An analysis of equation (9.18) shows that we are dealing with a scalar PDE and we have already shown the discretization of such PDEs via FEM. Therefore, we will not repeat it here and we will move directly over to some practical examples.

## 9.5. Transient 2D Thermal Analysis of a Micro AC/DC Thermo-converter

In this section we will present the transient thermal analysis of a micro AC[3]/DC[4] thermo-converter described in monograph [3] and in the original paper [4]. Due to its compact and geometrically accurate structure on a small silicon chip, this multijunction thermal converter minimizes the systematic errors in the transfer of AC voltage and current to equivalent DC quantities. In addition, due to its special structure, it offers a high (more than 100mV) and stable output DC voltage. This kind of AC/DC thermo-converter has been used for AC power measurement in microwave instrumentation, in true root-mean-square voltage measurement, and for AC/DC calibration [3].

The basic idea of the AC/DC thermo-converter is very simple. In the converter, the input electric power is converted into thermal power by an ohmic resistor or a so-called *heater*. The resulting thermal power is measured with a temperature sensor. The geometry of the device is presented in Figure 9.2.

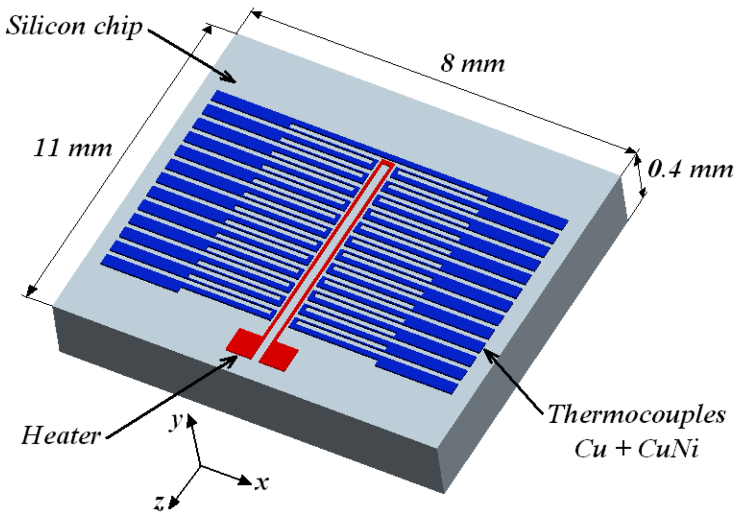


Figure 9.2. A simplified representation of the micro AC/DC thermo-converter described in [3, 4] is shown; The basic constitutive parts of the thermo-converter are the heater (red), the thermocouples (blue) and the silicon wafer (gray); Typical dimensions of the structure are given.

As one can see, over the surface of the silicon chip with a tiny layer of $SiO_2$, the heater and the thermocouples are sputtered step by step using appropriate masks and the "lift-off" technique [4]. The input AC signal is fed into the heater. Since the heater is made of some conductive material, Ohmic losses will develop within it. Those losses are the heat source of the structure. Thus, the input AC electric power is converted into the thermal power that heats up the surrounding space, including the thermocouples[5]. Here, a serial combination of 26 thermocouples is used in order to produce sufficiently high output DC voltage due to the thermoelectric effect. In order to achieve the needed temperature gradient for the thermocouples, the silicon wafer beneath the heater and thermocouples is etched away. This is visible in Figure 9.3. Thus, the heater and the hot side of the thermocouples (hot junctions) are placed on a tiny $SiO_2$ membrane. On the other side of the thermocouples (cold junctions), the

[3] AC represents Alternating Currents

[4] DC represents Direct Currents

[5] In 1821, the German-Estonian physicist Thomas Johann Seebeck discovered that when any conductor (such as a metal) is subjected to a thermal gradient, it will generate a voltage. A pretty significant voltage has been observed for a certain metal combination, i.e. a metal couple (two different conductive materials). This is now known as the thermoelectric effect and such couples are called thermocouples.

silicon wafer is left as a heatsink producing a necessary temperature gradient for the thermocouples. Our goal here is to numerically compute the time constant of the structure, i.e. the time that is needed with the given AC power input to reach thermal equilibrium (thermal steady state). Therefore, we need to perform a transient thermal analysis of the structure, i.e. we have to solve the BVP (9.18 - 9.22) using FEM. To find an accurate solution, we have to discretize the 3D structure shown in Figure 9.2. This requires significant knowledge of both theory and modern computer algorithms for handling of 3D geometry, mesh generation and 3D post-processing. The solution itself would require large hardware resources (memory and CPU speed). For educational purposes, we will use a simplified 2D approach to roughly estimate the transient thermal behavior of the structure. The equivalent 2D model is given in Figure 9.3.

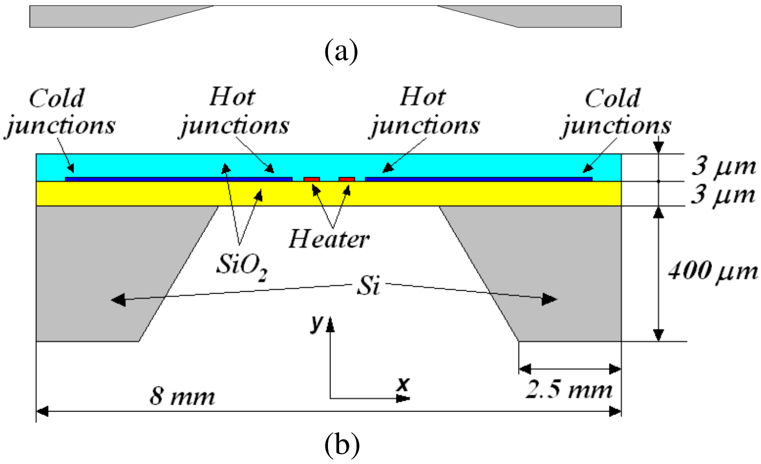


Figure 9.3. A 2D representation of the micro AC/DC thermo-converter shown in Figure 9.2; The width of the structure is around 8mm and the height is around 0.406mm. Due to such a large disproportion of the structure its figure in real proportions (a) is not useful because the details of the structure are not visible. Therefore, for visualization purposes, the structure is significantly enlarged in the y-direction and the details are visible (b); It is visible that the heater and the thermo-elements are placed on the $SiO_2$ membrane (yellow) and everything is protected with $SiO_2$ coating (light-blue).

To solve the BVP (9.18-9.22) we have to know the physical properties of the involved materials. According to reference [5], our materials have the following physical properties important for transient thermal simulation:

1. Silicon: $k = 124\frac{W}{mK}$, $\rho = 2300\frac{kg}{m^3}$, $c_p = 794\frac{J}{kgK}$, $T_0 = (273.15 + 25)K$
2. Silicon dioxide: $k = 1.4\frac{W}{mK}$, $\rho = 300\frac{kg}{m^3}$, $c_p = 732\frac{J}{kgK}$, $T_0 = (273.15 + 25)K$
3. Copper: $k = 401\frac{W}{mK}$, $\rho = 8960\frac{kg}{m^3}$, $c_p = 385\frac{J}{kgK}$, $T_0 = (273.15 + 25)K$

It is worth mentioning that all materials are assumed to be homogenous and isotropic. The heater is considered to be made of copper which is not so in reality. However, the heat generation over the volume of the heater is kept realistic ($Q = 6.93W/mm^3$ following [4]). The bottom of the silicon chip is assumed to be thermally connected to a large surface with a temperature equal to the ambient temperature $T_a = 298.15K = 25°C$, thus defining the Dirichlet boundary condition (9.19). All outer surfaces of the structure are supposed to be in contact with air. Therefore, the convective boundary condition (9.21) is defined there with the convection coefficient $h = 15W/(m^2K)$ and the ambient temperature $T_a = 298.15K = 25°C$. Initial condition (9.22), i.e. the initial temperature over the entire structure is set to be equal to the ambient temperature $T_0 = T_a = 298.15K = 25°C$ .

The FEM solution of the transient BVP in the time domain has already been described in Section 5.8 and therefore will not be repeated here.

Due to the large aspect ratio of the structure (the thickness is much smaller than the length) we have used here a regular mesh, i.e. rectangular elements as shown in Figure 9.4.

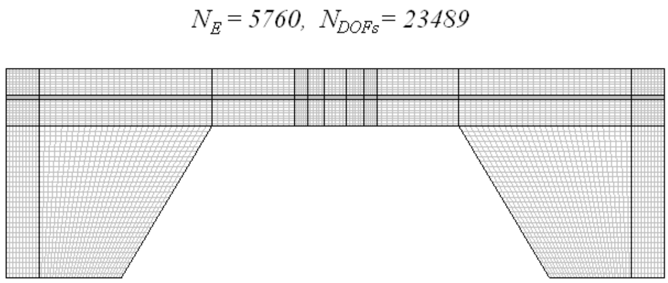


Figure 9.4. A regular rectangular mesh is depicted; The number of degrees of freedom is much larger then the number of elements due to a choice of second order shape functions over the element (8 nodes per rectangular element).

The time-step chosen for the transient analysis was $\Delta t = 1ms$ and the simulation was performed for the interval $t \in [0,120]ms$ because after 120ms steady state was reached as shown in Figure 9.5 and Figure 9.6.

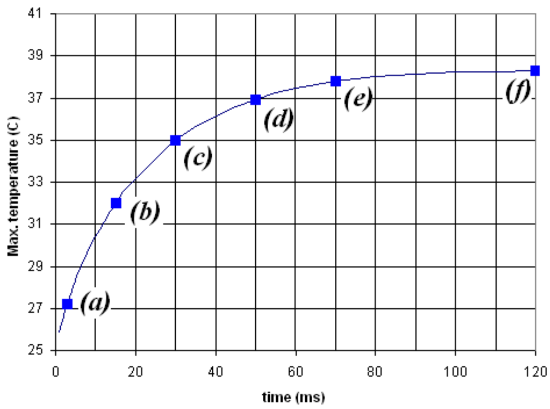


Figure 9.5. The heating diagram of the structure is depicted; The maximum temperature in the structure has been recorded for each time step and visualized (blue line); The characteristic moments of time have been chosen (a-f) and the temperature distributions for each particular case are depicted in Figure 9.6.

As one can see in Figure 9.5, the temperature in the structure increases quickly at the beginning of the heating process. After 30ms it gets slower and after 100ms it turns into a horizontal line (steady state). This practically means that the time constant of our structure can be estimated from this transient simulation to be 100ms. This estimation was our goal. It shows how important thermal analysis can be in the design of micro-devices. A similar analysis can be performed for the problem of microchip cooling. In combination with electromagnetic and mechanic analysis (coupling), thermal analysis can answer all major questions arising in development of new products based on a digital (virtual) prototype.

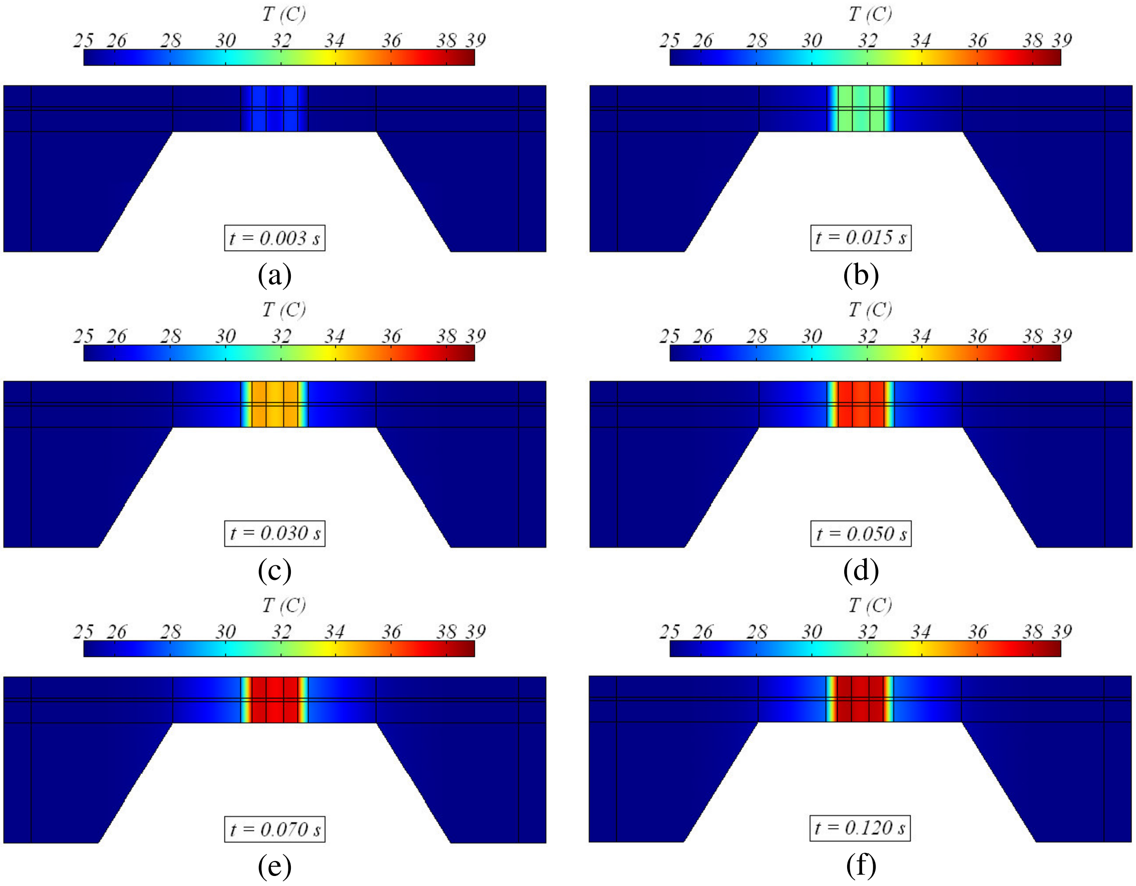


Figure 9.6. Temperature distribution over the structure for different moments in time is shown; The time-moments (a-e) are marked on the time-diagram of heating in Figure 9.5.

## 9.6. Concluding Remarks

In this chapter we have presented the basic theoretical statements of heat transfer analysis. Since the thermal design has a significant importance in a complete chain of a new product development, it is worth investing some time in studying its theory and practical aspects of its application. Through the example of the 2D transient analysis of the micro AC/DC thermo-converter, the basic application aspects of such an analysis for micro structures have been explained. It is important to mention that an accurate thermal analysis can be performed only with a full coupling with the source field. Namely, temperature, for example, influences the electromagnetic parameters of conductors (mainly the conductivity). Thus, the corresponding electromagnetic analysis is sensitive to the output of the thermal analysis and vise versa. Therefore, field coupling has to be taken into account. In the subsequent chapters of this script the coupling between electromagnetic and thermal analysis will be discussed.

## 9.7. References

[1] R. W. Lewis, P. Nithiarasu, K. N. Seetharamu, “Fundamentals of the Finite Element Method for Heat and Fluid Flow”, John Wiley & Sons, Chichester, England, 2004.
[2] A. Bejan, “Heat Transfer”, John Wiley & Sons, New York, 1993.

[3] J. G. Korvink, O. Paul, Eds., “MEMS: A Practical Guide to Design, Analysis, and Applications”, William Andrew Publishing and Springer Verlag GmbH, Norwitch, NY, 2006.
[4] M. Klonz, Th. Weimann, “Accurate Thin Film Multijunction Thermal Converter on a Silicon Chip”, IEEE Transactions on Instrumentation and Measurement, Vol. 38, pp. 335-337, 1989.
[5] MatWeb - The Online Materials Information Resource, www.matweb.com.