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Modeling and Simulation of MEMS Components: Challenges and Possible Solutions

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1. Introduction

Micro-electro-mechanical systems (MEMS) represent a very important class of systems having applications ranging from small embedded sensors and actuators, passive components in RF and microwave fields, and micro-mirrors in the optical range. The importance of MEMS stems from their many advantages, among which are, their small compact size amendable to integration with other components, low loss and parameter variability.

From structural point of view, each MEMS component is, by itself, a very small electromechanical system of heterogeneous structure composed of materials with different chemical composition (dielectric substrate, metal alloys and conducting wire) and different physical (electrical, thermal, mechanical) properties. Moreover, MEMS components may represent static systems or they may contain some moving parts, such as in variable capacitor, moving membranes and cantilevers. The dimensional scale of the different parts of MEMS components may vary from very small (microns or even nanometers) in one dimension, such as thickness of a plate, to comparatively large of few hundred microns in other dimensions, thus resulting in large aspect-ratios.

When MEMS components are put into oration, they constitute systems, in which electrical, thermal, mechanical, and other physical phenomena take place and interact with each other. From mathematical modeling and simulation point of view, this calls for multi-physics treatment, in which coupled systems of differential equations of different combinations of electromagnetic, mechanical, fluid, heat transfer and/or transport equations, are formulated then solved depending on the type of boundary conditions imposed by MEMS component under investigation.

Mathematical modeling and simulation has been used in all fields and disciplines of engineering for decades, for theoretical characterization of devices and systems before manufacturing, or even before prototyping, for a number of reasons among which are reduction in manufacturing cost and time. However, the heterogeneous nature of MEMS structures, coupled with multi-physics phenomena that take place during their operation, makes modeling and simulation of MEMS components, a complex and challenging task.

The main objectives of this chapter are to outline the nature of MEMS componets, from both the structural and physical points of view and identify the difficulties that these heterogeneous structures impose on modeling and simulation of these systems and to give a comprehensive account of different modern modeling methods and techniques used to overcome MEMS modeling and simulation difficulties, with illustrative examples. From here onwards, the word ‘components’ will be suppressed and refer to MEMS component just as MEMS for brevity.

The chapter starts with some basic definitions, then shed light on the use and advantages of mathematical modeling and simulation in MEMS design and manufacturing, investigates the nature of MEMS and the main challenges facing researchers in their modeling and simulation. It presents systematic approach to MEMS modeling and simulation, gives a survey coverage of different methods and techniques used for simulation of MEMS, such as finite-differences time-domain (FDTD), finite-element (FE) and their different variants proved to be successful in their applications to such microstructures. A detailed illustrative MEMS modeling and simulation example is given and other examples developed by other active research workers, are cited. The chapter concludes with future outlook and new trends in MEMS modeling and simulation.

2. Background

Over the last few years, extensive research work in modeling and simulation of MEMS took place, and a large number of techniques appeared in the literature to tackle this complicated modeling problem, each having its own advantages and limitations (Bushyager et al., 2003; Lynn Khine & Moorthi, 2006; Khine A. et. al., 2008; Yong Zhu & Espinosa, 2003; Shanmugavalli et. al. 2006; Heung-Shik Lee et. al., 2008; Fengyan and Vaughn, 2009; Chiao & Liwei, 2000).

Bushyager and his coworkers considered modeling electro-statically actuated RF passive components, such as parallel–plate capacitors and tuners (Bushyagers & Tenzeris, 2002; Bushyager et .al 2003; Bushyager, Mc Garvey & Tenzer 2000). They used finite-difference time-domain technique (FDTD) or its variant MRTD, with adaptive gridding to tackle the problem of large aspect ratio and moving boundary conditions (see section 4).

Fengyan and Vaughn (2009) developed an on-line tool for simulating micro scale electro-thermal actuators (ETA), using both distributed and lumped analysis. The model allows the user to input the electrical Current of ETA to compute both temperature distribution and the displacement of the ETA. Finite–Element method was used to find temperature distribution due to joule heating and the average temperature across the beam is used to find the displacement by lumped analysis. The Model takes into account both properties’ variation with temperature as well as radiation effects at high temperature. The main characteristics of their model is the use of computationally expensive distributed analysis for modeling electro thermal phenomenon and the computationally efficient lumped analysis for the modeling the thermo mechanical phenomenon thus improving the overall computational efficiency, accessibility and ease of use. The last two properties (accessibility and ease of use) are due to on-line availability of model for remote users.

Chiao & Liwei (2000) Considered self buckling behavior of micromechanical clamped-clamed micro beams under resistive heating using both analytical and finite-difference technique. Their model consisted of electro-thermal part in which electric current flowing through the beam gives rise to Joule Heating effects, and thermo-mechanical part which deals with the mechanical buckling of the beam due to thermal expansion. Results was verified by measurements with good agreement. They considered the effected of residual stress and found that when compressive residual is considered in the analysis the critical current causing bulking of the beams, decreased where as tensile residual stress hinders the actuation of the beams. They also considered the effect of process variation such as the width and the thickness of the beam, and found that they affect the performance of the beams such as the current–deflection curves, however variation expansion and Young's modulus with temperature, were not considered and called for characterization of these properties' variation in order to improve the accuracy of MEMS Models.

Most, if not all, of these attempts relied on numerical (computational), rather than analytical techniques, due to ability of numerical methods to model structures with arbitrarily complex geometrical shapes. Despite the advantages of numerical techniques researchers were faced with a number of difficulties when trying to use commercial simulation packages and adapt traditional numerical methods, such as finite-difference, time-domain (FDTD) and finite-element (FE), used in modeling structures at macro-scale. The main difficulties and challenges are highlighted in section 4.

3. Modeling & simulating definition & advantages

3.1 Definitions

Before we go into further details of this chapter definition of some of the main concepts is in order. In the following are given, definitions of the main keywords of this chapter; modeling and simulation.

Modeling: Modeling, and a model, has different meanings depending on the context or field of application. In engineering science and technology, Modeling refers to mathematical representation of a physical phenomenon, system or device. Usually mathematical models can take many forms such as dynamic system models, statistical models, game models, differential equation…etc. But for the purpose of this chapter, we will be mainly concerned with mathematical models that are represented by differential equations.

Simulation: Similar to modeling, simulation also has different meanings depending on the context and type of application and it can take many forms. However for the purpose of this chapter, we will concentrate on computer simulation or computational modeling, which is defined as: a computer program, or package, that attempts to simulate or imitate an abstract model of a particular system or device. Computer simulations have become very much related and integrated with mathematical modeling, and usually modeling and simulation are taken as being one discipline that can be used to explore and gain insight into the new technology and predict and estimate behavior of complex systems and devices that are too much complicated for analytical solutions.

Modeling and Simulation generally have iterative nature. A model is first developed then simulated to gain some understanding. The Model is then revised, and simulated again and this process goes on until an adequate level of understanding is developed for the system/device under consideration.

3.2 Need for MEMS modeling and simulation

There are many reasons why we need modeling and simulation for MEMS, among which are:

a. Due to small dimensions of MEMS, direct experimentation for determination of some physical properties of MEMS is difficult, and measurement errors occur when dealing with these micro-level systems.

b. Time reduction: Designers need simulation tools that allow them try "what If "experiments in hours instead of days and weeks, thus reducing time to market.
c. Production cost reduction: Modeling and simulations are needed in order to study the behavior of the design under different experimental conditions and different level of parameters, before prototyping, thus reducing production cost.
d. MEMS are usually embedded within other systems or packaged with other micro-machined components and systems. Therefore modeling and simulation is needed at macro or system level as well as micro-level.
e. Modeling and simulation can render fast design cycle that allows extensive scoping for more and accurate decision making.
f. Modeling and simulation allows better understanding of the device/system operation and gives scope for optimization of its operation.
g. Modeling and simulation enable designers and system developers to see and further investigate systems behavior which could have not been discovered otherwise.

4. MEMS modeling challenges

The difficulties and challenges that face MEMS modeling and simulation experts are due to the very nature of MEMS and can be related to the following MEMS features: Physical principle of operation, geometrical structure, miniaturization, packaging, manufacturing and processing of MEMS, and environmental conditions. These are detailed in the following:

a. Physical Principles:

As mentioned earlier, MEMS are characterized by interaction of many physics domains in a single device or system. This is pictorially represented in Fig. 2. Interaction of many physical phenomena in MEMS needs dealing with different types of equations, each governing a certain physical phenomenon e.g. electrical, mechanical or thermal. Moreover these governing equations are always coupled sometimes strongly and sometimes weakly, thus calling for solution of coupled system of equation a phenomenon called multi- physics approach. Depending on the number of physics domains involved, we can further classify these multidomain systems as: Double-Physics (interaction of two physics domain, Triple-Physics (interaction of three physics domains), Quadruple-Physics (interaction of four physics domains) and so on. In section 7.2 , we show specific modeling and simulation examples illustrating these different physics categories.

b. MEMS geometrical structure:

One of the main obstacles facing accurate modeling of micro-systems is proper definition (construction) of the system geometry, one of the main first requirements in any modeling and simulation process. This is due to different deformations and irregularities during MEMS operation, such as in the case of tuners and microbeams that contain moving parts. In order to tackle this problem, Peyrou David et.al, 2004, proposed a reverse engineering technique, whereby the model is first built using the real shape of the device, then a virtual model is made from the deformed shape, using different software packages. This method was applied for simulation of RF-MEMS capacitive switch and electrical contact resistance of RF MEMS, with satisfactory results (Peyrou David et.al, 2004).

c. Large Aspect Ratio:

Many MEMS, such as metallic sheets on top of large substrate (e.g. capacive stub tuners), have very small dimension in one direction (thickness) compared to relatively large dimension (length) in other direction, thus leading to large aspect ratio. Large aspect ratio, in turn lead to creation of large number of computations cells thus leading to long computation time (Ali, I. Kabula M. & Hartnagel H. L., 2010).

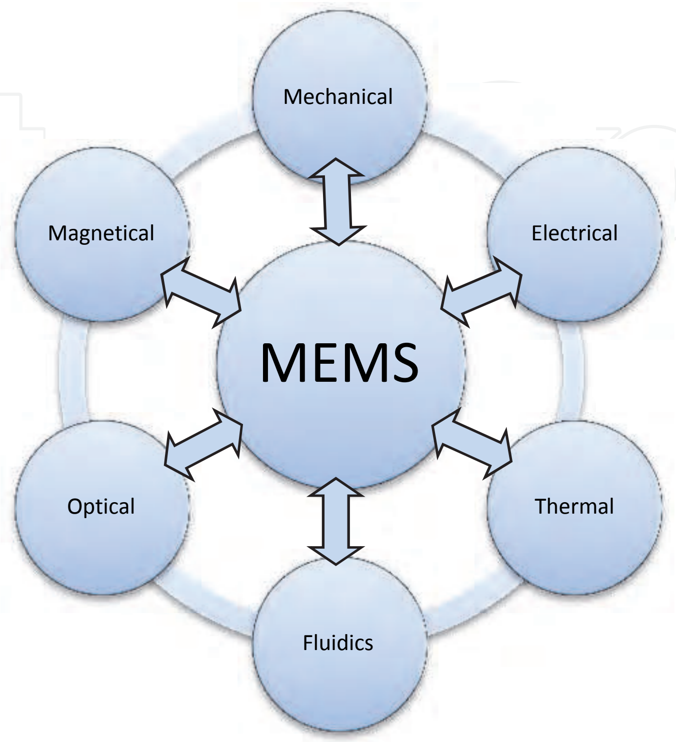

Fig. 1. Multiphysics nature of MEMS

d. Geometry change due to moving parts:
Some MEMS components, such as electrostatic and thermal actuators, contain moving parts, which lead to moving boundary conditions.Commercially available traditional frequency domain simulators are not adequate to handle these features, due to many approximations that are more to simplify modeling and time-domain techniques, are more appropriate (Bushyagers & Tenzeris. 2002; Bushyager et. al., 2003). However even the well-known time–domain techniques such as FDTD, are not adequate as they stand and some sort of modification are needed to deal with large grid size and moving boundary conditions. These are solved by using adaptive gridding in both space and time, which are included in FDTD technique with variable gridding capability or the use of multi resolution time domain technique known as MRTD for short.
e. Miniaturization:
Due to the very small dimensions of MEMS many physical phenomena such as surface tension from humidity, become significant at micro-level. Downscaling of the dimensions of MEMS structures, which are usually three-dimensional makes the scale of these effects (force, displacement … etc.) also significantly small which, in turn lead to accumulation of numerical errors.
f. Packaging:
In many cases MEMS are assembled and packaged with other electronic components and devices, and this calls for proper modeling and simulation at systems level taking into consideration all input/output feedback etc.

g. Manufacturing and processing:
Manufacturing and process uncertainties which result from the fact that the dimensions and properties used in simulation of the MEMS cannot be exactly produced during fabrication.
h. Environmental Conditions:
MEMS are sometimes needed to work at different environmental conditions, such as sensors on the surface of the aircraft wings or sensors and actuators in nuclear power plants or under sea. Being tiny components at micro level, these systems are much affected by these external conditions. This calls for careful considerations of these conditions when modeling.

5. MEMS modeling and simulation process, techniques and tools

In this section, we show a systematic procedure for modeling and simulation process of MEMS, and give a survey of techniques and software tools proved to be successful in tackling many of the modeling and simulation challenges illustrated in the last section.

5.1 Modeling and simulation process cycle

The process of modeling and simulation goes through a defined number of steps, briefly described and depicted graphically in Fig.1 below:

Step 1: Description of the Physical Problem:

The first step in the modeling and simulation process is the physical description of the problem under investigation in order to understand its geometrical structure and the entire physical phenomenon involved in its operation.

Step 2: formulation of governing equations:

Depending on the physical principles governing operation of the device/system, all equations and mathematical expressions governing this operation are setup together with appropriate boundary and/or initial conditions.

Step 3: approximation of governing equations:

At this step, some approximations that facilitate solution with adequate effort and/or resources are made. If more than one equation is involved, the degree of coupling between different types of equations is determined at this step.
Steps 2 and 3 are usually very much interrelated, and the process of approximation and formation of governing equations are done iteratively in one step.

Step 4: Method(s) of solution:

Here all adequate methods of solutions of the governing equations are explored, and the most appropriate one identified. Appropriateness here calls for proper consideration of all available computation resources (both hardware and software), and selection of the most efficient one in terms of computational resources.

Step 5: Solution of the governing equation(s):

The method(s) identified in step 4 is applied to find the solution of the system of equations under specified boundary/initial conditions.

Step 6: Verification of Results:

After finding the general solution in step 5, some simplified standard cases which can be verified by experimental measurements or for which analytical or known solutions are

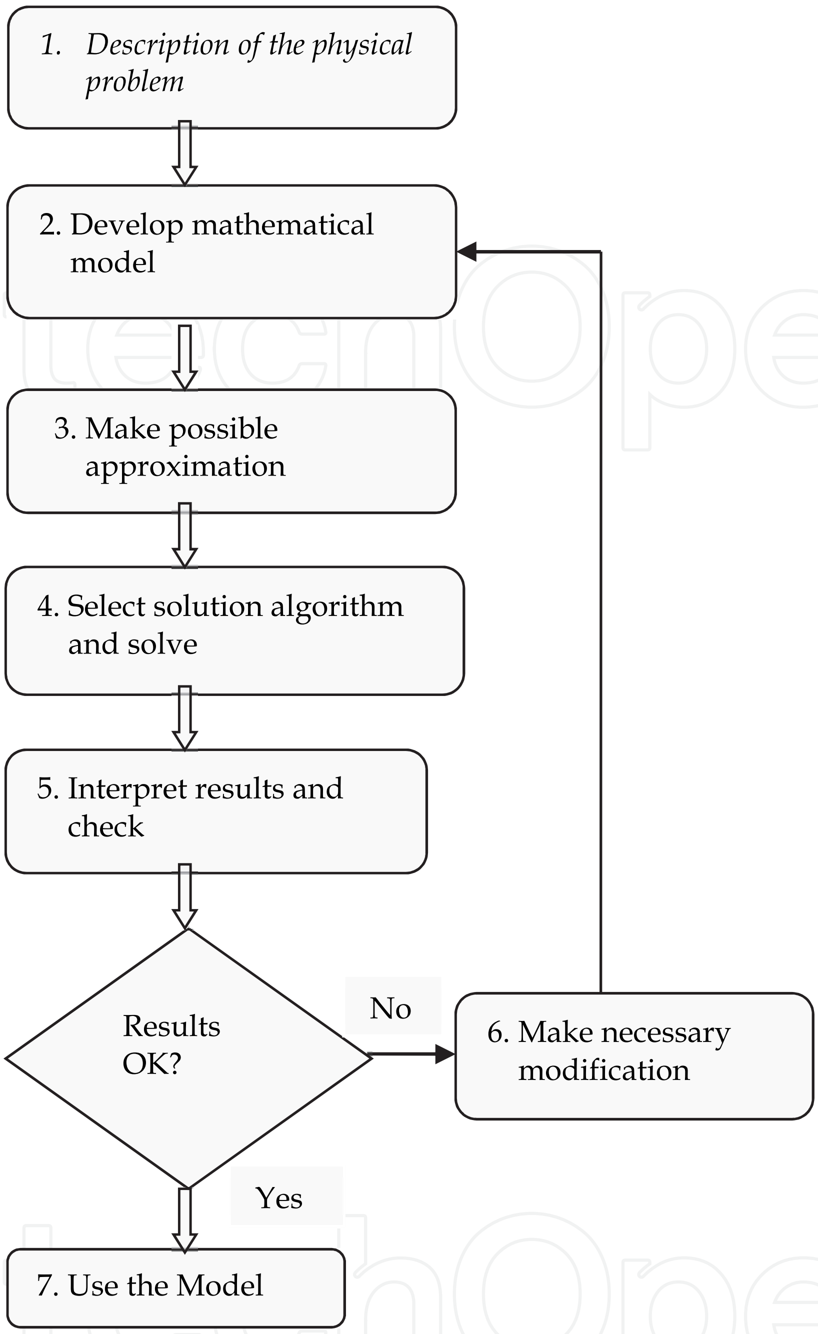

Fig. 2. The main Steps of Modeling and Simulation process (details of each step are given in the main text)

identified for comparison reasons. If adequate solution that agree with measurements or known solution is obtained, move to the following step or otherwise go back to check method of solution or even the model itself. This checking process goes on until adequate solution is obtained (see decision block in the flowchart of Fig.2.

Step 7: Use model for exploration and design optimization:

This is the last step at which you make use of your efforts in modeling and simulation. Here the model is used for analysis of varied situation under different conditions i.e. change of input parameters and study of what-if conditions.

5.2 MEMS modeling techniques

There are a number of modeling techniques, with different facilities and capabilities, for modeling and simulation of MEMS at both component and system levels. However, we will concentrate on two mostly used techniques; the finite difference time domain (FDTD) and Finite Elements techniques and their variants.

5.2.1 Finite – Difference – Time Domain (FDTD)

FDTD technique is direct method of Solution of Maxwell's curt equation (Taflove, A. & Hagness, S., 2001):

$$\nabla \text{ X } \bar{\mathrm{E}} = -\mu \frac{\partial \boldsymbol{H}}{\partial t} \tag{1}$$

$$\nabla \text{ X } \boldsymbol{H} = \sigma\bar{\mathrm{E}} + \epsilon \frac{\partial \boldsymbol{E}}{\partial t} \tag{2}$$

where **E** and **H** are the vector electric and magnetic fields, μ, ϵ and σ are the respectively, permeability, permittivity and conductivity of the medium.

FDTD method is a full-wave time stepping procedure that uses simple central—Difference approximation to evaluate the space and time derivatives. FDTD method has been successfully used for simulation of complex structure at macro scale, however one of the most constraints of FDTD is the requirement that cell size be equal to or smaller than the smallest feature of the device or system being simulated. This leads to large grid size when simulating structures consisting of several different elements or structure with large aspect ratios, such as MEMS circuits. The large grid size leads, in turn to large computing time.

In order to overcome this difficulty, a number of modification and /or addition have been proposed, among which are the method of sub gridding, and the use of non-uniform grid (Shanmugavalli et. al., 2006; Bushyager et. al., 2001). The first, subgridding method subdivides sections of the FDTD grid, thus creating finer grids in areas of large field variation or interfaces between areas of different properties. This method can be used when small complex devices are embedded in a coarse grid, such as small passive compounds (compactors' or inductors) connected by micro strip lines or when MEMS are packaged. Here a subroutine is needed to interface grids of different sizes. In the non uniform grid technique, each direction of the structure under investigation is treated separately, thus allowing each axis to be divided into a number of sections each having a different cell size.

5.2.2 Multiresolution Time Domain (MRTD) technique

MRTD employs multiresolution principles to discretize Maxwell's equations in wavelet expansions, which provide a set of functions with adaptive resolution. Higher resolution functions can be added and subtracted during simulation. Accordingly MRTD has built-in gridding capability in both time and time and space

1. MRTD can model changes in structure over time because it is a time-domain simulator for example: variable parallel-plate capacitor.
2. Variable grid capability and ability to arbitrarily place metals in structures allow for modeling of a structure that changes configuration during simulation.
3. Adaptive (variable) gridding allows modeling of MEMS in packages such as variable capacitor connected to large feed lines .In this case the surrounding structure can be modeled with a comparatively coarser grid, while the MEMS is modeled with a fine grid (higher resolution).

When MRTD is applied to Maxwell's Curl equations (1 and 2 above), the orthogonality of the wavelets provides an efficient discretization that results in an explicit time marching scheme similar to that of FDTD technique. Due to this property and the characteristics of MRTD stated in 1-3 above, MRTD has been successfully applied by Bushyager and his co-workers to a number of modeling and simulation of RF MEMS structures, such as parallel-plate capacitor (Bushyager & Tentzeris 2001), MEMS tunable capacitors (Bushyager et. al. 2002), analysis of MEMS embedded components in multilayer packages (Tentzeria et. al. 2003), for intracell modeling of metal/dielectric interfaces (Bushyager & Tentzeris, 2003), for static MEMS capacitor (Bushyager, McGarvey & Tentzeris, 2001).

5.2.3 Finite Element Technique

The **finite element method (FEM)** is a numerical technique for finding approximate solutions of partial differential equations (PDE) and integral equations. The solution approach is based either on eliminating the differential equation completely (steady state problems), or rendering the PDE into an approximating system of ordinary differential equations, which are then numerically integrated using standard techniques such as Euler's method, Runge-Kutta, etc. Historically, finite element method originated from the need for solving complex material and structural problems by civil and mechanical engineers.

The first step in finite-difference analysis is to divide the structure under consideration into small homogeneous pieces or elements with corners called nodes. The nodes define the boundaries of each element and the entire collection of elements defines the analysis region or the geometry of the structure. These elements can be small where detailed geometric properties are required and much larger elsewhere. A simple variation of the field is assumed in each element and the main goal of FEA is to determine field quantities at each node. In general, FEA techniques solve for the unknown field quantities by minimizing an energy functional using variational techniques. The energy functional is an expression describing all the energy associated with the structure under consideration. For instance, this functional for 3-dimentional time-harmonic electromagnetic fields E and H is represented as:

$$F = \int_v \frac{\mu|H|^2}{2} + \frac{\epsilon|E|^2}{2} + \frac{JE}{2j\omega} dv \tag{3}$$

Where the first two terms represent energy stored in the magnetic and electric fields and the third is the energy dissipated or supplied by the conduction currents.

Eliminating H using relation between E and H, and setting derivatives of this functional with respect to E to zero (for minimization), an equation of the form f(J,E)=0 is found. Appling K^{th} order approximation of F at each of the N nodes and enforcing boundary conditions results in a system of equations of the form:

$$\begin{bmatrix} J_1 \\ \\ J_n \end{bmatrix} = \begin{bmatrix} y_{11} & \cdots & y_{1n} \\ \vdots & \ddots & \vdots \\ y_{n1} & \cdots & y_{nn} \end{bmatrix} \begin{bmatrix} E_1 \\ \\ E_n \end{bmatrix} \tag{4}$$

Here J_i and y_{ij} (i=1,2,..n and j=1,2,..,n) are known quantities and the electric fields E at each node are the unknowns to be determined. This needs inversion of the y matrix and the larger the number of nodes, the larger the size of the matrix and hence more computational requirements. For example a mesh of a 3-D cube with 1000 nodes (10 nodes per side) and 3 degree of freedom creates a 3000 by 3000 matrix. Doubling the number of nodes per side gives a system of 24000 by 24000 matrix. Therefore it is necessary to as fewer as possible number of nodes is preferable from the point of view of computer resources. On the other hand the more the number of nodes the more is the result accuracy. Usually a compromise is made between required accuracy and computational resources. For proper grasp of this useful technique, the reader is referred to any of the many text books on finite element analysis (see for instance Silvester & Ferrari (1990)).

5.3 MEMS simulation software tools

During the last decade, and specially in the period 2002-2010, there were a lot of research activities and developmental in the area of modeling and simulation tools dedicated to MEMS, and a number of such software simulation tools moved from research centers to the commercial world. These tools can be classified broadly as: *system level modeling and simulation tools* and *detailed device–level tools known as field solvers*. Technique used in type of tools, have been in use at macro level for some time and have gained maturity. the micro level , however . There tools are still going some modification due to the nature of MEMS, which comprises many physical domains such as; mechanical, thermal, electrical and optical domains. In the following sections, we give a brief overview of these techniques and tools.

5.3.1 System level tools

These tools predict the main behavior of the MEMS, using a set of ordinary differential equations and non linear functions at block diagram level in terms of input and output of each block. These tools are usually required by MEMS Designers for accurate prediction of the overall performance of these systems when connected or operated with other circuit components and for proper optimization (Lynn Khine & Moorthi P., Hine A. et. al. 2008). In addition they enable the designer predict the performance of the device under consideration for a set of defined input parameters, it allows him/her to study the effect of variation of one or a certain set of parameters relative to other parameters on the overall performance of the device, thus leading to optimized design.

5.3.2 Field solvers

The majority of these solvers are based on the well-known numerical techniques of finite elements (FE) or finite–difference time–domain, methods briefly out lined in the lost section, with only few tools based on analytical or asymptotic solution of the governing equation. These methods are virtual and can analyze complex geometric shapes.

Finite-Elements–based tools

The majority of MEMS software tools now available in the market are based on the well – established FE technique. These include ANSYS (COMSOL), ConvectorWare, Intellisuite, ABAQUS, and DELEN, to mention only some example. In the following we give a brief account of their mostly used tools in the field of MEMS analysis and design.

a. ConventorWare

This is a fully integrated MEMS Design environment, the latest version of which is convectorWare2010. It runs on PCS and work Stations based on sun Solaris and windows
This package consists of four main parts; Designer, Architect, Analyzer and Integrator. Designer is concerned with design specification and modeling of the MEMS Structure including two-dimensional layout, process emulation and finite elements meshing. It

includes a full- featured layout editor, foundry access kits , 2D and 3 D import/export capabilities, mesh generator and a library of 3D models of standard MEMS packages. It is tightly integrated with the other two modules ARCHITECT and ANALYZER, but it can also be used as stand- alone package to be integrated with other third-party FEA tools.

   i. ARCHITECT 3D: This module creates schematic models of MEMS designs using MEMS component Library, perform fast system level simulations with finite elements accuracy and significantly reduce product development time by mean of fast simulation speeds.
   ii. ANALYZER: This Module provides a single unified interface to a complete suite of 3D field solver such as coupled Electro-Mechanics, Piezo–Electric or Microfluuidics. With this module the designer can perform: parametric studies to optimize design, Incorporate packaging effects such as ambient temperature and peruse, Predict and validate experimental measurements, Investigate manufacturing effects such as residual stress.
   iii. INTEGRATOR: This module extracts reduced-order models of physics effects for use in ARCHITECT. For Example it can be used to add gas damping effects on a ARCHITECT model. Similarity it can extract mechanical stiffness of structural components such as tethers that can be modeled as a linear or non linear mechanical springs a electro statistic forces between electrodes and combs that can be modeled as electrostatic springs.

b. IntelliSuite:

This is an integrated design environment specifically developed to link the entire MEMS organization together. It enables designers to manage their MEMS product throughout it life cycle. Intellisuite consists of a number of advanced tools that work together, each covering a certain MEMS development stage. The main components of Intellisuite are:

   i. Synble: that allows the designer to capture MEMS at a schematic level, explore his/her design, then optimize and synthesize. It has a powerful schematic editor specifically developed for MEMS and other multiphysics modeling.
   ii. Synthesis: these are sophisticated algorithms that automatically convert schematics into mask layouts or a meshed structure for multiphysics analysis.
   iii. Blueprint: a physical design tool that includes advanced layouts, cross section exploration and automated mask to hex mesh.
   iv. CleanRoom: used for creation of process flow and mask set before entering the physical clean room thus allowing visual prototype before actual fabrication.
   v. Fastfield: a collection of multiphysics tools featuring coupled electrostatic, electromagnetic and electromechanic engines.
   vi. Extraction: collection of techniques that capture electromechanical and damping behavior into compact models.

c. COMSOL Multi-physics

COMSOL Multiphysics is a simulation software specifically designed to tackle multi physics problem, usually encountered all disciplines in Engineering Design starting from the definition of geometry, through meshing and material property definition and ending with solving and visualization of results. It is based on solution of the partial differential equations that given different physical phenomenon be it electromagnetic, heat transfer, structural mechanics, magnetostatics, simultaneously or sequentially solved using finite element analysis.

By its very nature of structure it is particularly appropriate module for MEMS, modeling and simulation, and in addition , it has a specialized module for MEMS, called MEMS Module that simulates standard MEMS problems, such as piezoelectric and thin film damping problems.

Finite difference time domain tools

a. XFDTD Package:
This is based on finite difference time domain technique (FDTD), for the solution of vector Maxwell's equations developed by REMCOM Inc. It is an easy to use package, but it does not have the capability of dealing with multidomain (multiphysics) problems.

5.3.3 Other tools

In addition to the above mentioned main MEMS Simulation software tools, there are other tools most important of which is the hybrid approach in which both system-level and field solvers in circuit simulation environment. They rely on a new class of parameterized behavioral method that can automatically access relational databases that contain field software solution results. These models have been successfully used for analyzing packaging effects of inertial sensors and design of PZR pressure sensors (Lorenz G., Greiner, K., & Breit S. 2006).

6. Selected MEMS-based Modelling Examples

Modeling and simulation can not only be acquired by reading and studying different methods and techniques, but through actual involvement in building models, simulating and practicing. This is similar to driving a car. Car driving can be learned through reading instructors notes, books and articles about car driving, but can only mastered by actually driving a car.

In this section, we illustrate the process of modeling and simulation described in section 2.2, by going through an actual case carried out by the author and his coworkers, and highlight some few successful cases done by other research workers.

6.1 Detailed illustrative example on modeling and simulation process

Micromachined DC and high frequency power sensors

In order to show how the modeling and simultion process described in section 3.3 is implemented in practice, modeling and simulation of micromachined power sensors at both the dc and high frequencies (microwave and millimeter waves) is presented. The sensor fabrication techniques is based on bulk and surface micromachining of AlGaAs/GaAs heterostructures, and the sensor concept is based on transduction principle that converts the RF into thermal power, which is then measured by thermoelectric means (Mutamba et al., 2001; Ali, I. Kabula M. & Hartnagel H., 2010)).

Modeling and simulation is based on the solution of the coupled electromagnetic field and heat transfer equations, using hybrid finite-element/finite-difference techniques. The model can be used as an effective tool for adjustment of design parameters, such as geometric configuration of the sensor resistive element, and arrangement of thermocouples around the resistor for optimum sensitivity and noise figure.

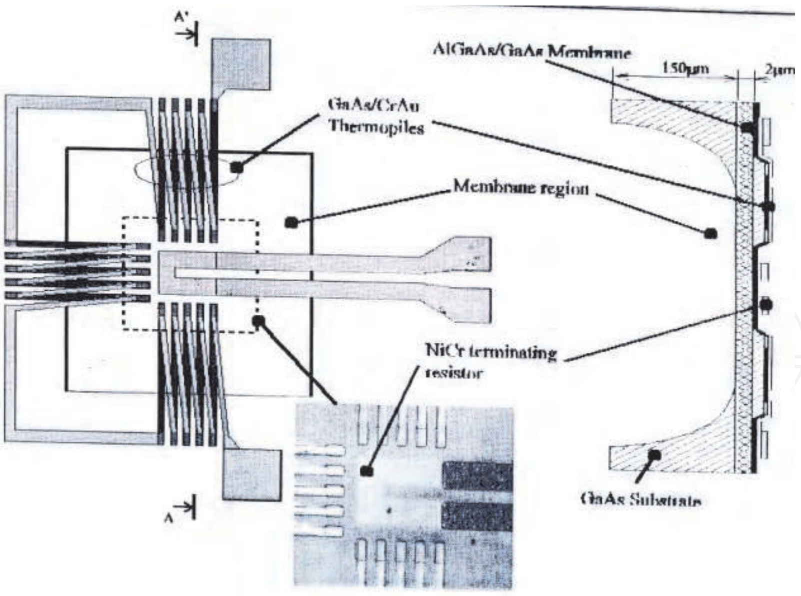

Fig. 3. The structure of the power sensor. left-hand : top view, right-hand-side sectional view along A-A'.

Step 1: Description of the Physical Problem:

A sectional view of the configuration of the sensor to be modeled is depicted in Fig. 3. The sensor is composed of a thermally isolated thin (2 µm) AsGaAs/GaAs membrane region with a terminating resistor, in which heat generated by DC or RF power is dissipated and converted into heat. A high-thermally resistive membrane region is obtained by selective etching of the GaAs against AlGaAs. This helps to increase temperature gradient between the resistor region and the rest of the chip, thus leading to high sensitivity. Temperature increase in the resistor region is sensed by a set of Gs/Au-Cr thermoelements, whose dc output is proportional to the input RF power. Detailed description of technical realization of this sensor is given by Mutamba et al., (2001).

Steps 2,3: The Governing Equations and Approximations:

Here we consider both the thermal and the electric models. The mathematical model is required to be simple enough to be handled by known methods which demand reasonable time and cost, and at the same time give an adequate description of the physical problem under investigation.

Thermal model

A simplified pictorial view of the sensor is shown in Fig. 3 for the purpose of thermal modeling. Here the thermocouple wires are not shown, and heat generated by the NiCr resistor, is assumed to be distributed throughout the sensor structure mainly by conduction. Due to axial symmetry of the sensor structure about it longitudinal axis, we only consider half of its geometry as shown in Fig.4. We select Cartesian coordinates (x,y,z) with its origin at the sensor input and the direction of power transmission along the positive z-direction.

In order to obtain a simple and manageable model, the following simplifying assumptions, are made:

i. The presence of the thermocouples is ignored as the metallic part (gold) is very small compared to other dimensions.

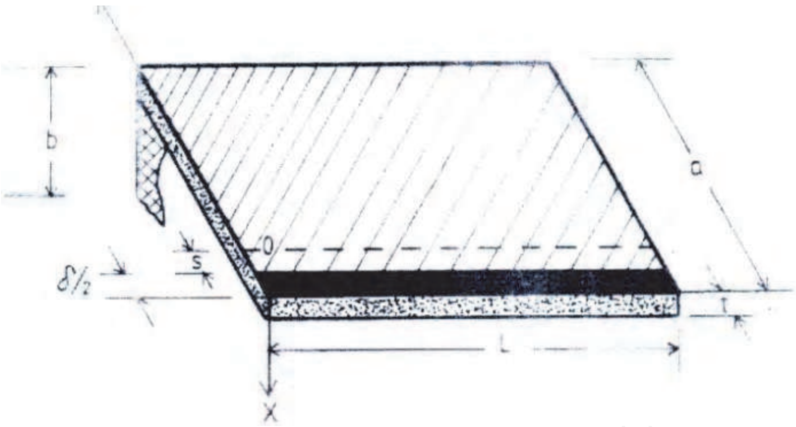

Fig. 4. Simplified half-section used for modeling.

ii. As a first approximation, heat distribution is assumed to be two-dimensional (in Y-Z plane). This assumption can be justified due to the presence of the thermally isolated thin membrane whose area dominates the horizontal dimensions of the sensor.
iii. Constant thermal properties. Although thermal properties, especially thermal conductivity of GaAs vary with temperature, these properties were assumed to be constant due to the expected moderate temperature rise.
iv. Radiation losses are ignored as the sensor were to work in a very confined region and the expected temperature rise is limited.

The equation governing heat flow as a result of microwave or dc heating is the well-known heat conduction equation, also known as Fourier equation:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + Q / \rho C \tag{5}$$

where T is the temperature, α is thermal diffusivity , Q heat generation term, ρ is the density and C is the specific heat of the medium .

Thermal boundary conditions

These conditions can be obtained from the prevailing thermal conditions at the boundaries and the interface between different material layers of the sensor.

i. Convective heat transfer at boundaries y=0 and y=a.
ii. Specified temperature at boundaries z=0 and z=L.
iii. At the interface between different sensor material layers: assuming perfect thermal contact leads to the continuity of heat flux and temperature at these interfaces between layers.
iv. Assume initially that the sensor is at a constant temperature To.

The heat source term, Q, in equation (5), is determined by solving either of two different sets of equations, depending on the operation mode of the sensor (dc or high frequency) as shown below.

Electric model

Here we consider the case of AC and DC case separately, because of their different governing equations.

DC Operation Mode:

In the case of the dc operation mode, the electrostatic potential equation is used:

$$-\nabla(\ \sigma\nabla V)=q_i \tag{7}$$

where V is the electrical potential, σ is the electrical conductivity, and q_i is the current source. In the case of constant electrical conductivity, equation (7) reduces to the simple Poisson's equation:

$$\nabla^2 V=q_i\ /\ \sigma \tag{8}$$

Boundary conditions assumed for solution of equation (8) were that a constant voltage +V applied at one arm and –V at the other arm of the CPS With the symmetry condition along the longitudinal axis of the sensor, +V was assumed at one arm at input of the sensor and zero voltage at the end of the resistor (see Fig. 3). Having found V from equation (8), the heat generation term, Q, is obtained as:

$$Q=\sigma\left|E^2\right| \tag{9}$$

where E is the electric field intensity, given by:

$$\bar{E}=\nabla V \tag{10}$$

High Frequency Mode:

In the case of high frequency operation mode, the heat generation term, Q, is obtained from the solution of Vector Maxwell's equations:

$$\nabla X\bar{E}=-\mu\frac{\partial\bar{H}}{\partial t} \tag{11}$$

$$\nabla X\bar{H}=\sigma\bar{E}+\varepsilon\frac{\partial\bar{E}}{\partial t} \tag{12}$$

in which $\bar{E}$ and $\bar{H}$ are electric and the magnetic field vectors, and ε, μ ,σ are respectively the permittivity, the permeability and the conductivity of the material (medium) through which electromagnetic wave propagation takes place.

Steps 4 & 5: Solution of Governing Equations:

If the simplifying assumption (i) – (iv) are used, equation (1) with boundary conditions ii), iii) and iv) can be solved analytically using the method of separation of variables. However, in the more general case of three-dimensional form of equation (1) with boundary conditions (i) to (iv), the versatile numerical methods of finite difference in time-domain or finite elements are more appropriate, since they can deal with any sensor structure. Investigation of available software packages revealed that XFDTD package, based on finite difference time domain technique, is most appropriate for the solution of vector Maxwell's equations and FEMLAB, a package based on FEM for solution of the heat equation. As the two packages (XFDTD and FEMLAB) are based on different solution techniques using different simulation tools, it was necessary to have an interface that links the two packages. This was achieved by a special script file written using MATLAB built-in functions. Material properties used in the simulation are shown in table 1.

Material	*Thermal conductivity (W/m K)*	*Specific heat (J/kg K)*	*Density (kg/m^3)*	*Relative permittivity*	*Electrical conductivity (mho)*
GaAs	*44*	*334*	*5360*	*12.8*	$5x10^{-4}$
NiCr	*22*	*450*	*8300*	-	$9.1x10^{5}$
Au	*315*	*130*	*1928*	-	$4.5x10^{7}$
Al/GaAs	*23.7*	*445*	*3968*	-	$5x10^{-4}$

Table 1. Electrical and thermal properties used in the simulation.

Step 6: Verification of Solution:

Due to the small dimensions of the sensor structure, it was difficult to determine temperature distribution by direct temperature measurements. Therefore, a technique based on thermal imaging was used. The top surface of the test structures were coated with a thin film of liquid crystal (R35CW 0.7 from Hallcrest Inc, UK), that changes color with the changes in the sensor surface temperature. This change in temperature was monitored by a CCD camera connected to a microscope and a personal computer was used to store the recorded shots for later analysis. For dc operation mode, a stable current source was used, and both the input voltage and current were monitored for accurate determination of input power. For RF mode of operation, the current source was replaced by an RF probe that connected directly to the input pads of the CPS (see Fig.3).

In order to show how closely the simulated results resemble the actually expected temperature distribution, we compare simulated current density distribution in Fig.5 with the an experimental shots of the sensor while it was burning shown in Figs 6,7; one with thermocouple (Fig. 6) and the other without thermocouples (Fig. 7). The experimental results were obtained by increasing the input power level at small increments until the resistor was destroyed at an input power level of about 80 mW. The accumulation of current density around the inner corner of the resistor in the simulated result (Fig. 5), explains the destruction of the resistor at one of its sharp inner corners. furthermore experimental results show that the degree of destruction is more severe (as illustrated by the size of the elliptical shape surrounding the resister) when the thermocouples are removed (Fig. 7). This can be attributed to spreading of heat away from the resistive termination by thermocouples when they present, thus decreasing level of destruction.

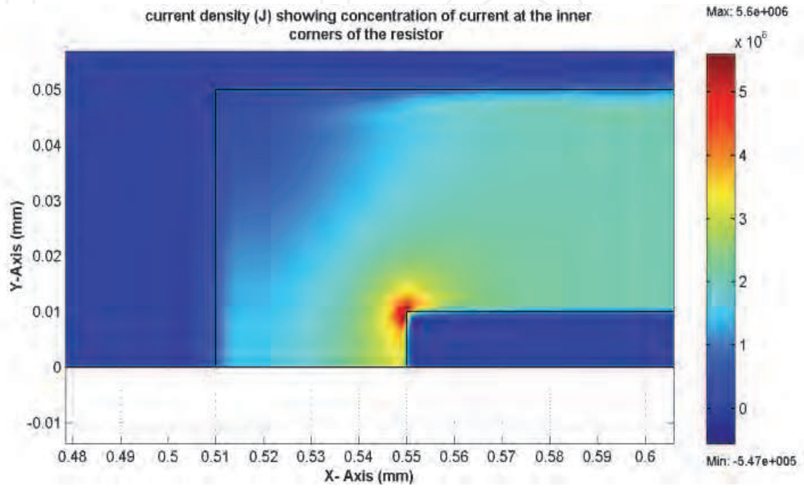

Fig. 5. Current density (J) at the inner corner of the resistive element

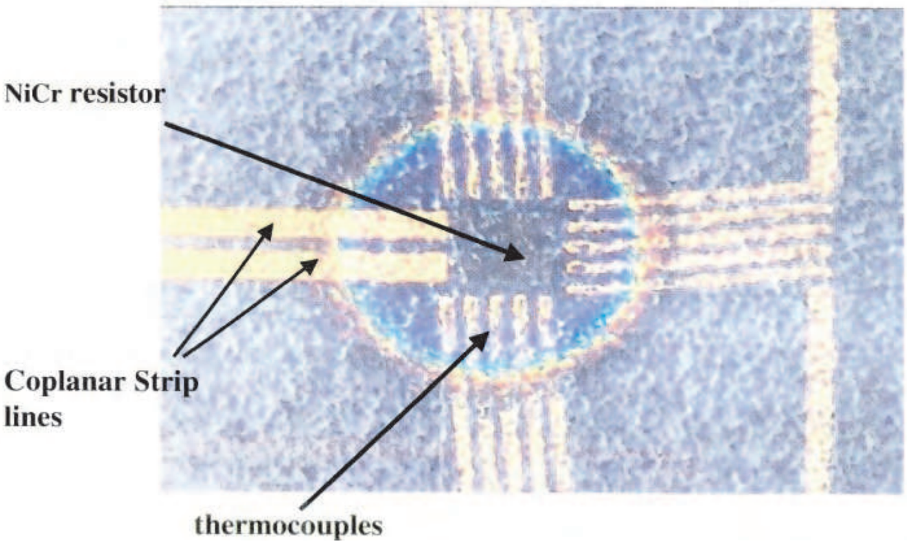

Fig. 6. Measured temperature distribution on the top surface of the sensor structure including thermocouple s

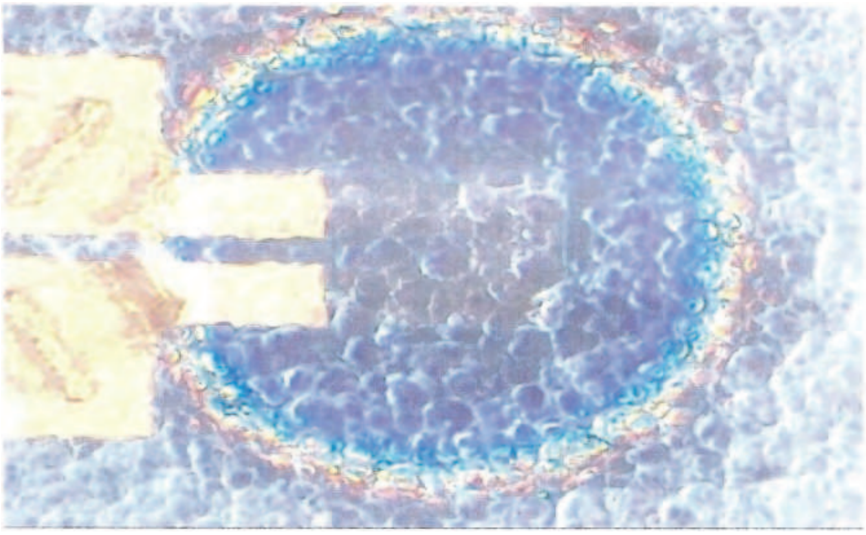

Fig. 7. Measured temperature distribution on the top surface of the sensor structure without thermocouples

Step 7: Using the Model

2-D simulation

Results obtained from 2-D simulation are shown in figure 8 through 11. Fig. 8 shows a 3D color plot of the normalized temperature distribution on the top surface of the sensor. It is shown here how temperature is concentrated in the Ni.Cr. resistor region with sharp decrease with distances from the resistor edges. In order to have a more quantitative picture, an enlarged view of the temperature contour around the resistor region is shown in Fig. 9. It can be seen that temperature decreases to about 67% of the peak value (at the resistor) at a distance of about 20 µm from the side arm of the resistor (y-direction). Further away from the resistor, temperature level reaches about only 33% of its peak value at a distance of about 180 µm. Along the x-axis away from the short arm of the resistor, the drop in temperature level is even more sharp reaching 67% at 10 µm, and 33% at 105 µm.

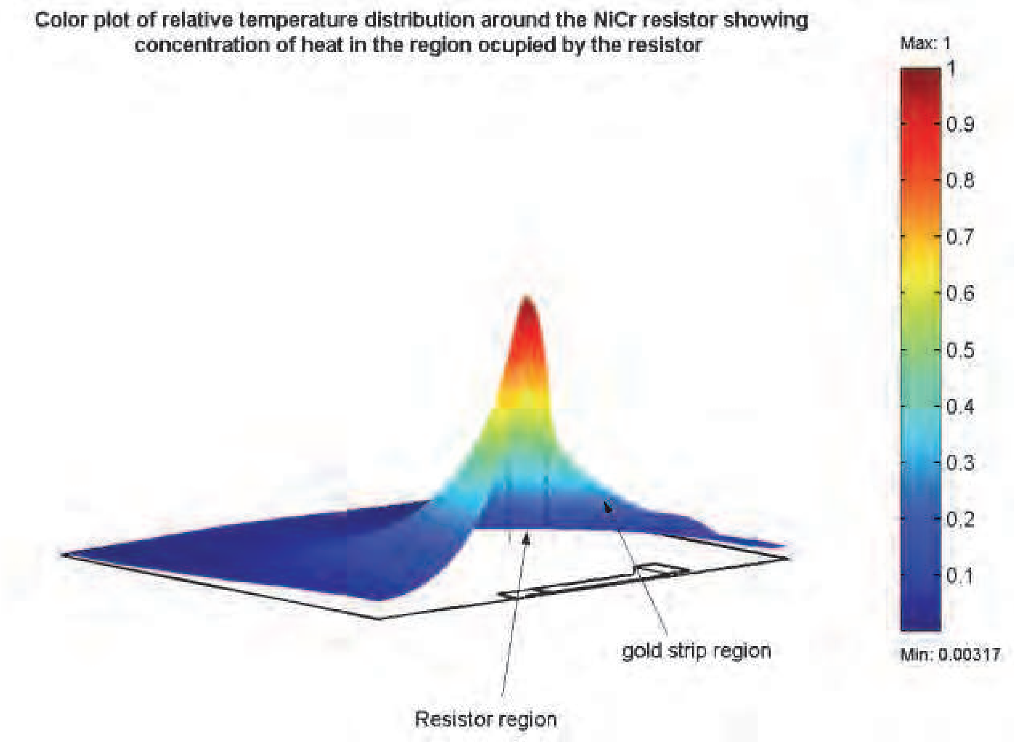

Fig. 8. Color plot of relative temperature distribution around the NiCr. Resistor.

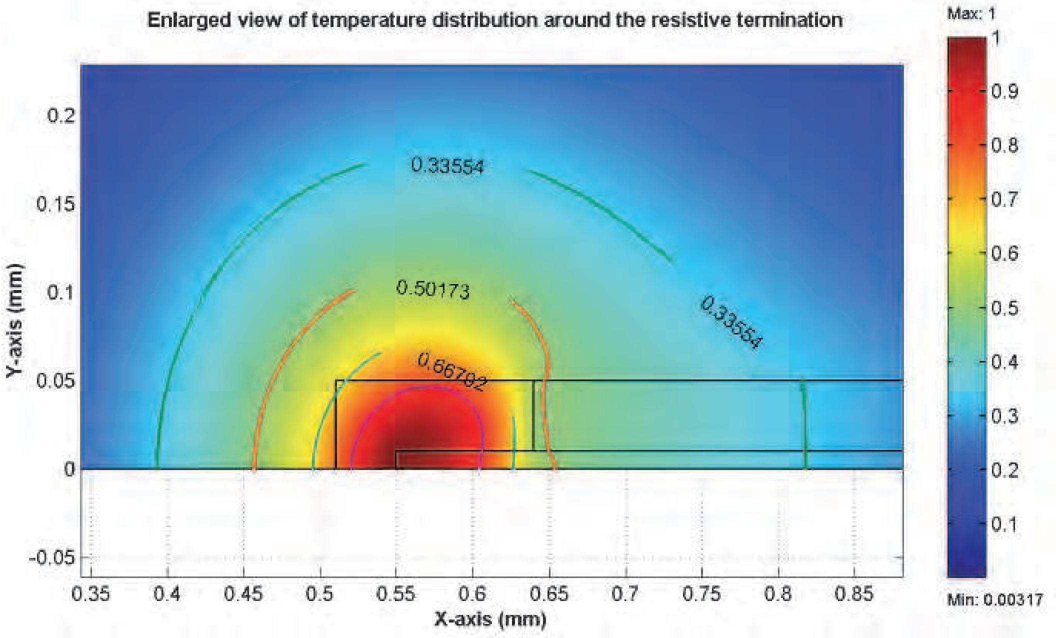

Fig. 9. Enlarged view of temperature distribution around the corner of the resistive termination

3-D simulation

The three-dimensional form of equations (5-8) were solved with the assumption of negligibly small resistor thickness. Fig. 10 shows a color plot of the temperature distribution on the top surface of a thin resistor on bulk substrate 150 μm thick. This figure compares very well with the experimentally obtained result of Fig. 9. 6,7, and clearly illustrates the elliptic form of surface temperature distribution. To see the effect of the third, z-dimension, temperature distribution on a plane cut along the line y-y on Fig. 10 is plotted in Fig.11. This figure illustrates the diffusion of heat through the GaAs substrate with peak values of temperature directly under the two long arms of the resistor. Thus it shows the effect of the bulk substrate that leads to the spreading of temperature away from the resistor region and down into substrate. This reinforces the idea behind using thin membrane technology, in which case the bulk substrate is removed, in the construction of thermoelectric power sensors.

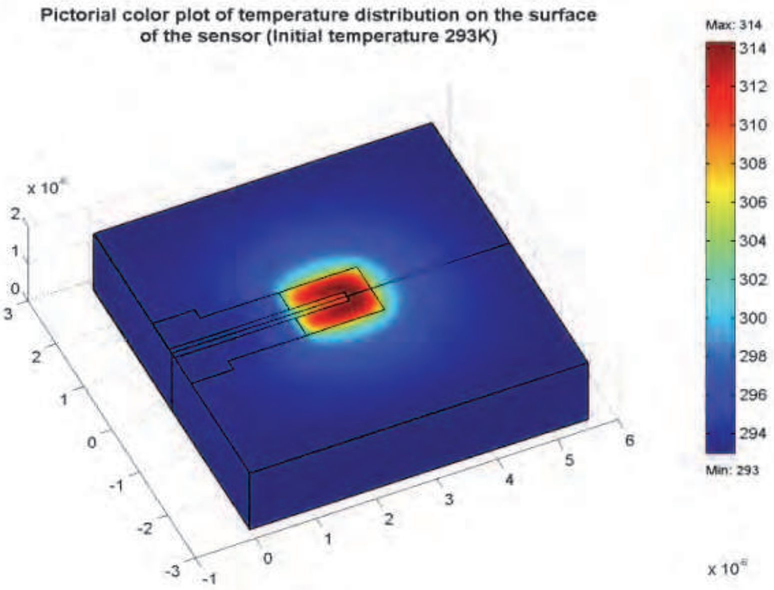

Fig. 10. Pictorial color plots of temperature distribution on the surface of the sensor (initial temperature 293K)

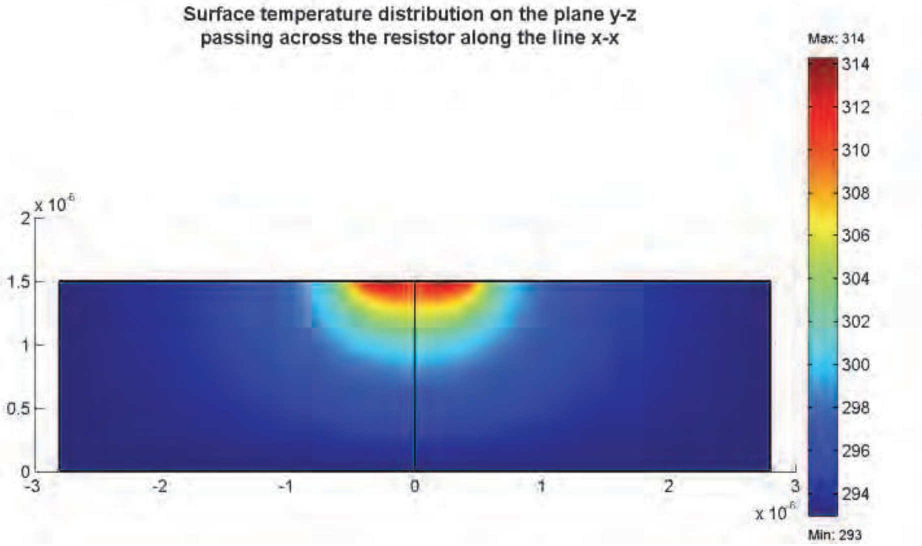

Fig. 11. Simulated temperature distribution on the top surface of the sensor structure along x-x

6.2 Other examples

Table 2a,b show respectively selected double and triple physics illustrative examples showing the type of MEMS, physical phenomena on which their operations are based, type of equations involved in their model and the technique and/or software tools used for their simulation. Information given in these tables are only highlights on the main principles and the interested reader is advised to consult cited references for more details.

Physical Phenomenon	*MEMS type*	*Type of Equations*	*Simulation Software tool/ technique*	*Reference*
Electromagnetism and Thermal	*Thermal convertors for gas sensors*	*Electric current flow + heat equation*	*IntelliSuite TM*	*Ijaz et. al. (2005)*
	Microwave power sensors	*Maxwell's + heat equation*	*XFDTD+ FEMLAB (FDTD+ FEM method)*	*Ali, I.et. al. (2010)*
	Fingerprint sensors	*Maxwell's + heat equation*	$\propto -Flow$	Ji-Song, et. al., (1999)
Electromagnetism and Mechanics	*Parallel-plate capacitors*	*Maxwell's + Transport equation*	*FDTD method*	Bushyager et. al. (2002)
	Stub tuners	*Maxwell's + equation of motion*	*FDTD method*	Bushyager et. al. (2001)
	Antennas with moving parts	*Maxwell's + equation of motion*	FDTD method	Yamagata, Michiko Kuroda & Manos M. Tentzeris (2005)
Magnetostaticts And Mechanics	*Magneto- sensitive Elastometers*	*Stress tensor + magnetic field equation*	COMSOL Multiphysics (F.E.M)	Bohdana Marvalova (2008)
	Magnetostrictive thin-film actuators	*Stress tensor + magnetic field equation*	Shell–Element Method	Heung-Shik Lee et. al. (2008)
Optics And Mechanics	*Ring laser and fiber optic gyroscopes*			*Riccardo & Roberto (2008)*

Table 2.a. Double-Physics Problems

Physical Phenomenon	*MEMSMEMS type*	*Type of Equations*	*Simulation Software tool/ technique*	*Reference*
Electromagnetism Thermal and Mechanical	*Electrothermal Actuators (ETA)*	*Electric current flow (Jule heating)+ heat equation+ Mechanical deflection*	COMSOL Multiphysics (F.E.M)	Fengyuan & Jason Clark (2009)
Electrical, Thermal and Mechanical	Self –Buckling of Micromechanical beams under resistive heating	*Voltage equation + heat equation + Mechanical deformation*	Analytical+ F.E.M	Chiao, Mu & David Lin, (2000)

Table 2.b. Triple-Physics Problems

7. Concluding remarks and future outlook

In this chapter we carefully looked at all MEMS features and nature which make their modeling and simulation a challenging task have been identified and summarized in the following:

1. Multidomain nature of MEMS calls for consideration of many interacting physical phenomena, thus leading to involvement of many types of equations that are coupled weakly or strongly depending on the type of MEMS.
2. Miniaturization: MEMS are by their nature tiny systems, sometimes with very large aspect ratios that make meshing a challenging task and demand considerable computer resources.
3. MEMS are very much affected by environmental conditions and need proper packaging, which in turn, complicates their modeling and simulation.

Different types of simulation techniques, as well as software tools based on these techniques, have been considered with advantages and limitations of each type. A detailed case study that illustrate proper modeling and simulation steps was made and some other successful modeling and simulation examples have been highlighted with proper reverence to their sources for interested reader.

The field of MEMS is very promising and much work is needed in the following areas:

1. The interdisciplinary nature of MEMS and the difficulties that face researchers and designers in this ever expanding field, calls for collaborative group work that comprises scientists and engineers with different background, such as electrical, mechanical, structural (civil) engineers and material scientists together with IT specialists in computer modeling and simulation.
2. Modified Finite difference time domain (FDTD) as well as the multiresolution time domain (MRTD) considered among the simulation techniques in this chapter, are promising due to their simplicity and efficiency compared to more mature finite element technique and more work is needed in development of software tools based on these techniques and specifically targeted to MEMS modeling and simulation.

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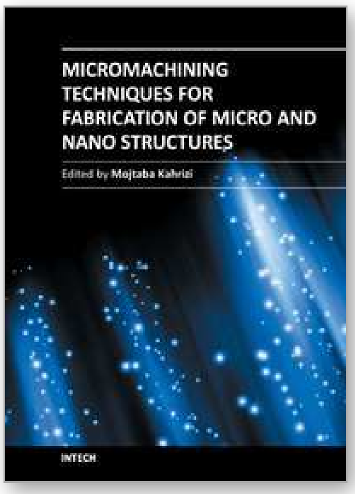

Micromachining Techniques for Fabrication of Micro and Nano Structures
Edited by Dr. Mojtaba Kahrizi

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Micromachining is used to fabricate three-dimensional microstructures and it is the foundation of a technology called Micro-Electro-Mechanical-Systems (MEMS). Bulk micromachining and surface micromachining are two major categories (among others) in this field. This book presents advances in micromachining technology. For this, we have gathered review articles related to various techniques and methods of micro/nano fabrications, like focused ion beams, laser ablation, and several other specialized techniques, from esteemed researchers and scientists around the world. Each chapter gives a complete description of a specific micromachining method, design, associate analytical works, experimental set-up, and the final fabricated devices, followed by many references related to this field of research available in other literature. Due to the multidisciplinary nature of this technology, the collection of articles presented here can be used by scientists and researchers in the disciplines of engineering, materials sciences, physics, and chemistry.

Idris Ahmed Ali (2012). Modeling and Simulation of MEMS Components: Challenges and Possible Solutions, Micromachining Techniques for Fabrication of Micro and Nano Structures, Dr. Mojtaba Kahrizi (Ed.), ISBN: 978-953-307-906-6, InTech, Available from: http://www.intechopen.com/books/micromachining-techniques-for-fabrication-of-micro-and-nano-structures/modeling-and-simulation-of-mems-components-challenges-and-possible-solutions-

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