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Multi-Physics Modelling for Microelectronics and Microsystems - Current Capabilities and Future Challenges

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Abstract

At present the vast majority of Computer-Aided-Engineering (CAE) analysis calculations for micro-electronic and microsystems technologies are undertaken using software tools that focus on single aspects of the physics taking place. For example, the design engineer may use one code to predict the airflow and thermal behavior of an electronic package, then another code to predict the stress in solder joints, and then yet another code to predict electromagnetic radiation throughout the system.

The reason for this focus of mesh-based codes on separate parts of the governing physics is essentially due to the numerical technologies used to solve the partial differential equations, combined with the subsequent heritage structure in the software codes.

Using different software tools, that each requires model build and meshing, leads to a large investment in time, and hence cost, to undertake each of the simulations.

During the last ten years there has been significant developments in the modelling community around multi-physics analysis. These developments are being followed by many of the code vendors who are now providing multi-physics capabilities in their software tools.

This paper illustrates current capabilities of multi-physics technology and highlights some of the future challenges.

1. Introduction

Increasing global competition is a significant factor impacting the design of modern products. While the product development time in the early 1980s was often years, portable computing and consumer products today have a time-to-market of only a few months. Such rapid times-to-market do not leave room for time-consuming trial and error approaches that have been the normal practice in the past.

Virtual prototyping, or computational modelling, tools that predict thermal, electrical and mechanical phenomena are now playing a key part at the early design stage and impacting delivery of reliable products to market as illustrated in figure 1. Exploitation of these software technologies benefits companies by:

- ✓ minimising the amount of physical prototyping
- ✓ improving quality and performance
- ✓ identifying optimal properties and process conditions
- ✓ generating knowledge of the process
- ✓ getting products to market earlier
- ✓ reducing overall development costs

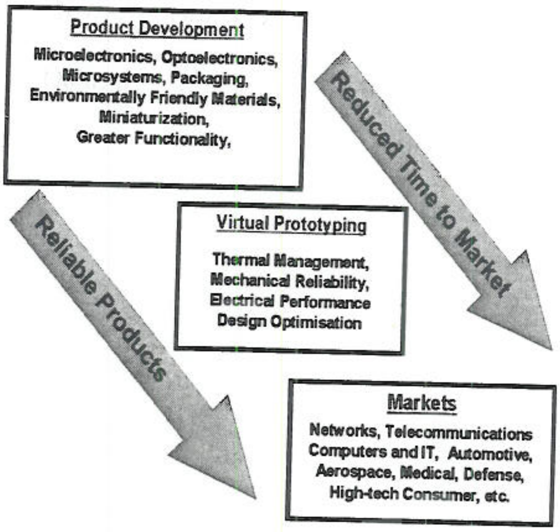

Figure 1 : Virtual Prototyping impact on Product Development

The development of heterogeneous systems that combine digital, analogue, RF, and even fluidic functions into a single piece of silicon has proved difficult and extremely costly. Although major advances are continuing to be made in the semiconductor industry, for highly complex systems containing multi-functional components (i.e. digital, analogue, RF, MEMS, Optics, etc) the System-on-Chip (SoC) option will be very costly if it can be achieved at all.

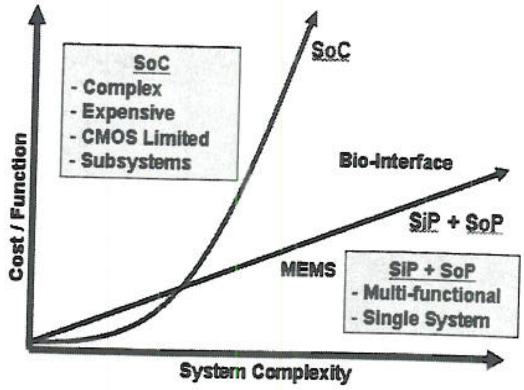

Figure 2: SOC, SIP and SOP

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Simulation and Analysis tools have traditionally focused on one aspect of the design requirement; for example: thermal, electrical or mechanical.

System-in-Package and System-on-Package technologies require analysis and simulation tools that can easily capture the complex three dimensional structures and provided integrated fast solutions to issues such as thermal management, reliability, electromagnetic interference, etc.

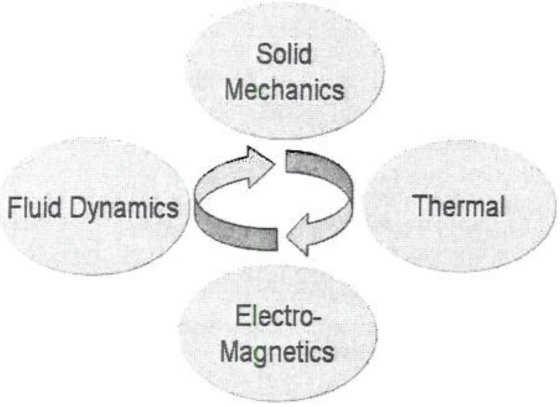

Figure 3: Multi-physics modelling

Technology roadmaps (i.e. ITRS, iNEMI) emphasize the requirement for improved design tools that permit integrated modeling and simulation of materials and processes to accommodate the rapid advancements in technology. Modeling tools can help industry identify potential defects very early in the design cycle and more importantly that can be used to provide optimal process conditions and material properties that will ensure success.

1. Multi-Physics Simulation Strategies

Until recently most of the Computer-Aided Engineerig analysis software tools have been developed in the context of single disciplinary groups such as:

- *Computational Fluid Dynamics (CFD)* solving phenomena such as fluid flow, heat transfer, combustion, solidification, etc
- *Computational Solid Mechanics (CSM)* solving deformation, dynamics, stress, heat transfer, and failures in solid structures
- *Computational Electromagnetics (CEM)* used to solve electromagnectis, electro-statics and magneto-statics.

One reason for this is the underpinning discretisation and solver technolgies used in each discipline. For computational fluid dynamics these have been based on control volume (or finite volme) techniques using segredated iterative solvers. For computational solid mechanics the solver techniques have been finite element based with the resulting matrices solved using direct solvers. For computational electromagnetics a mixture of finite volume, finite element and even boundary element techniques have been used [1-4].

The distinctive features of the above solver technologies and subsequent software developments over the last thirty years has meant that coupling the physics between the different disciplines has been challenging.

Many of the software vendors now claim a multi-physics or multi-discplinarity capability. In this context the term multi-discplinary means that data generated by one code (i.e. a traditional CFD solver) is transferred to another code (i.e. a traditional CMS solver) to undertake thermal-stress calculations for example. Here data from one code is used as input to the other code either as boundary conditions, loadings or volume sources.

Depending on the class of problem being solved this exchange of data can be classified as one-way or two-way. When the classification is one-way then the calculations from the first solver will influence the calculations in the second solver but not vice-versa. An example of this may be the temperatures calculated from a CFD solver, such as FLOTHERM, which influence the thermal-stress calculations in a solder joint calculated by a CSM solver, such as ABAQUS, MARC or ANSYS, but not vice versa. Figure 4 illustrates this type of approach.

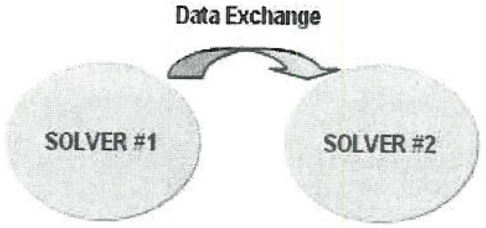

Figure 4: Multi-Physics: One-Way Coupling

Figure 5 highlights this type of one-way coupling where the CFD predictions for airflow and temperature are transferred to a CMS solver in terms of temperature changes, and then the CMS solver will calculate stress due to these changes.

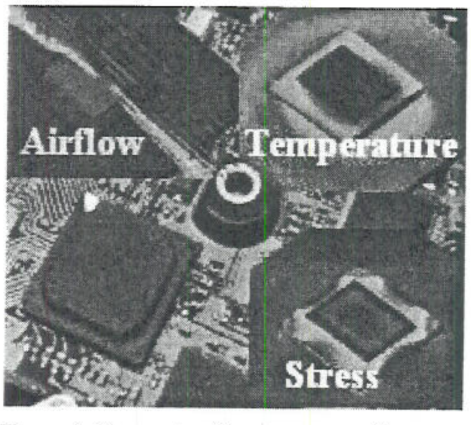

Figure 5: Example of one-way coupling

True multi-physics capability is defined by a much tighter integration between the solvers and this in general requires a two-way exchange of data between each as the predictions of one solver influences the other and vice-versa.

Such technology may be emebedded into a single software enviuronement. Multi-physics solvers may require the two-way exchange of data in both time and space. Figure 6 details this type of approach.

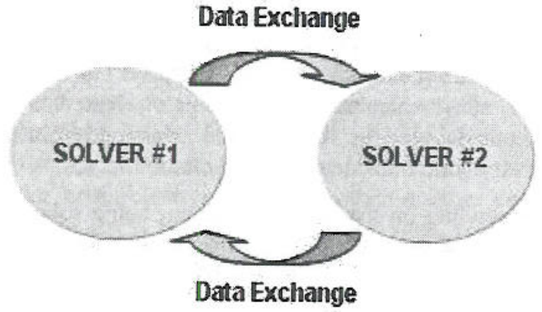

Figure 6: Multi-Physics: Two-Way Coupling

Figure 7 illustrates a process that will require two-way coupling capabilities. This is a simulation of the electrodeposition process, which requires integrated calculations between CFD, CSM and CEM. This work is further explained in the paper by Hughes-et-al in these proceedings.

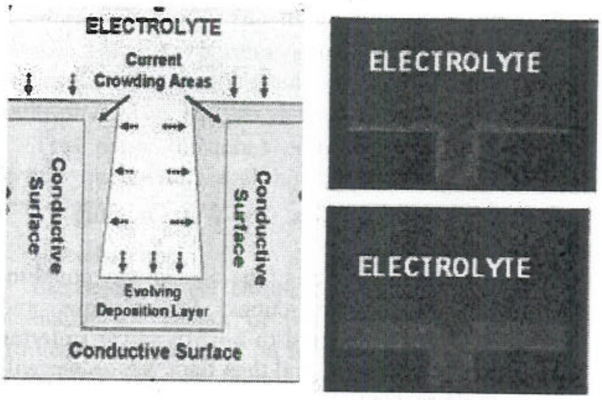

Figure 7: Example of Two-Way Coupling

Simulations that require one-way coupling can be undertaken by some form of file transfer between the solvers. For those that require two-way coupling the complexity increases as each solver may require mesh compatibility and time constraints.

In the last couple of years there have been a number of projects targeted at creating high performance computing tools to facilitate the coupling of distinct mesh-based solvers. For example coupling a CFD code and a CMS code to undertake multi-physics calculations. Some projects include:

- MDICE; a US Airforce funded project to develop a integrated computing environment led by CFDRC [5]
- ICE; a US Army funded project targeted at coupled multi-discplinary simulations across a GRID environment [6]
- MpCCI; an EU funded project to develop a suite of tools to enable the coupling of a wide variety of commercial codes [7]

The other approach is to try and solve all of the physics, and its coupling, within a single high performance computing software framework. This avoids the complexities of coupling different codes as outlined above.

The following table lists a number of software vendors in the microelectronics and microsystems market who have multi-physics or multi-disciplinary capabilities.

Software	Web Address
ANSYS	www.ansys.com
COMSOL	www.comsol.com
ANSOFT	www.ansoft.com
FLOMERICS	www.flomerics.com
PHYSICA	www.physica.co.uk

Table 1: Some Multi-physics codes

3. Fabrication and Assembly

Fabrication and assembly technologies for micrelectronics and microsystems can be complex and governed by interacting physical phenomena. One example is the formation of solder joints [8,9]. This takes place by first printing solder paste onto a printed circuit board and then reflowing the solder in a reflow furnace. The first calculations detailed in figure 8 illustrate CFD calculations for the printing of solder paste across a stencil.

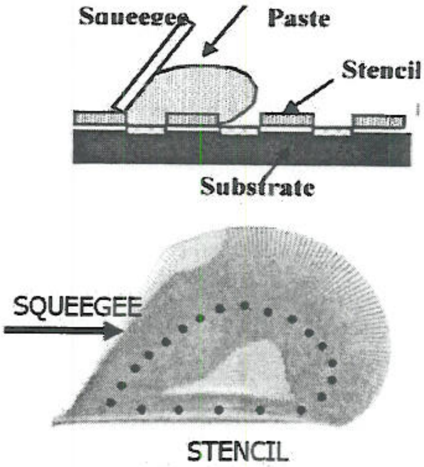

Figure 8: CFD Predictions for Solder Paste Printing

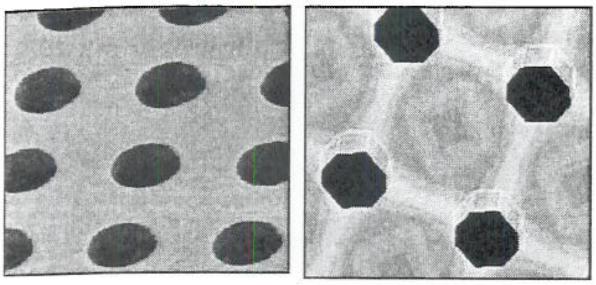

Figure 9: Stress Calculation in the Stencil

Figure 9 illustrates CSM calculations for stress in the stenncil due to the mounting and printing processes. These calculations of provide an insight into stencil behavior over time and its impact on final print quality. Full integration between CFD and CSM calculations for solder print predictions and stencil deformation is a two-way analysis as the fluid dyanmics of the paste places pressure on the stencil and the movement of the stencil impacts the manner in which the paste enters the apertures.

Once the solder is deposited onto a circuit board, and the component is place on the board, then this assembly is passed through a reflow furnace. The shape that the solder takes during this process can be predicted using the code SURFACE EVOLVER. These solder shapes can then be used by a computational mechanics code, such as PHYSICA, to model other interesting physics such as temperature and stress. This is an example of one-way coupling where in this case it is assumed that temperature, and stress does not affect the solder joint shape.

The shapes predicted using Evolver are represented using a surface triangular mesh. This is adequate to capture the evolving surface of the solder. For subsequent PHYSICA simulations of heat flow and stress a volume mesh is required. The interface developed between Evolver and PHYSICA uses PATRAN to generate a three-dimensional mesh from the two-dimensional surface mesh generated by Evolver. The surface to volume mesh procedure is:

1. Equilibrium geometry from Evolver is output into PATRAN format, one file for each body (i.e. solder, board, lead). In addition, a file containing boundary conditions is saved.
2. PATRAN produces a volume mesh from an Evolver surface mesh and the volume mesh files are output in PHYSICA format.
3. PHYSICA input files are created. PHYSICA simulations (temperature, stress, etc) can begin on the predicted solder shape using this volume mesh.

Figure 10 details comparisons between real solder joints and those predicted by Evolver. The top two pictures show the real solder bump and that predicted by Evolver. To illustrate the comparison between the two, the lower plots show the Evolver predictions overlaid onto the picture of the real joint. Clearly, we can see that the Evolver calculations give good agreement with the solder shapes found in reality.

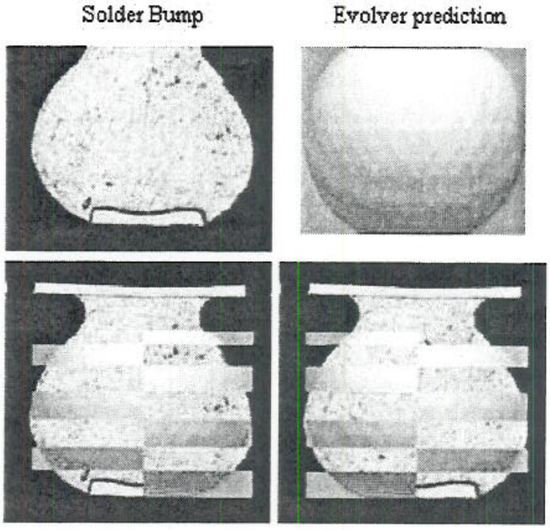

Figure 10: Evolver Calculation for Solder Joint Shape

Once we have the solder joint shape, then we can investigate other important physical phenomena, using in this case the PHYSICA software. Figure 11 shows void formation in solder joints with blind vias. At the very small micro-via dimensions being used, there is a concern that, during the printing process, not all of the micro-via is being filled with solder paste. Therefore, at the start of the reflow process, a void may already be present which, when the solder melts, will rise and form the void observed in the following photograph.

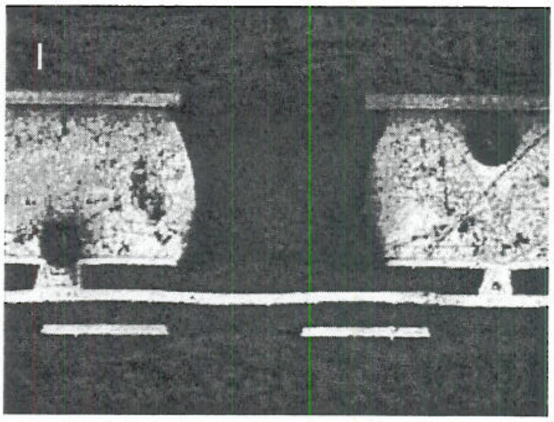

Figure 11: Observed Voids in Solder Joints

To test if the solder printing process is the cause of the final void observed, numerical simulations have been undertaken using the level set method to capture the movement of a void through liqiud solder. Figure 12 details the results from these simulations where solder is assumed to have penetrated the micro-via during printing and wetted its base. Clearly we can see that the void rises over time, due to buoyancy forces. Also presented is the magnitude of marangoni convection which is driven by surface tension gradients along the surface of the solder. .

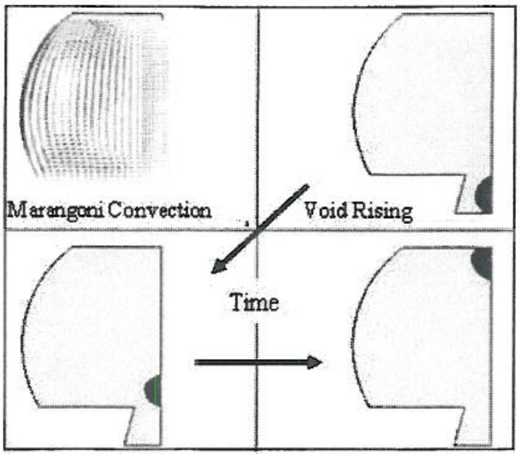

Figure 12: CFD Calculations of Void Movement

These simulations have shown that if the solder material does not wet the base of the micro-via, then it will not be able to rise. This is due to the high surface tension along the solder-void interface at the micro-via exit. Therefore, as long as solder wets the base of the micro-via and the void diameter is smaller than the micro-via diameter then the void will be able to rise into the solder mass from the micro-via. This requires a low initial void volume and a contact angle between the solder and micro-via wall near to zero. Obviously, these initial simulations are ignoring other effects such as gas from the flux that may also result in void formation

The next stage in solder joint formation is its solidification. This can be calculated using CFD techniques. Figure 13 shows the solidification fronts (light region is liquid) of the solder bumps during cool down. The solidification results show the corner (edge) bump solidifying first. The power connections, which are connected to the copper plate in the substrate, solidify locally at a faster rate than the ground connections. These results for solidification time can feed into the previous simulations on void movement to see how long a void has to rise through the solder bump and possibly escape.

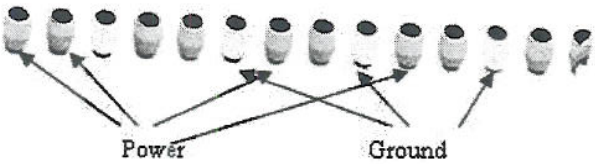

Figure 13: CFD Calculations of Solidification

Figure 14 shows the CMS calculations of stress in the solder joints at the end of the reflow process.

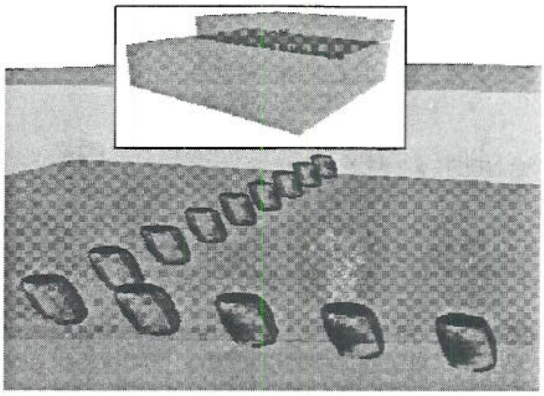

Figure 14: CSM Calculations of Stress after Reflow

4. Test and Reliability

Under test conditions microelectronic and Microsystems components are subjected to extreme environmental conditions, which are meant to promote the failures that would be observed in the field. The type of environmental conditions that a component can be subjected to is changes in temperature, humidity and vibration.

Given that the device may exhibit electrical, optical and fluidic behavior then the performance of the component under accelerated test conditions; the resulting stresses imposed; and the likelihood of failure is a multi-physics process.

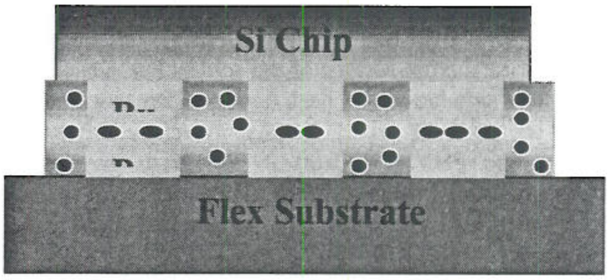

Figure 15: Anisotropic Conductive Film

As an exmaple of a test condition consider the pressure cooker test for anisotropic condictive adhesives [10]. The pressure cooker (or Autoclave) test is one of the most severe tests that polymer or adhesive materials can be subjected to. It involves placing the package into a humid environment (100% RH) at increased pressure (2 atm) and high temperature (120 C) for a period of time and measuring the change in contact resistance between polymer particles in an anisotropic conductive adhesive.

In this simulation the moisture diffusion analysis is coupled with the stress analysis so that the displacement field and the moisture concentration are solved simultaneously. Figure 16 shows the wetness fractions distribution in the Anisotropic Conductive Film (ACF) layer placed between a flexible substrate and die at 1 hour, 3 hour and 12 hours during the autoclave test. The results show that for this flip-chip assembly it is expected that the adhesive will be nearly fully saturated with moisture after 3 hours at 120C, 100%RH and 2atm conditions.

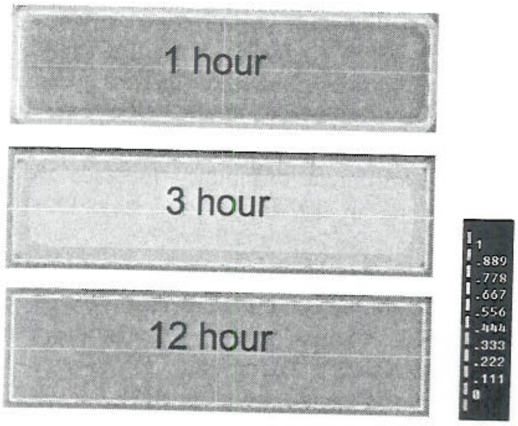

Figure 16: Moisture Ingress during Humidity Test

The above calculations have been undertaken on the whole flip-chip assembly. At the conductive particle scale there is also interest in predicting phenomena taking place. In this case it is the temperature and moisture induced stresses and the effect these can have on the contact resistance between the particle and pad surface. Figure 17 details a finite element model of the bump region which includes conductive particles.

A micro-macro modelling approach is adopted here where moisture and deformation results from the above model are transferred to this local model to predict the stresses around the particle.

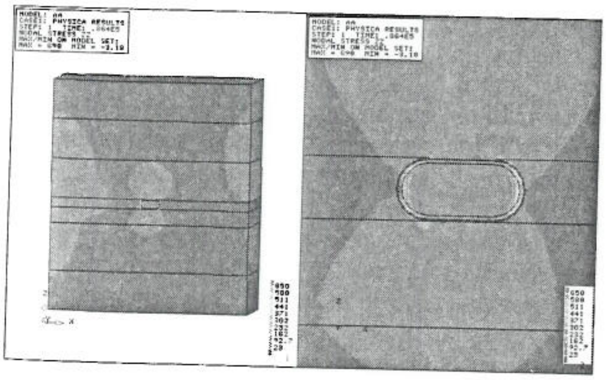

Figure 17: Stress around Conductive Particle due to Temperature and Moisture

The normal stress distribution around the conductive particle is shown in Figure 17. Higher stress was found at the interfaces between the conductive particle and adhesive matrix. This is an example of two-way coupling analysis as the temperature and moisture affect the stress calculations and the stress calculations, if cracking occurs, will affect the moisture calculations and to some degree the thermal behavior. .

As a second example, consider the following VCSEL device that is flip-chip assembled onto an organic substrate with embedded optical waveguides. The performance of the VCSEL device is governed by the thermal, mechanical and optical characteristics of this assembly. Figure 18 illustrates this package [11, 12].

During operation, the VCSEL device will heat up and the thermal change together with the CTE mismatch in the materials will result in potential misalignment between the VCSEL apertures and the waveguide openings in the substrate. Any degree of misalignment will affect the optical performance of the package.

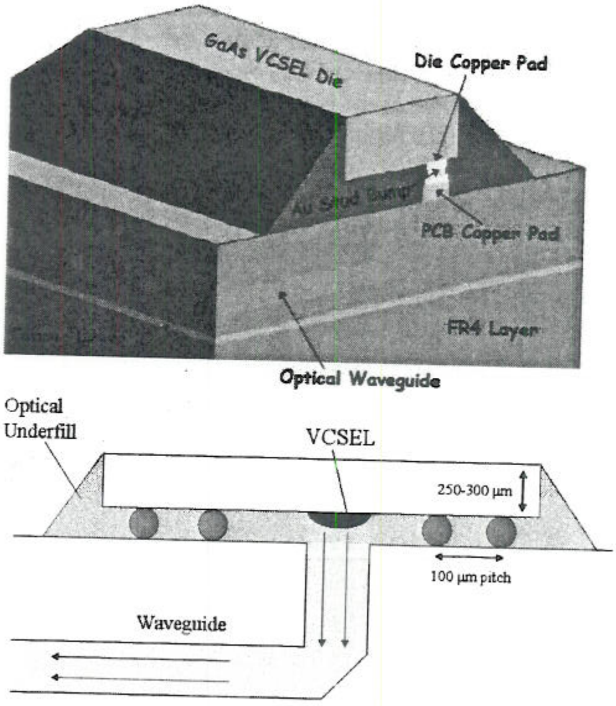

Figure 18: VCSEL Package

The amount of attenuation will depend on the degree of deformation between VCSEL aperture and waveguide entrance. The thermo-mechanical model simulates the VCSEL array heating up due to normal operation. Localised heating in the area surrounding each VCSEL device is seen at around the expected temperature of 85°C.

With the correct heating profile, the resultant stresses can be seen due to the effects of the heating and the CTE mismatch between the various materials present. The thermo-mechanical model showed the greatest general deformation in a single direction, along the horizontal direction as illustrated in figure 19.

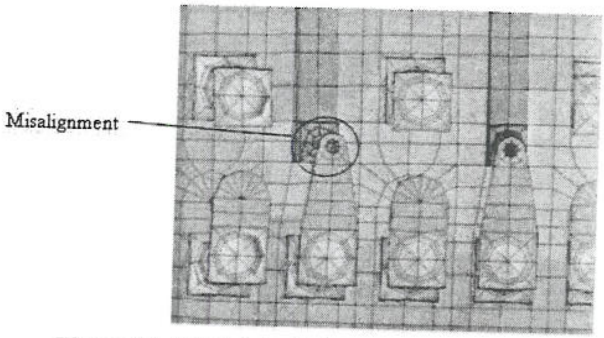

Figure 19: CSM Calculations of VCSEL Opening during Thermal Cycling

From the above simulation results, the misalignment values for these VCSELs were taken into account (i.e. maximum deformation) and used in a subsequent optical model. This is an example of again a one-way coupling simulation where the thermal model will affect the structural behavior of the package but this will not in tern affect the thermal behavior. For the optical calculations, the structural behavior will affect this although the optical calculations will not affect the structural behavior.

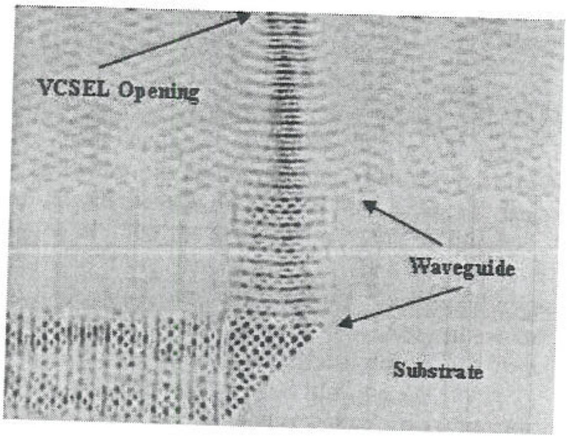

Figure 20: CEM calculations of optical performance of VCSEL Waveguide and Underfill

The objective of the optical simulations is to predict the coupling efficiency of the VCSEL beam to the waveguide entrance. This is characterised by the attenuation value, which is calculated by comparing the level of the optical signal as it leaves the VCSEL aperture, to that leaving the waveguide exit. Any attenuation observed will be because of the misalignment between VCSEL and waveguide; geometry of the waveguide; and the polymer material properties used. Fig. 20 shows a typical propagation contour plot of the optical signal travelling through the waveguide model.

5. Future Trends and Requirements

Although numerical modeling tools, based around CFD, CSM and CEM, are now routinely used in the design of microelectronic and Microsystems devices there are a number of key capability challenges for these tools need to address in the future.

1) Closer Coupling: Microsystems processes are generally governed by close coupling between different physical processes. As seen above numerical modelling tools are now addressing the need for multi-physics calculations, but more work is required to capture the physics accurately and to identify relevant failure models. Applications that involve complex fluid-structure interaction, including large amounts of mesh movement, are particularly challenging.

2) Multi-Discipline Analysis: Codes that can provide ease in data transfer between thermal, electrical, mechanical, environmental, and other designers important. Tools that accomplish this will allow design engineers from different disciplines to trade-off their requirements early in the design process and this will dramatically reduce lead times.

3) Multi-Scale Modelling: Much of the illustrations shown above have used continuum mechanics to solve the governing physics. Some of these calculations can be governed by phenomena taking place at the nano-scale. Multi-physics and multi-scale analysis is a very challenging area and will see a great deal of development in the near future. Modelling techniques that provide seamless coupling between simulation tools across the length scales are required.

4) Faster Calculations: Multi-physics software that solves highly coupled non-linear partial differential equations is compute intensive and slow. There is a need for reduced-order-models (or compact models) to be developed and used at the early stage of design. Although not as accurate as high fidelity models, these provide the design engineer with the ability to quickly eliminate many unattractive designs early in the design process.

To allow fast calculations the porting of multi-physics solvers to high performance computing clusters can result in dramatic speed-up in simulation times and the ability to run very large problems.

5) Life-Cycle Considerations: Life-cycle factors such as reliability, maintenance and end-of-life disposition receive limited visibility in numerical modelling tools. Future multi-physics and multi-scale models will aim to include all life-cycle considerations, such as product greenness, recycling, disassembly and disposal.

6) Variation Risk Mitigation: Microelectronic and microsystem simulations usually ignore process variation, manufacturing tolerances, and uncertainty in the input data. Future models will include these types of parameters to help provide a prediction of manufacturing and reliability risk. This can then be used by the design engineers to enable them to implement a mitigation strategy.

7) Integration with Optimisation Tools: Numerical optimisation techniques bring enormous advantages by offering an automated, logical and time efficient approach to identify the best process/design parameters for reliable components and products. Figure 21 illustrates the link between optimization and process modeling.

Although different design problems have been solved using optimisation procedures, fully integrated or coupled simulation-optimisation software modules are only just appearing and much more is required to fully capture process variation and uncertainty into these optimisation calculations.

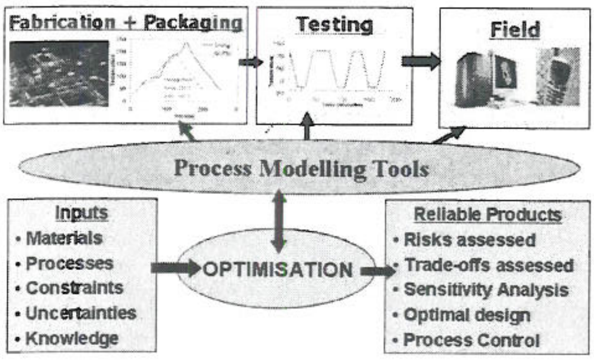

Figure 21: Integrated Process Modelling

8) Modelling through the Supply Chain: Numerical modelling tools require high quality input data in terms of materials data and failure models. Many companies are now using these modelling tools and there is an increasing requirement for companies within each others supply chain to gather and provide relevant modelling data. This is now starting to take place but much more effort is required.

9) Close integration with CAD. There is a trend in the analysis community to closely integrate analysis with Computer-Aided-Design (CAD). Users are demanding this capability with current software and the demand will also be there for new multi-physics software.

6. Conclusions

CAE analysis tools are now being used to underwrite the design of many microelectronic and microsystems components. The demand for greater capability of these tools is increasing dramatically because the user community is faced with the challenge of producing reliable products in ever shorter lead times.

This leads to the requirement for analysis tools to represent the interactions amongst the distinct phenomena and physics at multiple length and time scales. Multi-physics technology is now becoming a reality with many code vendors providing some capability in this area. The strategy in developing a multi-physics framework has been outlined above. Coupling seperate codes together is one appraoch. The other is to provide close coupling of the solvers within a single software framework.

But much still needs to be done to satisfy future user requirents. This paper has highlighted some of the current capabilities of Multi-physics technology and the trends and requirements for the future.

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