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Thermal Stress Analysis of Electronic Packaging

by

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A thesis submitted to

the Faculty of Graduate Studies and Research

in partial fulfillment of the requirements for the degree of

Master of Applied Science

Department of Mechanical and Aerospace Engineering

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Thermal Stress Analysis of Electronic Packaging

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Thesis Supervisor, J. A. Goldak

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Abstract

The objective of this thesis is to estimate the life of a package, i.e., the number of thermal cycles before solder balls in BGAs reach the 100 ppm failure level.

An FEM linear thermal stress analysis of the PCB assembly with heat sinks and required hardware is performed. Then a high resolution 3D FEM thermo-visco-plastic stress of one BGA package is performed. Part of the PCB was included in the analysis. The solder balls were treated as visco-plastic material, all other materials were elastic. Adhesive between Si die and lid was modeled with contact elements. The local deformation of the PCB and substrate around each solder ball was computed. The effective plastic strain increment was evaluated for each solder ball. The point with the maximum effective plastic strain increment was assumed to be the most likely failure point in that solder ball. The Coffin-Manson equation was used to predict the solder ball life. Several transient visco-plastic analyzes of solder balls were performed by applying prescribed displacement boundary conditions to the top and bottom of the solder balls. These analyzes showed that in the holding stages at high and low temperatures, the stress almost fully relaxes. This suggests that the linear thermo-elastic stress analysis of a module provides a useful estimate of which solder balls will fail first and possibly solder ball life.

To my son, Andrei.

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Chapter 1

Electronic Packaging

1.1 Introduction

The packaging of electronic devices and systems represents a significant challenge for product designers and managers. Performance, efficiency, cost considerations, dealing with the newer IC packaging technologies, and EMI/RFI issues all come into play. Electronics packaging continues to include expanding and evolving topics and technologies, as the demands for smaller, faster, and lighter products continues without signs of abatement. Thermal-stress considerations at both the device and the systems level are necessary to increase the reliability of today's electronics. There are three main levels of electronic packaging:

1. First Level Packaging - individual semiconductor devices packaged as part of a single chip module (SCM) or multichip module (MCM).
2. Second Level Packaging - refers to Printed Circuit Board (PCB) assemblies which include the PCB and required discrete components, Application Specific Integrated Circuits (ASIC), connectors, hardware.
3. Third Level Packaging - includes the assemblies of PCB's, cooling units, cables, cases.

1.2 IC Packaging Technology

Different packaging technologies are required for different semiconductor Integrated Circuit (IC) devices and applications. The following are four of the most common IC devices:

1. Solder-bumped flip chip technologies

Flip chip microelectronic assembly is the direct electrical connection of face-down (flipped) electronic components onto substrates, circuit boards, or carriers, by means of conductive bumps on the chip bond pads. In contrast, wire bonding, the older technology which flip chip is replacing, uses face-up chips

with a wire connection to each pad.

The boom in flip chip packaging results both from flip chip's advantages in size, performance, flexibility, reliability, and cost over other packaging methods and from the widening availability of flip chip materials, equipment, and services.

Flip chip assembly has significant advantages over other microelectronic packaging. Several varieties of flip chip assembly, including solder bump, plated bump, gold stud bump, and adhesive bump suit flip chip to a wide range of applications.

Figure 1.1: Wire bonding and flip chip package types (source: Siliconware Precision Industries).

2. Ball grid array (BGA) technologies

The BGA package construction is different from conventional leaded packages (wire bond) in several ways. BGA typically uses a BT-resin based organic

substrate (similar to PCB) for die and wire attachment. This substrate incorporates metalized trace routing for connection of the die to the system board through solder balls, instead of metal leads used in leaded packages. However, BGA packages also have several common features with the conventional leaded packages. These include similar chip level assembly techniques for die attach, wire bond, and overmolding. BGA packages also use conventional test, packing, handling, and PC board assembly methods. Depending on their substrates, there are ceramic BGA (CBGA), plastic BGA (PBGA), metal BGA (MBGA), etc.

Ceramic Substrate/AlSiC Lid

Organic Substrate/AlSiC Lid

Organic Substrate/Copper Alloy Lid

Figure 1.2: Different types of BGA packages (source: Siliconware Precision Industries).

3. TSOP and PQFP packages

Plastic quad flat packs (PQFP) are the most cost effective packages for Surface Mount Technology (SMT). They have been used extensively for ASICs and low speed microprocessors. Thin small outline package (TSOP) is a very low profile plastic package which is specially designed for memories (SRAM, DRAM, etc.), devices for space-limited applications.

4. Chip-scale package (CSP)

Chip Scale Package (CSP) are commonly designed and used for devices like DRAM, SRAM, flash memories, not so high pin count ASIC, and microprocessors. The main difference of a CSP as compared with other package technology is that the package area is less than 1.20 times the chip area. The unique feature of most CSP is the use of a substrate (interposer, or carrier or substrate carrier, or metal layer) to redistribute the very fine pitch (as small as $75\text{ }\mu\text{m}$) peripheral array pads on the chip to a much larger pitch (1mm, 0.8mm, 0.75mm, and 0.5mm) area array pads on the printed circuit board (PCB). Basically most of the CSP's uses either wire bonding or solder bumped flip-chip technology. From a generic classification of CSPs, they are typically classified into the following five categories:

- (a) Interposers with a flex circuit interconnect.
- (b) Interposers with rigid substrates.
- (c) Lead on Chip (LOC).
- (d) Wafer-level assembly packages.
- (e) Wafer-level process with redistribution.

5. Board Level Packaging Technology Issues

Traditional through-hole package assemblies have reached their limits in terms of improvements in cost, weight, volume, and reliability. SMT allows production of more reliable assemblies with higher I/O, increased board density, and reduced weight, volume, and cost. The weight of printed board assemblies (PBAs) using SMT is reduced because surface mount components (SMCs) can weigh up to 10 times less than their conventional counterparts and occupy about one-half to one-third the space on the printed board (PB) surface. SMT also provides improved shock and vibration resistance due to the lower mass of components. The smaller lead lengths of surface mount components reduce parasitic losses and provide more effective decoupling. The smaller size of SMCs and the option of mounting them on either or both sides of the PB can reduce board real estate by four times. A cost savings of 30% or better can also be realized through a

reduction in material and labor costs associated with automated assembly.

As surface mount technology (SMT) migrates toward smaller package dimensions, the physical and thermal characteristics of each packaging material become more critical. Significant differences between properties within a package (from layer to layer or between the carrier and the die) can cause extensive internal stresses. Once mounted to a PCB, the solder joint typically must absorb all strains induced by the expansion of the package and PCB in thermal excursions. For traditional SMT devices, such as quad flat packages, the leads and solder joints provide the compliance needed to compensate for the mismatch in coefficient of thermal expansion (CTE) of the package and PCB. However, in area array devices, such as ball grid arrays (BGAs) and chip scale packages (CSPs), the joint alone must provide CTE mismatch compliance. As joints become smaller, their quality becomes more critical. Physical defects (e.g., poor solderability, excessive intermetallic formation and voids) can have a negative impact on joint robustness and soldering yields.

Factors that affect area array assembly yields can be classified into several main categories, including assembly materials, PCBs and components, process methods, joint quality and human performance.

The assembly materials category can be subdivided further into solder paste and flux-related parameters, such as applied volume, reflow parameters, fluxing and solder paste deposition methods, and handling and storage conditions. The most critical issue within this category is the proper fluxing of the attachment surfaces and the creation of proper metallurgical bonds during the reflow operation.

The PCB category contains many influences on the overall solder joint reliability, including pad metallurgy, board thickness, pad size, base material, via formation technology, routing method (via-in-pad vs. fan-out), PCB layer count, solder mask technology, and pad definition vs. mask definition. The PCB parameters that influence CSP reliability will be the focus of this article. The components subgroup parameters that influence the assembly reliability may include construction (flex vs. rigid carrier, etc.), die-size-to-package ratio, solder ball size, attachment pad size and definition, base materials, package size, and ball configuration.

The process methods category is influenced heavily by the individual steps in the assembly (i.e., standard double-side assembly or mixed assembly with solder wave pass). Factors such as reflow methodology (convection vs. infrared (IR) radiation) and atmosphere will affect solder-wetting, joint formation/shape and

the presence of voids. Joint quality is affected by almost all assembly variables but is influenced strongly by the type of paste/flux, attachment pad metallurgy and reflow conditions. Highly irregular-shaped joints, excessive voiding and poor solderability can lead to early failures. Human performance factors that often are overlooked may include operator education and training, in addition to human error.

1.3 Design for solder attachment reliability

Following are some of the design parameters that have been identified to have influence on surface mount solder attachment fatigue reliability.

1. *Component Size:* The physical size of the component determines the amount of displacement a solder joint experiences during thermal expansion/contraction of the component and the substrate to which it is soldered. Larger components are larger threats to reliability.
2. *Attachment Type:* The choice of attachment type determines the maximum stress level that can be experienced in a solder joint during thermal cycling. The stiff leadless attachments typically stress the solder beyond the yield strength, whereas compliant leaded attachments typically do not. This choice determines

the reliability model that needs to be applied and affects the statistical failure distribution (Weibull slope). Leaded attachments provide larger reliability margins, which increase with decreasing lead stiffness.

3. *Solder joint height*: The solder joint height determines the strain level experienced in the solder joint for a given component displacement. It results from the solder-filled gap between the component metalization or component lead and the substrate pad. Higher solder columns reduce the strains in the solder joints and increase reliability.
4. *Lead stiffness*: The lead stiffness determines the forces resulting from a given component/substrate displacement. Because the corner solder joints experience the largest displacements and the displacements are in the direction of the component center (neutral point), it is the diagonal lead stiffness which is of primary importance. Lower lead stiffness results in increased reliability.
5. *CTE mismatch*: The CTE-mismatch is the difference between the coefficients of thermal expansion (CTE) of two materials or parts joined together. In most instances it is the CTE mismatch between component and substrate that is most important while the CTE mismatch between the solder and the materials to which it is bonded (ceramic, Alloy 42, Kovar) plays a smaller, but not negligible,

role. In some designs (ceramic component on ceramic or silicon substrate), this CTE mismatch assumes primary importance. Large CTE mismatches pose large reliability threats.

6. *Cyclic temperature swing:* The cyclic temperature swing (δT) of components and substrate is the difference in the maximum and minimum steady-state temperatures experienced during either externally (daily) imposed temperature variations or operationally (on/off, load fluctuations) imposed variations. It needs to be realized that the temperature swing of the components is typically not the same as the temperature swing of the substrate due to the power dissipated in active devices. An effective temperature swing (δT_e) can be used for simplicity by incorporating the CTE mismatch between component and substrate. Smaller δT_s will result in improved reliability.

Chapter 2

Finite Element Theory for Thermal Analysis

Heat transfer theory aims to predict the energy transfer taking place between material bodies. If there is a temperature difference between material bodies, the heat energy will flow from the body with a high temperature to the body with a low temperature. The science of heat transfer tries to explain how heat energy may be transferred and tries to predict the heat transfer rate and temperature field. The objective of heat transfer theory is different from thermodynamics. Thermodynamics deals with systems in equilibrium and it may be used to predict how much energy is required to change the system from one equilibrium state to another equilibrium state. Heat

transfer theory is used to predict how fast a change will occur when the system is not in equilibrium state during the process.

Exact analytical solutions of the equations of heat transfer can only be obtained for problems which have relatively simple geometry, material properties and boundary conditions. But practical problems often have complex geometries, material properties and boundary conditions. Then there is no option but to seek a numerical method to analyze practical problems. The Finite Element Method is one kind of numerical method that can be used to obtain an approximate solution of differential equations for practical problems.

There are three modes of heat transfer: conduction, convection and radiation. In the this thesis, the domain is the electronic package and the velocity of material points is zero in the electronic package. In this case, the convection and radiation heat transfer modes appear in the boundary conditions. This chapter will present a brief description of the heat transfer by conduction in the electronic package domain together with boundary conditions that include the convection and radiation heat transfer modes. The Finite Element Method with be introduced to analyze conductive heat transfer in the electronic package with convection and radiation boundary conditions.

2.1 Heat Transfer Modes

2.1.1 Conduction Heat Transfer

Conduction transfers energy from hot to cold regions of a substance by molecular interaction. In fluids, the exchange of energy is primarily by direct impact. In solids, the primary mechanism is relative lattice vibrations, enhanced in the case of metals by drift of free electrons through the lattice. Thus, good electrical conductors are also good heat conductors. Both the molecular and the free-electron interactions are well founded in theoretical atomic physics. We may also speak of the transfer of energy by molecular motion as diffusion of energy [1]. This phenomenon is known as conduction heat transfer, and is described by Fourier's Law (named after the French physicist Joseph Fourier),

$$q''_{cond} = -k \cdot \nabla T \quad (2.1)$$

Where:

$\nabla T(x, y, z)$ is the temperature gradient. (K/m)

$T(x, y, z)$ is the scalar temperature field.

∇ is the gradient operator and, in Cartesian coordinates, is defined as follows:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \quad (2.2)$$

k is the thermal conductivity, a material property that describes the rate at which heat flows within a body for a given temperature gradient. ($W/m K$),

q''_{cond} is the heat flux (W/m^2), the rate of heat per unit area flowing parallel to ∇T .

The minus sign ensures that heat flows down the temperature gradient.

The temperature profile within a body depends upon the rate of its internally-generated heat, its capacity to store some of this heat, and its rate of thermal conduction to its boundaries (where the heat is transferred to the surrounding environment).

Mathematically the conservation of energy is stated by the Heat Equation,

$$k\nabla^2 T - c_p \frac{\delta T}{\delta t} = -q_{gen} \quad (2.3)$$

along with its initial condition $T(x,0)$ and its boundary conditions, equations that prescribe either the temperature T on, or the heat flux q through, all of the body boundaries Ω ,

$$T(\Omega_D) = T_{prescribed} \quad (2.4)$$

$$q(\Omega_N) = q_{prescribed}, q_{conv}, q_{rad} \quad (2.5)$$

$$\Omega_D \cup \Omega_N = \Omega \quad (2.6)$$

$$\Omega_D \cap \Omega_N = \emptyset \quad (2.7)$$

For steady state problems, the heat equation simplifies to,

$$K\nabla^2 T = -q_{gen} \quad (2.8)$$

2.1.2 Convection Heat Transfer

Heat energy transfers between a electronic package and a fluid when there is a temperature difference between the fluid and the electronic package. This is known as convection heat transfer. Generally, convection heat transfer cannot be ignored when there is a significant fluid motion around the electronic package. The temperature of the electronic package due to an external field such as fluid buoyancy can induce a fluid motion. This is known as natural convection and it is a strong function of the temperature difference between the electronic package and the fluid. Blowing air over the electronic package by using external devices such as fans and pumps can also generate a fluid motion. This is known as forced convection.

Fluid mechanics plays a major role in determining convection heat transfer. For

each kind of convection heat transfer, the fluid flow can be either laminar or turbulent. Laminar flow generally occurs in relatively low velocities in a smooth laminar boundary layer over smooth small objects, while turbulent flow forms when the boundary layer is shedding or breaking due to higher velocities or rough geometries.

There are essentially two kinds of mechanism of heat transfer in convection heat transfer. One kind is diffusion in which energy is transferred by random molecular motion. The other kind is advection in which energy is transferred by bulk fluid motion. In nature, both phenomena occur simultaneously.

In electronic packaging convection heat transfer occurs between the surface of a electronic package and the fluid which may be moving relative to the electronic package surface. This region in the fluid is called a boundary layer. There are three different boundary layers: velocity boundary layer, thermal boundary layer and concentration boundary layer. The velocity boundary layer profile begins at the solid surface where the velocity of the liquid is zero. The velocity gradually increases until the velocity profile reaches a uniform value, the ambient velocity value u_∞ . Also, the thermal boundary layer occurs in a similar fashion. This kind of layer begins at the solid surface where the temperature is T_w and ends at the outer flow where the temperature is T_∞ , which is the ambient temperature. Between the two temperatures limits, there will be a varying gradient. The concentration boundary layer will develop

from the surface, where the concentration of species A is $C_{A,s}$, to the free stream, where the concentration of species A is $C_{A,\infty}$. A concentration gradient will exist in this region. In this thesis, concentration boundary layers are not considered.

The essential ingredients of forced convection heat transfer analysis are given by Newton's Law of Cooling,

$$q = h(T_w - T_\infty). \quad (2.9)$$

Where:

q is the convective heat flux(W/m^2),

h is the convection coefficient, ($W/m^2 K$),

T_w is the temperature of the surface,

T_∞ is the temperature of the ambient fluid.

The rate of heat q transferred to the surrounding fluid is proportional to the object's exposed area A , and the difference between the object temperature T_w and the fluid free-stream temperature T_∞ . The constant of proportionality h is termed the convection heat-transfer coefficient.

2.1.3 Radiation Heat Transfer

Radiation heat transfer is concerned with the exchange of thermal radiation energy between two or more bodies. Thermal radiation is defined as electromagnetic radiation in the wavelength range of 0.1 to 100 microns (which encompasses the visible light regime), and arises as a result of a temperature difference between 2 bodies. No medium need exist between the two bodies for heat transfer to take place (as is needed by conduction and convection). Rather, the intermediaries are photons which travel at the speed of light.

The heat transferred into or out of an object by thermal radiation is a function of several components. These include its surface reflectivity, emissivity, surface area, temperature, and geometric orientation with respect to other thermally participating objects. In turn, an object's surface reflectivity and emissivity is a function of its surface conditions (roughness, finish, etc.) and composition.

Radiation heat transfer must account for both incoming and outgoing thermal radiation. Incoming radiation can be either absorbed, reflected, or transmitted. This decomposition can be expressed by the relative fractions,

$$1 = \varepsilon_{reflected} + \varepsilon_{absorbed} + \varepsilon_{transmitted} \quad (2.10)$$

Since most solid bodies are opaque to thermal radiation, we can ignore the transmission component and write,

$$1 = \varepsilon_{reflected} + \varepsilon_{absorbed} \quad (2.11)$$

To account for a body's outgoing radiation (or its emissive power, defined as the heat flux per unit time), one makes a comparison to a perfect body that emits as much thermal radiation as possible. Such an object is known as a blackbody and the ratio of the actual emissive power E to the emissive power of a blackbody is defined as the surface emissivity ε ,

$$\varepsilon = \frac{E}{E_{blackbody}} \quad (2.12)$$

Considering that a body's surface emissivity is equal to its absorption fraction,

$$\varepsilon = \varepsilon_{absorbed} \quad (2.13)$$

The heat emitted by a blackbody (per unit time) at an absolute temperature of T is given by the Stefan-Boltzmann Law of thermal radiation,

$$Q = A\sigma T^4 = AE_{blackbody} \quad (2.14)$$

Where:

Q is the emission of a black surface (W),

A is the total radiating area,

T is the absolute temperature in Kelvin (K),

σ is the Stefan-Boltzmann constant, whose value is

$$\sigma = 5.669 \times 10^{-8} W/m^2 K^4. \quad (2.15)$$

Bodies that emit less thermal radiation than a blackbody have surface emissivities less than 1. If the surface emissivity is independent of wavelength, then the body is called a “gray” body, in that no particular wavelength (or color) is favored.

The Stefan-Boltzmann equation can be linearized to create an effective convection coefficient for radiation

$$\begin{aligned} q_{rad} &= \varepsilon \sigma (T_w^4 - T_\infty^4) = \varepsilon \sigma (T_w^2 - T_\infty^2)(T_w^2 + T_\infty^2) = \\ &\varepsilon \sigma (T_w + T_\infty)(T_w^2 + T_\infty^2)(T_w - T_\infty) = h_{rad}(T_w - T_\infty) \end{aligned} \quad (2.16)$$

Where:

q_{rad} is the radiated flux (W/m^2),

ε is the hemispheric emissivity and it depend on the type of the material and surface condition. The value of ε is between zero and one. If the body is a black body, then $\varepsilon = 1$, which is an ideal case. If the body is a grey body, the value ε is between 0 and 1.

2.2 Finite Element Method (FEM)

2.2.1 Introduction to Finite Element Method

The finite element method (FEM) is a numerical technique for solving problems which are described by partial differential equations, a variational formulation or a functional minimization. A domain of interest is represented as an assembly of finite elements. Approximating functions in finite elements are determined in terms of nodal values of a physical field which is sought. A continuous physical problem is transformed into a discretized finite element problem with unknown nodal values. For a linear problem a system of linear algebraic equations should be solved. Values inside finite elements can be interpolated from nodal values and element basis functions.

Two features of the FEM are worth mentioning: 1) Piece-wise approximation of physical fields on finite elements provides good precision even with simple approximating functions (increasing the number of elements we can achieve high precision). 2)

Locality of approximation leads to sparse equation systems for a discretized problem. This makes it feasible to solve problems with very large number of nodal unknowns.

To summarize how the finite element method works we list the main steps of the finite element solution procedure below.

1. Discretize the continuum.

The first step is to divide a solution region into finite elements. The finite element mesh is typically generated by a preprocessor program. The description of mesh consists of several arrays. The main arrays are nodal coordinates and element connectivities.

2. Select interpolation functions.

Interpolation functions are used to interpolate the field variables over the element. Often, polynomials are selected as interpolation functions. The degree of the polynomial depends on the number of nodes assigned to the element.

3. Find the element properties.

The matrix equation for the finite element should be established that relates the nodal values of the unknown function to other parameters. The first step is to evaluate the following element level matrices and vectors:

$$\{F^e\}, \quad [K^e], \{x^e\} \quad (2.17)$$

where the superscript “e” indicates the element stiffness matrix, $[K^e]$, element load vector $\{F^e\}$ and the vector of nodal values of the unknown $\{x^e\}$. Note that in a linear problem, only the Dirichlet boundary condition values of x^e could be known at the element level. In a non-linear problem, an initial guess or trial values of the unknown x^e are required. The matrix and vectors are a function of the material properties, element geometry and the interpolation function.

4. Assemble the element equations.

To find the global equation system for the whole solution region we must assemble all the element equations to form the global system of equations. In other words we must combine local element matrices $[K^e]$ and load vectors $\{F^e\}$. The global system of equation is:

$$\{F\} = [K]\{x\} \quad (2.18)$$

Where the $[K]$ is the global stiffness matrix, which is assembled from the local stiffness matrix.

$\{x\}$ is the global vector of the field variable for all the nodes.

$\{F\}$ is global vector of the load variable at each node.

Element connectivities are used for the assembly process.

5. Apply the Boundary Conditions and Initial Conditions.

The boundary conditions are applied to the global equations in this step. There are two kind of Boundary Conditions: essential and natural. For time dependent or transient problems, initial conditions must be assigned.

6. Solve the global equation system.

The finite element global equation system is typically sparse, symmetric and positive definite. Direct and iterative methods can be used to solve the system of equations. The nodal values of the sought function are produced as a result of the solution.

7. Compute additional results.

In many cases we need to calculate additional parameters. For example, in mechanical problems strains and stresses are of interest in addition to displacements, which are obtained after solution of the global equation system.

2.2.2 Differential Equation of Heat Conduction

The differential form of the heat conduction equation is

$$\begin{aligned} \frac{\partial}{\partial x} \left(k_x \frac{\partial T(r, t)}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T(r, t)}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial T(r, t)}{\partial z} \right) + q'''(r, t) \\ = \rho C_p \frac{\partial T(r, t)}{\partial t} \end{aligned} \quad (2.19)$$

Where:

$q'''(r, t)$ is the rate energy generation per unit volume, per unit time at point $r(x, y, z)$ at time t ,

$T(r, t)$ is the temperature at point $r(x, y, z)$ at time t ,

r is the point in three dimensions (x, y, z) .

If the conductivity is constant in (x, y, z) , then Equation 2.19 will be reduced to

$$k \left(\frac{\partial^2 T(r, t)}{\partial x^2} + \frac{\partial^2 T(r, t)}{\partial y^2} + \frac{\partial^2 T(r, t)}{\partial z^2} \right) + q'''(r, t) = \rho C_p \frac{\partial T(r, t)}{\partial t} \quad (2.20)$$

If we use the Laplacian operator $\nabla \cdot \nabla$ in this equation, it becomes

$$k \nabla \cdot \nabla T(r, t) + q'''(r, t) = \rho C_p \frac{\partial T(r, t)}{\partial t} \quad (2.21)$$

The following integral of this equation times a space of test functions ϕ over a volume v is the integral form equation of heat conduction.

$$\int_v \phi \left[\nabla \cdot k \nabla T(r, t) + q'''(r, t) - \rho C_p \frac{\partial T(r, t)}{\partial t} \right] dv = 0 \quad (2.22)$$

Apply Green's identity to Equation 2.22

$$\int_{\Omega} \left[-\nabla \phi \cdot k \nabla T(r, t) + \phi q'''(r, t) - \phi \rho C_p \frac{\partial T(r, t)}{\partial t} \right] dv = \int_{\partial \Omega} \phi q \cdot n d\Gamma \quad (2.23)$$

Equation 2.23 is the integral form of the energy equation. The FEM software will solve this equation to compute nodal temperatures as a function of time.

Chapter 3

Finite Element Theory for Stress Analysis

3.1 Fundamental Equations of Continuum Mechanics

3.1.1 Conservation of momentum.

$$\operatorname{div} \sigma + b = \rho \ddot{u}.$$

σ is the stress tensor.

b is the body force vector.

u is the displacement vector.

$\dot{u}$ is the velocity vector.

$\ddot{u}$ is the acceleration vector.

This partial differential equation (PDE) can be defined at every point in a domain, i.e., some simply connected subset of Euclidean space with a sufficiently smooth boundary which means that all required derivatives exists and are bounded. With appropriate boundary conditions, and the addition of a constitutive equation, i.e., a relationship between stress and strain, and the conservation of mass or continuity equation, there are conditions under which this PDE is a well posed problem whose solution exists and is unique. However, if the domain is unstable, e.g., if buckling occurs, then the solution might not be unique. If the domain fractures, the solution to this problem as it is posed here might not exist.

3.1.2 Displacement

$$u(X, t) \equiv x(X, t) - X.$$

$$x(X, t) \equiv X + u(X, t).$$

The displacement of material point X at time t , $u(X, t)$, is defined to be the position of the point at time t $x(X, t)$ minus its original position X . The displacement gradient is defined to be

$$\nabla u \equiv u_{,X} \equiv \begin{pmatrix} u_{1,X_1} & u_{1,X_2} & u_{1,X_3} \\ u_{2,X_1} & u_{2,X_2} & u_{2,X_3} \\ u_{3,X_1} & u_{3,X_2} & u_{3,X_3} \end{pmatrix}. \quad (3.1)$$

The displacement gradient is closely related to the deformation gradient described below. The deformation gradient is more convenient for theoretical discussions.

3.1.3 Deformation Gradient

The deformation gradient, F , is defined to be the operator

$$F \equiv x_{,X} \equiv \begin{pmatrix} x_{1,X_1} & x_{1,X_2} & x_{1,X_3} \\ x_{2,X_1} & x_{2,X_2} & x_{2,X_3} \\ x_{3,X_1} & x_{3,X_2} & x_{3,X_3} \end{pmatrix}.$$

The deformation gradient evaluated at the point X maps a vector $dX = (X + xX) - X$ to a vector $dx = x(X + dX) - x(X)$, i.e., $dx = F dX$. For finite Green's strain with deformation gradient F ,

$$\varepsilon = \frac{1}{2} (F^T F - I).$$

Using the identity, $F = I + \nabla u$, this can be written in the useful form

$$\varepsilon = \frac{1}{2} \left(\nabla u^T + \nabla u + \nabla u^T \nabla u \right).$$

The simplest definition of strain is infinitesimal strain.

$$\varepsilon = \frac{1}{2} \left(\nabla u^T + \nabla u \right).$$

∇u is the displacement gradient.

T denotes the transpose operator. Infinitesimal strain implies the assumption that the deformation did not change the geometry of the body, i.e., that the displacements are small enough that changes in the geometry of the body can be neglected. Finite strain measures are more rigorous definitions of strain that do not assume that the displacements are small.

3.1.4 Stress Strain Constitutive equation.

For an isotropic linear elastic material, the relationship between stress and strain can be written in the form

$$\sigma = \lambda I^2 \varepsilon_{vol} + 2\mu G \varepsilon + (3\lambda + 2\mu) \alpha I (T - T_0).$$

In indicial notation

$$\sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2\mu G \varepsilon_{ij} + (3\lambda + 2\mu) \alpha \delta_{ij} (T - T_0).$$

λ is Lamé's constant.

I^2 is the 3×3 identity tensor.

ε_{vol} is the volumetric strain.

μ is Poisson's ratio.

G is the shear modulus.

α is the coefficient of thermal expansion.

T is the temperature, usually in degrees absolute.

T_0 is a reference temperature at which the thermal strain is zero.

$\alpha \delta_{ij} (T - T_0)$ is the volumetric strain due to thermal expansion.

3.2 Element Stiffness Matrices and Vectors

3.2.1 Basis Functions and Gradient of Basis Functions

We define the basis functions of the 8-node brick.

$$R = (N_1 \quad N_2 \quad N_3 \quad N_4 \quad N_5 \quad N_6 \quad N_7 \quad N_8).$$

A typical basis function is the basis function that we associate with the node $(r, s, t) = (-1, -1, -1)$ is a trilinear polynomial $N(r, s, t) = (1 - r)(1 - s)(1 - t)/8$ The gradient

matrix of the basis functions with respect to (r, s, t) is a 3×8 matrix.

$$\begin{pmatrix} G_r \\ G_s \\ G_t \end{pmatrix} = \begin{pmatrix} N_{1,r} & N_{2,r} & N_{3,r} & N_{4,r} & N_{5,r} & N_{6,r} & N_{7,r} & N_{8,r} \\ N_{1,s} & N_{2,s} & N_{3,s} & N_{4,s} & N_{5,s} & N_{6,s} & N_{7,s} & N_{8,s} \\ N_{1,t} & N_{2,t} & N_{3,t} & N_{4,t} & N_{5,t} & N_{6,t} & N_{7,t} & N_{8,t} \end{pmatrix}.$$

The Jacobian for a general curvilinear element is

$$J = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial s} & \frac{\partial y}{\partial t} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial s} & \frac{\partial z}{\partial t} \end{pmatrix}.$$

The Jacobian for an brick element in a regular grid is

$$J = \begin{pmatrix} \frac{dx}{2} & 0 & 0 \\ 0 & \frac{dy}{2} & 0 \\ 0 & 0 & \frac{dz}{2} \end{pmatrix}.$$

$$\det J = (dxdydz)/8$$

The inverse Jacobian for a regular grid is

$$J^{-1} = \begin{pmatrix} \frac{2}{dx} & 0 & 0 \\ 0 & \frac{2}{dy} & 0 \\ 0 & 0 & \frac{2}{dz} \end{pmatrix}.$$

The gradient of the basis functions with respect to (x, y, z) or

$(x(r, s, t), y(r, s, t), z(r, s, t))$ for an element in a regular grid can be represented as

a matrix

$$\begin{pmatrix} G_x \\ G_y \\ G_z \end{pmatrix} = \begin{pmatrix} G_r 2/dx \\ G_s 2/dy \\ G_t 2/dz \end{pmatrix} = \begin{pmatrix} N_{1,x} & N_{2,x} & N_{3,x} & N_{4,x} & N_{5,x} & N_{6,x} & N_{7,x} & N_{8,x} \\ N_{1,y} & N_{2,y} & N_{3,y} & N_{4,y} & N_{5,y} & N_{6,y} & N_{7,y} & N_{8,y} \\ N_{1,z} & N_{2,z} & N_{3,z} & N_{4,z} & N_{5,z} & N_{6,z} & N_{7,z} & N_{8,z} \end{pmatrix}.$$

3.2.2 Displacement Gradient and Deformation Gradient

The displacement gradient is

$$\begin{pmatrix} u_{x,x} & u_{x,y} & u_{x,z} \\ u_{y,x} & u_{y,y} & u_{y,z} \\ u_{z,x} & u_{z,y} & u_{z,z} \end{pmatrix} = \begin{pmatrix} \bar{u}_x^T \\ \bar{u}_y^T \\ \bar{u}_z^T \end{pmatrix} (G_x^T \quad G_y^T \quad G_z^T).$$

Here $\bar{u}_x^T$ is a 1×8 vector and G_x^T is a 8×1 vector. The deformation gradient $F = I + \nabla u$ is

$$F = I + \begin{pmatrix} u_{x,x} & u_{x,y} & u_{x,z} \\ u_{y,x} & u_{y,y} & u_{y,z} \\ u_{z,x} & u_{z,y} & u_{z,z} \end{pmatrix}.$$

I is the 3×3 identity matrix.

The polar decomposition of the deformation gradient is $F = RU$ where R is a rotation matrix. R is orthogonal and has $\det R = 1$. U is the right stretch tensor. It is symmetric positive definite.

3.2.3 B Matrix

The B matrix that maps the nodal displacement vector to the infinitesimal strain vector at a point is

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \end{pmatrix} = \begin{pmatrix} G_x & 0 & 0 \\ 0 & G_y & 0 \\ 0 & 0 & G_z \\ G_y & G_x & 0 \\ 0 & G_z & G_y \\ G_z & 0 & G_x \end{pmatrix} \begin{pmatrix} \hat{u}_x \\ \hat{u}_y \\ \hat{u}_z \end{pmatrix} = [B] [u].$$

3.2.4 Element Body Force Nodal Vector

The nodal vector due to body forces acting on the volume of an element are now computed. The body force is a force per unit volume (b_x, b_y, b_z) acting on a point (x, y, z) , i.e., $b \in R^3 \times R^3$. The vector of basis functions $R(r, s, t)$ is a function of (r, s, t) . The nodal force vector due to body forces acting on the element is

$$[\bar{b}_\rho] = \int_{\Omega_{Element}} \begin{pmatrix} R^T & 0 & 0 \\ 0 & R^T & 0 \\ 0 & 0 & R^T \end{pmatrix} \begin{pmatrix} \rho g_x \\ \rho g_y \\ \rho g_z \end{pmatrix} \det J d\Omega.$$

3.2.5 Element Traction Vector

The traction vector at point on a surface with outward normal n is $\tau = \sigma \cdot n$ where σ is the Cauchy stress at that point. If a surface has a Neumann boundary condition with an applied traction, it generates a nodal force on all nodes on that surface. This nodal force can be evaluated by

$$[\bar{b}_\rho] = \int_{\partial\Omega_{Element}} \begin{pmatrix} R^T & 0 & 0 \\ 0 & R^T & 0 \\ 0 & 0 & R^T \end{pmatrix} \begin{pmatrix} \tau_x \\ \tau_y \\ \tau_z \end{pmatrix} \det J_\Gamma d\Gamma.$$

$J_\Gamma(r, s)$ is the Jacobian at a point on this face of the brick. For the 32-node brick, R could be R_{32} for the complete element or it could be R_{12} for the face. If it is R_{12} for the face, then the nodal loads from each face with $dim = 12$ have to be assembled into the element nodal load, $dim = 96$.

3.2.6 Elasticity D Matrix

The 6×6 D matrix represents the 4th order elasticity tensor that maps the second order strain tensor to the second order stress tensor where the strain and stress tensors are represented as vectors of dimension six.

$$[\sigma] = [D] [\varepsilon].$$

The elasticity tensor for isotropic materials is characterized by two parameters.

The two parameters can be chosen from the following table.

	λ, G	k, G	G, ν	E, ν	E, G
$\lambda =$	λ	$k - \frac{2G}{3}$	$\frac{2G\nu}{1-2\nu}$	$\frac{\nu E}{(1+\nu)(1-2\nu)}$	$\frac{G(E-2G)}{3G-E}$
$G =$	G	G	G	$\frac{E}{2(1+\nu)}$	G
$k =$	$\lambda + \frac{2G}{3}$	k	$\frac{2G(1+\nu)}{3(1-2\nu)}$	$\frac{E}{3(1-2\nu)}$	$\frac{EG}{3(3G-E)}$
$E =$	$\frac{G(3\lambda+2G)}{\lambda+G}$	$\frac{9kG}{3k+G}$	$2G(1+\nu)$	E	E
$\nu =$	$\frac{\nu}{2(\lambda+G)}$	$\frac{G(3k-2G)}{Gk+2G}$	ν	ν	$\frac{E}{2G} - 1$

The 3D D matrix for isotropic materials $[\sigma] = [D] [\varepsilon]$ is

$$\begin{pmatrix} D_{11} & D_{12} & D_{13} & 0 & 0 & 0 \\ D_{21} & D_{22} & D_{23} & 0 & 0 & 0 \\ D_{31} & D_{32} & D_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & D_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & D_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & D_{66} \end{pmatrix}.$$

where

$$D_{11} = D_{22} = D_{33} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}, \quad D_{44} = D_{55} = D_{66} = \frac{E}{2(1+\nu)}$$

and

$$D_{12} = D_{13} = D_{21} = D_{23} = D_{31} = D_{32} = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

The inverse of the 3D D matrix maps stress or stress rate to strain or strain rate. We

define $C \equiv D^{-1}$ and $[\varepsilon] = [C] [\sigma]$.

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{31} & C_{32} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix}.$$

where $C_{11} = C_{22} = C_{33} = \frac{1}{E}$, $C_{44} = C_{55} = C_{66} = \frac{-\nu}{E}$

and

$$C_{12} = C_{13} = C_{21} = C_{23} = C_{31} = C_{32} = \frac{2(1+\nu)}{E}$$

For elasto-plasticity and viscoplasticity, the 6×6 matrix is usually dense. For isotropic elasticity, it is more efficient to develop this in terms of the shear modulus μ and Lamé's constant $\lambda = \left(K - \frac{2}{3}G\right)$.

$$D = G \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} + \left(K - \frac{2}{3}G\right) \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

3.2.7 Initial Strain

The linear elastic stress strain relationship is

$$\sigma = D(\varepsilon - \varepsilon_0) + \sigma_0$$

where ε_0 is an external or initial strain that could be due to thermal expansion, phase changes, pore formation or composition changes. It can occur during the time step and need not be initial. It is simply strain that is not elastic and is not due to stress. σ_0 is an initial stress that could be due to residual stress. It must be such that

$\text{div } \sigma_0 + b = 0$, i.e., it must self-equilibrating.

3.2.8 Rate Independent and Rate Dependent or Visco-plastic Deformation

In rate independent plasticity, there exists a surface called a yield stress in stress space such that if the stress state attempts to exceed this surface, it is prevented by the formation of plastic strain. The yield stress may increase due to strain hardening and it may soften due to annealing. This plastic strain is independent of the strain rate or stress rate. In rate dependent plasticity, there exists a surface in stress space called a deformation resistance such that if the stress exceeds this this surface, then it is returned to the closest point on this surface at a stress rate proportional to the viscosity and the distance from the surface.

3.2.9 Stress Divergence K Matrix

The divergence of the stress, $\nabla \cdot \sigma$ is a force in the space $\nabla \cdot \sigma \in R^3 \times R^3$. Applying the D matrix, this can be expressed as $\nabla \cdot \sigma = \nabla \cdot (D\varepsilon)$. Expressing strain in terms

of the B matrix, we have $\nabla \cdot \sigma = \nabla \cdot (D B \hat{u})$.

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \end{pmatrix} = \begin{pmatrix} G_x & 0 & 0 \\ 0 & G_y & 0 \\ 0 & 0 & G_z \\ G_y & G_x & 0 \\ 0 & G_z & G_y \\ G_z & 0 & G_x \end{pmatrix} \begin{pmatrix} \hat{u}_x \\ \hat{u}_y \\ \hat{u}_z \end{pmatrix} = [B] [\hat{u}].$$

The divergence of the stress at a point is

$$\begin{pmatrix} b_{x\sigma} \\ b_{y\sigma} \\ b_{z\sigma} \end{pmatrix} = \begin{pmatrix} G_x^T & 0 & 0 & G_y^T & 0 & G_z^T \\ 0 & G_y^T & 0 & G_x^T & G_z^T & 0 \\ 0 & 0 & G_z^T & 0 & G_y^T & G_x^T \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{xz} \end{pmatrix}.$$

The projection of the divergence of the stress onto the space of nodal force vectors is

$$\begin{pmatrix} \bar{b}_{x\sigma} \\ \bar{b}_{y\sigma} \\ \bar{b}_{z\sigma} \end{pmatrix} = \int_{\Omega_{Element}} B^T \sigma \det J d\Omega.$$

The implementation is of the form

$$\begin{pmatrix} \bar{b}_{x\sigma} \\ \bar{b}_{y\sigma} \\ \bar{b}_{z\sigma} \end{pmatrix} = \sum_{GP} \begin{pmatrix} G_x^T & 0 & 0 & G_y^T & 0 & G_z^T \\ 0 & G_y^T & 0 & G_x^T & G_z^T & 0 \\ 0 & 0 & G_z^T & 0 & G_y^T & G_x^T \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{xy} \\ \sigma_{yz} \\ \sigma_{xz} \end{pmatrix} w_{GP} \det J.$$

The volumetric strain is the trace of the strain tensor.

$$\varepsilon_V = (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$\sigma_h = k\varepsilon_V$$

where k is the bulk modulus. The bulk modulus can be written in the form

$$k = \frac{E}{2(1 + \nu)}.$$

3.3 External Strain Nodal Load Vector

The external strain generates a volumetric stress whose divergence projects onto the space of nodal force vectors is

$$\begin{pmatrix} \bar{b}_{x\sigma} \\ \bar{b}_{y\sigma} \\ \bar{b}_{z\sigma} \end{pmatrix} = \int_{\Omega_{Element}} B^T D \varepsilon \det J d\Omega.$$

$$\bar{b}_{x\sigma} = \sum_{GP} G_x^T \sigma_h \det J \quad (3.2)$$

$$\bar{b}_{y\sigma} = \sum_{GP} G_y^T \sigma_h \det J \quad (3.3)$$

$$\bar{b}_{z\sigma} = \sum_{GP} G_z^T \sigma_h \det J. \quad (3.4)$$

3.4 Thermal Strain

We follow G. Mase, Continuum Mechanics [7]. The total strain tensor at a point can be considered to be the sum of the elastic strain due to the stress and the thermal strain due to temperature changes from the reference state. (This note will have to redone in terms of increments of displacements, strain and stress.)

$$\varepsilon_{ij} = \varepsilon_{ij}^S + \varepsilon_{ij}^T$$

The thermal strain in an unconstrained body with linear coefficient of thermal expansion α and bulk modulus $k = \frac{E}{2(1+\nu)}$ is

$$\varepsilon_{ij}^T = \alpha \delta_{ij} (T - T_{ref})$$

Inserting Hooke's law for an isotropic material into the above, we have

$$\varepsilon_{ij} = \frac{1}{2\mu} \left(\sigma_{ij} - \frac{\lambda}{3\lambda + 2\mu} \delta_{ij} \sigma_{kk} \right) + \alpha (T - T_{ref}) \delta_{ij}$$

Inverting this equation, the stress is

$$\sigma_{ij} = [2\mu \varepsilon_{ij} + \lambda \delta_{ij} \varepsilon_{kk}] - 3k\alpha \delta_{ij} (T - T_{ref})$$

The term in square brackets can be interpreted as the stress for this displacement field and hence strain if there was no thermal strain. The last term on the right is the hydrostatic stress due to the volumetric thermal strain.

3.5 Residual in Equilibrium Equation for Stress

The virtual work equation can be written in the form

$$\begin{aligned}\frac{\partial \pi}{\partial \bar{\delta}} &= \int_{\Omega} R^T b + \int_{\partial \Omega} R^T \tau - \int_{\Omega} B^T D B \bar{\delta} = \mathcal{P} - K \bar{\delta} = \mathcal{R} \\ \mathcal{R} &= \mathcal{P} - \int B^T \sigma = \mathcal{P} - \int B^T D B \delta\end{aligned}$$

where $\bar{\delta}$ is the trial nodal displacement vector,

R is the row vector of global basis functions,

D is the 6×6 matrix representing the 3D elasticity tensor,

B is the discrete gradient operator that maps the nodal displacement vector to the strain tensor at a point. The strain tensor is represented as a 6-vector,

b is the body force field and

τ is the traction field on the Neumann boundary of the domain.

$\mathcal{R} = \mathcal{P} - K \bar{\delta}$ is the residual. The residual $\mathcal{R}$ is the nodal load due to external forces $\mathcal{P}$ minus the nodal load due to internal nodal forces $K \bar{\delta}$ or $\int B^T \sigma$. We define the residual $\mathcal{R}$ to be

$$\mathcal{R} = \mathcal{P} - \sum_{\mathcal{EL}} \sum_{\mathcal{GP}} \mathcal{B}^T(\sigma) \quad (3.5)$$

where $\mathcal{P}$ is the external load vector and σ is the stress. This is the condition that the current configuration is in equilibrium where stress is Cauchy stress. Note this is the full Cauchy stress, not the increment and the external load is the full external load and not the increment. This is the condition of equilibrium. However, we use the residual to compute an increment in the nodal displacement vector.

$$[K] [\Delta \hat{u}] = \mathcal{R}.$$

In terms of the elastic displacement increment the residual is

$$\mathcal{R} = - \sum_{\mathcal{GP}} \text{Div}(\mathbf{D}\mathcal{F}(\Delta \mathbf{u})) + \mathcal{P}.$$

This is only true for linear elastic problems with infinitesimal strain. For nonlinear material or nonlinear geometry, the divergence of stress must be evaluated using the Cauchy, Kirchhoff, first Piola-Kirchhoff or second Piola-Kirchhoff stress measure.

1. Nodal force due to internal forces. $\int B^T \sigma(t3)$ where $\sigma(t3)$ which is computed in the stress model code using the initial stress, $\sigma(t1)$, and the current values of any internal variables and the current trial displacement increment dU for this

time step, i.e.,

$$\sigma(t3) = \sigma(t1) + D_{evp} dU.$$

D_{evp} is the tangential or algorithmic D matrix which is evaluated in the stress model code.

2. Nodal forces due to external forces: Ideally these would be evaluated on the deformed or current configuration. This would allow a pressure BC to follow the changes in geometry.

- (a) Total body force $\int R^T b$ where b is the body force vector.
- (b) Total Neumann BC $\int R^T \tau$ where τ is the Neumann traction vector.
- (c) Increment in applied volumetric strain, $\int B^T D d\varepsilon_{vol}$ where $d\varepsilon_{vol} = \varepsilon_{vol}(t3) - \varepsilon_{vol}(t1)$.
- (d) Increment in Dirichlet BCs which equals $dU_D = U_D(t3) - U_D(t1)$.

Chapter 4

Solder Balls Damage Mechanisms

4.1 Stress Strain Behavior of Solder

We take the following constitutive equation for solder (4.1) [2]. The first two terms on the right are the elastic strain rate. The third term is the change in the elastic strain rate because of the rate of change of Young's modulus. In this case, this term is very small because Young's modulus changes very little in the temperature ranges and it is neglected. The term on the second line is the plastic strain rate due to the rate of change of the deviatoric stress. In this case, this term is very small above 25 deg C and it is neglected in this analysis. The term on the last line is the viscoplastic strain rate due to the deviatoric stress S_{ij} . It is included in the analysis.

$$\begin{aligned}
\frac{d\epsilon_{ij}}{dt} = & \frac{1+\nu}{E} \frac{d\sigma_{ij}}{dt} - \frac{\nu}{E} \frac{d\sigma_{kk}}{dt} \delta_{ij} + \\
& \left(\frac{\nu}{E^2} \sigma_{kk} \delta_{ij} - \frac{1+\nu}{E^2} \sigma_{ij} \right) \frac{dE}{dt} + \frac{\alpha A m}{2\tau_p} \left(\frac{\sigma_{eff}}{\sqrt{3}\tau_p} \right)^{m-1} \frac{dS_{ij}}{dt} + \\
& \frac{C_0}{2\tau_0} \left[\left(\frac{\sigma_v}{\sqrt{3}\tau_0} \right)^{n_1-1} + \left(\frac{\sigma_{eff}}{\sqrt{3}\tau_0} \right)^{n_2-1} \right] S_{ij}
\end{aligned} \tag{4.1}$$

where

$d\epsilon_{ij}/dt$ is the strain rate tensor.

E is Young's modulus.

ν is Poisson's ratio.

S_{ij} is the deviatoric stress tensor.

δ_{ij} is the Kronecker delta.

σ_{eff} is the effective stress $= (3J_2)^{1/2}$ where $J_2 = S_{ij}S_{ij}/2$

τ_0 is defined as $\tau_0 = [\tau \exp [U/T]]^{1/(n_2-n_1)}$

C_0 is defined as $C_0 = k \exp [Q_c/T]$

The material constants $A, m, C_1, C_2, \tau, U, k, Q_c, n_1$ and n_2 are listed in Table 4.1 below.

Table 4.1: Material Parameters for 37Pb/63Sn and 90Pb/10Sn [2].

Solder	n_1	n_2	k	Q_c	τ	U	A	m	C_1	C_2
37Pb/63Sn	2	7.1	8.31	5790	7.42	3940	1	2	-2.067	913.04
90Pb10Sn	0	4.0	1.00	0	1.08	7300	1	2	-0.0827	66.28

4.2 Low Cycle Fatigue Life of Solder Balls

Low cycle fatigue life with rate independent plastic strain, is best estimated by the Coffin-Manson equation. At high enough temperatures, such as 100 °C, creep or viscoplastic strain also contributes to failure. It is not clear how low cycle fatigue and creep should be combined to estimate the number of cycles to failure. Plastic strain rate or more precisely rate independent plastic strain rate is a function of stress rate. Creep or more generally, viscoplastic strain rate or rate dependent plasticity, is a function of stress, not stress rate. Rate dependent plasticity involves dislocation climb and other processes that depend on diffusion, particularly vacancy diffusion. The temperature dependence of rate dependent plasticity is largely due to the diffusivity being a function of temperature. The rate independent plastic strain rate is zero if the stress rate is zero. Therefore there is no stress relaxation and viscosity is zero in rate independent plasticity. Rate independent plasticity involves dislocation glide.

However, given a configuration of dislocations at time t_1 and another configuration of dislocations at time $t_1 + \delta t$, it is not clear how to decide what part of the dislocation motion was due to glide and what part was due to climb. This phenomena is not well understood and no simple answers should be expected.

We use the following equation proposed by Engelmaier [3] for estimating the life of a solder ball subjected to both low cycle fatigue and creep. Other choices are possible. We choose it because to our knowledge it represents the best correlation with known experimental results. It modifies the Coffin-Manson equation by making the exponent, c , a function of temperature and time.

$$N_f (x\%) = \frac{1}{2} \left[\frac{2\epsilon_{eff}}{F} \frac{h}{L_D \Delta \alpha \Delta T_e} \right]^{-\frac{1}{c}} \left[\frac{\ln(1 - 0.01x)}{\ln(0.5)} \right]^{\frac{1}{\beta}}$$

$$c = -0.442 - 6 \times 10^{-4} T_{SJ} + 1.74 \times 10^{-2} \ln \left(1 + \frac{360}{t_D} \right)$$

where

ϵ_{eff} is the effective plastic strain to failure in one load cycle. This could be determined from a uniaxial tensile test.

F as Engelmaier [3] stated, is an empirical factor indicative of deviations of real solder joints from idealizing assumptions and accounting for secondary and fre-

quently intractable effects such as cyclic warpage, cyclic transients, non-ideal solder joint geometry, brittle intermetallic compounds, Pb-rich boundary layers, and solder/bonded-material expansion differences as well as uncertainties in the parameters in equation 1. Engelmaier recommends $1.5 > F > 1.0$ for column-like leadless solder attachments.

$L_D \Delta \alpha \Delta T_e / h$ is the increment in effective plastic strain in a thermal load cycle for a Distance From Neutral Point (DNP) model. We replace this factor by the maximum effective strain increment at a point in a solder ball.

$[\ln(1 - 0.01x) / \ln(0.5)]^{\frac{1}{\beta}}$ is the Weibull factor for $x\%$ failure probability with Weibull slope β .

T_{SJ} is the mean cyclic solder joint temperature $= (T_C + T_S + T_{C,0} + T_{S,0}) / 4$ where

T_C is steady state component temperature during high temperature dwell,

T_S is steady state substrate temperature during high temperature dwell,

$T_{C,0}$ is steady state component temperature during low temperature dwell,

$T_{S,0}$ is steady state substrate temperature during low temperature dwell.

t_D is the half-cycle dwell time in minutes, the average time available for stress relaxation at T_C/T_S and $T_{C,0}/T_{S,0}$.

x cumulative failure probability for the component after N cycles expressed as %.

4.2.1 SED Method

Liu [4] proposes another method for estimating the life of a solder ball subject to low cycle fatigue and creep uses the strain energy density (SED) per load cycle.

SED over a load cycle with period from time t_1 to t_2 and stress $\sigma_{ij}(t)$ and strain rate $\dot{\epsilon}_{ij}(t)$ is defined by

$$SED = \int_{t_1}^{t_2} \sigma_{ij} \dot{\epsilon}_{ij} dt.$$

For low cycle fatigue, the SED is evaluated neglecting the elastic strain. Then the equation becomes

$$SED = \int_{t_1}^{t_2} \sigma_{eff} \dot{\epsilon}_{eff} dt.$$

σ_{eff} is the effective stress or second invariant of the stress tensor or von Mises stress and $\dot{\epsilon}_{eff}$ is the second invariant of the deviatoric strain rate tensor.

Although the term SED is used in the literature for cyclic loading, the name is rather misleading. As SED is usually used in low cycle fatigue analysis it refers to the energy dissipated per load cycle per unit volume. It is a pointwise measure. This means that it is computed over a small volume around the desired point and then

divided by the volume around the point. The point chosen is usually the point that has the maximum SED because this is the point most likely to fail.

Liu [4] has proposed the following equation to estimate solder joint life.

$$N_f(x\%) = \frac{2 \times 10^{-8}}{SED}$$

For the cases that Liu analyzed, his results have been encouraging. However, in the BGA's considered in this study, SED is roughly 2 times smaller in the 75 – 150 deg C load cycle than in the 25 – 100 deg C load cycle. This is easily seen because the strain is driven primarily by the thermal distortion of the package. With elastic properties being approximately constant with temperature, the strain rates are similar for both load cycles but the stress is about 2x smaller in the higher temperature load cycle. Thus a naive application of Liu's SED formula would suggest that the higher temperature load cycle would have the longer life. This is contrary to experience and to tests. In order for Liu's SED methodology to succeed in this case, the numerator 2×10^{-8} would have to be a function of the load cycle temperature and time.

4.3 Stress Life Approach to High Cycle Fatigue Life

This chapter presents a very brief summary of theory available for estimating fatigue life.

4.3.1 Basquin's equation

Basquin's equation [6] estimates the number of cycles to failure in the high cycle fatigue for a fully reversed, constant amplitude fatigue test with number of load reversals to failure, N_f , and stress amplitude $\sigma_a = \Delta\sigma/2$

$$\frac{\Delta\sigma}{2} = \sigma'_f (2N_f)^b. \quad (4.2)$$

σ_f is the true stress, i.e., corrected for necking, in monotonic tensile loading. For most metals, the Basquin exponent b lies in the range of -0.05 to -0.12.

σ'_f is the fatigue strength coefficient

σ_y yield strength for tensile loading.

σ_{TS} tensile strength for tensile loading.

stress range $\Delta\sigma = \sigma_{max} - \sigma_{min}$.

stress amplitude $\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2}$

mean stress $\sigma_m = \frac{\sigma_{max} + \sigma_{min}}{2}$.

$N_f|_{\sigma_m=0}$ Number of cycles to failure for zero mean stress.

4.3.2 Soderberg Relation

$$\sigma_a = \sigma_a|_{\sigma_m=0} \left(1 - \frac{\sigma_m}{\sigma_y} \right) \cdot [6] \quad (4.3)$$

$$(4.4)$$

This provides a conservative estimate of fatigue life for most engineering materials.

4.3.3 Modified Goodman Relation

$$\sigma_a = \sigma_a|_{\sigma_m=0} \left(1 - \frac{\sigma_m}{\sigma_{TS}} \right) \cdot [6] \quad (4.5)$$

This matches experimental observations for brittle materials but is conservative for ductile materials. Because it is generally non-conservative for compressive mean stresses, one may assume that compressive mean stresses provide no beneficial effects on fatigue life.

4.3.4 Modified Morrow Relation

$$\sigma_a = \sigma_a|_{\sigma_m=0} \left(1 - \left(\frac{\sigma_m}{\sigma_{TS}} \right)^2 \right). \quad (4.6)$$

This is generally good for ductile materials for tensile mean stresses. Morrow modified Basquin's equation to account for mean stress effects

$$\begin{aligned} \sigma_a &= (\sigma'_f - \sigma_m) (2N_f)^b. \\ N_f &= \left(1 - \frac{\sigma_m}{\sigma'_f} \right)^{1/b} N_f|_{\sigma_m=0}. \end{aligned} \quad (4.7)$$

4.4 Strain Life Approach to Fatigue Life

Coffin and Manson [6] proposed the following equation to estimate low cycle fatigue life based on the plastic strain amplitude, $\Delta\varepsilon_p/2$, per load cycle

$$\frac{\Delta\varepsilon_p}{2} = \varepsilon'_f (2N_f)^c \quad (4.8)$$

where ε'_f is the fatigue ductility coefficient and c is the fatigue ductility exponent. Usually ε'_f is equal to the true fracture ductility and c is in the range of -0.5 to -0.7 for most metals. Cyclic Strain Life data for some engineering metals and alloys

is presented in table (4.2) [6]. In a constant strain amplitude test, the total strain amplitude, $\Delta\varepsilon/2$, can be written as the sum of the the elastic strain amplitude, $\Delta\varepsilon_e/2$, and the plastic strain amplitude, $\Delta\varepsilon_p/2$,

$$\frac{\Delta\varepsilon}{2} = \frac{\Delta\varepsilon_e}{2} + \frac{\Delta\varepsilon_p}{2}. \quad (4.9)$$

Noting that

$$\frac{\Delta\varepsilon_e}{2} = \frac{\Delta\sigma}{2E} = \frac{\sigma_a}{E}. \quad (4.10)$$

Substituting for the stress amplitude in Basquin's equation

$$\frac{\Delta\varepsilon_e}{2} = \sigma'_f (2N_f)^b. \quad (4.11)$$

The Coffin-Manson equation and Basquin's equation can be combined

$$\frac{\Delta\varepsilon}{2} = \frac{\sigma'_f}{E} (2N_f)^b + \varepsilon'_f (2N_f)^c. \quad (4.12)$$

The transition from strain-based to stress-based failure can be estimated by equating the number

$$(2N_f)_t = \left(\frac{\varepsilon'_f E}{\sigma'_f} \right)^{1/(b-c)}. \quad (4.13)$$

Morrow assumed that a tensile mean stress reduces fatigue life such that

$$\sigma_a = (\sigma'_f - \sigma_m) (2N_f)^b. \quad (4.14)$$

and modified equation (4.12)

$$\frac{\Delta \varepsilon}{2} = \frac{\sigma'_f - \sigma_m}{E} (2N_f)^b + \varepsilon'_f (2N_f)^c. \quad (4.15)$$

Table 4.2: Cyclic Strain Life data for some engineering metals and alloys.

Material	Condition	σ_y	σ_f	ε_f	b	c
Al Alloys						
Al 1100	annealed	97	193	1.80	-0.106	-0.69
Al 2014	T6	462	848	0.42	-0.106	-0.65
Al 2024	T351	379	1103	0.22	-0.124	-0.59
Al 5456	H311	234	724	0.46	-0.110	-0.67
Al 7075	T6	469	1317	0.19	-0.126	-0.52
Steels						
1015	air cooled	228	827	0.95	-0.110	-0.64
4340	tempered	1172	1655	0.73	-0.076	-0.62
Ti Alloys						
Ti-6Al-V	solution treated	1185	2030	0.841	-0.104	-0.69
Ni-base Alloys						
Inconel X	annealed	760	2255	1.16	-0.117	-0.75

4.5 Thermal Cycling Damage Mechanisms

The reliability of the solder joint attachment of electronic components surface mounted to printed circuit boards requires explicit attention during design and manufacturing. During use, solder joints can be subjected to a variety of loading conditions which can lead to premature failure [10]:

1. Cyclic differential thermal expansion
2. Vibration
3. Thermal shock during cooling from the soldering operation or from severe use environments
4. Mechanical shock

The failure mechanism of primary concern for surface mount solder joint reliability is cyclic differential thermal expansion causing fatigue damage. These thermal expansion differences result from changing temperatures due to power dissipation internal to the component and differences in the coefficient of thermal expansion in combination with system internal or external temperature variations caused by component or system load fluctuations.

The primary damage mechanism in thermal cycling is the creep/ stress-relaxation-enhanced fatigue of the solder joints. When loaded from a zero-stress, zero-strain condition, the solder joint first undergoes elastic deformation followed by plastic yielding if the loading continues beyond the yield strength of the solder. The elastic-plastic yielding portion of the loading response is followed by the temperature and stress-dependant relaxation/creep response of the solder joint. The difference between stress relaxation and creep is that the former occurs when the solder joint strain is held constant and the stress decreases and the latter occurs when the stress is held constant and the strain changes with time. Microstructurally, creep and stress relaxation behave similarly and together cause the simultaneous time-dependant changes in the stresses and strains experienced by the solder joints. The relaxation/creep process occurs in the dwell period of thermal cycle where the solder joint will relax towards its maximum possible plastic strain. The extent of strain is primarily time dependent although at high temperature dwells (around 100°C), relaxation can occur in a matter of minutes. The loading response described represents half of the thermal cycle. The other half of the loading cycle is represented by a temperature ramp down and a low temperature dwell period resulting in a stress reduction proceeding in the opposite direction. The solder joint response is characterized by hysteresis loops in the shear stress-strain plane as shown in figure 4.1.

Figure 4.1: Hysteresis Loops Characterizing the Solder Joint Response under Cyclic Loading.

Such loops have been obtained experimentally and numerical simulations of these loops form the basis of many of the reliability models. The general shape of these loops gives a meaningful insight into the solder joint deformation and stress history. The area of the hysteresis loop is representative of the viscoplastic strain energy density dissipated per cycle, which represents the fatigue damage accumulating per cycle. During the dwell at higher temperature, creep and stress relaxation occur

along a steep isothermal stress reduction line. The length of the line is dependent on the dwell time used. If full stress reduction is permitted, zero stress and maximum plastic strain is obtained by the end of the dwell period. In some cases, like some of the accelerated tests, the stress reduction is incomplete. For ball solder attachments, the limits of the loop envelope are determined by the solder yield strength during the initial elastic loading, plastic yielding, creep and stress relaxation. The yield strength of solder is highly dependent on temperature, loading rate, solder composition and grain structure. Some of these variables are controllable (e.g., temperature), and some are difficult to control (e.g., grain structure). Although solder fatigue is best represented by a stress-strain hysteresis loop, the strain range is usually taken to quantify solder damage. The reason for using just the strain range is because of the significant time spent beyond the yield point by the solder during each thermal cycle. Since solder spends a small proportion of its cycle in its elastic state, the strain energy density due to elasticity can be omitted from the stress-strain hysteresis loop.

Chapter 5

Thermal Stress Analysis of ASIC's

5.1 Electronic Data Exchange

Electronic data exchange represents a very important link for integrating PCB electrical layout and mechanical design. The Intermediate Data Format (IDF) is the most used file format for exchanging printed circuit assembly (PCA) data between electrical and mechanical CAD/CAE systems and for allowing users of these systems to participate concurrently in the design of electro-mechanical products.

5.1.1 The Intermediate Data Format

Excellent data exchange standards exist for communicating raw 3D geometric data such as IGES, DXF, STL and more rich data formats such as STEP. However, with the exception of STEP, none of these standards go much beyond geometric data and they are unsuitable for the application specific data exchange required for PCA design. The Intermediate Data Format (IDF) bridges the gap that exists between ECAD (Electrical Computer-Aided Design), MCAD (Mechanical Computer-Aided Design) and CAE software. IDF has become a de facto industry standard for PCA data exchange and is now supported by most of the MCAD and ECAD vendors.

5.1.2 Integrated Product Design

Integrated Product Design (IPD) is key to shortening electronic product design schedules. One of the difficulties is linking together the different MCAD, ECAD and CAE software packages used by engineers and designers. At the heart of most electronic products is copper-clad FR4 based printed circuit board assemblies. The PCA design touches all aspects of the product design process; examples include mechanical and electrical packaging, schematic capture, component placement, board routing, thermal engineering and EMI. Using the IDF facilitates the design data transfer process

between MCAD and ECAD. In most cases, the product packaging constrains the shape, size, and position of the PCAs used. Based on these package constraints, the mechanical designer determines the board outline and the size and locations of mounting holes for the board. Usually, the mechanical designer knows where to place certain critical components, such as connectors, LEDs, displays, and switches, because their locations are determined by the product packaging itself. Components preplaced by the designer can include mechanical components, such as standoffs, stiffeners, and other mechanical supports. Detailed 3D component models are used for preplacement in the mechanical CAD application. During the transfer, these reference the 2D footprints required by the ECAD application. Often, the mechanical designer indicates areas on the board where components cannot be placed, or where placement is limited by other obstructions in the overall assembly. The most common information transferred initially from MCAD to ECAD includes:

- Board outline
- Board mounting holes
- Component mounting holes
- Placement keepouts
- Placement of critical components

The layout designer uses the initial information from MCAD as the basis for creating the board part in ECAD. Often the layout designer adds additional placement and routing restriction areas, tooling holes, and fiducials. With the preplaced components from MCAD as a start, the layout designer places additional components. The locations of the preplaced components may need to be modified to accommodate routing considerations. For those components that do not have detailed 3D models in MCAD, the MCAD IDF translators create extrusions of the ECAD component outlines by their height. Mounting holes defined in the components are transferred, resulting in holes in the board at appropriate locations. The information typically transferred back to MCAD from ECAD includes:

- Board outline
- Additional placement and routing areas
- Component shapes
- Component placement
- Component mounting holes

Figure 5.1 shows the board assembly with the initial MCAD model. The new model containing additional placement areas and new components is shown in figure

5.2

Figure 5.1: View of a PCB assembly - MCAD input.

Another essential part of the PCB data exchange process is to coordinate component part information between ECAD and MCAD systems. The data exchange tool must provide simple methods to allow matching and filtering component data between MCAD and an ECAD system. Component mapping helps to maintain different component part names and numbers between MCAD and ECAD software. Filtering helps to remove small components and small board features such as pin holes for more efficient assembly modeling in MCAD. During the process of filtering,

Figure 5.2: View of a PCB assembly - ECAD input.

the data exchange tool should interactively preview IDF files and visualize the data exchange process in order to verify content before committing to revisions.

5.1.3 Thermal Representation in IDF

PCB thermal data and component thermal characterization data are needed to compute the thermal stress. For the board, the thermal properties can be defined based on a stack of physical layers as well as conductors:

- Conductor pads and traces
- Thermal vias
- Conductive filled areas
- Physical layers, used to represent the physical characteristics and arrangement of the physical layers that make up a board part
- Thermal material properties used to define the material characteristics of board or physical layers

For components, the thermal data can be associated with individual component parts as well as component instances. This way, a component can have global prop-

erties, all or some of which can be overwritten by the component's instance in the PCA. The following component properties to support thermal analysis are provided:

- Material properties for the component; isotropic or orthotropic with surface properties such as emissivity and roughness
- Specific physical and thermal properties, such as heat dissipation (min, max, nominal), thermal resistances (R_{jc} , R_{jb} , R_{cb}), thermal capacitance, and the thickness of the air-gap between the component and board
- Mounting type, surface or through-hole, as well as pin quantity, size (length and area), locations and pin material

5.2 Description of Domain and Problem

The domain chosen for the analysis here is that of an application specific to electronic packaging. Depending on the EMI shielding and environmental requirements, the circuit packs can be fully enclosed or open. For our analysis a fully enclosed type pack has been considered. A general view of such a circuit pack (ProE model) is presented in figure 5.3.

Since some of the hardware parts such as latches, face plate, etc., have little effect on thermal and structural performance of the circuit pack, these parts have

Figure 5.3: View of a circuit pack.

been removed from the model to be analyzed to simplify the mesh and to save in computational expense. A simplified ProE model of the pack used for thermal/stress analysis is presented in figure 5.4. This model has been used to generate the stereolithographic files (STL) which are the input files for the mesh generation program (SmtFramework mesher). Figure 5.5 is an exploded view of the simplified circuit pack. Note that the electronic components are not meshed from STL files. All the meshes required for the components included in thermal/stress domain are obtained directly from data contained in board assembly IDF file.

Figure 5.4: View of a simplified circuit pack.

Figure 5.5: Exploded view of a simplified circuit pack.

Figure 5.6: Inside view of a simplified circuit pack.

The stress analysis of the solder ball was performed using the multigrid technique. A series of thermal analysis followed by stress analysis were performed on progressively finer meshes. Following are the steps performed in order to get accurate solutions:

1. Thermal analysis of the circuit pack
2. Stress analysis of the circuit pack
3. Thermal analysis of a detailed ASIC model
4. Stress analysis of a detailed ASIC model
5. Stress analysis of refined solder ball(s)

5.2.1 Thermal analysis of the circuit pack

A thermal analysis of the simplified circuit pack is performed. The domain includes all the hardware parts (heat sinks, end caps, standoffs, pedestals, overfill) and the printed circuit assembly. From the PCA only the components that were considered to impact the thermal result were included in the analysis. Figure 5.7 shows the printed circuit assembly mesh (pedestals and overfill parts are shown as well). A side view of the full mesh is shown in figure 5.8

Figure 5.7: PCB assembly mesh - top view.

For this analysis all the electronic components are meshed with two layers of elements through the thickness. Separate material properties are assigned to each layer based on component geometry and thermal resistances R_{jc} and R_{jb} . A flux boundary condition is applied between the two layers to represent the component dissipation power. A convection boundary condition was placed on the fin side of both heat sinks using data from thermal experiments.

5.2.2 Stress analysis of the circuit pack

The domain for circuit pack stress analysis includes all the hardware parts (heat sinks, end caps, standoffs, pedestals, overfill) and the printed circuit board. For all

Figure 5.8: Circuit Pack Mesh.

components that require a cooling path to the heat sink, a soft interface material is used to eliminate the risk of damaging the component due to heat sink warpage. We assume that, for this design, the components will not affect the stress results and are not included in the stress analysis. If stiffeners or other big components that may affect PCA stiffness are present, they should be included in the stress analysis. Temperature results from previous analysis are used as thermal load for the current stress analysis.

5.2.3 Thermal analysis of a detailed ASIC model

For this analysis the domain includes the detailed ASIC mesh together with overfill, pedestal and part of the printed circuit board. Dirichlet boundary conditions were applied to the top surface of the pedestal (the surface that comes in contact with the heat sink) and to the side surfaces of the printed circuit board part. The values for the prescribed temperatures were taken from the previous thermal analysis of the entire circuit pack. A flux boundary condition was applied between the silicon die and the copper lid above it to represent the power generation from the silicon die. Figures 5.9, 5.10 and 5.11 show different views of the mesh used for this analysis.

Figure 5.9: Section of a simplified ASIC mesh.

Figure 5.10: Section of a simplified ASIC (iso view).

5.2.4 Stress analysis of a detailed ASIC model

The domain for this analysis includes the detailed ASIC mesh together with part of the printed circuit board. It is assumed that the overfill, because of its softness, does not affect the ASIC deformation. Therefore the pedestal and overfill parts were not included in the stress analysis. Dirichlet boundary conditions were applied to the side surfaces of the printed circuit board part. The values for the prescribed displacement were taken from the previous stress analysis of the entire circuit pack.

Figure 5.11: Section of a simplified ASIC mesh (detail with dimensions added).

5.2.5 Stress analysis of refined solder ball(s)

The domain of the subsequent analysis is changed from the entire ASIC to just a solder ball or a set of solder balls. The location and number of solder balls to be analyzed depends on the position and size of the region of interest (the region with high effective plastic strain). These solder balls were taken out of the full ball grid array along with sections of the attached PCB and substrate. Figure 5.12 is a detailed view of a refined solder ball mesh and figure 5.13 shows the same solder ball mesh with attached PCB and substrate regions. Dirichlet boundary conditions were applied to the edges of the PCB and substrate. The values of the prescribed displacement were taken from the previous analysis of the entire ASIC.

Figure 5.12: Refined Mesh of a Solder ball.

Figure 5.13: Refined Mesh of a Solder ball with cut-outs from the substrate and PCB.

Chapter 6

Results and Discussions

6.1 Thermal Analysis of the Circuit Pack

A thermal analysis of the simplified circuit pack (the mesh shown in figures 5.7 and 5.8) followed by a thermal analysis of the detailed ASIC (the mesh shown in figures 5.9, 5.10 and 5.11) were performed to accurately predict the temperature distribution within the PCB and the ASIC under investigation. For the circuit pack analysis a convection boundary condition was placed on both heat sinks. The convection coefficient was assumed to be $50 \text{ W/m}^2\text{K}$ and the ambient temperature was set to 25°C . There was a flux boundary condition applied for each component to represent the dissipation power. Temperature distribution for the analyzed circuit pack is shown in

figure 6.1. We can see that most of the dissipated power is concentrated towards the right side of the circuit pack. This will cause higher PCB and heat sink deformations in that area and may cause the components to overheat. The standoffs placed in the affected area increase the assembly stiffness and also help to reduce the PCB temperature. The temperature results from this analysis may be used in subsequent stress analysis to predict PCB and heat sink deformation.

Figure 6.1: Temperature distribution in the circuit pack - steady state.

For the thermal analysis of the detailed ASIC a flux boundary condition was applied between the silicon die and the copper lid to represent the power dissipation (maximum power for the analyzed component is $30W$). Dirichlet boundary condition were applied on top surface of the pedestal. The obtained temperature distribution

in the ASIC is presented in figure 6.2. In this analysis, the maximum temperature achieved is approximately 371K, or about 98 °C. For most of the ASIC's the maximum operating temperature of the silicon die should not exceed 105 °C. For the size of the analyzed component and cooling strategy, the dissipating power should not exceed 30W. These temperature results may be used in subsequent stress analysis to predict the component deformation and to estimate the life of the analyzed component.

Figure 6.2: Temperature distribution in the ASIC.

6.2 Thermal Stress Analysis of the Circuit Pack

The stresses in the solder balls arise from the temperature variation and different coefficients of thermal expansion (CTE) between ASIC layers, printed circuit board (PCB) and heat sinks. To estimate the fatigue life of solder balls under accelerated test conditions, the following stress analysis were performed:

1. Stress analysis of the circuit pack.
2. Stress analysis of detailed ASIC model.
3. Stress analysis of solder ball layer.
4. Stress analysis of refined solder balls placed in regions of interest.

6.2.1 Stress analysis of the circuit pack

For this analysis the mesh described in figure 5.8 was used. The temperature variation was modeled after a prescribed furnace temperature cycle and was prescribed, for each time step, for all the elements in domain. The furnace temperature cycle involves subjecting the circuit packs alternately to high and low temperatures for predetermined dwell times in order to produce failure in less time than would be required during the field use conditions. The temperature variation vs time, for one

load cycle is presented in figure 6.12. We can see that the temperature linearly increases from the initial temperature of 300K (26.5 °C) to 375K (101.5 °C) in 15min, is held there for 15min, then linearly decreases to 300K and is held there for 15min. The stress analysis was done for two cycles, a total time of 120min with 80 time steps (90 seconds/time step).

Figures 6.3 through figure 6.5 show the deformed circuit pack. We can see that, for this type of circuit pack, the number of standoffs and their placement, as well as the heat sink design, have a very significant role in limiting the PCB deformation. Usually, large ASIC's are placed close to standoffs location in order to increase the component reliability by reducing PCB deformation. The PCB displacement results obtained in this analysis are applied as Dirichlet boundary conditions for the stress analysis of the detailed ASIC model.

6.2.2 Stress analysis of detailed ASIC model

The domain for the subsequent analysis is changed from the entire circuit pack to the entire ASIC along with a section of the PCB. Dirichlet boundary conditions (DBC's) were applied to the edges of the PCB. The values for the DBC's applied were taken from that of the previous analysis of the entire circuit pack, so these DBC's essentially deformed the ASIC as if it was analyzed together with the enclosure. The

Figure 6.3: Circuit pack stress analysis - deformed heat sinks.

Figure 6.4: Circuit pack stress analysis - deformed PCB.

Figure 6.5: Circuit pack stress analysis - section through deformed PCB.

stress analysis was done for the same number of steps and with the same temperature load cycle as for the entire circuit pack. Figure 6.6 and figure 6.7 show how the ASIC deforms during the thermal cycle. We can see how the heat sink does not remain planar but tries to bend like a bubble. This bending increase the plastic deformation in the inner and outer rows of solder balls. A consequence of this bending is that the top and bottom surface of the solder balls do not remain parallel.

Figure 6.6: View of deformed ASIC.

6.2.3 Stress analysis of solder ball layer

The domain for this analysis includes only the solder balls layer along with sections of the attached substrate and PCB. Dirichlet boundary conditions were applied to the PCB and substrate parts. The DBCs applied were from that of the previous analysis of the entire ASIC. The same number of time steps and the same temperature load cycle as for the entire ASIC were used. Figure 6.8 shows the solder balls layer deformation (displacement is magnified 200 times for emphasis).

The distribution of maximum effective plastic strain in solder balls is shown in figure 6.9. The far corner solder ball which has the greatest distance from the neutral point (DNP) is by far at greatest risk of failure. However, for other solder balls, the risk of failure is not a simple function of DNP.

Figure 6.10 show a tendency for solder balls on the outer row and the ones underneath the edges of the Si die to have a higher risk of failure than the other solder

Figure 6.7: Section through the deformed ASIC.

Figure 6.8: Solder balls layer stress analysis - deformed solder balls.

Figure 6.9: Effective Plastic Strain distribution in solder balls layer.

balls. This information could be used to allocate high risk solder balls functions to power and ground leads. The reason is that the heat sink does not remain planar but tries to bend like a bubble (see figures 6.6, 6.7, 6.8). This bending increase the plastic deformation of the solder balls underneath the deformed regions.

The number of cycles to failure is estimated using the Coffin-Manson equation. The increment in the effective plastic strain amplitude, i.e., the effective plastic strain in half a load cycle and the Coffin-Manson coefficients determine the number of cycles to failure. The analysis of the number cycles to failure is done with a script. The script checks all the nodes in each solder ball to determine the maximum effective plastic strain increment in a solder ball at the end of a specified load step. Then it determines the effective plastic strain at that point in that element for all time steps in the analysis and the increment in the effective plastic strain in the last load cycle. Finally, it evaluates the Coffin-Manson equation to estimate the number of cycles to failure. The estimated number of cycles to failure at the 3% level for the analyzed solder balls is presented in figure 6.10

Figure 6.10: Cycles to Failure distribution in solder balls layer.

6.2.4 Stress analysis of refined solder balls placed in regions of interest

In order to accurately determine the location of the effective plastic strain, which is the location of the initial crack, a stress analysis of refined solder balls placed in regions of interest is performed. For our analysis a solder ball furthest from the package center along with sections of PCB and substrate was chosen. DBCs were applied to PCB and substrate parts. Figures 6.11 show the deformation (displacements magnified 100 times for emphasis) and distribution of effective plastic strain in the solder ball farthest from the neutral point at the start of the 25 °C cold holding stage. At this time, the stress in the solder ball is maximal. We can see that the distribution of effective plastic strain is not homogeneous. It is concentrated at the top and bottom edges of the solder balls on sections facing toward and facing away from the neutral point. There is very little plastic deformation in the center of the solder ball on the top and bottom surfaces. This suggests that defects in the high plastic strain regions would be much more likely to lead to failure than defects in low plastic strain regions. This information could be used in devising inspection programs that classify defects by both their size and shape and their location in a solder ball.

The variation of temperature, effective stress, effective plastic strain and effec-

Figure 6.11: View of deformed solder ball and effective plastic strain distribution.

tive strain versus time are shown in figure 6.12 for the 25-100 °C test. The rather complex behavior is due to different relaxation rates during the hot and cold holding stages. One can see that the stress increase until time step 10 (900 sec) when the maximum temperature is achieved. We can see the stress relaxation during the hot holding stage. Once the high temperature dwell is over (time step 20), the ASIC is cooled and the solder viscosity increase. As this occurs, the package begin to warp more severely and thus there is a large increase in stresses as the solder ball is loaded as it hardens while cooling. When the cold holding stage begins the stress in the solder ball relaxes slowly. At high temperatures the relaxation times are much shorter than at lower temperatures. The solder balls are expected to fail due to low cycle fatigue. We can see as the effective strain and effective plastic strain increase during this time because of the creep effect.

Figure 6.12: Temperature (K), effective stress, effective strain and effective plastic strain plotted versus time for one load cycle of 25-100 $^{\circ}C$.

Chapter 7

Conclusions and Future Work

7.1 Conclusions

This thermal stress analysis of the package and circuit pack estimated that the maximum effective plastic strain increment at a point in a solder ball is 0.0081 for the 25 °C to 100 °C accelerated test. The Coffin-Manson equation predicts a life of 1495 load cycles for this thermal cycle.

Data was imported largely automatically from IDF files. This demonstrated an opportunity to improved collaboration between members of the design team for electronic packaging.

The analysis suggests that the adhesive joining the silicon die and copper heat

spreader could reduce the deformation of the heat spreader and affect the solder ball life. The results show a tendency for solder balls on the outer row and the ones underneath the edges of the silicon die to have a higher risk of failure than the other solder balls. This information could be used by ASIC designer to assign the high risk solder balls to ground or power functions.

A true fatigue life analysis should be performed that reaches cyclic steady state. In this thesis, to save computational time, the first two cycles were used in the analysis. We can consider this as being conservative in our cycle to failure calculations, as the cyclic stress and the plastic strain are expected to be greater at the beginning than during cyclic steady state.

The cycles to failure calculation using the Coffin-Manson equation has the disadvantage that one must have a good idea of the value of the Weibull exponent for that particular type of package because differences in the Weibull exponent can cause great differences in the estimated component life. This can only be achieved through experiments for that specific ASIC package.

The predicted solder ball life is not inconsistent with the test results. The analysis uses a full nonlinear analysis that accurately couples the nonlinear behavior of the solder balls with the package and PCB. This analysis uses contact elements that accurately captures the behavior of adhesives. A very fine mesh is used to captures

the local deformations where PCB and substrate join the solder ball.

The effective plastic strain is not uniformly distributed in each solder ball. It tends to be concentrated near the solder joint with PCB and substrate.

7.2 Future Work

From the viewpoint of estimating the in-service life of a package, it appears most important to do a transient analysis of deformation of packages, particularly the heat sinks and PCB due to temperature gradients during cooling and heating, that includes the heat loads on Si chips due to service conditions. This is a transient thermal stress analysis in which the thermal analysis is coupled to the stress analysis. These analyses would help to design test procedures that were more realistic simulations of service conditions and provide more accurate estimates of life. There is a need for a careful study of the statistical aspects of solder ball failures. Analyzes of any packages for which good experimental data is available, either for in-service operation or experimental test data would be very useful to determine failure criteria in terms of plastic strain increment for low cycle fatigue failure or due to time at temperature and stress for creep failure. The life of solder balls with defects could be studied as well as the life of solder balls with different shapes.

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