Finite element analysis of semiconductor package debonding due to thermal cycling

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Finite Element Analysis of Semiconductor Package Debonding Due to Thermal Cycling

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FINITE ELEMENT ANALYSIS OF SEMICONDUCTOR PACKAGE DEBONDING DUE TO THERMAL CYCLING

by

Ali Osman Ayhan

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Presented to the Graduate and Research Committee of Lehigh University in Candidacy for the Degree of Master of Science in Mechanical Engineering

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(Chairman of Department)
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Abstract

In this study, the problem of "debonding", which is a difficult issue due to various complex package configurations, material properties, different loading (thermal loading and moisture absorption) and constraint conditions, has been investigated. The finite element method was used both in two dimensions and three dimensions. In the analyses, deformation and stresses in the semiconductor package have been determined and fracture analysis for possible interface cracks has been performed.

Some of the problems encountered in this area are real three dimensional problems (i.e., corner cracks). Other problems can be partially three dimensional (modeling of solder balls, etc.). There is also a need to employ three dimensional finite element analysis to decide on where and when two dimensional finite element analysis can be used with confidence. Thus, in this study, Finite Element Analysis is performed by using a three dimensional finite element approach, in terms of both stresses and fracture parameters. For this purpose, a three dimensional finite element program was developed, and the theoretical aspects are given in this thesis. As a first step in understanding the behavior of semiconductor packages in 3-D, and to be able to make comparisons between the 2-D and 3-D results, an additional capability has been added to the three dimensional finite element program, "Generalized Plane Strain".

Comparisons in terms of stresses and fracture parameters, have been made between the 2-D and 3-D analyses. These results showed, that for the problems that are encountered in semiconductor packaging, one cannot make a general statement which defines the relationship between 3-D (Generalized Plane Strain) analysis and 2-D calculations, i.e., it depends on the specific package configuration, material properties and boundary conditions.
Chapter 1

Introduction

1.1 WHAT IS A SEMICONDUCTOR PACKAGE?

In today's advanced electronic technology, it became a necessity to use compact semiconductor "chips" in a variety of areas, such as computers, electrical appliances, automotive, etc. Clearly, the need for more and more sophisticated packages is increasing.

A sample semiconductor package is shown in Fig. 1.1. As can be seen in the figure, an IC package mainly consists of four parts, silicon die (chip), polymeric substrate, plastic molding compound and connectivity parts; lead frames and bond wires. The silicon chip is assembled on a polymeric substrate, plastic molding compound surrounding both parts. Lead frames and bond wires provide electrical connectivity between the package and the board on which the assembly is made.

![Figure 1.1: A Sample Semiconductor Package.](image-url)
As the need for faster computers increases, design of denser and more complicated packages becomes unavoidable. More complicated package means that, the size of the chip more or less remains the same, but it has more electronic circuitry per unit surface area. This, of course, increases the temperature of the package and causes thermal stresses because of differences in the CTE's (Coefficient of Thermal Expansion) of the constituent materials. Thermal stresses ultimately may cause the failure of the device.

1.2 AN OVERVIEW OF THE PROBLEM

The interfacial integrity of an integrated circuit (IC) package is a very significant reliability issue for service life performance. Any sort of interface degradation can cause failure of the chip or if not, effects its efficiency resulting in substandard operation. In addition to delamination failure modes, other structural failures include: metal line deformation, passivation cracking, dielectric cracking, wire bond shear, and epoxy molding compound (EMC) cracking. These failures are generally due to thermal stressing, and the solder reflow process for printed circuit board (PCB) mounting. In addition, if moisture absorption is experienced by the package, the corrosion risk becomes greatly increased because of water-borne contaminants entering the package and diffusing into the material interfaces.

1.2.1 THERMAL CYCLING

Delamination between a silicon die and a polymeric substrate is often observed in semiconductor packages subjected to severe thermal shock and thermal cycles. Acoustic imaging techniques such as C-mode scanning acoustic microscopy (C-SAM), can be
used to visualize the extent of this delamination and relate damage to thermal processing conditions, e.g., IR solder reflow, and subsequent thermal cycling. In Fig. 1.2 some delaminations in an IC package are shown (red areas).

![Figure 1.2 (a) - Surface Delaminations, (b) - Small Surface Delaminations in An Electronic Package.](image)

The theory behind the detrimental effects suggests, that thin film cracking and metal line smearing result from inelastic deformations of the die surface. If perfect adhesion exists between the EMC and the die surface, any elastic deformation of one material will translate to the other. Due to the thermal mismatch, however, shear stresses are generated at the interface. Once the stress magnitude reaches a certain critical value above the yield strength of some films of the multilayer structure, surface damage can occur if good adhesion still exists, or else, interfacial adhesion is broken resulting in delamination [1].
used to visualize the extent of this delamination and relate damage to thermal processing conditions, e.g., IR solder reflow, and subsequent thermal cycling. In Fig. 1.2 some delaminations in an IC package are shown (red areas).

![Figure 1.2](image)

**Figure 1.2** (a)- Surface Delaminations, (b)- Small Surface Delaminations in An Electronic Package.

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1.2.2 PRINTED CIRCUIT BOARD (PCB) ASSEMBLY

Semiconductor package-board attachment methods, i.e. solder reflow, results in thermal stresses. The moisture absorbed within a package cannot desorb quickly enough, because the solder reflow procedure is performed at elevated temperatures (greater than 183°C for some packages) and at too fast ramp rate (greater than 1°C/s), to allow the solder to melt properly; which turns into steam within the package. It is sometimes the case that, the resulting pressure is greater than the strength of the compound, and the compound cracks to release the pressure, which causes the failure called "pop corning". The situation is shown in Fig. 1.3.

![Diagram](image)

**Figure 1.3**: Schematic of "Pop corning" Mechanism During Board Assembly.

There may occur more than one crack in the device, depending on the package type and constituent materials (Fig. 1.4), and these cracks can be located at the substrate-molding compound, die-molding compound interfaces, or within the die attach layer.
**Figure 1.4**: Possible Cracks in the Semiconductor Package

Although an external crack does not occur and the package seems intact externally, the stresses due to steam pressure can cause delamination between the epoxy molding compound and the backside of the die pad. The magnitude of the interfacial damage can vary with the package configuration, the constituent materials, the mounting process and solder reflow conditions.

To protect the semiconductor packages from cracking during the board assembly stage, they are shipped in dry bags and opened just before the process, or else baked before mounting, to maintain the humidity level as low as possible.

**1.2.3 MOISTURE ABSORPTION**

**Figure 1.5**: Moisture Absorption Induced Delaminations.
Moisture itself, in the presence of heat and/or pressure, can cause failure in the device. The adhesion between the molding compound and die depends on hydrogen bonds, or OH pairs. The moisture, becoming saturated, will concentrate at interfaces due to osmotic pressure, and if the effect of elevated temperature is taken into account the separations between different surfaces are expected [1]. The schematic of moisture absorption and some surface delaminations are depicted in Fig. 1.5.

1.3 SOLUTION TECHNIQUES TO DETERMINE THERMALLY INDUCED STRESSES IN IC PACKAGES

1.3.1 ANALYTICAL SOLUTIONS TO THE PROBLEM

The thermal stresses in semiconductor packages are caused by thermal expansion (contraction) mismatch of dissimilar materials and/or nonuniform temperature distribution within the package and may result in failure of the packages. Thermal stresses, the normal stresses, in a bi-material assembly ("bi-material thermostat") were examined by Timoshenko, 1925, using an elementary beam theory. In his analysis, it is assumed that, these stresses remain unchanged along the thermostat strips. Some other related work includes, Aleck, 1949, Bogy, 1970, Blech and Kantor, 1984, and others on the basis of the elasticity theory, and other various simplified approaches, using basically methods of Engineering Mechanics.

As an example of an analytical approach to the problem, V. Mishkevich and E. Suhir's work is given here. Extending Timoshenko's theory they were able to evaluate both the interfacial normal and shearing stresses from the two coupled differential equations, one second order equation for the shearing stress and one fourth order equation for the peeling stress. Without going into detail, the shearing, \( \tau(x) \) and peeling,
$p(x)$, stresses in an elongated bimaterial assembly subjected to uniform heating or cooling are represented by the following two coupled differential equations from Suhir's previous work (1989, 1991):

\[
\tau''(x) - k^2 \tau(x) = \frac{\mu}{K \kappa} \rho''(x),
\]

\[
\rho''(x) + 4 \alpha^4 \rho(x) = 4 \mu \alpha^4 \tau'(x),
\]

and they must satisfy the conditions

\[
\tau(0) = 0, \quad \int_{-l}^{l} \tau'(l) = \frac{\Delta \alpha \Delta t}{\kappa},
\]

\[
\tau(l) = 0, \quad \int_{0}^{l} \tau(x) dx = 0,
\]

\[
\rho''(l) = 0, \quad \int_{0}^{l} \rho(x) dx = 0.
\]

**Figure 1.6**: Bi-material Assembly.

Here, $l$ is the half of the assembly length, (Fig.1.6). Note that the shearing stress, $\tau(x)$, is an odd function, and the peeling stress, $p(x)$, is an even function which must satisfy the self equilibrium condition.
In Eq. (1.1),

\[ K = \left( \frac{1 - \nu_1^2}{E_1 h_1} + \frac{1 - \nu_2^2}{E_2 h_2} \right)^{-1} \]  \hspace{1cm} (1.3)

is the spring constant (through-thickness stiffness) of the composite (Suhir, 1989),

\[ \kappa = \frac{h_1}{3G_1} + \frac{h_2}{3G_2} \]  \hspace{1cm} (1.4)

is the interfacial compliance. \( E_1 \) and \( E_2 \) are Young's moduli of the materials, \( \nu_1 \) and \( \nu_2 \) are the Poisson's ratios.

\[ G_1 = \frac{E_1}{2(1 + \nu_1)} \quad , \quad G_2 = \frac{E_2}{2(1 + \nu_2)} \]  \hspace{1cm} (1.5)

are the shear moduli, \( h_1 \) and \( h_2 \) are the thicknesses of the composite plates,

\[ \mu = \frac{h_1 D_2 - h_2 D_1}{2D} \]  \hspace{1cm} (1.6)

is a parameter of the flexural rigidity of the plates,

\[ D_1 = \frac{E_1 h_1^3}{12(1 - \nu_1^2)} \quad , \quad D_2 = \frac{E_2 h_2^3}{12(1 - \nu_2^2)} \]  \hspace{1cm} (1.7)

are the flexural rigidities, \( D = D_1 + D_2 \) is the total rigidity,
\[ \alpha = \sqrt[4]{\frac{KD}{4D_1D_2}} \]  

is the parameter of the through-thickness compliance,

\[ k = \sqrt{\frac{\lambda}{\kappa}} \]  

is the parameter of the longitudinal compliance,

\[ \lambda = \frac{1 - \nu_1^2}{E_1h_1} + \frac{1 - \nu_2^2}{E_2h_2} \]  

is the longitudinal axial compliance of the plate.

Introducing a new variable \( \xi = \frac{\pi}{l} \) the equation (1.1) can be written as;

\[ \frac{d^2\tau(\xi l)}{d\xi^2} - \xi^2 K^2 \tau(\xi l) = \frac{\mu}{K\kappa l} p''(\xi l). \]  

(1.11)

Taking into account that, \( l \) is significantly larger than the thickness of the structure, \( \frac{\mu}{K\kappa l} \approx O(h/l) \ll 1 \), Eq. (1.11) can be reduced to homogeneous form;

\[ \tau''(x) - k^2 \tau(x) = 0. \]  

(1.12)

Solution of Eq. (1.12) yields,
\[ \tau(x) = k \frac{\Delta \alpha \Delta t}{\lambda \cosh kl} \sinh kx \] (1.13)

The maximum of the shearing stress, \( \tau_{\text{max}} \), occurs at the assembly end, \( x = l \)

\[ \tau_{\text{max}} = k \frac{\Delta \alpha \Delta t}{\lambda \cosh kl} \tanh kl \] (1.14)

Substitution of the solution for the shearing stress, \( \tau(x) \), into Eq. (1.2) to solve for the peeling stress, \( p(x) \), gives;

\[ p(x) = \mu k s^4 \frac{\Delta \alpha \Delta t}{\lambda} \frac{1}{1 + s^4} \left( \cosh kl \frac{\cosh kx}{\cosh kl} + A_0 V_0(\alpha x) + A_2 V_2(\alpha x) \right) \] (1.15)

where the parameter

\[ s = \frac{\alpha \sqrt{2}}{k}, \] (1.16)

represents the effect of the ratio of the through-thickness stiffness to the longitudinal stiffness. The functions \( V_0(\alpha x) \) and \( V_2(\alpha x) \), and the constants \( A_0 \) and \( A_2 \) are expressed as,

\[ V_0(\alpha x) = \cosh \alpha x \cos \alpha x, \quad V_2(\alpha x) = \sinh \alpha x \sin \alpha x, \] (1.17)

\[ A_0 = 2 \sqrt{2} \frac{V_3(v) - s^3 V_0(v) \tanh u}{s^2(\sinh 2v + \sin 2v)}, \] (1.18)

\[ A_2 = -2 \sqrt{2} \frac{V_1(v) + s^3 V_2(v) \tanh u}{s^2(\sinh 2v + \sin 2v)}, \] (1.19)

where
\[ V_1(\alpha x) = \frac{1}{\sqrt{2}} (\cosh \alpha x \sin \alpha x + \sinh \alpha x \cos \alpha x), \quad (1.20) \]

\[ V_3(\alpha x) = \frac{1}{\sqrt{2}} (\cosh \alpha x \sin \alpha x - \sinh \alpha x \cos \alpha x). \quad (1.21) \]

and

\[ u = kl \quad \text{and} \quad v = \alpha l. \quad (1.22) \]

After plotting the stress distributions according to above formulas and based on the performed FEA calculations for the same model, it has been concluded, that in an approximate engineering analysis the above solution gives a good estimation of the stress state in the thermostat-like structures. Nevertheless, when the geometry of the problem gets complicated, the above simplifications cannot be used and there is a need for other type of solution techniques, i.e., the finite element method.

### 1.3.2 THE FINITE ELEMENT METHOD

The finite element method is a numerical method for the evaluation of engineering problems often related to structures and continua. Generally, this technique is applied to problems which can not be solved by direct analytical methods because of complicated geometry and boundary conditions. Provided that the problem in question is modeled appropriately, geometric complexity can be handled in a straightforward manner using the finite element method. The finite element method produces many simultaneous algebraic equations, and the solution of these equations gives numerical values of the field of interest at pre-defined locations (nodal points).
1.3.2.1 Finite Elements Used in Electronic Packaging

The complicated geometrical structures and different material properties as well as the loading conditions have made it almost impossible to study the mechanical behavior of the semiconductor packages analytically. Therefore, the finite element method has become a useful tool for the evaluation of problems encountered in this area.

It would be very desirable to employ three-dimensional stress and fracture analysis to understand the reaction of a semiconductor package under different loading conditions, e.g., thermal cycling, effect of moisture alone and/or in the presence of pressure during thermal cycling. Thus, for this purpose a three-dimensional finite element program, capable of performing three-dimensional stress and fracture analysis (including interfacial crack), was written. In this thesis, the theoretical aspects of the finite element program are explained in detail, and some numerical examples are presented. Instead of doing a regular three-dimensional calculation, for comparison purposes with the two-dimensional analyses, an additional condition, "Generalized Plane Strain ", is introduced into the three-dimensional model, and the results from an example semiconductor package configuration are presented.
Chapter 2

Finite Element Formulation

2.1 INTRODUCTION

The equilibrium configuration of a system is found by analysis of its potential energy. Expressions for potential energy and other integral equations, "functionals", are introduced as a starting point for an approximation technique, namely the Rayleigh-Ritz method, whose modern form is the finite element method.

The Rayleigh-Ritz method has a classical form and a finite element form. In the classical form, an approximating field is defined over the entire region of interest. In the finite element form, the approximating field is defined in a piece-wise fashion. Finite elements use nodal values of the field as degrees of freedom. The term "Degrees of Freedom", means independent quantities that are used to define the configuration of a system, not violating compatibility and constraint conditions, e.g. support conditions. That is, these are the quantities used to define the spatial variation of an approximating field [4].

2.2 POTENTIAL ENERGY OF AN ELASTIC BODY

The potential energy of an elastic body consists of the strain energy contained in elastic deformations and the potential of forces that act within the structure or on its surface, and can be used to formulate element stiffness matrices and element load vectors.
Considering an elastic body that is exposed to conservative loads, and assigning \( V \) as its volume and \( S \) its surface, the potential energy can be written in the following form.

\[
\Pi_p = \int_V \left( \frac{1}{2} \{ \varepsilon \}^T [E] \{ \varepsilon \} - \{ \varepsilon \}^T [E] \{ \varepsilon^0 \} + \{ \varepsilon \}^T \{ \sigma^0 \} \right) dV \\
- \int_V \{ u \}^T \{ F \} dV - \int_S \{ u \}^T \{ \Phi \} dS - \{ D \}^T \{ P \},
\]

(2.1)

where

\( \{ u \} = [u, v, w]^T \), the displacement field,

\( \{ \varepsilon \} = [\varepsilon_x \varepsilon_y \varepsilon_z \gamma_{xy} \gamma_{yz} \gamma_{zx}]^T \), the strain field,

\([E]\) = the material property matrix,

\( \{ \varepsilon^0 \}, \{ \sigma^0 \} \) = initial strain and initial stress, respectively,

\( \{ F \} = [F_x \ F_y \ F_z]^T \), body forces,

\( \{ \Phi \} = [\Phi_x \ \Phi_y \ \Phi_z]^T \), surface tractions,

\( \{ D \} \) = nodal d.o.f. of the structure,

\( \{ P \} \) = external loads applied to d.o.f.,

\( S, V \) = surface area and volume of the structure.

2.3 FORMULAS FOR ELEMENT MATRICES, \([k]\) AND ELEMENT LOAD VECTOR, \( \{ r_e \} \)

In this section general expressions for the element stiffness matrix, \([k]\), and the element load vector, \( \{ r_e \} \), are given. Using these expressions, the procedure to formulate the element stiffness matrix and the load vector representing the existing loading conditions is described for a full three-dimensional finite element analysis.
Once the potential energy expression for an elastic medium is derived, derivation of finite element formulas is a straightforward procedure. Displacements are taken as the dependent variables. Therefore, the appropriate functional for a Rayleigh-Ritz solution is the expression for the potential energy, $\Pi_p$. We select an admissible displacement field, defined in piece-wise fashion so that displacements within any element are interpolated from the nodal d.o.f. of that element, then evaluate $\Pi_p$ in terms of the nodal d.o.f. Using the principle of stationary potential energy we write $d\Pi_p=0$, from which we obtain algebraic equations to be solved for the nodal d.o.f. [4]. The starting point is the expression for potential energy in a linearly elastic body which was given in Eq. (2.1).

Displacement fields within an element are interpolated from the element nodal d.o.f. $\{d\}$,

$$\{u\} = [N]\{d\}, \quad (2.2)$$

where $[N]$ is the shape function matrix.

Strains are obtained from displacements by differentiation. Thus,

$$\{\varepsilon\} = \partial \{u\} \text{ yields } \{\varepsilon\} = [B]\{d\}, \text{ where} \quad (2.3)$$

$$[B] = [\partial][N], \quad [\partial] = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 & 0 \\
0 & \frac{\partial}{\partial y} & 0 \\
0 & 0 & \frac{\partial}{\partial z}
\end{bmatrix}, \quad (2.4)$$
The differential operator matrix is defined by Eq. (2.4), and its size is 6 by 3 for three dimensional problems. Substitution of the expressions for \{u\} and \{ε\} into Eq. (2.1) yields,

\[ Π_p = \frac{1}{2} \sum_{n=1}^{\text{numel}} \{d\}^T_n \{k\} \{d\} - \sum_{n=1}^{\text{numel}} \{d\}^T_n \{r_e\} - \{D\}^T \{P\}, \quad (2.5) \]

where summation symbols indicate that we include contributions from all elements (numel) of the structure. Element stiffness matrix \([k]\) and element load vector \([r_e]\) are defined by,

\[ [k] = \int_{V_e} [B]^T [E] [B] dV, \quad (2.6) \]

\[ [r_e] = \int_{V_e} [B]^T [E] \{ε^0\} dV - \int_{V_e} [B]^T \{σ^0\} dV + \int_{S_e} [N]^T \{F\} dS + \int_{S_e} [N]^T \{Φ\} dS, \quad (2.7) \]

where \(V_e\) denotes the volume of an element and \(S_e\) its surface. In the surface integral, \([N]\) is evaluated on \(S_e\).

To complete the derivation we must determine the algebraic equations to be solved for the nodal d.o.f. Every d.o.f. in an element vector \(\{d\}\) also appears in the vector of global (i.e. structural) d.o.f. \(\{D\}\). Therefore, \(\{D\}\) can replace \(\{d\}\) in Eq. (2.5) if \([k]\) and \([r_e]\) of every element are conceptually expanded to structure size. Thus, Eq. (2.5) becomes
\[ \Pi_p = \frac{1}{2} \{D\}^T \{K\} \{D\} - \{D\}^T \{R\}, \] (2.8)

where

\[ [K] = \sum_{n=1}^{\text{numel}} [k]_n \quad \text{and} \quad \{R\} = \{P\} + \sum_{n=1}^{\text{numel}} \{r_e\}_n. \quad (2.9) \]

Summations indicate assembly of element matrices by addition of overlapping terms. Now, \( \Pi_p \) is a function of d.o.f. \( \{D\} \). Making \( \Pi_p \) stationary with respect to small changes in the \( D_i \) by use of convenient differentiation, i.e.,

\[ \left\{ \frac{\partial \Pi_p}{\partial D} \right\} = 0, \quad \text{yields} \quad [K] \{D\} = \{R\}, \quad (2.10) \]

the latter matrix equation is a set of simultaneous algebraic equations to be solved for d.o.f. \( \{D\} \) [4].

### 2.3.1 FORMULATION OF THE ELEMENT STIFFNESS MATRICES FOR THE THREE DIMENSIONAL ELEMENTS USED

In this study isoparametric 32-node cubic brick and 24-node collapsed cubic triangular prism elements are used and the element types are shown in Fig. 2.1. More information about utilization of isoparametric formulation can be found in the finite element books. Here, cubic element means that, it has cubic interpolation functions. In the next two sections the formulation of element stiffness matrices for a 32-node brick element and for a 24-node triangular prism, respectively, is described.
2.3.1.1 Formulation of Element Stiffness Matrix for 32-Node Brick Elements

The general expression for the element stiffness matrix was given previously as:

$$[k] = \int_{V_e} [B]^T[E][B]dV,$$

(2.11)

but, this formula is given in terms of global coordinates, that is one needs to evaluate the integral with respect to global coordinates, $x, y, z$. However, by utilization of the isoparametric formulation, the above integral can be rewritten as the following:

$$[k] = \int^{-1}_{-1} \int^{-1}_{-1} \int^{-1}_{-1} [B]^T[E][B] J d\xi d\eta d\rho.$$

(2.12)

Note that, the integrand is now with respect to isoparametric coordinates, $\xi, \eta, \rho$, values of which can vary between -1 and 1, and as it will be shown, this is accomplished by introducing the determinant of the "Jacobian" matrix, $J$, into the integrand. In Eq. (2.12), $[B]$ contains the derivatives of the shape (interpolation) functions and generally is known as the "strain-nodal displacement" matrix, $[E]$ is the elastic property matrix.
The formulation of $[B]$, which contains the appropriate derivatives of shape functions, is critical to obtaining the proper element stiffness matrix.

![Figure 2.2: The 32-Node Cubic Brick Element and Nodal Order.](image)

### 2.3.1.2 Shape Functions for a 32-Node Cubic Brick Element

In order to make use of interpolation functions one needs to choose a nodal order in which the shape functions and the nodal d.o.f.'s are defined. This can be any order in terms of node labeling, but the appropriate shape functions should match with the node in turn, i.e., whether it is a midside node or a corner node, and if it is, on which edge? The selected nodal order is shown in Fig. 2.2.

The shape functions of corner nodes for a 32-node brick element $(i = 1, 2, 3, \ldots, 8)$ are given by:

$$N_i = \frac{1}{64} (1 + \xi \xi_i)(1 + \eta \eta_i)(1 + \rho \rho_i) \left[ 9(\xi^2 + \eta^2 + \rho^2) - 19 \right], \quad (2.13)$$
where, $\xi_i, \eta_i, \rho_i$ are the local (isoparametric) coordinates of the corner nodes, $\mp 1$. For the midside nodes that are on the edges parallel to the $\xi$ axis ($i = 9, 10, 13, 14, 17, 18, 21, 22$) the shape functions have the following form ($\xi_i = \mp \frac{1}{3}, \eta_i = \mp 1, \rho_i = \mp 1$),

$$N_i = \frac{9}{64} (1 - \xi^2)(1 + 9\xi\xi_i)(1 + \eta\eta_i)(1 + \rho\rho_i). \quad (2.14)$$

For the nodes ($i = 11, 12, 15, 16, 19, 20, 23, 24$), $\xi_i = \mp 1, \eta_i = \mp 1, \rho_i = \pm \frac{1}{3}$, the shape functions are defined as;

$$N_i = \frac{9}{64} (1 - \rho^2)(1 + 9\rho\rho_i)(1 + \eta\eta_i)(1 + \xi\xi_i). \quad (2.15)$$

Finally, for $i = 25, 26, ..., 32$, $\xi_i = \mp 1, \eta_i = \mp \frac{1}{3}, \rho_i = \pm 1$, the shape functions are;

$$N_i = \frac{9}{64} (1 - \eta^2)(1 + 9\eta\eta_i)(1 + \xi\xi_i)(1 + \rho\rho_i). \quad (2.16)$$

### 2.3.1.3 Formulation of Strain-Nodal Displacement Matrix, $[B]$}

As can be understood from its name, $[B]$ gives the relationship between the strain field of the element and the nodal displacements, that is;

$$\{\epsilon\} = [B]\{d\} \quad (2.17)$$
and can be written in vector form as the following;

\[
\begin{pmatrix}
\varepsilon_x \\
\varepsilon_y \\
\varepsilon_z \\
\gamma_{xy} \\
\gamma_{yz} \\
\gamma_{xz}
\end{pmatrix} =
\begin{pmatrix}
\frac{\partial u}{\partial x} \\
\frac{\partial v}{\partial y} \\
\frac{\partial w}{\partial z} \\
\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \\
\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \\
\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}
\end{pmatrix}
\]

(2.18)

where, displacement and coordinate values at a given point (isoparametric point) within the element is given by,

\[
\begin{align*}
\mathbf{u} &= \sum_{i=1}^{32} N_i \mathbf{u}_i, & \mathbf{v} &= \sum_{i=1}^{32} N_i \mathbf{v}_i, & \mathbf{w} &= \sum_{i=1}^{32} N_i \mathbf{w}_i \\
x &= \sum_{i=1}^{32} N_i x_i, & y &= \sum_{i=1}^{32} N_i y_i, & z &= \sum_{i=1}^{32} N_i z_i.
\end{align*}
\]

(2.19)

In the above equations, \( \mathbf{u}_i, \mathbf{v}_i, \) and \( \mathbf{w}_i \) are the nodal displacements, and \( x_i, y_i, z_i \) are the nodal coordinate values in the \( x, y, \) and \( z \) directions, respectively. The required derivatives of the displacement field in Eq. (2.18) can be found by simply applying the chain rule, for example, for the \( x \)-direction displacement field,
\[ \frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial u}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial u}{\partial \rho} \frac{\partial \rho}{\partial x}, \]

\[ \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial u}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial u}{\partial \rho} \frac{\partial \rho}{\partial y} \quad (2.20) \]

\[ \frac{\partial u}{\partial z} = \frac{\partial u}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial u}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial u}{\partial \rho} \frac{\partial \rho}{\partial z}, \]

and, it can be expressed in matrix form as

\[
\begin{bmatrix}
\frac{\partial u}{\partial x} \\
\frac{\partial u}{\partial y} \\
\frac{\partial u}{\partial z}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial u}{\partial \xi} \\
\frac{\partial u}{\partial \eta} \\
\frac{\partial u}{\partial \rho}
\end{bmatrix} \begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} & \frac{\partial \rho}{\partial x} \\
\frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} & \frac{\partial \rho}{\partial y} \\
\frac{\partial \xi}{\partial z} & \frac{\partial \eta}{\partial z} & \frac{\partial \rho}{\partial z}
\end{bmatrix},
\]

where, \([\Gamma] = \begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \eta}{\partial x} & \frac{\partial \rho}{\partial x} \\
\frac{\partial \xi}{\partial y} & \frac{\partial \eta}{\partial y} & \frac{\partial \rho}{\partial y} \\
\frac{\partial \xi}{\partial z} & \frac{\partial \eta}{\partial z} & \frac{\partial \rho}{\partial z}
\end{bmatrix}\]

(2.21)

The matrix, \([\Gamma]\), in Eq. (2.21) is called the "inverse of the Jacobian matrix", and the Jacobian matrix, \([J]\), can be expressed by simply applying the chain rule for differentiation in the other way.

\[
\begin{bmatrix}
\frac{\partial u}{\partial \xi} \\
\frac{\partial u}{\partial \eta} \\
\frac{\partial u}{\partial \rho}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial u}{\partial x} \\
\frac{\partial u}{\partial y} \\
\frac{\partial u}{\partial z}
\end{bmatrix} \begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\
\frac{\partial x}{\partial \rho} & \frac{\partial y}{\partial \rho} & \frac{\partial z}{\partial \rho}
\end{bmatrix},
\]

where, \([J] = \begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\
\frac{\partial x}{\partial \rho} & \frac{\partial y}{\partial \rho} & \frac{\partial z}{\partial \rho}
\end{bmatrix}\]

(2.22)

Obviously, the relationship between \([\Gamma]\) and \([J]\) is such, that they are inverse of one another.
\[
[\Gamma] = [J]^{-1} \quad (2.23)
\]

Now, going back to the strain vector expression, and introducing a coefficient matrix, \([C]\), one can write the strains in terms of the derivatives of each displacement component, \(u, v, w\), with respect to \(x, y, z\).

\[
\begin{align*}
\{ \varepsilon_x \} &= \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \\
\{ \varepsilon_y \} &= \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0
\end{bmatrix} \\
\{ \varepsilon_z \} &= \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \\
\{ \gamma_{xy} \} &= \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \\
\{ \gamma_{yz} \} &= \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \\
\{ \gamma_{xz} \} &= \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\end{align*}
\quad (2.24)
\]

Employing \([\Gamma]\), the inverse of the Jacobian matrix, the derivatives of the displacement field with respect to global coordinate system at the end of Eq. (2.24) can be expressed in terms of the derivatives with respect to isoparametric coordinates as follows;

\[
\begin{align*}
\begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
\varepsilon_z \\
\gamma_{xy} \\
\gamma_{yz} \\
\gamma_{xz}
\end{bmatrix} &= \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u, x \\
u, y \\
u, z \\
v, x \\
v, y \\
v, z
\end{bmatrix},
\end{align*}
\quad (2.25)
\]

\[
\begin{align*}
\begin{bmatrix}
u, x \\
v, y \\
u, z \\
v, x \\
v, y \\
v, z
\end{bmatrix} &= \begin{bmatrix}D\end{bmatrix}
\begin{bmatrix}
u, \xi \\
v, \eta \\
u, \rho \\
v, \xi \\
v, \eta \\
v, \rho
\end{bmatrix},
\end{align*}
\quad (2.25)
\]

\[
\begin{align*}
\begin{bmatrix}D\end{bmatrix} &= \begin{bmatrix}[\Gamma] & [0] & [0] \\
[0] & [\Gamma] & [0] \\
[0] & [0] & [\Gamma]
\end{bmatrix}
\end{align*}
\]
null matrices. Now, up to this point we have been able to write the derivatives of the displacement field with respect to isoparametric coordinates. But, to get the "strain-nodal displacement" matrix, \([B]\), these derivatives must be related to the nodal displacements. From Eq. (2.19), we know that, utilization of interpolation functions, \(N_i\), enables one to express the displacement field within the element in terms of nodal displacements. Since the interpolation functions are expressed as local (isoparametric) coordinates, the differentiation of the shape functions with respect to isoparametric coordinates is a straightforward procedure. For example, considering \(u\) component of the displacement field one can write,

\[
\begin{align*}
\frac{\partial u_i}{\partial \xi} &= \sum_{i=1}^{32} N_{i,\xi} u_i, \\
\frac{\partial u_i}{\partial \eta} &= \sum_{i=1}^{32} N_{i,\eta} u_i, \\
\frac{\partial u_i}{\partial \xi} &= \sum_{i=1}^{32} N_{i,\xi} u_i.
\end{align*}
\]  

(2.26)

We now have the relationship between the derivatives and the nodal displacements. Introducing another matrix, \([F]\), the required derivatives can be expressed in terms of the displacements of 32 nodes in each direction, a total of 96 displacement values, which is the total d.o.f. of a 32-node brick element.

\[
\begin{pmatrix}
\begin{bmatrix}
u,_{\xi} \\
u,_{\eta} \\
u,_{\rho} \\
v,_{\xi} \\
v,_{\eta} \\
v,_{\rho} \\
w,_{\xi} \\
w,_{\eta} \\
w,_{\rho}
\end{bmatrix}
\end{pmatrix}
= [F]
\begin{pmatrix}
\begin{bmatrix}
u_1 \\
u_1 \\
u_1 \\
u_2 \\
u_2 \\
u_2 \\
u_32 \\
u_32 \\
u_32
\end{bmatrix}
\end{pmatrix}
\]  

(2.27)
where \([F]\) is defined by:

\[
\begin{bmatrix}
N_{1,\xi} & 0 & 0 & N_{2,\xi} & 0 & 0 & \ldots & N_{32,\xi} & 0 & 0 \\
N_{1,\eta} & 0 & 0 & N_{2,\eta} & 0 & 0 & \ldots & N_{32,\eta} & 0 & 0 \\
N_{1,\varphi} & 0 & 0 & N_{2,\varphi} & 0 & 0 & \ldots & N_{32,\varphi} & 0 & 0 \\
0 & N_{1,\xi} & 0 & 0 & N_{2,\xi} & 0 & \ldots & 0 & N_{32,\xi} & 0 \\
0 & N_{1,\eta} & 0 & 0 & N_{2,\eta} & 0 & \ldots & 0 & N_{32,\eta} & 0 \\
0 & N_{1,\varphi} & 0 & 0 & N_{2,\varphi} & 0 & \ldots & 0 & N_{32,\varphi} & 0 \\
0 & 0 & N_{1,\xi} & 0 & 0 & N_{2,\xi} & \ldots & 0 & 0 & N_{32,\xi} \\
0 & 0 & N_{1,\eta} & 0 & 0 & N_{2,\eta} & \ldots & 0 & 0 & N_{32,\eta} \\
0 & 0 & N_{1,\varphi} & 0 & 0 & N_{2,\varphi} & \ldots & 0 & 0 & N_{32,\varphi}
\end{bmatrix}
\]

Note that, the matrix, \([F]\), is 9 by 96 in size containing three contributions from each node of the element. Obviously, in the nodal displacements vector and in \([F]\), the spaces filled with dots contain the contributions from the remaining nodes, \(i = 3, 4, \ldots, 31\).

Since the nodal displacements have already been related to the strain field, \([B]\) can be written as a sequence of multiplications of the described matrices.

\[
[B] = [C] [D] [F]
\]

(2.28)

2.3.1.4 Integration for Calculation of Element Stiffness Matrix

The formula for the element stiffness matrix was given in Eq. (2.12) as,

\[
[k] = \int_{-1}^{1} \int_{-1}^{1} [B]^T [E] [B] J d\xi d\eta d\rho.
\]

(2.12)
Since we now have the strain-nodal displacement matrix and the elastic property matrix can easily be computed using the specified material properties, it only remains to perform the necessary integration. The method used for this integration is the Gauss Integration Method, and the formula, for a \(4 \times 4 \times 4\) integration, is given below,

\[
[k] = \sum_{i=1}^{4} \sum_{j=1}^{4} \sum_{k=1}^{4} W_i W_j W_k \phi(\xi_i, \eta_j, \rho_k) J
\]  

(2.29)

where \(W_i\)'s are the weight factor of the sampling Gauss points, and \(\phi(\xi_i, \eta_j, \rho_k)\) is a 96 by 96 matrix, obtained from evaluation of the matrices in the integrand, \([B]^T[E][B]\), at the sampled Gauss point locations. Note that, for a four-point integration scheme, Eq. (2.29) results in evaluation of the integrand \(4^3 (64)\) times. Finally, the stiffness matrix for a 32-node element is obtained as a 96 by 96 matrix in size (symmetric), i.e., the element has 96 independent d.o.f.

2.3.1.5 Formulation of Element Stiffness Matrix for 24-Node Collapsed Triangular Prisms

A sample 24-node collapsed triangular prism is shown in Fig. 2.3. As shown in the figure, there are 4 sets of nodes that are collapsing onto each other. In this case, these sets are defined with respect to local node numbers of the element as; (1, 4, 15, 16), (5, 8, 23, 24), (25, 28), and (29, 32). It is not significant to determine which specific corner is collapsed. We could have, of course, chosen one of the other corners. In addition, we could have also collapsed again the above tied nodes, forming the collapsed edge, and alternatively formed a pyramid. But this is not our purpose here, and only the first situation will be illustrated.
The term "collapsed" means that, specified nodes in each set are forced to move (tied) together, so that they have the same displacements in each direction. Note that, since there are 12 nodes tied together and in each set there will be a master node, the total d.o.f. of the element reduces from 96 to (96-(8)(3))=72. Thus, the stiffness matrix of the collapsed triangular prism is 72 by 72. This is achieved by adding the stiffness contributions of collapsed (slave) nodes to the stiffness contribution of the master node in each set. For example, for the first set given above, the stiffness contributions of 4th, 15th, and 16th nodes are added to the 1st node (for convenience the 1st node is assigned as the master of this set). The extension of the procedure to the other sets is obvious.

We also note here that, since we are eliminating d.o.f. of the collapsed nodes (eliminating nodes), relabeling of the nodes in the recently created element is necessary, and is shown in Fig. 2.4.
Recall Eq. (2.12) for the element stiffness matrix expression,

\[ [k] = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} [B]^T [E] [B] J \, d\xi d\eta d\rho \, . \]  

(2.12)

Calculation of element stiffness matrix is going to be the same, i.e., the same procedure will be applied, the same integration method and integration points will be used. The only difference is going to occur in the calculation of strain-nodal displacement matrix, \([B]\). And from before, we observe that this is going to affect only \([F]\) which contains the derivatives of shape functions. In the calculation of regular brick elements this matrix was 6 by 96. As we add the contributions of the slave nodes in the appropriate set, deleting these rows (the rows containing contributions of the slave nodes) \([F]\) matrix reduces in size to 6 by 72. One thing we should be aware of is that, inserting the
resulting contributions into the $[F]$ matrix according to new node labeling is very important.

The remaining part of the calculation is exactly the same as in previously defined procedure. Reviewing the integrand in Eq. (2.12), it is seen that the stiffness matrix is going to be a 72 by 72 symmetric matrix.

### 2.3.2 CONSISTENT ELEMENT NODAL FORCES, $\{r_e\}$, FOR DIFFERENT LOADING CONDITIONS

In this section the element load vector, $\{r_e\}$, is considered, and for different loading conditions calculation of representative (equivalent) nodal forces is explained. The formula for element load vector was given by Eq. (2.7).

$$\{r_e\} = \int_{V_e} [B]^T [E] \{\epsilon^0\} dV - \int_{V_e} [B]^T \{\sigma^0\} dV$$

$$+ \int_{V_e} [N]^T \{F\} dV + \int_{S_e} [N]^T \{\Phi\} dS \quad (2.7)$$

Eq. (2.7) converts loads distributed throughout an element or over its surface to the equivalent nodal forces which represents the loading condition on the element. Any of the four integrals in Eq. (2.7) may vanish. For example, the value of the surface integral is zero if there is no traction applied over any of the edges on the element. If there is a surface traction applied on an edge or edges, then it is integrated over those surfaces only. All four integrals vanish if externally applied nodal loads $\{P\}$ make up the entire load vector $\{R\}$.

The terms in Eq. (2.7) that contain $\{\epsilon^0\}$ and $\{\sigma^0\}$ account for initial strain and initial stress conditions. For these cases, heating or cooling of the element, swelling, and
initial lack of fit can be given as examples. These nodal loads are self-equilibrating, which means that, \( \{ r_e \} \) produces zero resultant force and zero resultant moment. To illustrate this situation, computation of equivalent nodal forces due to "Thermal Loading" will be explained.

Loads \( \{ r_e \} \) produced by body forces \( \{ F \} \) and surface tractions \( \{ \Phi \} \) are given by the latter two integrals in Eq. (2.7). These loads are called "work equivalent loads" for the following reason: work done by nodal loads \( \{ r_e \} \) in going through nodal displacements \( \{ d \} \) is equal to work done by distributed loads \( \{ F \} \) and \( \{ \Phi \} \) in going through the displacement field associated with the element shape functions. Work \( W \) done by loads \( \{ r_e \} \) during small nodal displacements \( \{ d \} \) is \( W = \{ d \}^T \{ r_e \} \). Taking for example the surface integral in Eq. (2.7), and substituting the displacement field \( \{ u \}^T = \{ d \}^T [N]^T \), we have

\[
W = \{ d \}^T \{ r_e \} = \int_{S_e} \{ d \}^T [N]^T \{ \Phi \} dS = \int_{S_e} \{ u \}^T \{ \Phi \} dS
\]

(2.30)

The latter integral sums the work of force increments \( \{ \Phi \} dS \) in going through displacements created by \( \{ d \} \) via shape functions \( [N] \). Calculation of consistent nodal forces due to normal pressure acting on the 32-node brick element is explained in Sec. (2.3.2.2).

Consistent nodal forces due to concentrated point loads acting not at the nodes, but anywhere within the element, can be also calculated from the surface integral in Eq. (2.7), by treating them as large surface tractions concentrated on single points. Denoting \( \{ p \} \) as a concentrated force that has three components, \( p_x, p_y, \) and \( p_z \), one can write \( \{ p \} = \{ \Phi \} dS \). Then, the integral of \( [N]^T \{ \Phi \} dS \) simply becomes \( [N]^T \{ p \} \), where the
concentrated force acts and zero elsewhere. Therefore, for \( n \) concentrated forces applied to an element, Eq. (2.7) gives

\[
\{ r_e \} = \sum_{i=1}^{n} [N]_i^T \{ p \}_i
\]  

(2.31)

where \([N]_i\) are evaluated at the location of \( \{ p \} \). This type of loading condition is studied in Sec. (2.3.2.3) in detail.

### 2.3.2.1 Thermal Loading

As mentioned in the previous section, the first term in Eq. (2.7) represents initial strains, and thermal loading is included in this part since it produces some initial strains in the element. Corresponding nodal forces are computed from

\[
\{ r_e \} = \int_{V_e} [B]^T [E] \{ \varepsilon^0 \} dV
\]  

(2.32)

In Eq. (2.32) the strain vector \( \{ \varepsilon^0 \} \) is given by

\[
\{ \varepsilon^0 \} = \begin{pmatrix}
\varepsilon^0_x \\
\varepsilon^0_y \\
\varepsilon^0_z \\
\varepsilon^0_{xy} \\
\varepsilon^0_{yz} \\
\varepsilon^0_{xz}
\end{pmatrix}
\]  

(2.33)
where the components in Eq. (2.33) are the normal and shearing strains due to temperature change or nonuniform temperature distribution. These strains are expressed in terms of "coefficients of thermal expansion" (CTE) in the following way;

\[
\begin{align*}
\varepsilon_x^0 &= \alpha_x \Delta T, \\
\varepsilon_y^0 &= \alpha_y \Delta T, \\
\varepsilon_z^0 &= \alpha_z \Delta T,
\end{align*}
\]

\[
\varepsilon_{xy}^0 = \alpha_{xy} \Delta T, \quad \varepsilon_{yz}^0 = \alpha_{yz} \Delta T, \quad \varepsilon_{zx}^0 = \alpha_{zx} \Delta T.
\]

(2.34)

In Eq. (2.34) \(\alpha\)'s are normal and shearing CTE's, and \(\Delta T\) is the temperature change.

Once the temperature differences at the nodes, \(\Delta T_i\), are known, like other field quantities, employing shape functions the temperature change anywhere in the element can be found. That is,

\[
\Delta T(\xi, \eta, \rho) = \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i.
\]

(2.35)

With this, Eq. (2.32) becomes

\[
\{r_e\} = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} [B]^T [E] \begin{bmatrix}
\alpha_x \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i \\
\alpha_y \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i \\
\alpha_z \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i \\
\alpha_{xy} \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i \\
\alpha_{yz} \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i \\
\alpha_{zx} \sum_{i=1}^{32} N_i(\xi, \eta, \rho) \Delta T_i \\
\end{bmatrix} J \, d\xi \, d\eta \, d\rho,
\]

(2.36)
and, according to the type of the element in consideration (regular or collapsed), evaluation of the above integral results in 96 or 72 load vector components. Note that, Eq. (2.36) is a volume integral, and can be integrated together with the element stiffness matrix using the same Gauss sampling points.

### 2.3.2.2 Distributed Surface Traction

In Eq. (2.7), evaluation of the last integral gives consistent nodal forces due to surface tractions applied over any of the faces on an element. In this case, integration involves only the loaded face, and only the shape functions associated with the nodes on that face are included (the other shape functions are going to be zero). Therefore, there is no need to calculate the other shape functions.

**Figure 2.5:** (a) Uniform Stress, $\sigma$, Acting on A Rectangular Face Area of $A$. 
(b) Consistent Nodal Forces on The Face.
In Fig. (2.5.a) a uniform traction acting normal to the top surface, which is horizontally placed and area of $A$, is shown. Since only evaluation of the shape functions associated with this face is needed, one can simply use the shape functions of a 12-node two dimensional cubic element (Note that, when distributed tractions are applied on a face of a perfectly rectangular three-dimensional element, shape functions of the face are equivalent to the shape functions of the corresponding element in two dimensions). Equivalent nodal forces are shown in Fig. (2.5.b), by $P$ and $Q$. Looking at the figure, it is seen that equivalent nodal forces for the corner nodes, $Q$, are directed in the opposite direction of acting pressure, whereas those of midside nodes are in the same direction of the surface traction, and they are given by,

$$ P = \frac{3\sigma A}{16}, \quad \text{and} \quad Q = \frac{\sigma A}{8} \quad (2.37) $$

and these nodal forces must satisfy the equilibrium condition, that is, summation of these forces must be equal to the mechanical load due to uniform pressure application.

$$ 8P - 4Q = \frac{3}{2} \sigma A - \frac{1}{2} \sigma A = \sigma A \quad (2.38) $$

If the face under consideration on the element is not perfectly rectangular and/or not flat, than the situation should be handled by using the isoparametric formulation, since it allows mapping of the fields to a standard unit volume. For example, if the above face on the top of the element were to be a curved face, that is not flat, then, creation of consistent nodal forces in $x$ and/or $z$ directions, as well as in the vertical direction is unavoidable. Again, utilization of the isoparametric formulation gives very
accurate resultant nodal forces for the above case, including nonuniformly distributed surface tractions.

Since evaluation of distributed surface tractions is performed only on the loaded face, from the programming point of view, it would be efficient to provide only the node numbers and pressure values on these nodes (which describe the distribution of distributed load on the surface) as input. Then the finite element program should determine the loaded surface using element connectivity data of the structure. Therefore, one needs to describe different faces on the element, and the finite element program should automatically find the loaded faces associating the given nodal pressures with the appropriate nodes on those faces. In this study, description of the faces are implemented into the finite element program dividing the element into 6 different parts as shown in Fig. 2.6.

![Figure 2.6: Illustration of Different Faces on A Three-Dimensional Element.](image)
Figure 2.7: Normal Pressure Acting on The 2nd Face of A Distorted 3-D Element.

Since implementation of the procedure is similar for different face loadings, in this thesis the method will be described employing isoparametric formulation in detail only for the 2nd face shown in Fig. 2.6. Extension of the method to the other faces on the element is a similar procedure. In Fig. 2.7, such a loading case, a uniform pressure, $p_n$, acting on the 2nd face of a distorted element (not rectangular), is depicted.

It is seen in Fig. 2.7 that, the loaded face is now not a rectangular flat plane. Therefore, according to distortion of the loaded face, the resultant nodal forces may have components in each direction, $x$, $y$ and $z$. This will be determined by coordinates of the nodes describing the face. For this loading case, from Eq. (2.7) we have,

$$\{r_e\} = \int_{S_e} [N]^T \{\Phi\} dS$$

(2.39)
and, in our case, surface traction vector, \( \{ \Phi \} \), is simply pressure, \( \vec{p}_n \), which is normal to the surface everywhere on the face. Then Eq. (2.39) becomes,

\[
\{ r_e \} = \int_{S_e} [N]^T \vec{p}_n dS
\]  

(2.40)

Furthermore, defining the type of pressure loading directed towards the surface as positive in sign, the expression can be rewritten as;

\[
\{ r_e \} = \int_{S_e} [N]^T p_n ( - \hat{n} ) dS
\]  

(2.41)

where, \( \hat{n} \) is unit vector, directed outwards and normal to the surface everywhere on the face. At this point, we need to define the normal vector of the face in terms of known quantities. Going back to basic principle of the isoparametric formulation, the mapping relationship in terms of coordinates, which defines the position of an arbitrary point within the element, can be written in vector form as follows;

\[
\vec{X}(\xi, \eta, \rho) = \begin{pmatrix} x(\xi, \eta, \rho), y(\xi, \eta, \rho), z(\xi, \eta, \rho) \end{pmatrix},
\]  

(2.42)

\[
\vec{X}(\xi, \eta, \rho) = x(\xi, \eta, \rho) \hat{i} + y(\xi, \eta, \rho) \hat{j} + z(\xi, \eta, \rho) \hat{k}.
\]  

(2.43)

In Eq. (2.43), \( \hat{i} \), \( \hat{j} \) and \( \hat{k} \) are unit vectors in \( x \), \( y \) and \( z \) directions respectively.

Since Eq. (2.43) defines the position of any point on the face, taking into account that, \( \xi = 1 \) on this face, the unit normal vector directed outwards from the face can be written in terms of appropriate derivatives of the mapping field vector \( \vec{X}(\xi, \eta, \rho) \).
\[ \hat{n} = \frac{\hat{X}_\eta \times \hat{X}_\rho}{\| \hat{X}_\eta \times \hat{X}_\rho \|}_{\xi=1} \]  

(2.44)

In Eq. (2.44), the evaluation of the numerator requires a vector cross product, and the denominator simply is the magnitude of the resulting vector from the cross product. Note, that this expression should be evaluated at \( \xi = 1 \) since the applied loads are on the second face. In the integrand, the term \( dS \) should also be written in terms of the above quantities, so that the integral can be evaluated. For an infinitesimal area element on the face, \( dS \) is given by,

\[ dS = \| \hat{X}_\eta \times \hat{X}_\rho \| d\eta d\rho. \]  

(2.45)

Then, the integral (2.41) becomes,

\[ \{ r_e \} = \int_{S_e} [N]^T p_n \left\{ - \frac{\hat{X}_\eta \times \hat{X}_\rho}{\| \hat{X}_\eta \times \hat{X}_\rho \|}_{\xi=1} \right\} \| \hat{X}_\eta \times \hat{X}_\rho \| d\eta d\rho, \]  

(2.46)

and cancellation gives,

\[ \{ r_e \} = \int_{S_e} [N]^T p_n \left\{ - (\hat{X}_\eta \times \hat{X}_\rho)_{\xi=1} \right\} d\eta d\rho. \]  

(2.47)

where,

\[ \hat{X}_\eta = \frac{\partial x}{\partial \eta} \hat{i} + \frac{\partial y}{\partial \eta} \hat{j} + \frac{\partial z}{\partial \eta} \hat{k} \quad \text{and} \quad \hat{X}_\rho = \frac{\partial x}{\partial \rho} \hat{i} + \frac{\partial y}{\partial \rho} \hat{j} + \frac{\partial z}{\partial \rho} \hat{k}. \]  

(2.48)
The vector product can be written,

\[-(\hat{\mathbf{x}}_\eta \times \hat{\mathbf{x}}_\rho) = \hat{\mathbf{x}}_\rho \times \hat{\mathbf{x}}_\eta, \quad (2.49)\]

\[
\hat{\mathbf{x}}_\rho \times \hat{\mathbf{x}}_\eta = \begin{vmatrix}
\hat{i} & \hat{j} & \hat{k} \\
\partial x & \partial y & \partial z \\
\frac{\partial x}{\partial \rho} & \frac{\partial y}{\partial \rho} & \frac{\partial z}{\partial \rho} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta}
\end{vmatrix},
\quad (2.50)
\]

\[
\hat{\mathbf{x}}_\rho \times \hat{\mathbf{x}}_\eta = \left( \frac{\partial y \partial z}{\partial \rho \partial \eta} - \frac{\partial z \partial y}{\partial \rho \partial \eta} \right) \hat{i} + \left( \frac{\partial z \partial x}{\partial \rho \partial \eta} - \frac{\partial x \partial z}{\partial \rho \partial \eta} \right) \hat{j}
\]

\[+ \left( \frac{\partial x \partial y}{\partial \rho \partial \eta} - \frac{\partial y \partial x}{\partial \rho \partial \eta} \right) \hat{k}. \quad (2.51)\]

Since the pressure distribution is given in terms the nodal values on the face, the pressure field on that face should also be written appropriately (using shape functions), i.e.,

\[
p_n(\xi, \eta, \rho) = \sum_{i=1}^{12} N_i(\xi, \eta, \rho) p_{ni} \quad (2.52)
\]

Note, that the summation is over 12 nodes that are located on the face, therefore, there is no need to compute the remaining shape functions.

Now, we can write the integral expression dividing it into three parts, namely; the parts that are giving nodal forces in \(x\), \(y\), and \(z\) directions separately.
\[
\{ r_{e_x} \} = \int_{-1}^{1} \int_{-1}^{1} [N]^T \left( \sum_{i=1}^{12} N_i(\xi, \eta, \rho)p_{ni} \right) \left( \frac{\partial y}{\partial \rho} \frac{\partial z}{\partial \eta} - \frac{\partial z}{\partial \rho} \frac{\partial y}{\partial \eta} \right) d\eta d\rho \quad (2.53)
\]

\[
\{ r_{e_y} \} = \int_{-1}^{1} \int_{-1}^{1} [N]^T \left( \sum_{i=1}^{12} N_i(\xi, \eta, \rho)p_{ni} \right) \left( \frac{\partial z}{\partial \rho} \frac{\partial x}{\partial \eta} - \frac{\partial x}{\partial \rho} \frac{\partial z}{\partial \eta} \right) d\eta d\rho \quad (2.54)
\]

\[
\{ r_{e_z} \} = \int_{-1}^{1} \int_{-1}^{1} [N]^T \left( \sum_{i=1}^{12} N_i(\xi, \eta, \rho)p_{ni} \right) \left( \frac{\partial x}{\partial \rho} \frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \rho} \frac{\partial x}{\partial \eta} \right) d\eta d\rho \quad (2.55)
\]

Evaluation of Eq. (2.53), Eq. (2.54) and Eq. (2.55) gives the consistent nodal forces due to pressure loading on the second face, Fig. 2.6, in \( x \), \( y \), and \( z \) directions, respectively. Using a 4 by 4 Gauss integration the above integrals can be written as;

\[
\{ r_{e_x} (j) \} = \sum_{k=1}^{12} \sum_{l=1}^{12} W_k W_l F_j(\eta_k, \rho_l), \quad (2.56)
\]

and the function \( F_j(\eta_k, \rho_l) \) is given as,

\[
F_j(\eta_k, \rho_l) = N_j(\eta_k, \rho_l) \left( \sum_{i=1}^{12} N_i(\eta_k, \rho_l)p_{ni} \right) \left\{ \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \rho} y(i) \right) \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \eta} z(i) \right) \\
- \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \rho} z(i) \right) \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \eta} y(i) \right) \right\} \quad (2.57)
\]

Similarly, nodal forces in the \( y \) and \( z \) directions are given by the following equations.

\[
\{ r_{e_y} (j) \} = \sum_{k=1}^{12} \sum_{l=1}^{12} W_k W_l G_j(\eta_k, \rho_l), \quad (2.58)
\]
\[ G_j(\eta_k, \rho_l) = N_j(\eta_k, \rho_l) \left( \sum_{i=1}^{12} N_i(\eta_k, \rho_l) p_m \right) \left\{ \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \rho} x(i) \right) \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \eta} y(i) \right) - \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \rho} x(i) \right) \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \eta} z(i) \right) \right\} \] (2.59)

\[ r_{e_k}(j) = \sum_{k=1}^{12} \sum_{l=1}^{12} W_k W_l H_j(\eta_k, \rho_l), \] (2.60)

\[ H_j(\eta_k, \rho_l) = N_j(\eta_k, \rho_l) \left( \sum_{i=1}^{12} N_i(\eta_k, \rho_l) p_m \right) \left\{ \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \rho} y(i) \right) \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \eta} x(i) \right) - \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \rho} y(i) \right) \left( \sum_{i=1}^{12} \frac{\partial N_i(\eta_k, \rho_l)}{\partial \eta} z(i) \right) \right\} \] (2.61)

In this section, for a selected face on a 3-D element, implementation of distributed loads into three-dimensional finite element programming has been explained in detail. With the caution to take the appropriate derivatives of the coordinate field on the face of interest, then using the same method, one can easily obtain formulas for the other faces. This detail is not given in this thesis.

### 2.3.2.3 Concentrated Loads

In Sec. (2.3.2) we stated that concentrated loads are regarded as surface tractions that are acting on single points within the element and can be calculated by using,

\[ \{ r_e \} = \int_{S_e} [N]^T \{ \Phi \} dS. \] (2.62)
We also explained that, for concentrated loads the above equation simply reduces to

\[ \{ r_e \} = \sum_{i=1}^{n} [N]_i^T \{ p \}_i, \quad (2.63) \]

where \( n \) is number of concentrated (point) forces acting on the element. We know that the term, \([N]_i\), must be evaluated at the coordinate points where the forces are located. Shape functions are given in terms of local (isoparametric) coordinates and require the conversion of global coordinate values to corresponding local coordinates. For an undistorted, \(2a \times 2b \times 2c\), rectangular prism, let

\[ \xi_p = \frac{x_p}{a}, \quad \eta_p = \frac{y_p}{b}, \quad \rho_p = \frac{z_p}{c}. \quad (2.64) \]

Conversion is a straightforward manner \((x_p, y_p, z_p\) are relative coordinates of the point where the force is located, and are measured from the centroid of the element). \(\xi_p, \eta_p\) and \(\rho_p\) are the corresponding local coordinate values at which the interpolation functions are evaluated.

It can be shown that, for a distorted element, i.e., not perfectly rectangular, including an element with curved boundaries, the situation is not so simple since we cannot introduce simple conversion formulas as given above. On the other hand, we know that utilization of the shape functions allows us to perform interpolation of any scalar field, including coordinate values. That is,

\[ x = \sum_{i=1}^{32} N_i x_i, \quad y = \sum_{i=1}^{32} N_i y_i, \quad \text{and} \quad z = \sum_{i=1}^{32} N_i z_i \quad (2.65) \]
If local coordinate values, \( \xi_p, \eta_p \) and \( \rho_p \), are known, evaluating shape functions at these points and summing over \( n=32 \) together with the nodal coordinate values, the corresponding coordinate values can easily be computed with respect to global structure. But, in our case we know global coordinate values of the point where the force is acting and we want to find corresponding local coordinate values for evaluation of the shape functions. This requires solution of the three nonlinear equations (2.65) simultaneously. Since the equations are nonlinear in \( \xi_p, \eta_p \) and \( \rho_p \) iteration is necessary.

2.4 FRONTAL SOLUTION TECHNIQUE FOR THE FINITE ELEMENT EQUATIONS

2.4.1 INTRODUCTION

The simultaneous equations produced by the finite element method can be solved by using several techniques, such as Gauss-Seidel method (iterative method) and direct Gauss elimination techniques, and the efficiency of the finite element program is dependent on the solution technique used. In this study, because the three dimensional finite element program requires a significant amount of memory, a special direct Gauss elimination technique, called a "Frontal Solver" is used. The general concept of this solution technique is explained with a simple example.

The frontal solution technique was originated by Irons [7] and has earned the reputation of being efficient and inexpensive to use. The technique can be considered as a particular technique for assembling finite element stiffnesses and nodal forces into a global stiffness matrix and load vector and then solving for the unknown displacements by the method of Gauss elimination and backsubstitution process. It is designed to minimize core storage requirements, the number of arithmetic operations and the use of
peripheral equipment. In the frontal solution that is used in this study, equation solution and other operations such as, element stiffness formations, were performed in a single integrated program, i.e., the element stiffness matrix is calculated at the time of assembly for the specific element introduced into the "front".

2.4.2 GENERAL DESCRIPTION OF THE FRONTAL SOLVER

The frontal solver that is described in this thesis is applicable only to the solution of symmetric systems of linear equations. The main idea of the frontal solution is to assemble the equations and eliminate the variables at the same time. As soon as the coefficients of an equation are completely assembled from the contributions of all relevant elements, the corresponding variable can be eliminated. Therefore the complete structural stiffness matrix is never formed as such, since after elimination the reduced equation is immediately transferred to back-up disc storage [6].

The core contains, at any-given instant, the upper triangular part of a square matrix containing the equations which are being formed at that particular time. These equations, their corresponding nodes and degrees of freedom are termed the "front". The number of unknowns in the front is the "frontwidth": this length generally changes continually during the assembly/reduction process. The maximum size of the problem which can be solved is governed by the "maximum frontwidth". The equations, nodes and degrees of freedom belonging to the front are termed "active"; those which are yet to be considered are "inactive", those which have passed through the front and have been eliminated are said to be "deactivated" [6].

During the assembly/elimination process, the elements are considered each in turn according to a prescribed order. Whenever a new element is called into the front, its
stiffness terms are calculated by calling another subroutine and summed either into existing equations, if the nodes are already active, or into new equations which have to be included in the front if the nodes are being activated for the first time. If some nodes are appearing for the last time, the corresponding equations can be eliminated and stored away on a disc file and are thus deactivated. In so doing they free space in the front which can then be employed during assembly for the next element. To illustrate the frontal solution technique, a simple three element numerical example is given in the next section.

2.4.3 NUMERICAL EXAMPLE

![Three-Element Finite Element Model](image)

**Figure 2.8:** Three-Element Finite Element Model.

In Fig. 2.8 a simple three-element finite element is shown. To keep the size of the problem small, one degree of freedom is assumed for each node, and it is further assumed that every element (Fig. 2.9) has the same stiffness matrix and load vector (Eq. 2.66). The nodal orders for every element are as shown in Fig. 2.8. In the given example, node \#3 undergoes a prescribed displacement \( u_3 = 2.0 \).
As explained previously, the frontal solver, element by element, assembles the element stiffness matrices into a triangular global (partially) stiffness matrix and eliminates the variables that are appearing in the front lastly. Because the problem to be considered is a relatively small one, the maximum frontwidth is taken as "5", and instead of assembling the element stiffness matrices into a triangular global stiffness matrix, to help visualize the procedure, the global stiffness matrix is shown as a 5 by 5 square matrix. The procedure can be explained step by step as follows.

At the beginning, the global stiffness matrix and the arrays which monitor the active variables and their positions are set to zero. We first assemble the stiffness matrix of the first element,

**Assembly of Element # 1;**

\[
\begin{bmatrix}
1 & -1 & 0 & 0 & 0 \\
-1 & 3 & -2 & 0 & 0 \\
0 & -2 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u_4 \\
u_1 \\
u_2 \\
u_3 \\
u_5
\end{bmatrix}
= 
\begin{bmatrix}
10 \\
10 \\
10 \\
0 \\
0
\end{bmatrix}
\] (2.67)
In the above system of equations, the d.o.f. that correspond to node #1 can be eliminated. This is because that node is appearing last in the structure as the front goes through the elements in the given order.

**Elimination of Node #1:**

\[
\begin{bmatrix}
\frac{2}{3} & 0 & -\frac{2}{3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
-\frac{2}{3} & 0 & \frac{2}{3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
u_4 \\
u_3 \\
u_2 \\
u_1 \\
u_0 \\
\end{bmatrix} =
\begin{bmatrix}
\frac{40}{3} \\
0 \\
\frac{50}{3} \\
0 \\
0 \\
\end{bmatrix}
\] (2.68)

And, the second equation which corresponds to the first node is written on the disk.

Eliminated Equation #1: \(- u_4 + 3u_1 - 2u_2 = 10\) (2.69)

We, now, can assemble the second element into the front.

**Assembly of Element #2:**

\[
\begin{bmatrix}
\frac{2}{3} & 0 & -\frac{2}{3} & 0 & 0 \\
0 & 1 & -1 & 0 & 0 \\
-\frac{2}{3} & -1 & \frac{11}{3} & -2 & 0 \\
0 & 0 & -2 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
u_4 \\
u_3 \\
u_2 \\
u_1 \\
u_0 \\
\end{bmatrix} =
\begin{bmatrix}
\frac{40}{3} \\
10 \\
\frac{80}{3} \\
10 \\
0 \\
\end{bmatrix}
\] (2.70)

This time, we observe that node #5 is appearing last, thus can be eliminated.
Elimination of Node # 5;

\[
\begin{bmatrix}
\frac{2}{3} & 0 & -\frac{2}{3} & 0 & 0 \\
0 & 1 & -1 & 0 & 0 \\
-\frac{2}{3} & -1 & \frac{5}{3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
u_4 \\
u_3 \\
u_2 \\
0 \\
0 \\
\end{bmatrix} =
\begin{bmatrix}
\frac{40}{3} \\
10 \\
\frac{110}{3} \\
0 \\
0 \\
\end{bmatrix}
\] (2.71)

Eliminated Equation #2: \(-2u_2 + 2u_5 = 10\) (2.72)

Since we do not have any more active variables which can be eliminated, the next step is to assemble the element stiffness and load vector of third element.

Assembly of Element # 3;

\[
\begin{bmatrix}
\frac{8}{3} & -2 & -\frac{2}{3} & 0 & 0 \\
-2 & 4 & -2 & 0 & 0 \\
-\frac{2}{3} & -2 & \frac{8}{3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
u_4 \\
u_3 \\
u_2 \\
0 \\
0 \\
\end{bmatrix} =
\begin{bmatrix}
\frac{70}{3} \\
20 \\
\frac{140}{3} \\
0 \\
0 \\
\end{bmatrix}
\] (2.73)

We have assembled all the elements in the structure, therefore, all the nodes in the front can now be eliminated.

Elimination of Node # 2;

\[
\begin{bmatrix}
\frac{5}{2} & -\frac{5}{2} & 0 & 0 & 0 \\
-\frac{5}{2} & \frac{5}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
u_4 \\
u_3 \\
0 \\
0 \\
0 \\
\end{bmatrix} =
\begin{bmatrix}
35 \\
55 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\] (2.74)
Eliminated Equation #3: \[ -\frac{2}{3} u_4 - 2u_3 + \frac{8}{3} u_2 = \frac{140}{3} \] (2.75)

Elimination of node #3 will be different than the other nodes, since it has a prescribed displacement. To do this, the contributions of this node in all equations are taken to the right hand side, and the equation for this d.o.f. is still needed for calculation of nodal reaction forces because of the prescribed displacement at that node.

\textit{Elimination of Node #3;}

\[
\begin{bmatrix}
\frac{5}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
u_4 \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
= 
\begin{bmatrix}
35 + 2 \times \frac{5}{2} \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\]
(2.76)

Eliminated Equation #4: \[ -\frac{5}{2} u_4 + \frac{5}{2} u_3 = 55 \] (2.77)

Eliminated Equation #5: \[ \frac{5}{2} u_4 = 40 \] (2.78)

Now, the elimination process has been completed, therefore we can start backsubstitution. Starting from the last eliminated equation, and taking the steps backwards, unknowns can be solved in turn;

\[ \frac{5}{2} u_4 = 40, \ u_4 = 16 \] (2.79)
As can be understood from the given example, the frontal solver technique is a very useful technique, especially for finite element programs which require a significant amount of memory, i.e., three dimensional finite element programs having high order elements. Therefore, in this study, the solution of the simultaneous equations is achieved using this technique. The procedure is given as a flow chart in Fig. 2.10.

### 2.5 STRESS COMPUTATION

Stresses, \( \{\sigma\} \), in an element can be calculated after the nodal d.o.f.'s associated with this element are known. The system of equations to be solved is; \( [K]\{D\} = \{R\} \), and a special solution technique (Frontal Solution) was explained in the previous section. The expression for stress computation can be expressed as follows;

\[
\{\sigma\} = [E]\left(\{\epsilon\} - \{\epsilon^0\}\right) + \{\sigma^0\}
\]  

(2.84)
Interpret Fixity data in vector form

Set a marker for the last appearance of each node before elimination

Assign positions in the front for the element degrees of freedom and adjust the frontwidth if necessary.

Assemble the element stiffnesses for the 1st load case and assemble the element loads.

Can the node be eliminated?

Yes

Extract the equation coefficients and the right hand side terms corresponding to the eliminated node for writing to file.

Deal with prescribed displacements or eliminate a free variable.

No

Read the equation in reverse sequence from file.

Backsubstitute in the current equation.

Store the solved variable in an array ready for output and stress calculations.

Loop over each element

Loop over each node

Loop over all eliminated variables

Output the nodal displacements and reactions at restrained nodal points

Figure 2.10: Operational Sequence for Frontal Equation Solution.
in which mechanical strains \( \{\epsilon\} = [B] \{d\} \) are produced by displacements of the nodes.

Ignoring the initial stress term \( \{\sigma^0\} \) and taking thermal loading term \( \{\epsilon^0\} \) into account, the above equation can be rewritten,

\[
\begin{pmatrix}
\sigma_x \\
\sigma_y \\
\sigma_z \\
\tau_{xy} \\
\tau_{yz} \\
\tau_{xz}
\end{pmatrix} = [E] \left( [B] \{d\} - \begin{pmatrix}
\alpha_x \Delta T \\
\alpha_y \Delta T \\
\alpha_z \Delta T \\
\alpha_{xy} \Delta T \\
\alpha_{yz} \Delta T \\
\alpha_{xz} \Delta T
\end{pmatrix} \right)
\] (2.85)

Matrix \([B]\) is a function of the coordinates and must be evaluated at the locations within the element where stresses are desired.

The calculation \( \{\epsilon\} = [B] \{d\} \) involves differentiation of the displacement field. Therefore, stresses are computed less accurately than displacements. In low-order elements, stresses are often most accurate at the element centroid, less accurate at midsides and least accurate at corners. Elements of higher order usually display multiple points of optimal accuracy for stresses. The location of these points depend on the element geometry and the displacement field, and can often be predicted before doing numerical calculations. Stresses at other locations are usually best found by extrapolation from the optimal points [4].

Here, in isoparametric elements, \([B]\) is a function of the natural (local) coordinates and \( \{\sigma\} \) contains stresses referred to the global coordinate system \( xyz \). Then, there arises the question, "Where in the element should stresses be calculated ?". For isoparametric elements, it often happens that stresses (especially shear stresses) are most accurate at Gauss points. In elements based on displacement fields, one expects stresses to be less accurate than displacements. However, when computed at the Gauss points they are "super accurate" or "super convergent". This conclusion is for undistorted
(rectangular) elements. For distorted elements, Gauss points may not be optimal locations but they still remain very good choices. Stresses at Gauss points can be interpolated or extrapolated to other points in the element. The result is usually more accurate than the result of evaluating the above equation at the point of interest. This procedure is called "stress extrapolation (smoothing)". Although there are several techniques (i.e. using shape functions of the element), in this study, in each direction \((x, y, z)\) a cubic variation is employed and it is described in the next section.

2.5.1 STRESS SMOOTHING

In the previous section it is said that the stresses are most accurate when computed at the Gauss points. In this study, for the stress calculation, the points of a \(4 \times 4 \times 4\) integration scheme are used, which means that one can get stress values at 64 different locations within the element. To extrapolate these stresses to nodal points one can use several methods, i.e. using shape functions of the three-dimensional element, other assumed stress variation techniques. To make use of shape functions, the stress values at 32 points out of 64 Gauss points, which are the closest points to the nodes can be used, but that way stress values at the remaining 32 points are not used which can contain useful information to define the stress state within the element. Therefore, one may want to make a stress variation assumption that uses all the computed stress values (at 64 points). The argument goes as the following. Let \(\phi\) be the stress state in the element, and for the stress distribution assume a variation of the form;

\[
\phi = a_1 + a_2 \xi + a_3 \eta + a_4 \rho + a_5 \xi \eta + \ldots + a_{64} \xi^3 \eta^3 \rho^3
\]  

(2.86)
Since we have stress values computed at 64 Gauss points, for each of those points the above expression can be written in the matrix form as \( \{ \phi \} = [C] \{ a \} \),

\[
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\vdots \\
\phi_{64}
\end{pmatrix} =
\begin{bmatrix}
1 & \xi & \eta & \cdots & \xi^3 & \eta^3 & \rho^3 \\
1 & \xi & \eta & \cdots & \xi^3 & \eta^3 & \rho^3 \\
1 & \xi & \eta & \cdots & \xi^3 & \eta^3 & \rho^3 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
1 & \xi & \eta & \cdots & \xi^3 & \eta^3 & \rho^3
\end{bmatrix}
\begin{pmatrix}
a_1 \\
a_2 \\
a_3 \\
\vdots \\
a_{64}
\end{pmatrix} \tag{2.87}
\]

Note that, in the above 64 x 64 matrix each row is evaluated at the location values of the corresponding Gauss points, and the unknowns are the 64 coefficients \( a_i \). To determine the unknowns, the matrix \([C]\) can easily be inversed. Once the inverse of \([C]\) is obtained, unknown coefficients \( a_i \) can be found by,

\[
\begin{pmatrix}
a_1 \\
a_2 \\
a_3 \\
\vdots \\
a_{64}
\end{pmatrix} = [C]^{-1}
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\vdots \\
\phi_{64}
\end{pmatrix} \tag{2.88}
\]

After \( a_i \)'s are determined, the necessary equation for stress smoothing within the element can be evaluated at desired locations. Note also that, the calculation of inverse of \([C]\) is necessary only once, i.e. for the first element only, and the same matrix can be used for the subsequent elements. Therefore, for every element in turn, the above matrix
multiplication is done to obtain $a_i$'s and observing that the nodes are located at the local points $\mp 1$ or $\mp \frac{1}{3}$, by evaluation of $\phi$ at the local coordinates of the corresponding node, the stress state at desired node is computed.

2.6 ENRICHED CRACK TIP ELEMENT FORMULATION

The finite element method has been used successfully to treat crack problems in fracture mechanics where the tip of the crack possesses a stress singularity. The enriched crack tip element formulation goes back to Benzley's work [8], and is generalized such that any singularity may be represented by including the proper near field terms. A 32-noded three-dimensional crack tip element is shown in Fig.1, where the crack tip has 4 nodes.

Figure 2.11: Enriched Crack Tip Element.

For the enriched crack tip elements, the asymptotic displacement field is given by as the following.
As one can see, in the formulation of the displacement field for the enriched crack tip elements, some additional unknowns (stress intensity factors) are included, i.e., for a 32-node three dimensional element, in addition to nodal displacements, there are 12 more unknowns (3 stress intensity factors for each of the crack tip nodes), and the contributions from these stress intensity factors are then assembled into the global matrix as unknowns in the same way it is done for the regular elements. The first summation terms in each equation refer to the regular part of the displacement field, i.e., they have the same field approximation used in regular isoparametric elements. $Z_0(\xi, \eta, \rho)$ is the "zeroing function" and it provides inter-element compatibility between the crack tip elements and the elements that are surrounding the enriched elements.
(transition elements). This incompatibility is due to the singular field defined in the enriched crack tip elements. The value of $Z_0$ is 1 in the enriched crack tip elements and it may take some other forms in the transition elements always satisfying the condition that, it is 1 at the nodal points where the transition element is adjacent to any of the crack tip elements, and it is 0 when adjacent to regular isoparametric elements. $K_I^1$, $K_{II}^1$ and $K_{III}^1$’s are the stress intensity factors, for mode I, mode II, and mode III, respectively. Note that, since there are four crack tip nodes on one element, they are associated with the corresponding interpolation function of each node (the variation of stress intensity factors in the $z$ direction is related to the shape function values of the crack tip nodes). The functions $f_1, f_2, g_1, g_2$ and $h$ are the asymptotic displacement terms that are coefficients of the mode I, mode II and mode III stress intensity factors, $K_I, K_{II}$ and $K_{III}$. The terms $f_{1j}, f_{2j}, g_{1j}, g_{2j}$ and $h_j$ are the asymptotic displacement expressions evaluated at the $j^{th}$ node.

The computation of element stiffness matrix for enriched and transitional elements is performed using the same procedure that is used for regular isoparametric elements. The only difference is that, now the element has more unknowns because of the stress intensity factors included in the formulation, and a higher order integration scheme is needed due to the non-polynomial asymptotic displacement terms. We, immediately, observe that the difference for the additional unknowns will show up, in the "strain-nodal displacement matrix", $[B]$. In the formulation of $[B]$, to account for the stress intensity factors as additional unknowns, $[F]$ will be computed including more d.o.f. Note that, for the three-dimensional triangular prism elements, the d.o.f. of the element were reduced from 96 to 72. In this case, the number of unknowns will increase from 96 to 108. $[F]$ will now be computed from the relation,
\[
\begin{bmatrix}
  u, \xi \\
v, \xi \\
u, \rho \\
v, \eta \\
\end{bmatrix} = \left[ F \right] \begin{bmatrix}
  u_1 \\
v_1 \\
w_1 \\
v_32 \\
\end{bmatrix} \text{ with } [K] = \begin{bmatrix}
  K_{I}^{I} & K_{I}^{I} & K_{III}^{I} \\
  K_{II}^{III} & K_{II}^{III} & K_{III}^{IV} \\
  K_{I}^{IV} & K_{I}^{IV} & K_{III}^{IV} \\
\end{bmatrix}^T
\]

(2.92)

Note—that, the matrix, \([F]\), is 9 by 108 in size containing three displacement contributions from each node of the element, and three stress intensity factor contributions for the 4 crack tip nodes. As in the regular isoparametric element formulation, the derivatives of the displacement components must be computed for the given displacement field, in this case, it is the asymptotic displacement expressions. Expanding the stress intensity variation term, for example, the \(u\) displacement can be rewritten as;

\[
u(\xi, \eta, \rho) = \sum_{j=1}^{32} N_j(\xi, \eta, \rho)u_j + Z_0(\xi, \eta, \rho)f_1^* \left\{ N_I K_I^I + N_{II} K_{II}^{III} + N_{III} K_{III}^{IV} + N_{IV} K_{IV}^I \right\} + Z_0(\xi, \eta, \rho)g_1^* \left\{ N_I K_{II}^I + N_{II} K_{II}^{III} + N_{III} K_{III}^{IV} + N_{IV} K_{IV}^I \right\}
\]

(2.93)

where,

\[
f_1^* = f_1(\xi, \eta, \rho) - \sum_{j=1}^{32} N_j(\xi, \eta, \rho)f_{ij} \text{ and }
\]

\[
g_1^* = g_1(\xi, \eta, \rho) - \sum_{j=1}^{32} N_j(\xi, \eta, \rho)g_{ij}
\]

(2.94)

(2.95)
Then, the first derivative component in the left-hand side becomes

\[
\frac{\partial u(\xi, \eta, \rho)}{\partial \xi} = \sum_{j=1}^{32} \frac{\partial N_j(\xi, \eta, \rho)}{\partial \xi} u_j
\]

\[
+ \left\{ \frac{\partial Z_0(\xi, \eta, \rho)}{\partial \xi} f_1^* + Z_0(\xi, \eta, \rho) \frac{\partial f_1^*}{\partial \xi} \right\} \left\{ N_I K_I^I + N_{II} K_I^{II} + N_{III} K_I^{III} + N_{IV} K_I^{IV} \right\}
\]

\[
+ Z_0(\xi, \eta, \rho) f_1^* \left\{ \frac{\partial N_I}{\partial \xi} K_I^I + \frac{\partial N_{II}}{\partial \xi} K_I^{II} + \frac{\partial N_{III}}{\partial \xi} K_I^{III} + \frac{\partial N_{IV}}{\partial \xi} K_I^{IV} \right\}
\]

\[
+ \left\{ \frac{\partial Z_0(\xi, \eta, \rho)}{\partial \xi} g_1^* + Z_0(\xi, \eta, \rho) \frac{\partial g_1^*}{\partial \xi} \right\} \left\{ N_I K_I^I + N_{II} K_I^{II} + N_{III} K_I^{III} + N_{IV} K_I^{IV} \right\}
\]

\[
+ Z_0(\xi, \eta, \rho) g_1^* \left\{ \frac{\partial N_I}{\partial \xi} K_I^I + \frac{\partial N_{II}}{\partial \xi} K_I^{II} + \frac{\partial N_{III}}{\partial \xi} K_I^{III} + \frac{\partial N_{IV}}{\partial \xi} K_I^{IV} \right\}
\]

The derivatives of the starred asymptotic terms are given by:

\[
\frac{\partial f_1^*}{\partial \xi} = \frac{\partial f_1}{\partial x} \left( \sum_{j=1}^{32} \frac{\partial N_j}{\partial \xi} x_j \right) + \frac{\partial f_1}{\partial y} \left( \sum_{j=1}^{32} \frac{\partial N_j}{\partial \xi} y_j \right) - \sum_{j=1}^{32} \frac{\partial N_j}{\partial \xi} f_1,
\]

and

\[
\frac{\partial g_1^*}{\partial \xi} = \frac{\partial g_1}{\partial x} \left( \sum_{j=1}^{32} \frac{\partial N_j}{\partial \xi} x_j \right) + \frac{\partial g_1}{\partial y} \left( \sum_{j=1}^{32} \frac{\partial N_j}{\partial \xi} y_j \right) - \sum_{j=1}^{32} \frac{\partial N_j}{\partial \xi} g_1.
\]

The other derivatives of displacements needed to define \([F]\) are similar to the above expression, containing the appropriate asymptotic displacement fields associated with the displacement component of interest. According to the above formulation, for the calculation of \([F]\), the first 96 columns are going to be the same as in the \([F]\) calculated for regular isoparametric elements. Additionally, we now have the last 12 columns that are accounting for the coefficients of the unknown stress intensity factors. When
inserting the elements in the last 12-column part of \([F]\), caution should be taken to match the corresponding unknown quantities in the right-hand side (stress intensity factors). For example, the element that is accounting for the mode I stress intensity factor for the first-crack-tip node, \(K^f_i\), in the first row of \([F]\) is given by the following expression.

\[
F(1,97) = \left( \frac{\partial Z_0(\xi, \eta, \rho)}{\partial \xi} f^* + Z_0(\xi, \eta, \rho) \frac{\partial f^*}{\partial \xi} \right) N_I + Z_0(\xi, \eta, \rho) f^* \frac{\partial N_I}{\partial \xi}
\]  

(2.98)

Once the matrix \([F]\) is computed, obtaining \([B]\) matrix is a straightforward computation using the relation,

\[
[B] = [C] [D] [F]
\]

\[
\begin{bmatrix}
B
\end{bmatrix}
= 
\begin{bmatrix}
C
\end{bmatrix}
\begin{bmatrix}
D
\end{bmatrix}
\begin{bmatrix}
F
\end{bmatrix}
\]

(2.99)

and, the element stiffness matrix for the enriched and transitional elements is given by the same integral expression as used for the regular isoparametric elements.

\[
[k] = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} [B]^T [E] [B] J d\xi d\eta d\rho
\]

(2.100)

The only difference, now, is that, we have 108 unknown quantities, therefore the element stiffness matrix for the enriched elements is going to be 108 by 108 in size. Once again, evaluation of the above expression must be performed using a higher order integration, i.e., more Gaussian integration points should be used, because of the singular terms that are introduced to account for the stress singularity at the crack tip.
2.7 IMPLEMENTATION OF GENERALIZED PLANE STRAIN INTO FINITE ELEMENT PROGRAMMING

The previous finite element formulations were based on full three-dimensional analysis. However, in this study an additional condition, "Generalized Plane Strain", is introduced into the three-dimensional finite element program. Some numerical examples of this case encountered in the modeling of semiconductor package debonding due to thermal cycling will be presented. To employ the necessary procedure for generalized plane strain case, one needs to introduce an additional constraint condition in the three-dimensional FE program. As will be explained, this is accomplished by tying all the nodes on the front face of the model together in the "z" direction, so that they would have the same displacement values in this direction. The generalized plane strain case, could also have been studied with the approach based on two-dimensional elements, but the three-dimensional analysis model presented here will allow comparison of results for the same model between full three-dimensional and generalized plane strain case.

The necessary condition for generalized plane strain can be expressed as the following; "Normal strain in the "z" direction, $\varepsilon_{zz}$, is a constant value throughout the model and there is no shearing distortion in the "z" plane". This can be written mathematically as,

$$
\varepsilon_{zz} = C, \quad \varepsilon_{xz} = 0, \quad \varepsilon_{yz} = 0 \quad (2.101)
$$

The necessary procedure for this constraint to be introduced into the finite element program is to tie the front face nodes in the "z" direction. To illustrate this, a simple example will be presented.
The three-dimensional program can also be used for plane strain and plane stress calculations for checking purposes. For the latter case, thickness of the model in the $z$ direction can be chosen so thin, that the problem can be considered as a plane stress problem. To obtain the appropriate plane strain condition, both front and back faces of the model should be constrained in the $z$ direction (zero displacements in "$z$"). The generalized plane strain condition, however, requires, that instead of constraining with zero displacement, both of the faces should be forced to have the same displacement in the $z$ direction, i.e. all the nodes on the front and back faces are tied together in the $z$ direction, creating two separate tied node sets. But, to achieve the same goal, it is possible that one can constrain the back face with zero displacements (symmetry condition) in the $z$ direction whereas the front face remains tied.

### 2.7.1 TYING THE NODES FOR CONSTRAINT CONDITIONS

As discussed previously, the finite element method produces linear algebraic equations of the form,

$$ [K]\{U\} = \{R\} $$

(2.102)

to be solved simultaneously for the unknown displacements. The global stiffness matrix, $[K]$, contains coefficients of the unknown displacement values, $\{U\}$ is vector of unknowns, and $\{R\}$ represents the nodal forces.

For generalized plane strain, we want to tie some specific nodes in the $z$ direction, which means, that there is constraint condition(s) to be introduced into the system of equations. Although there are several ways to accomplish this, i.e., transformations,
Lagrange multipliers, penalty functions and stiffness method, in this thesis Lagrange multipliers and stiffness method will be described.

2.7.1.1 Lagrange Multipliers Method

The constraint equation is written in the homogenous form as,

$$[C]\{U\} - \{Q\} = \{0\} \tag{2.103}$$

and it can be introduced into the system of equations in the following form;

$$\begin{bmatrix} K & C^T \\ C & 0 \end{bmatrix} \begin{bmatrix} U \\ \lambda \end{bmatrix} = \begin{bmatrix} R \\ Q \end{bmatrix} \tag{2.104}$$

The lower partition of the above equation, which must be solved for both \{U\} and \{\lambda\}, is the equation of constraint. The \lambda_i may be interpreted as forces of constraint.

The problem can be illustrated by the simple three-element model that is used in the frontal solver section as an example.

Fig. 2.8 shows a three-element finite element model, and to simplify the problem at each nodal point only one dimensional d.o.f. is assumed. Again for simplicity, the element stiffness matrix (3 by 3) and load vector (3 by 1) for each of the element in the structure are taken as the same. For an element shown in Fig.2.9 element stiffness matrix and load vector are defined,

$$\begin{bmatrix} k_{ii} & k_{ij} & k_{im} \\ k_{ji} & k_{jj} & k_{jm} \\ k_{mi} & k_{mj} & k_{mm} \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 3 & -2 \\ 0 & -2 & 2 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} R_i \\ R_j \\ R_m \end{bmatrix} = \begin{bmatrix} 10 \\ 10 \\ 10 \end{bmatrix} \tag{2.105}$$
For the above model configuration, if, for example, one wants to force the node 4 and 2 to have the same displacement value, then the assembled global system of equations (5 by 5), after including the constraint equation, will be,

\[
\begin{bmatrix}
3 & -1 & 0 & 0 & 1 \\
-1 & 3 & -2 & 0 & 0 \\
0 & -2 & 6 & -2 & -1 \\
0 & 0 & -2 & 2 & 0 \\
1 & 0 & -1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
U_4 \\
U_1 \\
U_2 \\
U_5 \\
\lambda
\end{bmatrix}
= 
\begin{bmatrix}
24 \\
10 \\
34 \\
10 \\
0
\end{bmatrix}
\quad (2.106)
\]

Note that, in the above finite element model, it is assumed that node 3 undergoes a prescribed displacement, \( U_3 = 2.0 \), and taking the prescribed displacement into account, the contribution of node 3 is already eliminated from the above system of equations. Then, it becomes a system of 5 linear equations to be solved for 5 unknowns, and the solution gives, \( x_1 = 22.833, \ x_2 = 19.5, \ x_4 = 19.5, \ x_5 = 24.5, \) and \( \lambda = -11.6667 \)

This technique is very attractive because of its simplicity, but from the solver point of view, for large system of equations it is not an efficient method. Depending on the solution method used, i.e., Gauss elimination, frontal solver, it increases either bandwidth or frontwidth, respectively, and because of memory problem, especially for three-dimensional finite element analysis, this is not desirable. Therefore, in this study, instead of using this technique, another method that does not require additional memory, stiffness method, is used.
2.7.1.2 Stiffness Method

Since the rows and columns of stiffness matrix contain stiffness contributions of the nodal d.o.f.'s and positions of these contributions are known in the stiffness matrix, tying the d.o.f.'s can also be accomplished by adding stiffness contributions to a pre defined "master" d.o.f. and eliminating the added contributions from the stiffness matrix. And, the mathematical explanation of this technique goes as the following.

Suppose that we have a system of three linear equations to be solved for three unknowns, $x$, $y$, and $z$,

\begin{align*}
a_1x + b_1y + c_1z &= A \\
a_2x + b_2y + c_2z &= B \\
a_3x + b_3y + c_3z &= C
\end{align*} \tag{2.107}

and, we want $y$ and $z$ to have the same values. To employ this condition, one can add the third equation to the second one, and it reduces to the following form.

\begin{align*}
a_1x + b_1y + c_1z &= A \\
(a_2 + a_3)x + (b_2 + b_3)y + (c_2 + c_3)z &= B + C
\end{align*} \tag{2.108}

At this point, we observe the condition that $y = z$, therefore the coefficients of the unknowns $y$ and $z$ can be combined, and the above system of equations becomes two linear equations with two unknowns,

\begin{align*}
a_1x + (b_1 + c_1)y &= A \\
(a_2 + a_3)x + (b_2 + b_3 + c_2 + c_3)y &= B + C
\end{align*} \tag{2.109}
Since, now, all the coefficients are known, the above equations can be solved for \( x \) and \( y \), and due to the imposed constraint condition it is known that, \( y = z \).

Observing that, the finite element method reduces the problem to system of linear equations of the above type, one could also use this method to embed constraint conditions into the problem. To illustrate this approach, the same simple example for the three-element structure shown previously will be solved using the stiffness method.

We recall the assembled global stiffness matrix,

\[
\begin{bmatrix}
3 & -1 & 0 & 0 \\
-1 & 3 & -2 & 0 \\
0 & -2 & 6 & -2 \\
0 & 0 & -2 & 2 \\
\end{bmatrix}
\begin{bmatrix}
U_4 \\
U_1 \\
U_2 \\
U_5 \\
\end{bmatrix}
= 
\begin{bmatrix}
24 \\
10 \\
34 \\
10 \\
\end{bmatrix}
\]

and our constraint condition was \( U_4 = U_2 \). Therefore we first add the third equation into the first one,

\[
\begin{bmatrix}
3 & -3 & 6 & -2 \\
-1 & 3 & -2 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & -2 & 2 \\
\end{bmatrix}
\begin{bmatrix}
U_4 \\
U_1 \\
U_2 \\
U_5 \\
\end{bmatrix}
= 
\begin{bmatrix}
58 \\
10 \\
0 \\
10 \\
\end{bmatrix}
\]

The next step is to add contributions from the third column to the first column and to delete the third row and third column from the system of equations, since the contribution of this d.o.f. has already been included to the master d.o.f. \( U_4 \).

\[
\begin{bmatrix}
9 & -3 & -2 \\
-3 & 3 & 0 \\
-2 & 0 & 2 \\
\end{bmatrix}
\begin{bmatrix}
U_4 \\
U_1 \\
U_5 \\
\end{bmatrix}
= 
\begin{bmatrix}
58 \\
10 \\
10 \\
\end{bmatrix}
\]

67
Note, that we reduced the number of equations from 4 to 3 due to the constraint condition. The above is, now, a system of equations with three unknowns and can be solved uniquely, and the solution gives the same values, when compared Lagrange multipliers method, as $x_1 = 22.833$, $x_2 = 19.5$, $x_4 = 19.5$, $x_5 = 24.5$. We could have performed the calculation by adding the corresponding columns first and then the rows. Both calculations give the same results.

The extension of the above example for tying more than two nodes is straightforward. Once the master d.o.f. is defined, the subsequent contributions of the d.o.f.'s to be tied (slave d.o.f.'s) are included into the master d.o.f. This approach is also not limited to one set of tied d.o.f.'s. There can be created multiple sets, that are tied separately in the desired direction, but again for every tied set one has to predefined a master d.o.f. to which the contributions of slave d.o.f.'s of that set are added.

In this study the necessary condition for "Generalized Plane Strain" is introduced into the finite element program using the stiffness method, and therefore the increase in the frontwidth which affects the necessary memory was prevented.
Chapter 3

Numerical Examples for Semiconductor Package Debonding Due To Thermal Cycling

3.1 INTRODUCTION

In this chapter, a finite element model suitable for the evaluation of semiconductor package debonding due to thermal cycling, using both two dimensional and three dimensional analyses is presented. In particular, for both analyses, the results from a fracture mechanics approach that utilizes enriched crack tip elements to model interfacial cracking are given. The enrichment methodology, which was explained in the previous chapter, can be used to characterize interface cracking due to thermal cycling and it is demonstrated with a simple IC package configuration. The behavior of the fracture parameters, (e.g., strain energy release rates and mixed mode stress intensity factors) is studied for different crack lengths and for different boundary conditions. In an effort to quantify the three dimensional nature of the problem, comparisons are made between 2-D and 3-D models.

Thermal cycling and thermal shock can severely stress polymeric semiconductor packages because of large thermal mismatches between the different materials - silicon (Si) or gallium arsenide (GaAs), metal alloys (Cu, Fe/Ni, Sn/Pb lead frame plating, etc.), polyimides, epoxies, and other organic materials [1]. Delamination between a silicon die and a polymeric substrate is often observed in semiconductor packages subjected to severe thermal shock and thermal cycles. It is often the case that a small amount of
delamination maybe unavoidable during fabrication of a semiconductor package and that this "damage" may not necessarily result in ultimate failure of the device. Therefore, it is highly desirable to develop predictive methodologies that can be used to estimate the life of a package based on some preexisting interfacial flaw size. In addition, in the absence of nondestructive inspection techniques that can determine the exact extent of initial debonding, it is still possible to devise "fail-safe" design methodologies based on fracture mechanics concepts. For example, to assist in the selection of geometries and material properties that minimize the likelihood of failure in actual packages, fracture mechanics calculations, in conjunction with interfacial fracture toughness measurements, can be used to assure that a hypothetical severe debond will not propagate to a critical length during the service life of the package. The application of interfacial fracture mechanics to predict debonding between layered materials has been intensively investigated and should serve a basis for structural design for damage tolerance.

Utilization of interface fracture mechanics methodology for life prediction, requires the accurate computation of such parameters as mixed mode stress intensity factors, $K_I$, $K_{II}$, and $K_{III}$, and strain energy release rates, $G$, for complex geometries and loading conditions. The finite element method, suitably modified, can be used to compute these quantities for the complex interface cracking problems encountered in semiconductor packaging. In particular, it will be demonstrated that a finite element approach that takes advantage of special "enriched" interface crack tip elements, can be highly efficient for computing the required fracture parameters performing both two-dimensional and three-dimensional analyses for thermal cycling problems in electronic packages. Therefore, in this study, for the same particular semiconductor package model, in terms of stresses and fracture parameters comparisons are made between the two-dimensional and three-dimensional analysis (generalized plane strain). For the three-dimensional analysis, one 3-D element is used in the thickness, "z", direction and the
necessary condition for the generalized plane strain case is imposed. As explained in the previous chapter, the front face nodes are tied in that direction. In such an analysis, cubic 32-node rectangular and 24-node triangular prisms are used.

3.2 DEVICE CONFIGURATION FOR NUMERICAL CALCULATIONS

In this chapter, using a simple example device configuration (Fig. 3.1), in addition to stress analysis, to demonstrate the application of enriched crack tip elements, interface fracture results are also presented. Interfacial debonding in a semiconductor package subjected to reversed thermal cycles, and the effect of crack length $a$ ($a/b=0.5$, $b$ is the half length of the silicon die) is studied for the case of positive temperature change considering two different boundary conditions.

![Diagram of Underfilled Semiconductor Package](image)

**Figure 3.1**: Underfilled Semiconductor Package.

The package to be analyzed is a Silicon die (0.686 mm thick, 20.32 mm wide), bonded to a substrate (1.016 mm thick, 23.0125 mm wide). The bond thickness between the die and the substrate is 0.0762 mm, with the bond is composed of solder balls (~2.5% by volume) and epoxy underfill. A realistic underfill fillet at the edge of the die is also included in the model (Fig. 3.1). The material properties for this package are given in Table 3.1 (note the orthotropic CTE for the substrate).
Table 3.1: Material Properties for The Example Package.

<table>
<thead>
<tr>
<th>Material</th>
<th>Young's Modulus</th>
<th>Poisson's Ratio</th>
<th>CTE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silicon Die</td>
<td>E=1.299e11 Pa</td>
<td>$\nu = 0.279$</td>
<td>$\alpha = 3.3\text{e-6}^\circ\text{C}$</td>
</tr>
<tr>
<td>Substrate</td>
<td>E=2.35e10 Pa</td>
<td>$\nu = 0.33$</td>
<td>$\alpha_x = 15\text{e-6}^\circ\text{C}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\alpha_y = 57\text{e-6}^\circ\text{C}$</td>
</tr>
<tr>
<td>Underfill</td>
<td>E=6.89e9 Pa</td>
<td>$\nu = 0.3$</td>
<td>$\alpha = 26\text{e-6}^\circ\text{C}$</td>
</tr>
<tr>
<td>Solder</td>
<td>E=2.35e10 Pa</td>
<td>$\nu = 0.35$</td>
<td>$\alpha = 26\text{e-6}^\circ\text{C}$</td>
</tr>
</tbody>
</table>

In an effort to simplify the calculations, an axisymmetric finite element model was created, with the bond layer material properties estimated from a proportional ratio (by volume) of solder and underfill properties. For an interfacial crack, the influence of material properties on the fracture solution is characterized by the nondimensional Dundur's bimaterial parameters [10]. In this particular case these parameters are given by, $\alpha = -0.534$ (not to be confused with CTE) and $\beta = -0.1593$. The bimaterial parameter $\epsilon = 0.0511$ [10].

3.3 THERMAL CYCLING UNDER DIFFERENT BOUNDARY CONDITIONS (AXISYMMETRIC)

3.3.1 UNRESTRAINED PACKAGE

Initial calculations were performed for an unrestrained package subjected to a uniform $\Delta T = -1.0^\circ\text{C}$ having an axisymmetric interface crack between the underfill and the substrate with radius $a = 2.54$ mm. The finite element model used in this fracture analysis contained 384 cubic elements and 1951 nodes (Fig. 3.2). In addition, the mesh close to the crack tip was refined as depicted in Fig. 3.3. Because of
differences in the coefficient of thermal expansion, the unrestrained package deforms as shown in the exaggerated view depicted in Fig. 3.2. The fracture results from this thermal stress calculation are given in Table 3.2. The definitions of $K_I$, $K_{II}$, $e$, and $G$ for interface crack can be found in ref. [10]. The phase angle, $\psi$, is defined by $\psi = \tan^{-1}(K_{II}/K_I)$.

![Finite Element Fracture Model - Uniform Cooling.](image)

**Figure 3.2:** Finite Element Fracture Model - Uniform Cooling.

<table>
<thead>
<tr>
<th>$\Delta T$ ($^\circ$C)</th>
<th>$K_I$ Pa-m$^{1/2}$</th>
<th>$K_{II}$ Pa-m$^{1/2}$</th>
<th>$\psi$</th>
<th>$G$ J/m$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1</td>
<td>2.765</td>
<td>-1.7</td>
<td>-31.58$^\circ$</td>
<td>8.357e-10</td>
</tr>
<tr>
<td>+1</td>
<td>1.6868</td>
<td>1.6937</td>
<td>45.11$^\circ$</td>
<td>4.5376e-10</td>
</tr>
</tbody>
</table>

**Table 3.2:** Fracture Results for Axisymmetric Interface Crack - a=2.54 mm.

![Close-up View of Crack Tip Refinement.](image)

**Figure 3.3:** Close-up View of Crack Tip Refinement.
It is important to note that in the $-\Delta T$ case, the mode I stress intensity factor has a positive value and the crack opens along its entire length. This is not the case when a uniform positive temperature is imposed on the package. (Fig. 3.4). If only the sign of $\Delta T$ is reversed, the calculation gives a $K_I$ of the same magnitude but of opposite sign. However, the crack surfaces, pass through one another. In this particular problem crack surface contact first occurs at $r = 0$ and progresses outward radially. Recomputing the fracture parameters by simulating frictionless crack surface contact, i.e., constraining the elements from passing through one another, but allowing them to slide radially, results in a nonlinear calculation, with the length of the contact zone an additional unknown. The final result for the $+\Delta T$ case is also given in Table 3.2 and again yields a positive $K_I$.

![Figure 3.4: Finite Element Fracture Model - Uniform Heating.](image)

The condition of no boundary constraint generally corresponds to the fabrication stage of the semiconductor package, where it can expand and contract freely. However, once the package is mounted to a board for service, some boundary conditions are introduced into the problem. In this thesis, two different boundary conditions are studied.
3.3.2 SUBSTRATE IS RESTRAINED IN THE VERTICAL DIRECTION ONLY

**Figure 3.5:** Finite Element Model Where The Substrate is Restrained in The Vertical Direction.

This particular boundary condition is shown in Fig. 3.5. As can be seen in the figure, the bottom of the substrate is restrained in the vertical direction and the whole model is free to move in the horizontal direction. The effect of this particular boundary condition is analyzed for different crack lengths ($a/b = 0 \sim 0.5$, $b$: half length of the Silicon die).

**Figure 3.6:** Strain Energy Release Rate ($J/m^2$) v.s. Different Nondimensional Crack Lengths ($a/b$) for The Boundary Condition Type Where The Substrate is Restrained in The Vertical Direction Only.

It can be seen in Fig. 3.6 that, for this type of boundary condition, strain energy release rate increases with increasing crack length and the values are almost three
orders of magnitude greater than those in the case where there was no boundary constraint (Table 3.2). Fig. 3.7 shows the behavior of the mixed mode stress intensity factors ($K_I$ and $K_{II}$). The stress intensity factors differ by an order of magnitude from the results given by the unrestrained package model.

![Graph showing stress intensity factors $K_I$ and $K_{II}$ vs. $a/b$.](image)

**Figure 3.7**: Stress Intensity Factors, $K_I$ and $K_{II}$ (Pa$\cdot$m$^{1/2}$), v.s. Different Nondimensional Crack Lengths ($a/b$) for the Boundary Condition Type Where the Substrate is Restrained in the Vertical Direction Only.

### 3.3.3 Substrate is Restrained in Both Directions

![Finite element model with boundary conditions](image)

**Figure 3.8**: Finite Element Model Where the Substrate is Restrained in Both Directions.

It can be seen in Fig. 3.8 that, for this type of constraint condition, which is a more realistic representation of the situation that corresponds to the package/board assembly; the bottom of the substrate is restrained in both vertical and horizontal directions.
Again, for different crack lengths \((a/b = 0 - 0.5)\), the effect of this boundary condition can be observed in Fig. 3.9 and Fig. 3.10.

**Figure 3.9**: Strain Energy Release Rate \((J/m^2)\) v.s. Different Nondimensional Crack Lengths \((a/b)\) for The Boundary Condition Type Where The Substrate is Restrained in Both Directions.

**Figure 3.10**: Stress Intensity Factors, \(K_I\) and \(K_{II}\)(Pa-m\(^{1/2}\)) vs Different Nondimensional Crack Lengths \((a/b)\) for The Boundary Condition Type Where The Substrate is Restrained in Both Directions.
In Fig. 3.9, the strain energy release rate again increases with increasing crack length, but this time is two orders of magnitude greater than the first type of constraint condition. For this particular type of constraint condition, the shearing component, $K_{II}$, of the mixed mode stress intensity factor becomes dominant because of the severe restraint condition imposed in the horizontal direction (Fig. 3.10). $K_{II}$ is now not only greater than $K_I$, but also greater than $K_{II}$ computed for the previous type of boundary condition.

3.4 THREE DIMENSIONAL FINITE ELEMENT ANALYSIS

The above calculations were based on axisymmetric analyses. The same type of semiconductor package geometry, will now be examined using a three dimensional model with one element through the thickness in the "z" direction. Instead of performing general three dimensional analysis of the problem, "Generalized Plane Strain" case is examined in this study. This is done by creating a three dimensional model with one element through the thickness. To achieve the appropriate condition for the generalized plane strain, the back part of the model ($z = 0$) is restrained from moving in the $z$ direction (symmetry) whereas all the nodes on the front face are constrained to move with the same displacement in that direction, e.g., all the nodes on the front face of the model are tied together in the $z$ direction.

Comparisons between the stress distributions for the two dimensional analyses (Plane Strain, Plane Stress and Axisymmetric) and for the generalized plane strain case are made, and it is also shown that the three dimensional finite element calculations yield the plane strain and plane stress results as limiting cases.
3.4.1 COMPARISON BETWEEN THE 2-D AND GENERALIZED PLANE STRAIN FINITE ELEMENT ANALYSIS IN TERMS OF STRESSES

The same type of package configuration is used and comparisons of $\sigma_{xx}$ stress distribution on the top edge of the silicon die (chip) and shearing stress, $\sigma_{xy}$, distribution in the underfill layer are made between the results of 2-D calculations and those of generalized plane strain. The calculations are performed, using a $+10 \degree C$ uniform temperature change applied to the model, with no boundary constraints.

In Fig. 3.11, $\sigma_{xx}^* = \sigma_{xx}/E_{\text{chip}}$, nondimensional $\sigma_{xx}$ stresses are plotted with the $x$ axis representing the nondimensional location (the stresses and the $x$ location are nondimensionalized by the elastic modulus and the length of the chip, respectively). It can be seen from the figure that, plane stress conditions underestimate (in magnitude) the $\sigma_{xx}$ stress distribution on the top edge of the chip, whereas plane strain yields an overestimate. It can also be seen that the generalized plane strain case lies between plane strain and axisymmetric analyses. As expected, in all cases the stress magnitude remains relatively constant along the edge and becomes zero at the free end.

In Fig. 3.12, $\sigma_{xy}^* = \sigma_{xy}/E_{\text{underfill}}$, the nondimensional shearing stress is plotted for the different cases. Along the underfill layer the shearing stress remains zero until close to the end of the chip. In the neighborhood of the free end, it increases (in magnitude) dramatically, for all the cases. The plane stress case exhibits a small deviation from the other three cases in this region. It is obvious that, when the sign of temperature change is reversed the exact stress distributions, but this time with reversed signs, occur.

In Fig. 3.13, 3.14, 3.15 and 3.16, for the same temperature loading, different stress distributions ($\sigma_{xx}$, $\sigma_{xy}$, $\sigma_{yy}$ and $\sigma_{zz}$ respectively) are shown in three dimensions. Blue areas represent negative stresses, whereas red areas show positive stresses.
Figure 3.11: A Comparison Between the 2-D and Generalized Plane Strain Finite Element Analysis (For the $\sigma_{xx}$ Stress Distribution on the Top Edge of the Chip).

Figure 3.12: $\sigma_{xy}$, Shearing Stress Distribution Along the Underfill Layer.
Figure 3.13: $\sigma_{zz}$ Stress Distribution.

Figure 3.14: $\sigma_{xy}$ Stress Distribution.
Figure 3.13: $\sigma_{xx}$ Stress Distribution.

Figure 3.14: $\sigma_{zy}$ Stress Distribution.
Figure 3.15: $\sigma_{yy}$ Stress Distribution.

Figure 3.16: $\sigma_{zz}$ Stress Distribution.
Figure 3.15: $\sigma_{yy}$ Stress Distribution.

Figure 3.16: $\sigma_{zz}$ Stress Distribution.
3.4.1.1 Recovery of Two Dimensional Results From Three Dimensional Finite Element Calculations

As a check on the 3-D formulation, two dimensional (plane strain and plane stress) calculations were performed using the three dimensional program. For the plane strain case this was achieved by restraining both, back and front faces of the model in the $z$ direction. For the plane stress case, the model was made very thin in the $z$ direction, so that the problem can be considered as essentially a plane stress problem. As can be seen in Fig. 3.17, exactly the same results were obtained for the $\sigma_{xx}$ stresses on the top of the chip.

![Comparison of Stresses for Plane Strain and Plane Stress Conditions from Two Dimensional and Three Dimensional Calculations](image_url)

**Figure 3.17:** Comparison of Stresses for Plane Strain and Plane Stress Conditions from Two Dimensional and Three Dimensional Calculations.
3.4.2 THREE DIMENSIONAL FRACTURE ANALYSIS

For the same underfilled package shown in Fig. 3.1, fracture analyses under the same type of boundary conditions were performed three dimensionally and comparisons between Generalized Plane Strain (3-D) and the 2-D calculations were made. There were some differences in the results in terms of fracture parameters, and they are illustrated with the graphs and tables in the following two sections. For the first type of constraint condition (the substrate is restrained in the $y$ direction only), and for the second type of boundary condition (the substrate is restrained in both vertical and horizontal directions) the effect of crack length is studied.

3.4.2.1 Substrate is Restrained in The Vertical Direction Only

This type of boundary condition was shown in Fig. 3.5, and the substrate was fixed in the vertical direction only from its bottom edge. Axisymmetric calculations showed, that in terms of fracture parameters this type of constraint condition was relatively safe condition when compared to the second type of constraint condition where the substrate was restrained in both directions. For this type of boundary condition, the three dimensional finite element calculations have been performed for various crack lengths and comparisons of the results are shown in the following graphs. The numerical values of the fracture parameters are also given as tables.

Looking at the graphs, it is observed that the fracture parameters ($G, K_I, K_{II}$) increase with the increasing crack length and for this particular type of boundary condition, in terms of fracture parameters, the generalized plane strain case falls between plane strain and axisymmetric calculations.
Figure 3.18: Comparison of Strain Energy Release Rate Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.

Figure 3.19: Comparison of Mode I Stress Intensity Factor Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.
Figure 3.20: Comparison of Mode II Stress Intensity Factor Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.

Figure 3.21: Comparison of Phase Angle Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.
Table 3.3: Strain Energy Release Rates (J/m$^2$) for Different Solution Cases.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.471E-10</td>
<td>0.208E-10</td>
<td>0.642E-09</td>
<td>0.765E-09</td>
</tr>
<tr>
<td>0.250</td>
<td>0.379E-08</td>
<td>0.189E-08</td>
<td>0.133E-07</td>
<td>0.628E-08</td>
</tr>
<tr>
<td>0.375</td>
<td>0.407E-07</td>
<td>0.156E-07</td>
<td>0.101E-06</td>
<td>0.503E-07</td>
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<tr>
<td>0.500</td>
<td>0.121E-06</td>
<td>0.464E-07</td>
<td>0.207E-06</td>
<td>0.131E-06</td>
</tr>
</tbody>
</table>

Table 3.4: Mode I Stress Intensity Factors (Pa·m$^{1/2-i\pi}$) for Different Solution Cases.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.605E-01</td>
<td>0.139E+00</td>
<td>0.647E+00</td>
<td>0.157E+01</td>
</tr>
<tr>
<td>0.250</td>
<td>0.244E+01</td>
<td>0.145E+01</td>
<td>0.522E+01</td>
<td>0.405E+01</td>
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<tr>
<td>0.375</td>
<td>0.132E+02</td>
<td>0.734E+01</td>
<td>0.224E+02</td>
<td>0.146E+02</td>
</tr>
<tr>
<td>0.500</td>
<td>0.389E+02</td>
<td>0.226E+02</td>
<td>0.510E+02</td>
<td>0.405E+02</td>
</tr>
</tbody>
</table>

Table 3.5: Mode II Stress Intensity Factors (Pa·m$^{1/2-i\pi}$) for Different Solution Cases.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.768E+00</td>
<td>0.470E+00</td>
<td>0.277E+01</td>
<td>0.268E+01</td>
</tr>
<tr>
<td>0.250</td>
<td>0.646E+01</td>
<td>0.444E+01</td>
<td>0.118E+02</td>
<td>0.792E+01</td>
</tr>
<tr>
<td>0.375</td>
<td>0.184E+02</td>
<td>0.112E+02</td>
<td>0.277E+02</td>
<td>0.205E+02</td>
</tr>
<tr>
<td>0.500</td>
<td>0.271E+01</td>
<td>-0.480E+01</td>
<td>-0.209E+01</td>
<td>0.385E+01</td>
</tr>
</tbody>
</table>

Table 3.6: Phase Angles, $\psi = \tan^{-1} \frac{K_{II}}{K_f}$, for Different Solution Cases.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>85.495</td>
<td>73.455</td>
<td>66.087</td>
<td>59.611</td>
</tr>
<tr>
<td>0.250</td>
<td>69.325</td>
<td>71.961</td>
<td>55.429</td>
<td>62.907</td>
</tr>
<tr>
<td>0.375</td>
<td>54.307</td>
<td>56.765</td>
<td>40.297</td>
<td>54.578</td>
</tr>
<tr>
<td>0.500</td>
<td>39.925</td>
<td>-11.984</td>
<td>-13.106</td>
<td>5.4328</td>
</tr>
</tbody>
</table>
3.4.2.2 Substrate is Restrained in Both Vertical and Horizontal Directions

This type of constraint condition was shown in Fig. 3.8, i.e., the substrate is restrained in both directions. It can be considered as a relatively good approximation of the appropriate constraint after board assembly. Of course, the printed circuit board is not a perfectly rigid base, but this approximate boundary condition should provide an upper bound solution. For this type of restraint condition, the three dimensional finite element analysis is compared with the two dimensional analyses.

Figure 3.22: Comparison of Strain Energy Release Rate Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.
Figure 3.23: Comparison of Mode I Stress Intensity Factor Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.

Figure 3.24: Comparison of Mode II Stress Intensity Factor Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.
Figure 3.25: Comparison of Phase Angle Between The Two Dimensional Analyses and Generalized Plane Strain for Various Crack Lengths.

Once again, comparing the fracture parameter values with the first constraint case, we observe that this type of constraint condition is a more severe condition, especially with respect to shearing component of the stress intensity factor, and this is due to the additional $x$ direction constraint introduced at the bottom edge of the substrate. For this type of restraint condition, the three dimensional generalized plane strain approach underestimates the situation when compared with the other three cases. Again, we have an increasing strain energy release rate and increasing mode II stress intensity factor (dominant component when compared with mode I stress intensity factor). For all the cases phase angle, $\psi = \tan^{-1} \frac{K_{II}}{K_I}$, increases at the beginning and becomes almost a constant value for the subsequent increasing crack lengths. The numerical values of fracture parameters for this type of boundary condition are given below as tables.
Table 3.7: Strain Energy Release Rates ($J/m^2$) for Different Solution Cases.

<table>
<thead>
<tr>
<th>$a/b$</th>
<th>PIn. Strain</th>
<th>PIn. Stress</th>
<th>Axisymmetric</th>
<th>Gen. PIn. Strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.161E-05</td>
<td>0.853E-06</td>
<td>0.235E-05</td>
<td>0.558E-06</td>
</tr>
<tr>
<td>0.250</td>
<td>0.886E-05</td>
<td>0.461E-05</td>
<td>0.112E-04</td>
<td>0.303E-05</td>
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<tr>
<td>0.375</td>
<td>0.298E-04</td>
<td>0.155E-04</td>
<td>0.351E-04</td>
<td>0.102E-04</td>
</tr>
<tr>
<td>0.500</td>
<td>0.779E-04</td>
<td>0.410E-04</td>
<td>0.854E-04</td>
<td>0.267E-04</td>
</tr>
</tbody>
</table>

Table 3.8: Mode I Stress Intensity Factors (Pa·m$^{1/2}$) for Different Solution Cases.

<table>
<thead>
<tr>
<th>$a/b$</th>
<th>PIn. Strain</th>
<th>PIn. Stress</th>
<th>Axisymmetric</th>
<th>Gen. PIn. Strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.100E+02</td>
<td>-0.194E+01</td>
<td>0.229E+02</td>
<td>0.715E+01</td>
</tr>
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<td>0.250</td>
<td>-0.741E+01</td>
<td>-0.257E+02</td>
<td>0.310E+01</td>
<td>-0.221E+01</td>
</tr>
<tr>
<td>0.375</td>
<td>-0.297E+02</td>
<td>-0.581E+02</td>
<td>-0.195E+02</td>
<td>-0.152E+02</td>
</tr>
<tr>
<td>0.500</td>
<td>-0.500E+02</td>
<td>-0.967E+02</td>
<td>-0.392E+02</td>
<td>-0.200E+02</td>
</tr>
</tbody>
</table>

Table 3.9: Mode II Stress Intensity Factors (Pa·m$^{1/2}$) for Different Solution Cases.

<table>
<thead>
<tr>
<th>$a/b$</th>
<th>PIn. Strain</th>
<th>PIn. Stress</th>
<th>Axisymmetric</th>
<th>Gen. PIn. Strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.142E+03</td>
<td>0.992E+02</td>
<td>0.171E+03</td>
<td>0.835E+02</td>
</tr>
<tr>
<td>0.250</td>
<td>0.334E+03</td>
<td>0.229E+03</td>
<td>0.377E+03</td>
<td>0.195E+03</td>
</tr>
<tr>
<td>0.375</td>
<td>0.612E+03</td>
<td>0.419E+03</td>
<td>0.664E+03</td>
<td>0.358E+03</td>
</tr>
<tr>
<td>0.500</td>
<td>0.990E+03</td>
<td>0.681E+03</td>
<td>0.104E+03</td>
<td>0.580E+03</td>
</tr>
</tbody>
</table>

Table 3.10: Phase Angles, $\psi = \tan^{-1}\frac{K_{II}}{K_{I}}$, for Different Solution Cases.

<table>
<thead>
<tr>
<th>$a/b$</th>
<th>PIn. Strain</th>
<th>PIn. Stress</th>
<th>Axisymmetric</th>
<th>Gen. PIn. Strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>85.958</td>
<td>91.122</td>
<td>71.616</td>
<td>85.107</td>
</tr>
<tr>
<td>0.250</td>
<td>91.269</td>
<td>96.389</td>
<td>78.768</td>
<td>90.648</td>
</tr>
<tr>
<td>0.375</td>
<td>92.776</td>
<td>97.903</td>
<td>80.919</td>
<td>92.433</td>
</tr>
<tr>
<td>0.500</td>
<td>92.893</td>
<td>98.082</td>
<td>81.407</td>
<td>91.983</td>
</tr>
</tbody>
</table>
Chapter 4

Conclusion

In this study, the problem of "debonding" in semiconductor IC (Integrated Circuit) packages has been investigated by employing three dimensional finite element analysis restricted to cases where "Generalized Plane Strain" conditions are assumed. In the thesis, theory of three dimensional finite elements is given. Also, solutions are provided that illustrate the solution technique for specific package types. These are analyzed for different thermal conditions and different boundary conditions. Comparisons between the two dimensional and three dimensional (generalized plane strain) finite element analyses are made in terms of stresses and fracture parameters.

As a general statement, for the three dimensional finite element analysis the following can be concluded. Some of the problems that are related to semiconductor package debonding have to be evaluated three dimensionally, whereas some others are adequately handled as two dimensional problems. Although it requires some computational effort, one reason for performing three dimensional finite element analysis, is to check the applicability of 2-D results. That is, use of two dimensional analysis can still be a good approach, but to have confidence in the solution and to know how accurate the 2-D model is, the results should be compared with each other. In the numerical examples section, we have shown that, even for the specific 3-D case, "Generalized Plane Strain", there are observed differences in the results. However, the nature of the problem is very dependent on the specific package geometry and loading conditions, as well as types of imposed constraints. For the underfilled package that was chosen as the numerical example, the results can be summarized as follows;
1) The fracture results for positive $\Delta T$ are significantly different than those for a negative $\Delta T$ (from the fracture results for an unrestrained package). This is reflected in mode I stress intensity factor, phase angle, and the total strain energy release rate and is due to the effect of crack surface contact. In this particular example, cooling the semiconductor package results in a more severe fracture condition than heating the package. Thus, fracture calculations for cyclic thermal loading that assume equal severity on cooling and heating, would likely predict a higher crack growth rate than would be predicted by the more accurate nonlinear analysis described in this study.

2) It is also shown that boundary conditions have a significant effect on the solution of the problem. The second type of boundary condition described, where the substrate is restrained in both vertical and radial directions, results in the most severe fracture condition.

3) In terms of stresses ($\sigma_{xx}$, on the top edge of the chip), it was shown that the generalized plane strain (3-D) solution for this type of problem is bounded by the axisymmetric and plane strain results.

4) For the first type of constraint case (the substrate is restrained in the vertical direction only), in terms of fracture parameters the generalized plane strain results fall between those of axisymmetric and plane strain.

5) When the second type of constraint condition is considered (the substrate is restrained in both directions), the fracture results of generalized plane strain condition are lower compared with the 2-D results.

Considering the results for the described two different boundary conditions and for the different solution cases, the following general conclusion can be made: In semiconductor packaging, the model of interest is essentially a composite structure. And, especially when performing thermal stress analysis, there is a need to employ three dimensional calculations. Performing three dimensional analysis can be useful for several
reasons. First of all, we need to know the relationship between the 3-D solution and the related 2-D analyses. Second, using the comparisons, we need to answer the following questions: "Are the 2-D analyses valid for the problems encountered in this area?", "If applicable, which ones and how close are they to the 3-D analyses?". From the given underfilled package configuration and the results, we can conclude the following: Although there exists a difference between "Generalized Plane Strain" and two dimensional analyses, the differences (in terms of fracture parameters and stress distributions) are small. Therefore, "Plane Strain" and "Axisymmetric" solutions are still good approximations for this particular class of problems.
References


Vita

Ali Osman Ayhan was born in Karabük, Turkey on the 8th of January, 1972. He is the only son of Muzaffer Ayhan and Mükerrerem Ayhan.

He finished his primary school education in Safranbolu, the secondary and high school education in Karabük, Turkey. After graduating from the high school in 1989, he started his undergraduate study and obtained his B.S. degree from Mechanical Engineering Faculty, Istanbul Technical University, Turkey as the first ranking graduate in July, 1993. After graduation, he has been a trainee for two weeks in Renault Automotive Corp., Paris, France. Having worked for a year in The Turkish State Railways, Haydarpaşa, Istanbul, Turkey, he joined Lehigh University in August 1995 for his graduate study.
END OF TITLE