Chapter 2
Overview of the Simulation Methodology

2.1 Introduction

This chapter presents an overview of the simulation methodology that comprises both the art and science involved in simulating physical phenomena. It adequately summarizes the various aspects of simulation, including identification of the physical problem of interest, determination of material properties and behavior through mechanical testing, and formulations of governing equations for the finite element (FE) method. The chapter also introduces a numerical experiment framework along with a description of a typical problem solving process using FE simulation. In addition, it elaborates generic steps in performing FE simulation of structural engineering problems. Examples related to assessment of solder joint reliability are illustrated.

2.2 Simulation of Physical Phenomena

The central problem being addressed throughout this book relates to the assessment of solder joint reliability in microelectronic packages and assemblies. A quantitative assessment of reliability covers the establishment of the mechanics of solder joints under temperature and mechanical cycles, a description of the fracture process in critical solder joints and a determination of the fatigue lives of the solder joints. The small physical dimensions of solder joints found in a typical BGA package render direct measurements of parameters and property values of the solder joint difficult if not impossible. In this respect, the hybrid experimental-computational approach offers an indirect assessment of package reliability. Such methodology calls for the simulation of various phenomena exhibited by solder joints in the package and assembly during reliability testing and field operation.

Simulation is a process of recreating physically occurring phenomena of interest for a better understanding of the behavior of the system and materials, or for
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establishing their characteristics. Examples of these phenomena are viscoplastic deformation of metals, creep-fatigue interaction, brittle fracture of the bi-material interface, convective heat transfer and fluid-structure interaction. Simulation of any of these phenomena for a specific problem, such as fatigue failure of solder joints in a BGA package, is often accomplished using combinations of experimental characterization, mathematical equations and/or computational methods. An example of the experimental-computational concept involving a simulation of a solder ball shear push test of a reflowed solder joint specimen is illustrated in Fig. 2.1 and described in the following paragraphs.

The solder ball shear push test is a common test performed on reflowed solder specimens to partly quantify intrinsic properties of solder/intermetallic (IMC) interfaces. It is challenging to fabricate a standard shear test specimen with similar solder/IMC interface in the gage section as one found in reflowed solder joints. Such solder/IMC interface is a result of a chemical reaction between the solder and Ball Limiting Metallurgy (BLM) layers of the substrate during the solder reflow process, thus forming a thin intermetallic layer. Since the type of the intermetallic phase and grain structure of the adjacent reflowed solder dictate the resulting strength properties of the interface, the solder specimen is prepared using a similar reflow process to that of the package with BGA solder joints.

The experimental part of the hybrid experimental-computational approach consists of the solder ball shear push test. The test is performed on a reflowed solder joint specimen under displacement-controlled conditions. The test setup is illustrated in Fig. 2.1a. The resisting force and shear tool displacement data pairs
are recorded throughout the test. A schematic of a measured force-displacement curve for a solder joint with a relatively brittle solder/IMC interface is represented in Fig. 2.1b by the solid line. A sudden drop in the force value at the peak of the curve indicates the onset of solder/IMC interface fracture. The corresponding stress in a critical point on the solder/IMC interface should have reached the shear strength of the interface. The nominal shear strength of the interface can be defined as the recorded peak force, $F_i$ divided by the measured sheared area of the solder joint. However, it is argued that the inherent shear tool clearance in the test setup induces significant bending stress on the interface, thus the measured force constitutes the combined effects of shear and bending stresses on the interface [8].

An FE simulation of the shear push test is then employed to gain insight into the stress states at the critical point on the interface corresponding to the measured peak force. An accurate FE model of the shear push test setup is designed, as explained in Chap. 3. Comparable force-displacement curves, as predicted by the FE model (illustrated by the dashed line in Fig. 2.1b) and that measured experimentally should be ensured. Equivalent shear stress at the interface is represented, in this example, by the absolute maximum shear stress quantity. The typical distribution of the absolute maximum shear stress on Sn-40Pb solder/Ni$_3$Sn$_4$ interface corresponding to the measured peak force is illustrated in Fig. 2.2. The stress field exhibits a gradient of the absolute maximum shear stress values at the leading edge of the interface. The highest magnitude of the absolute maximum shear stress at the edge of the solder/IMC interface is taken as the shear strength of Sn-40Pb solder/Ni$_3$Sn$_4$ bi-material interface at the test temperature. It is noted that the nominal shear strength calculated based on the observed peak force over the sheared area corresponds to the predicted minimum magnitude of the absolute maximum shear stress in the central portion of the interface plane [8]. Fractographic analysis of the fractured interface should reveal that shear failure initiated at the solder/IMC interface. Such observation provides validation of the interface shear strength determined using the experimental-computational approach.

A similar concept of combining experimental methods with a computational approach by FE simulation is employed in various studies in conjunction with the assessment of solder joint reliability. This hybrid experimental-computational approach is incorporated within a numerical experiment framework.

### 2.3 Numerical Experiment Framework

The numerical experiment framework encompasses several requirements in addressing an engineering problem. The framework is schematically illustrated in Fig. 2.3. Emphasis is placed on the complete identification and synthesis of the real-world problem of interest. Utilization of computational tools such as FE analysis software and spreadsheets are central to the problem solving process. Oftentimes, controlled experiments are required both in establishing parameter values of the material model and validating predicted results.
The solder joint reliability assessment is used as an example of the real-world problem in describing the numerical experiment framework, shown in Fig. 2.3. Synthesis of the problem calls for a thorough understanding of the failure process of solder joints in a BGA package during reliability temperature cycles. Reliability temperature cycles range typically from −40 to 125 °C along with relatively high heating and cooling ramps. The high homologous test temperature activates creep deformation of the solder, especially when dwell time period at a peak temperature level is incorporated into the cycle. The large temperature range induces plasticity through mismatches in the coefficients of thermal expansion among the various types of materials making up the assembly. The fast temperature ramp rates induce viscoplastic deformation while the temperature cycles promote fatigue and creep-fatigue interaction of the solder joints. These mechanical responses should be represented by appropriate constitutive models for the stress–strain behavior of a material point under loading. Damage-based models may be required for fracture prediction of the solder joints.
The solution approach should integrate various physical laws including equilibrium of forces, strain-displacement compatibility conditions, minimum potential energy requirements and plastic flow rule in the solution process. These governing laws have been formulated into numerical procedures such as the finite element method (FEM), the finite difference method and the boundary element method. While details of these methods are beyond the scope of this book, essential features of the FEM will be discussed in relation to the accuracy of computation, validity of prediction and limitation of the solution.

The choice of suitable and valid constitutive models is central in ensuring accurate prediction of the stress–strain response of the solder joint material to load. In view of the anticipated temperature- and strain rate-dependent response of the solder alloy, the viscoplastic constitutive model, the creep and the fatigue model of the material can be employed in the simulation. Several constitutive models such as the Anand [2] and the Johnson-Cook [6], and the creep models, including hyperbolic sine and Arrhenius equations, have been coded in commercial finite element analysis (FEA) software. In addition, continuum damage-based material models are useful in simulating the fatigue failure process in bulk solder joints. The challenge in employing any of these material models lies in determining the values of the model parameters over the temperature and strain range of interest.

Values for the material model parameters need to be extracted from test data for the material under controlled experimental conditions. A comprehensive experimental program is required to establish uniaxial stress–strain diagrams for the solder alloy at different test temperature levels and applied strain rates. These curves
are then used to establish values of the set of constitutive model parameters for the solder alloy. An additional discussion on extracting model parameter values from test data is included in Chap. 4. Similarly, a series of creep-rupture curves at combinations of applied stress and test temperature levels are required for determination of the creep model parameter values. An additional set of test data is needed for use in validating the newly established model.

An FE model can be developed to incorporate relevant constitutive and damage models for solder joints. These models predict the evolution of stresses and strains in the solder joints throughout reliability temperature cycles. Characteristic stress–strain hysteresis in the critical solder joint is then employed in the fatigue life prediction of the assembly. To this end, both phenomenological- and mechanism-based fatigue life models have been developed. Selected models are discussed with respect to solder joint reliability in this book.

The accuracy and validity of the prediction through numerical experiments rely on the capability of the simplified numerical model employed, the accuracy of the input parameters and good engineering judgment on the calculated results. Challenges in employing numerical experiments in the evolution of technology are derived from the requirements to realistically mimic physical phenomena. These include modeling the compounding effect and the various effects of microstructure features, the long-term response and degradation of materials, and the processing-structure-property relationship. The success of numerical experiments strongly depends on the solid foundation of physics, analytical capability, and the added advantage of parallel computing capabilities on multi-core, multi-processor computers.

### 2.4 Deriving Finite Element Equations

The finite element method (FEM) is a numerical analysis technique for obtaining approximate solutions to a wide variety of engineering problems. The basic premise of the method is that a solution region can be analytically modeled or approximated by replacing it with an assemblage of discrete elements, as illustrated in Fig. 2.4. Within each element, the field or dependent variables of interest such as displacement, temperature and damage are governed by relevant differential equations, while specified boundary conditions are satisfied at the boundary of the solution region. Extensive treatment of FEM is beyond the scope of this book and covered in numerous publications (e.g. [3–5, 7]). This section provides a basic understanding of FEM by examining how finite element equations are derived from problems in solid mechanics.

The formulation of the displacement-based finite element (FE) method can be based on several approaches, including the variation method, the use of the principal of virtual displacement, the Galerkin method and the Ritz method. The following derivation of FE equations is illustrated using the variational approach in establishing the governing equilibrium equations of a system. The requirements
and assumptions for deriving the element equations are discussed in the following. The basic 3-node triangular element along with the linear elastic material response is used in this illustration, which aims at providing a quick overview of the steps in deriving FE equations. The element equations are dedicated for plane stress and plane strain problems in solid mechanics.

FE equations for this element are expressed in the matrix form as:

$$ [k] \{q\} = \{f\} $$

(2.1)

where $[k]$ is the stiffness matrix, vector $\{q\}$ consists of nodal displacement values and vector $\{f\}$ is the corresponding element nodal forces. Derivation of the FE equations begins with the assumed displacement field within an element. One such element is shown in Fig. 2.5 along with nodal coordinates and displacement variables. The displacement component in the $x$- and $y$-axis is denoted as $u$ and $v$ respectively.

### 2.4.1 Variation of Field Variables

Displacements within the element are assumed to vary according to the prescribed interpolation or shape functions, $N_i \ (i = 1, 2, 3)$ such that:

$$ \{u\} = \begin{bmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \end{bmatrix} $$

(2.2)

The shape functions for the 3-node triangular element can be expressed in terms of Cartesian coordinates of the element nodes:

$$ N_i = \frac{1}{2\Delta}(a_i + b_ix + c_iy), \quad i = 1, 2, 3 $$

(2.3)
Indices \( i \) in Eq. (2.3) refer to the assigned node number for the element while \( \Delta \) represents the area of the element that could also be computed using nodal coordinates of the element (refer to Fig. 2.5). In addition, the coefficients, \( a_i \), \( b_i \) and \( c_i \) are also functions of nodal coordinates of the element, as included in Fig. 2.5.

Requirements for the choice of the shape functions including continuity and compatibility conditions are deliberated elsewhere (e.g. [3, 4]).

Alternate forms of the shape functions can also be prescribed using generalized or local coordinates (\( \xi, \eta \)) as:

\[
\begin{align*}
N_1 &= \xi \\
N_2 &= \eta \\
N_3 &= 1 - \xi - \eta
\end{align*}
\]  

(2.4)

Both coordinates values vary, such that \( 0 \leq (\xi, \eta) \leq 1 \). The shape functions in Eq. (2.4) should also satisfy the condition \( N_1 + N_2 + N_3 = 1 \). Each shape function takes a value of unity at the respective node and varies linearly to zero at the other two nodes. Schematic representations of the shape functions are shown in Fig. 2.6.

**Fig. 2.5** A 3-node triangular element shown with element nodal displacements. An element nodal connectivity is defined to provide the connection between local and global node numbers for each element.
The strain-displacement relationship or compatibility conditions, based on small strain theory, can be expressed as:

$$\{\varepsilon\} = \left\{ \begin{array}{c} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{array} \right\} = \left\{ \begin{array}{c} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \end{array} \right\} = \left[ \begin{array}{ccc} \frac{\partial N_1}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_2}{\partial x} & 0 \\ \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial x} \end{array} \right] \left\{ \begin{array}{c} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \end{array} \right\}$$

(2.5)

It is noted that only three independent strain components are included in the strain vector, $\{\varepsilon\}$ and sufficient for the plane elasticity problem. The last equality follows from the form of the displacement field, as defined in Eq. (2.2). Partial differentiation of Eq. (2.3) with respect to the respective coordinate variable $x$ and $y$ results in the following:

$$\frac{\partial N_i}{\partial x} = \frac{b_i}{2\Delta}; \quad \frac{\partial N_i}{\partial y} = \frac{c_i}{2\Delta}; \quad i = 1, 2, 3$$

(2.6)
Thus, the strain-displacement relationships can be expressed in terms of nodal coordinate as:

\[
\begin{bmatrix}
\varepsilon_x \\
\varepsilon_y \\
\gamma_{xy}
\end{bmatrix} =
\begin{bmatrix}
(y_2 - y_3) & 0 & (y_3 - y_1) & 0 & (y_1 - y_2) & 0 \\
0 & (x_3 - x_2) & 0 & (x_1 - x_3) & 0 & (x_2 - x_1) \\
(x_3 - x_2) & (y_2 - y_3) & (x_1 - x_3) & (y_3 - y_1) & (x_2 - x_1) & (y_1 - y_2)
\end{bmatrix}
\begin{bmatrix}
u_1 \\
v_1 \\
u_2 \\
v_2 \\
u_3 \\
v_3
\end{bmatrix}
\]

or alternately:

\[
\{ \varepsilon \} = [B] \{ q \} \tag{2.7a}
\]

The resulting strain-displacement matrix, \([B]\) consists only of nodal coordinate values for the element, which leads to a constant strain field within the element. Thus the element is also known as a constant-strain-triangular (CST) element.

### 2.4.2 Constitutive Equations

The constitutive equations for linear elasticity of numerous metallic materials are given by the generalized Hooke’s law:

\[
\{ \sigma \} = [C] \{ \varepsilon \} \tag{2.8}
\]

The Cartesian stress and strain components are as defined in Chap. 4 [Eqs. (4.1a), (4.1b) and (4.2)]. The general form of the elasticity matrix \([C]\) is presented in Eq. (4.1a), while the specific form for the idealized plane stress or plane strain condition is shown by Eqs. (4.4) and (4.6), respectively.

### 2.4.3 Total Potential of the System: The Functional

The variational approach is employed in this illustration to derive the governing equilibrium equations, i.e. the FE equations of the continuous system. In this approach, the total potential, \(\Pi\) of the system is calculated and the stationary of \(\Pi\) is invoked with respect to the state variables. The total potential or functional of the problem in solid mechanics is represented by the total potential energy of the solid:

\[
\Pi(u, v) = U(u, v) - W(u, v) \tag{2.9}
\]

where \(U(u, v)\) is the strain energy of the system and \(W(u, v)\) is the potential of the applied loads. Considering elastic deformation of the solid (with area, \(A\) and
2.4 Deriving Finite Element Equations

thickness, \( t \) under the acting body force, \( \{ F_b \} \) and applied traction, \( \{ T \} \) along the edge length, \( S_1 \). Eq. (2.9) can be written as:

\[
\Pi(u, v) = \frac{1}{2} \int_A \left[ [q] [B]^T [C] [B] [q] \right] tdA - \int_A \{ F_b \} [q] tdA - \int_{S_1} \{ T \} [q] dS
\]

Eq. (2.10)

In invoking the principle that the total potential of the system must be stationary i.e. the variation, \( \delta \Pi = 0 \) implies the total potential energy of the deforming solid must be at a minimum for equilibrium conditions. The total potential energy for a discretized elastic domain is the sum of energies from all elements in the domain. Thus the minimum potential energy theorem requires that the displacement field \( q(u, v) \) that satisfies the equilibrium of forces and the conditions at the boundary surface also minimizes the total potential energy of the system. Such requirements can be written as:

\[
\delta \Pi(u, v) = \sum_{e=1}^{M} \delta \Pi^{(e)}(u, v) = 0
\]

Eq. (2.11)

\[
\delta \Pi^{(e)}(u, v) = 3 \sum_{i=1}^{3} \frac{\partial \Pi^{(e)}}{\partial u_i} \delta u_i + 3 \sum_{i=1}^{3} \frac{\partial \Pi^{(e)}}{\partial v_i} \delta v_i = 0
\]

Since \( \delta u_i \) and \( \delta v_i \) are independent variations and not necessarily zero, thus:

\[
\frac{\partial \Pi^{(e)}}{\partial \{ q \}} = \left\{ \frac{\partial \Pi^{(e)}}{\partial u_i}, \frac{\partial \Pi^{(e)}}{\partial v_i} \right\} = 0; \quad i = 1, 2, 3
\]

Eq. (2.12)

Operating on Eq. (2.10) yields the FE equations for the element (the superscript \( ^{(e)} \) has been omitted for convenience):

\[
\int_A \{ B \}^T [C] [B] tdA [q] = \int_A N_i \{ F_b \} tdA + \int_{S_1} N_i \{ T \} dS
\]

Eq. (2.13a)

which can be expressed in the familiar form shown in Eq. (2.1).

2.5 Procedures for Finite Element Simulation

Finite element (FE) simulation refers to a series of related problem solving activities; while employing FEM for solving the governing equations to arrive at the solution of the identified engineering problem. Figure 2.7 illustrates the process flow in the simulation of physical problems employing FEM as a computational tool. FE simulation consists of a mathematical modeling phase, an FE modeling and solution phase, and an analysis phase. As part of problem identification, mathematical modeling scopes the complex physical problem with adequate details
for FE simulation. These simplifications, while ensuring a correct and accurate predicted response of the model, limit the application of calculated results with respect to the various assumptions employed. In considering the relatively complex phenomenon of interacting surfaces, for example, a linear Coulomb’s friction model is commonly employed. The assumption of an analytically rigid body is often used to model parts with high stiffness relative to the adjacent softer deformable part of interest. Such rigid body assumption reduces computational time and cost during the solution phase through reduction of active degrees of freedom. Other simplifications and assumptions on applied loading, material laws and boundary conditions are discussed with respect to specific examples in Chaps. 5, 6, 8 and 9.
The FE modeling phase is described on the assumption that one is using the commercially available finite element analysis (FEA) software. The FE modeling phase refers to the process of setting-up a geometrical model, specifying initial and boundary conditions, and prescribing load and load cases for the analysis, as required by the software. This phase is also called a pre-processing phase. The essential steps in FE modeling and the corresponding procedures performed by the pre-processor of FEA software are listed in Table 2.1. Although different commercial FEA software provides different Graphical User Interfaces (GUI) for
Table 2.2  The types of problems for implicit and explicit analysis in FE simulation

<table>
<thead>
<tr>
<th>Implicit analysis</th>
<th>Explicit analysis</th>
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<tbody>
<tr>
<td>• Static stress/displacement analysis</td>
<td>• Rate independent/dependent response</td>
</tr>
<tr>
<td>• Linear dynamics</td>
<td>• Eigenvalue buckling load prediction</td>
</tr>
<tr>
<td>• Linear/nonlinear dynamics</td>
<td>• Natural frequency extraction</td>
</tr>
<tr>
<td>• Heat transfers/acoustics, mass diffusion, steady-state transport problems</td>
<td>• Modal superposition</td>
</tr>
<tr>
<td>• Multiphysics analysis</td>
<td>• Response spectrum analysis</td>
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<td>• Random loading</td>
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<td></td>
<td>• Implicit/explicit transient dynamics</td>
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<td></td>
<td>• Thermal-mechanical analysis</td>
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<td></td>
<td>• Structural-acoustic</td>
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<td></td>
<td>• Fluid-structure interaction</td>
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<td></td>
<td>• Fully/partially saturated pore fluid flow-deformation</td>
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<tr>
<td>Explicit analysis</td>
<td></td>
</tr>
<tr>
<td>• Simulation of high speed dynamic events</td>
<td>• e.g. Product drop test, board-level drop test</td>
</tr>
<tr>
<td>• Quasi-static metal-forming simulations</td>
<td>• e.g. Sheet metal drawing process</td>
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<tr>
<td>• Thermal-mechanical with adiabatic heating effects</td>
<td></td>
</tr>
<tr>
<td>• Adaptive meshing using ALE (Adaptive Langrangian-Eulerian)</td>
<td></td>
</tr>
<tr>
<td>• Coupled Eulerian-Langrangian (CEL)</td>
<td>• For flow problems of structural problems with extensive deformations</td>
</tr>
</tbody>
</table>

setting-up an FE model, these steps are essentially the same. A typical sequence of steps in an FE simulation is illustrated and briefly described in Fig. 2.8. The simulation steps cover the setting-up of an FE model for the solution phase, submission of the job in the solution phase and visualizing the results as part of the analysis phase. Accurate data and information gathered about the problem during the mathematical modeling phase is input into the FE model through GUI of the FEA software used.

In the solution phase, the system of linear equations for the problem are simultaneously assembled and solved for the unknown degrees of freedom. These FE equations should have been coded in the commercial FEA software. However, users have some control over the type of analysis, the choice of solution methods, the rate of convergence and the associated level of numerical accuracy. A selected list of these choices and their brief descriptions are summarized in Table 2.2. Detailed descriptions should be available in users’ manuals of the FEA software.

The FE analysis phase deals with post-processing of numerical results into meaningful graphical presentation and visualization. A strong background in physics, the mechanics of materials and materials science is required to extract meaningful information through interpretation of the calculated outcomes. Previous related experience should guide engineers in exercising good judgment and lots of common sense when extracting FE-predicted results for solutions of the problem.
Some obvious checks that can be performed immediately upon successful completion of the FE simulation job are listed in Table 2.3. Additional discussion on validating the FE model is discussed in Chap. 3 with emphasis on the solder joint reliability assessment.

### References

Solder Joint Reliability Assessment
Finite Element Simulation Methodology
Tamin, M.N.; Shaffiar, N.M.
2014, XIII, 174 p. 119 illus., 55 illus. in color., Hardcover
ISBN: 978-3-319-00091-6