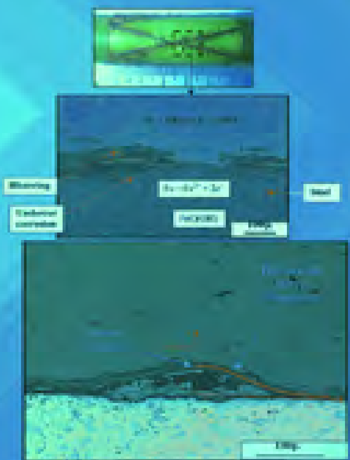
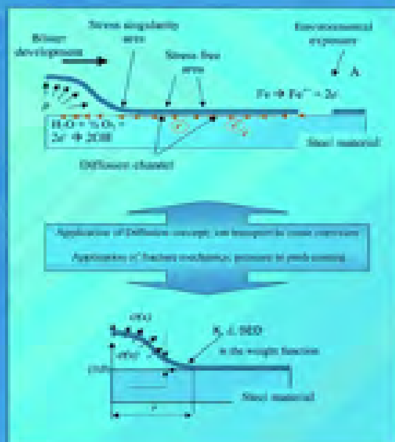
Integration of Mechanics into Materials Science Research

A Guide for Material Researchers in Analytical, Computational and Experimental Methods



Integrate the Mechanics Concepts



Yunan Prawoto

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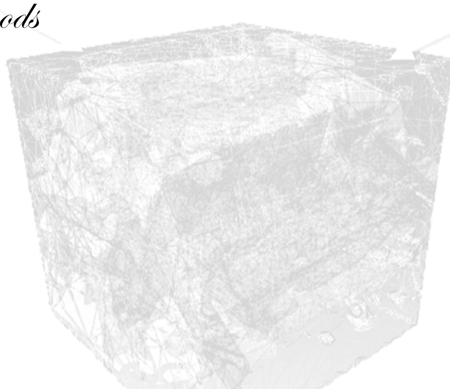

Yunan Prawoto
Faculty of Mechanical Engineering
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To my wife Anita, my daughters Almas and Alya. To all of you who cares about environment.

Preface

THIS book is written for my students. As an academician who returned to education after 15 years working in industry and business, I can understand the hardship and difficulties for master and PhD students, as well as young researchers wanting to adopt the knowledge outside their area.

While my formal education was in mechanics from bachelor until doctorate degree, I was lucky enough to work as an R&D manager/technician at the same time, responsible for the metallurgical department in an automotive supplier in its Detroit headquarters. I was also lucky enough to have worked for a laboratory that supports the metallurgical division of an oil company back in my early career. As a result, I can easily integrate the mechanics concept into materials science area. Among the students that I supervised, I noticed that students with pure materials background are commonly have great difficulties getting their works published, while the ones with mechanics background were able to publish their works with hardly any difficulties. Usually, it doesn't take long for me to teach basic mechanics again, they can integrate the concept of mechanics into their research after that. By doing so, they can publish their work easier in high impact journals. This book was prepared for them to get a jump start to be familiar with a mechanics concept.

The fact that solid mechanics applications are scattered as an array of proceedings, scientific journals and monographs are making it even more difficult for young researchers with pure materials science background to study and to know the advances of materials sciences when aspects of mechanics and mesomechanics are involved. Researchers new to the field or individuals interested in discovering applications of mechanics in materials science and engineering also need a book that bridges the gap since the undergraduate curriculum in mechanics for materials science department is typically weak, if not only skin deep. This book contributes in helping students in my study group and those young researchers who have focused on applications of mechanics in materials science. Although there are numerous books on Mechanics, their main focus is on the macroscale mechanical behavior of materials. Mechanics of materials has been dominated and used mostly by design engineers not for materials scientists and engineers who want to apply the mechanics concept.

This book does not replace the mechanics textbook. Instead it is an introductory book for non-mechanics engineers. It is written mainly for the audience with the background of materials science. In any way, the author does not claim that this book is a complete book of mechanics. It gives materials engineers and scientists alike the fundamental of mechanics. It bridges the materials scientists to the mechanics world with the intention of utilizing mechanics in their research. Should they need different topics of mechanics, this book is useful for building the foundation in their mechanics knowledge. Although the book uses mainly steel materials, the principle should be applicable to other similar materials with some adjustments.

I used LaTeX for the whole process of preparations. Thanks to the technology that enables me to do everything myself with my decade old Macbook. This book follows a format such that readers can use each chapter independently. Although it also aims to prepare new researchers starting their career in mechanics usage in materials science and engineering. It is a combination of a textbook and a monograph. My private collection to teach my research students.

You never achieve real success unless you like what you are doing, said Dale Carnegie, an Engineer that was very successful in almost everything. You and I all believe in what he said. The same person also said, *Have you seen unhappy wild horses? Have you seen unhappy wild birds? Birds that feeling blue?.. Well they never feel unhappy because they never try to impress others...* These two quotes are a perfect description for me when preparing this book. I love what I do. I don't want to and I don't need to impress others. Many parts of this book are NOT my original knowledge. They are extracted from various sources, just like other textbooks are.

I would like to thank my employer, the Universiti Teknologi Malaysia for accepting me as a faculty member after being away from academic for a while. I would also like to thank my working colleagues, whom co-authored in writing my publications that I adapted in this book. Profs and Doctors: Nasir Tamin, Nazri Kamsah, Joy Rizky, Zaini Ahmad, Azizi, Amran Alias from UTM. Prof Emmanuel Enemuoh from Univ of Minnesota Dulluth, and Mark Martin Fanone from Mubea USA. Also Prof. Aizawa from the University of Tokyo and SIT Japan. Prof Winholtz from the University of Missouri was my PhD supervisor. It was Prof Emiritus Krawitz's class in *Writing intensive course* that made me addicted to writing. Also more friends who I might have forgotten to mention here. Also I thank all the authors whom their works are cited here. I also owe thanks to ex UTM students: Roslinda, Irwan, Shima, Hazley, and many more students whom their works are adopted in this book. Essentially this book is a collection of more than *four hundred references* that I read over

the past years that relate to mechanics and materials, mesomechanics. **Never** have I claimed that this book is my original work. **It is a compilation for limited group usage**. Many examples presented in this book are already published in journals. Of course majority are authored by myself and my working colleagues as co-author(s). If you are reading the printed version of this, it is just that I want to leave my legacy. BTW the original version of this is a pdf version, and it is FREE turn to the very last page on how to get the free copy. But then students of mine told me that a pdf file will be lost easily. Therefore, I decided to make the pdf version to be printed.

You may find some language errors in my writings. I would like to apologize for my lack of proficiency. As you could probably tell, English is not my native language. But remember, not writing in a perfect English means that I am perfect in some other languages at least one; that means I am a bilingual person ⌣ Lastly, I would like to share one of his favorite poems by Kalil Gibran, I hope you can ponder it too :

- Say not, *I have found the truth,* but rather, *I have found a truth.* Say not, *I have found the path of the soul.* Say rather, *I have met the soul walking upon my path. For the soul walks upon all paths. The soul walks not upon a line, neither does it grow like a reed. The soul unfolds itself, like a lotus of countless petals.*

May the knowledge that the author shares with the readers be one of the lights that enlightens.

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Contents

Part I

REVIEW OF BASIC THEORIES

Chapter 1

Introduction: What is Solid Mechanics?

Solid mechanics. What is it? This chapter is a compilation of several resources [88; 119; 158; 204; 408] and my own definition. It is the branch of classical mechanics that studies the deformation and motion of solid materials under external actions such as external forces, temperature changes, applied displacements, etc. A material is called solid rather than fluid if it can also support a substantial shearing force. Shearing forces are directed parallel, rather than perpendicular, to the material surface on which they act.

Solid mechanics is part of a broader study known as continuum mechanics. One of the most common practical applications of solid mechanics is the Euler-Bernoulli beam equation. Solid mechanics extensively uses tensors to describe stresses, strains, and the relationship between them. It is one of the fundamental applied engineering sciences, in the sense that it is used to describe, explain and predict many of the physical phenomena around us.

The term is sometimes used in a narrow sense to include only solid materials and deformable bodies. However, often times it includes structural elements and entire structures (such as bridges, ship hulls and offshore platforms, etc.), the study of which is often referred to as structural mechanics.

It is also relevant here to clarify that the major division of the mechanics discipline are classical mechanics from quantum mechanics. Historically, classical mechanics

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1.1 Notations

Unlike the traditional books in mechanics, this book was written for material scientists, who usually are not familiar with tensor notation. Therefore, the notation is gradually introduced. By the time the readers finished the basic theories they will understand the common notation used in mechanics perfectly. Although the notations are made in such a way that are easy for the readers to follow, in some equation derivations, regular summation convention notations are used. For example, the following expressions refer to identical thing:

$$\begin{aligned} T_j &\equiv \mathrm{e}_j \cdot \mathrm{T} \\ &= n_1\sigma_{1j} + n_2\sigma_{2j} + n_3\sigma_{3j} \\ &= \begin{bmatrix} n_1\sigma_{11} + n_2\sigma_{21} + n_3\sigma_{31} \\ n_1\sigma_{12} + n_2\sigma_{22} + n_3\sigma_{32} \\ n_1\sigma_{13} + n_2\sigma_{23} + n_3\sigma_{33} \end{bmatrix} \\ &= \sum_{i=1}^{3} n_i\sigma_{ij}, \quad (j = 1, 2, 3) \\ &= n_i\sigma_{ij} \leftarrow \text{Summation convention.} \\ &\ \text{(repeating index means to be summed).} \end{aligned} \tag{1.3}$$

It is worth noting that almost always, when there is a sum over an index, the index on which it is summed is repeated precisely twice but other indices appear only once (see the last of the above equation, i appeared twice). Thus, readers should understand that many researchers prefer to drop the summation signs and adopt the summation convention that one always understands a repeated index to denote a sum.

Chapter 2

Statics of Rigid Bodies

Equilibrium condition of a body larger than a particle can be treated as a particle under either of two possible conditions: **The first one** is F the forces acting on the body were concurrent, that is, if they were directed toward a single point, the body could be treated as if it were a particle. **The second one** is if the body moved with uniform translational motion in which every particle of the body moved in the same fixed direction with uniform speed, the whole body could be treated as though it were a particle.

Many of the problems of the equilibrium of extended bodies do not fulfill these conditions. The forces acting on the body do not pass through a single point, and the motion of the body is not one of uniform translational motion but may include rotation as well. The motion of a body is often quite complicated, as in the case of a spiraling (American) football. The ball is generally thrown so that it spins about its longer axis, but, in addition to its spinning motion, the axis of rotation itself rotates, and the ball has a general translational projectile-like motion superimposed upon the rotational motions.

While all material bodies deform somewhat under the action of applied forces, it is convenient to think of them as non-deforming, or as rigid; we shall define a rigid body as one in which all dimensions remain the same, regardless of the nature of the applied forces. With this concept the statics of material bodies can be greatly simplified, instead of having to study the body as though it were a vast collection of

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particles to which the conditions of equilibrium must be applied to one particle at a time, the entire body may be treated as a single object, and its equilibrium may be studied through the introduction of a new concept called torque.

The sources for this chapter are also my own knowledge combined with the literatures, including but not limited to the following books [154; 236; 238; 302].

2.1 The Fundamental Concepts and Principles of Mechanics

The basic concepts used in mechanics are: space, time, mass, and force. These concepts cannot be truly defined; they should be accepted on the basis of intuition and experience and used as a mental frame of reference for our study of mechanics. The concept of space is associated with the notion of the position of a point P. Three lengths measured from a certain reference planes having a common point called origin in three given directions may define the position of P. These lengths are known as the coordinates of P. The space is assumed to be uniform. To define an event, it is not sufficient to indicate its position in space. The time of event should also be given. The concept of mass is used to characterize and compare bodies based on certain fundamental mechanical experiments. Two bodies of the same mass, for example, will be attracted by the earth in the same manner; they will also offer the same resistance to a change in translational motion.

A force represents an action of one body in another. It may be exerted by actual contact or at a distance, as in the case of gravitational forces and magnetic forces. A force is characterized by its point of application, its magnitude, and its direction; a force is represented by a vector. In Newtonian mechanics, space, time, and mass are absolute concepts, independent of each other. This is not true in relativistic mechanics, where the time of event depends upon its position, and where the mass of a body varies with its velocity. On the other hand, the concept of force is not independent of the other three. Indeed, one of the fundamental principles of Newtonian mechanics listed below indicates that the resultant force acting on a body is related to the mass of the body and the manner in which its velocity varies with time. We shall study the conditions of rest or motion of particles and rigid bodies in terms of the four basic concepts we have introduced. By particle we mean a very small amount of matter, which may be assumed to occupy a single point in space. A rigid body is a combination of a large number of particles occupying fixed positions with respect to each other. The study of the mechanics of particles is obviously a prerequisite to that of rigid bodies. Besides, the results obtained for a particle may be used directly in a large number of problems dealing with the conditions of rest or motion of actual

Chapter 3

Stress and Strain

STRESS is defined as force per unit area. A measure of the internal forces acting within a deformable body. It has the same units as pressure, and in fact pressure is one special variety of stress. However, stress is a much more complex quantity than pressure because it varies both with direction and with the surface it acts on. The stress field is the distribution of internal *tractions* that balance a given set of external tractions and body forces. While, strain is defined as the amount of deformation an object experiences compared to its original size and shape.

Quantitatively, stress is the average force per unit area of a surface within the body on which internal forces act. These internal forces usually arise as a reaction to external forces applied to the body. Because the loaded body is assumed to behave as a continuum, these internal forces are distributed continuously within the volume of the material body, and result in deformation. A strain field results from a stress field induced by applied forces or is due to changes in the temperature field inside the body. For linear elastic materials, the relation between stresses and induced strains is expressed by constitutive equations of *Hooke's law*. Deformations which are recovered after the stress field has been removed are called elastic deformations.

The sources for the chapter came from the following books [4; 34; 47; 48; 153; 211].

3.1 Body Forces

A body force is a force that acts throughout the volume of a body, in contrast to contact forces or applied forces. Gravity and electromagnetic forces are examples of body forces. Centrifugal force can also be viewed as body forces. This can be put into contrast to the classical definition of surface forces which are supposed to be exerted to the surface of an object. Shear forces and normal forces occurring in physical and engineering circumstances are supposed to be surface forces and exerted to the surface of an object. All cohesive surface attraction and contact forces between objects are also considered as surface forces.

3.2 Internal and Normal Stresses

An axially loaded body, such as a bar subjected to tension loading passing through its center, the stress σ, can be obtained by dividing the total normal force F_{N} by the bar's cross-sectional area A. In the case of a prismatic bar axially loaded, the stress is represented by a scalar called engineering stress or nominal stress that represents an average stress σ_{avg} over the area, meaning that the stress in the cross-section is uniformly distributed.

$$\sigma \approx \frac{F_{\mathrm{N}}}{A} \tag{3.1}$$

and

$$\sigma_{\mathrm{avg}} = \frac{F_{\mathrm{N}}}{A} \tag{3.2}$$

Graphical depiction of the situation is shown in Figure 3.1. The normal force can be a tensile force if acting outward from the plane, or compressive force if acting inward to the plane. Normal stress can be caused by several loading methods, the most common being axial tension and compression, bending, and hoop stress. For the case of axial tension or compression, the normal stress is observed in two planes and of the axially loaded prismatic bar. The stress on plane, which is closer to the point of application of the load F, varies more across the cross-section than that of plane. On the other hand, the variation of shear stress across the section of a prismatic bar cannot be assumed to be uniform.

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3.5 Practice Problems for Chapter 3

#1

The state of stress at a point is given by σ_x = 14, σ_y = 10, σ_z = 35, σ_{xy} = 7, σ_{xz} =-7 and σ_{yz} = 0. You are to evaluate the normal and shear stresses for a plane whose normal is defined by l = 2/$\sqrt{14}$, m = - 1/$\sqrt{14}$ and n = 3/$\sqrt{14}$.

#2

The state of stress at a point is given by:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \begin{bmatrix} 1 & 5 & -5 \\ 5 & 0 & 0 \\ -5 & 0 & -1 \end{bmatrix}$$

After transformation of coordinate that first and the second axes are **K=2u**$_1$**+4u**$_2$**+6u**$_3$ and **L=4u**$_1$**+4u**$_2$**-4u**$_3$. You are to compute the third axis vector and the stress after transformation

$$\begin{bmatrix} \sigma'_{11} & \sigma'_{12} & \sigma'_{13} \\ \sigma'_{21} & \sigma'_{22} & \sigma'_{23} \\ \sigma'_{31} & \sigma'_{32} & \sigma'_{33} \end{bmatrix}$$

(Answers are available in the Appendix, Chapter 25, use the provided answer wisely ◡).

Chapter 4

Differential Equations for Solid Mechanics

THE differential equations are typically needed to comprehend the problems of varying stress and strain fields in materials. In this chapter, some differential equations relating the stresses and body forces, the strains and displacements will be derived. These equations are derived from physical principles. It is also preceded with the introduction to the notations that the readers need to get familiar with. In this chapter readers are expected to get familiar with the tensor notations too, see also Appendix on Vectors and Tensors, Chapter 22.

The sources of this chapter includes the following reading materials [44; 119; 314; 408] and some OCW courses scattered from participant universities worldwide.

4.1 Be Familiar with Common Notations used in Mechanics

Since one of the goals of this book is to provide a brief introduction to mechanics of materials for those researchers with little or no previous knowledge on continuum mechanics but are interested in studying the mechanics of materials, now it is a chance to introduce notations that often used in the world of mechanics. The French mathematician *Augustin Louis Cauchy* was the first to formulate such models and notations in the 19^{th} century. A particular particle within the body in a particular configuration is characterized by a position vector

$$\mathrm{x} = \sum_{i=1}^{3} x_i \mathrm{e}_i \tag{4.1}$$

where e_i is the coordinate vectors in some frame of reference chosen. This vector can be expressed as a function of the particle position X in some reference configuration, for example the configuration at the particular time Ω_t so that

$$\mathrm{x} = \Omega_t(X) \tag{4.2}$$

When engineers and researchers in mechanics are analyzing the deformation or motion of solids, they describe the sequence or evolution of configurations throughout time. One description for motion is made in terms of the material or fixed referential coordinates, and is called a material description or the **Lagrangian description**. The other description for motion is made in terms of the spatial or current coordinates, called a spatial description or **Eulerian description**. An intuitive comparison of these two descriptions would be that in the Eulerian description one places the coordinate or reference system for motion of an object on the object as it moves through a moving fluid (e.g., on a boat in a river) while in the Lagrangian description one observes and describes the motion of the object from a fixed vantage point (e.g., motion of the boat from a fixed point on a bridge over the river or on the side of the river.)

4.1.1 Lagrangian description

In a Lagrangian description an observer standing in the referential frame observes the changes in the position and physical properties as the material particles move in space as time progresses. In other words, this formulation focuses on individual particles as they move through space and time. In Lagrangian description, the motion of a continuum is expressed by the mapping function $\chi(\cdot)$

$$\mathrm{x} = \chi(X, t) \tag{4.3}$$

or, the other way around can be expressed in its inverse, typically used in Eulerian description:

$$X = \chi^{-1}(\mathrm{x}, t) \tag{4.4}$$

which is a mapping from initial (undeformed/material) configuration Ω_0, to the present (deformed/spatial) configuration Ω_t. For example, in a Lagrangian coordinate sys-

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Chapter 5

Linear Elasticity

CONSTITUTIVE equations, such as Hooke's law for linear elastic materials, describe the stress-strain relationship in linear elasticity calculations. When a structure is expected to deform elastically and resume its original shape, a boundary-value problem based on the theory of elasticity is applied, with infinitesimal strains, under design loads. When the applied loads permanently deform the structure, the theory of plasticity applies.

The sources for this chapter comes from the books that are basically introduction to linear elasticity and some journal articles [34; 47; 48; 99; 119; 131; 133; 306].

5.1 Hooke's Law for Plane Stress

In Chapter 3, the simplification using the concept of plane stress was discussed. In this section, that simplification is discussed further. For simplicity, the stresses in the z direction are considered to be negligible here. The stress-strain relationship for an

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Chapter 6

Energy and Virtual Work

IN this chapter, the concept of energy and virtual work are discussed. They include the conservation of work and energy, the principle of virtual work, the principle of complementary virtual work, the principle of stationary total potential energy, the principle of stationary total complementary potential energy, the reciprocal theorem, Castigliano's 1^{st} theorem, and Castigliano's 2^{nd} theorem.

This chapter is an extraction of several sources from the OCW materials and reading materials available in your library too [131; 133; 253; 305].

6.1 Energy in Deforming Materials

Energies can be grouped into kinetic energies, which are due to movement and potential energies, which are stored energies. Elastic strain energy is a potential energy. Elastically deforming a material is in many ways similar to raising a weight off the ground; in both cases the potential energy is increased. Elastic energy can be increased by giving work towards the system. When a small load is given on a large metal slab, the slab will undergo small strains. When the load is removed, the slab uses the internally stored strain energy to return to its initial state.

In a real material undergoing deformation, some of the supplied energy is converted into heat. However, with the ideal elastic material under study in this chapter,

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becomes:

$$\left.\begin{aligned}\delta W_C &= \sum_{i=1}^{n} u_i \delta P_i + \sum_{i=1}^{m} u_{si} \delta R_i \\ &= \sum_{i=1}^{n} u_i \delta P_i + \sum_{i=1}^{m} u_{si} \left(\sum_{j=1}^{n} \frac{\partial R_i}{\partial P_j} \delta P_j \right) \\ &= \sum_{i=1}^{n} \left(u_i + \sum_{j=1}^{m} \left(u_{si} \frac{\partial R_j}{\partial P_i} \right) \right) \delta P_i \\ &= \sum_{i=1}^{n} \left(u_i + \frac{\partial W_{Cs}}{\partial P_i} \right) \delta P_i \end{aligned}\right\} \tag{6.35}$$

where W_{Cs} is the complementary work of support reaction $\sum_{i=1}^{m} u_{si} R_i$. Since the displacement and strain of the actual structure at the same state are essentially compatible, the principle of complementary virtual work implies that the complementary virtual work is equal to the complimentary virtual strain energy. Therefore,

$$\sum_{i=1}^{n} \left(u_i - \frac{\partial U_C}{\partial P_i} + \frac{\partial W_{Cs}}{\partial P_i} \right) \delta P_i = 0 \tag{6.36}$$

or,

$$u_i = \frac{\partial U_C}{\partial P_i} - \frac{\partial W_{Cs}}{\partial P_i} \tag{6.37}$$

the second term on the right hand side is the displacement due to the support settlements. For the special case when there is no movement of all supports, the complementary work W_{Cs} and the relation simply reduces to:

$$u_i = \frac{\partial U_C}{\partial P_i} \tag{6.38}$$

This is called Castigliano's second theorem. It stated that for a given elastic structure that is compatible, the partial derivative of the complementary strain energy minus the complementary work due to the support movements with respect to the applied concentrated load is equal to the displacement or rotation at the location and in the direction of that load.

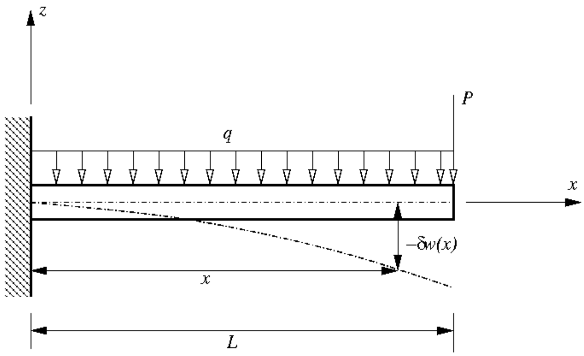

Figure 6.7 A beam deflected due to the loading.

6.4 Practice Problem for Chapter 6

Figure 6.7 is referred for this problem. On the beam, point loading P and distributed loading q are applied. You are to derive the deflection using the principle of virtual work based on

$$\delta W_{ext} = \delta W_{int} \tag{6.39}$$

(Answer is available in the Appendix, Chapter 25, use the provided answer wisely ◡).

Chapter 7

Viscoelasticity

VISCOELASTIC materials are materials for which the relationship between stress and strain depends on time or, in the frequency domain, on frequency. The effect of speed/rate of stretching shows that the viscoelastic material depends on time. This contrasts with the elastic material, whose constitutive equation is independent of time, for example it makes no difference whether an elastic material is loaded to some given stress level for one second or one day, the resulting strain will be the same.

This chapter is intended for researchers working on materials like polymers and polymer-matrix composites viscoelastic response is often used as a probe in polymer science, since it is sensitive to the material's chemistry and microstructure. The concepts and techniques presented here are important for this purpose, readers can find how linear viscoelasticity can be incorporated into the general theory of mechanics of materials, so that structures containing viscoelastic components can be designed and analyzed. The sources for this chapter are mainly from the continuum mechanics books [42; 89; 266].

7.1 Introduction

In viscoelastic materials, the slope of a plot of stress vs. strain depends on strain rate. Inelastic solids represent a subset of viscoelastic materials: they have a unique equilibrium configuration and ultimately recover fully after removal of a transient

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Chapter 8

Plasticity

FOR materials researchers, plasticity usually refers to the deformation of a material that is non-reversible. In this chapter the complexity of crystallographic deformation mechanisms and evolving dislocation substructures is not considered and the plastically deforming material is replaced by a homogeneous continuum. Although plasticity mechanisms are the result of atomic defect processes a continuum phenomenological approach is simpler from the mechanics point of view. As the material is loaded beyond its elastic limit, Hooke's law does not apply, the material yields, begins to flow and residual, permanent deformation results after unloading.

The mechanisms for plastic deformation can vary widely. At the crystal scale, plasticity in metals is known to be the consequence of dislocations. In brittle materials such as rock, concrete, and bone, plasticity is caused predominantly by slip at microcracks, while for ductile materials, once the load exceeds the yield strength, the extension increases more rapidly than in the elastic region, and when the load is removed, some amount of the extension remains. This chapter discuss plasticity more from mechanics point of view rather than from metallurgical one. It intends to provide motivations and basic hypotheses of elastoplastic theory and presents some of the more classical results of the theory with the hope that the readers, materials researchers, benefit of this chapter too.

This chapter is compilation of several introductory materials for plasticity [64; 83; 156; 176; 222; 231; 254; 397].

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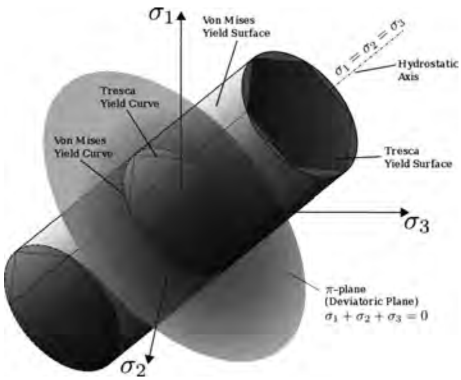


Figure 8.2 Yield locus.

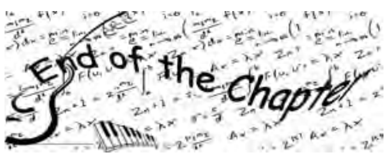
reality there are much more theories out there. This chapter should give you a start so that you can slowly immerse yourself in the mechanics world. Only that way can you be familiar with the concept and eventually have no barrier when reading the papers consisting mechanics elements.

8.7 Practice Problems for Chapter 8

Unlike the linear elasticity problems, problems in plasticity is almost impossible to be solved without the help of a computer. Prof. Louie L. Yaw from Walla Walla University (Washington State) compiled an easy to implement examples of 1D plasticity problems. So, here the exercise is adopted from his works (http://people.wallawalla.edu / louie.yaw/plasticitypublications/1Dplasticity.pdf). The task is to develop algorithm for

- Perfect plasticity
- Isotropic hardening

(Answers are available in the Appendix, Chapter 25, and from his website. Thank you prof Prof. Louie L. Yaw)



Chapter 9

Mechanical Properties of Materials

IN this chapter, the discussion is dominated mainly by metals rather than other materials. It is intended as a review of certain fundamental aspects of mechanics of materials using the material's response to provide an overview of mechanical properties without addressing the complexities of stress states. A property may be a constant or may be a function of one or more independent variables, such as temperature. Properties of materials often vary to some degree according to the direction in the material in which they are measured, referred to as anisotropy. Materials properties that relate two different physical phenomena often behave linearly in a given operating range, and may then be modeled as a constant for that range. This linearization can significantly simplify the differential constitutive equations that the property describes. The properties discussed here are limited to that of basic ones that typically used for basic characterization. ASTM specifies test procedures for determining the various properties of a material. It is usually used as a guideline by experimentalists to obtain reproducible results for material properties needed. This chapter is extracted from various sources of literatures [157; 229; 334; 370]

9.1 Density

The mass density or density of a material is its mass per unit volume:

$$\rho = \frac{m}{V} \tag{9.1}$$

where ρ is the density, m is the mass, and V is the volume. In the case of volumic thermal expansion at constant pressure and small intervals of temperature the dependence of temperature of density is :

$$\rho = \frac{\rho_{T_0}}{(1 + \alpha \Delta T)} \tag{9.2}$$

where ρ_{T_0} is the density at a reference temperature T_0 and α is the thermal expansion coefficient of the material.

9.2 Tensile Strength and Tensile Stress

The most natural test of a material's mechanical properties is the tension test, in which a strip or cylinder of the material, having length L and cross-sectional area A, is anchored at one end and subjected to an axial load P at the other end. As the load is increased gradually, the axial deflection δ of the loaded end will also increase. If the value of the axial force P is less than the breaking load P_f, the tensile stress is defined by:

$$\sigma = \frac{P}{A_0} \tag{9.3}$$

The special case for this is when the material brakes,

$$\sigma_f = \frac{P_f}{A_0} \tag{9.4}$$

where the σ_f is the ultimate tensile stress, abbreviated as UTS, P_f is the load at fracture and A_0 is the original cross sectional area. Specific terminology for the case of using the original area is engineering strength. Figure 9.1 shows typical characteristics obtained by the tensile test.

9.3 Hardness

Hardness measurements quantify the resistance of a material to plastic deformation.. Macroscopic hardness is generally characterized by strong intermolecular bonds, but

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9.6.2 Fracture Toughness

It is an indication of the amount of stress required to propagate a preexisting flaw. Flaws may appear as cracks, voids, metallurgical inclusions, weld defects, design discontinuities, or some combination of them. For elastic approach, a parameter of critical stress-intensity factor (K_{Ic}), with the unit of $[Pa\sqrt{m}]$ is usually used to determine the fracture toughness of most materials, while for elastic-plastic approach the fracture toughness is denoted by J_{Ic}, with the unit of $[Joule/cm^2]$.

9.6.3 Plane Stress vs. Plane Strain

When a material with a crack is loaded in tension, the materials develop plastic strains as the yield stress is exceeded in the region near the crack tip. Material within the crack tip stress field, situated close to a free surface, can deform laterally because there can be no stresses normal to the free surface. The state of stress tends to biaxial and the material fractures in a characteristic ductile manner. This condition reflects *plane-stress*and it occurs in relatively thin bodies where the stress through the thickness cannot vary appreciably due to the thin section. However, material away from the free surfaces of a relatively thick component is not free to deform laterally as it is constrained by the surrounding material. The stress state under these conditions tends to triaxial and there is zero strain perpendicular to both the stress axis and the direction of crack propagation when a material is loaded in tension. This condition reflects *plane-strain*and is found in thick plates. Under plane-strain conditions, materials behave essentially elastic until the fracture stress is reached and then rapid fracture occurs.

The most common test specimen configurations are the single edge notch bend (SENB or three-point bend), and the compact tension (CT) specimens. Plane-strain fracture toughness requires a specimen whose thickness exceeds some critical thickness (B).

$$B \geq 2.5 \left(\frac{K_{Ic}}{\sigma_y} \right)^2 \tag{9.12}$$

where σ_y is the yield strength. Table 9.4 shows the typical toughness values for some engineering materials.

Stress Corrosion Cracking

In the corrosive environment, cracks develop and propagate well below K_{Ic}. In fact, the subcritical value of the stress intensity, designated as K_{Iscc}, may be much less

Table 9.4 Approximate fracture toughness for commonly known engineering materials.

Material	**Fracture Toughness** [$MPa\sqrt{m}$]
Aluminum alloy	24-30
Steel alloy	50-70
Titanium alloy	44 - 66
High Purity of Aluminum	14 - 28
Aluminium oxide	3 - 5
Silicon carbide	3 - 5
Soda-lime glass	0.7-0.8
Concrete	0.2 - 1.4
Polymethyl methacrylate	0.7 - 1.6
Polystyrene	0.7 - 1.1
Mullite-fibre composite	1.8 - 3.3
Silica aerogels	0.0008 - 0.0048

than that of K_{Ic}. The crack initiates at K_{Ic} and subsequently propagates at a rate governed by the slowest process, which most of the time is the rate at which corrosive ions can diffuse to the crack tip. As the crack advances and finally it reaches K_{Ic}. Stainless steels, for example, are employed because under most conditions they are passive. Very often one finds a single crack has propagated whiles the left metal surface stays apparently unaffected.

9.7 Brittle vs. Ductile Materials

The behavior of materials can be broadly classified into two categories; brittle and ductile. Steel and aluminum usually fall in the class of ductile materials, while glass and cast iron fall in the class of brittle materials. The material response for ductile and brittle materials are exhibited by both qualitative and quantitative differences in their respective stress-strain curves. Ductile materials will withstand large strains before the specimen ruptures; brittle materials fracture at much lower strains. The yielding region for ductile materials often takes up the majority of the stress-strain curve, whereas for brittle materials it is nearly nonexistent. Ductile materials exhibit large strains and yielding before they fail. On the contrary, brittle materials fail suddenly and without much warning.

Ductility is especially important in metalworking, as materials that crack or break therefore:

$$\begin{aligned} E_1 &= \frac{\sigma_1}{\varepsilon_1} \\ &= V_f E_f + V_m E_m \end{aligned} \tag{9.18}$$

This is similar with the *series* and *parallel* concept, Equation (9.18) is when the loading direction is the same with the fiber direction, while the following equation is when the loading direction is perpendicular to the fiber direction:

$$E_2 = \frac{V_f}{E_f} + \frac{V_m}{E_m} \tag{9.19}$$

In more complicated composites, for instance those with fibers in more than one direction or those having particulate or other nonfibrous reinforcements, Equation (9.18) provides an upper bound to the composite modulus, while Equation (9.19) is a lower bound. One of the most popular models is an empirical one known as the Halpin-Tsai equation:

$$E = \frac{E_m[E_f + \xi(V_f E_f + V_m E_m)]}{V_f E_m + V_m E_f + \xi E_m} \tag{9.20}$$

ξ is an adjustable parameter that results in series coupling for ξ = 0 and parallel averaging for very large ξ.

Chapter 10

Steel Materials and Metallurgy

STEEL metallurgy studies the physical and chemical behavior of elements comprising steel, their intermetallic compounds, and their mixtures, which are typically called ferrous alloys. It is also the technology of steels, the way in which science is applied to their practical usage. In this chapter, the discussion is kept minimal because the book is written for audience familiar with materials science and engineering. This chapter is only intended to refresh the knowledge on steel materials used in the example parts discussed in the later chapters.

This chapter is extracted from various sources of literatures [38; 40; 51; 53; 62; 80; 81; 87; 135; 148; 149]

10.1 Brief History

The first evidence of human metallurgy dates from the 6000 yrs BC, and was found in the archaeological sites of Majdanpek, Yarmovac and Plocnik, all three in Serbia. While all of those were non ferrous, the ferrous metallurgy began approximately

1000 years after that. The earliest surviving iron artifacts, from 5000 yrs BC in Iran and 2000 yrs BC in China, were made from meteoritic iron-nickel. By the end of the 2nd millennium BC iron was being produced from iron ores from South of the Saharan Africa to China [135]. During the medieval period, means were found in Europe for producing wrought iron from cast iron using finery forges. For all these processes, charcoal was required as fuel. Meanwhile, the earliest surviving iron

Figure 10.1 One of the world largest iron meteorites, weight of more than 15 tons.

artifacts were extracted from iron-nickel meteorites, which consists about 6% of all meteorites that fall on the earth, see Figure 10.1. That source can be often identified with certainty because of the unique crystalline features of Widmanstätten. Those artifacts include the ones 5000yrs BC found in Iran, 4000 yrs BC from Ancient Egypt and 2000 yrs BC in China. The man made steel was first appears long after that, in 500 yrs BC China, while new methods of producing it by carburizing bars of iron in the cementation process were devised in the 1700s. In the Industrial Revolution, new methods of producing bar iron without charcoal were formulated. In the late 1850s, Henry Bessemer invented a new steel making process, involving blowing air through molten pig iron, to produce mild steel. Bessemer patented *a decarbonization process, utilizing a blast of air* in 1855. Modern steel is made using technology based on Bessemer's process. Bessemer was knighted in 1879 for his contribution to science. Sir Henry Bessemer (19 January 1813 - 15 March 1898) was an English engineer, inventor, and businessman. Bessemer's name is known in connection with the Bessemer process for the mass manufacturing of steel. *The Bessemer process* for mass producing steel, was named after him, see Figure 10.2 [40].

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cubic crystal structure is again the more stable form of delta-ferrite (δ-Fe). Ferrite above the critical temperature A_2 (Curie temperature) of 771 °C (1,044 K; 1,420 °F), where it is paramagnetic rather than ferromagnetic, is beta ferrite (β-Fe). The term beta iron is seldom used because it is crystallographically identical to, no more than 0.021 wt% at 723 °C (1,333 °F), and only 0.005% at 0 °C (32 °F).

Only a very small amount of carbon can be dissolved in ferrite; the maximum solubility is about 0.02 wt% at 723 °C (1,333 °F) and 0.005% carbon at 0 °C (32 °F). This is because carbon dissolves in iron interstitially, with the carbon atoms being about twice the diameter of the interstitial vacancy, so that each carbon atom is surrounded by a strong local strain field. Hence the enthalpy of mixing is positive (un favorable), but the contribution of entropy to the free energy of solution stabilises the structure for low carbon content. 723 °C (1,333 ° F) also is the minimum temperature at which iron-carbon austenite (0.8 wt% C) is stable; at this temperature there is a eutectoid reaction between ferrite, austenite and cementite.

Acicular ferrite is a microstructure of ferrite that is characterized by needle shaped grains when viewed in two dimensions. The grains, actually three dimensional in shape, have a thin lenticular shape. This microstructure is advantageous over other microstructures because of its chaotic ordering, which increases toughness. Lenticular ferrite Acicular ferrite is formed in the interior of the original austenitic grains by direct nucleation from the inclusions, resulting in randomly oriented short ferrite needles with a 'basket weave' appearance. This interlocking nature, together with its fine grain size, provides maximum resistance to crack propagation by cleavage. Acicular ferrite is also characterized by high angle boundaries between the ferrite grains. This further reduces the chance of cleavage, because these boundaries impede crack propagation. It is reported that nucleation of various ferrite morphologies is aided by nonmetallic inclusion; in particular oxygen rich inclusions of a certain type and size are associated with the intragranular formation of acicular ferrite. Acicular ferrite is a fine Widmanstätten constituent, which is nucleated by an optimum intragranular dispersion of oxide/sulfide/silicate particles. Figure 10.5 shows the typical ferrite structures.

10.4.2 Martensite

The martensite is formed by quenching of austenite which traps carbon atoms that do not have time to diffuse out of the crystal structure. This martensitic reaction begins during cooling when the austenite reaches the martensite start temperature (M_s) and the parent austenite becomes mechanically unstable. At a constant temperature below M_s, a fraction of the parent austenite transforms rapidly, then no further transforma-

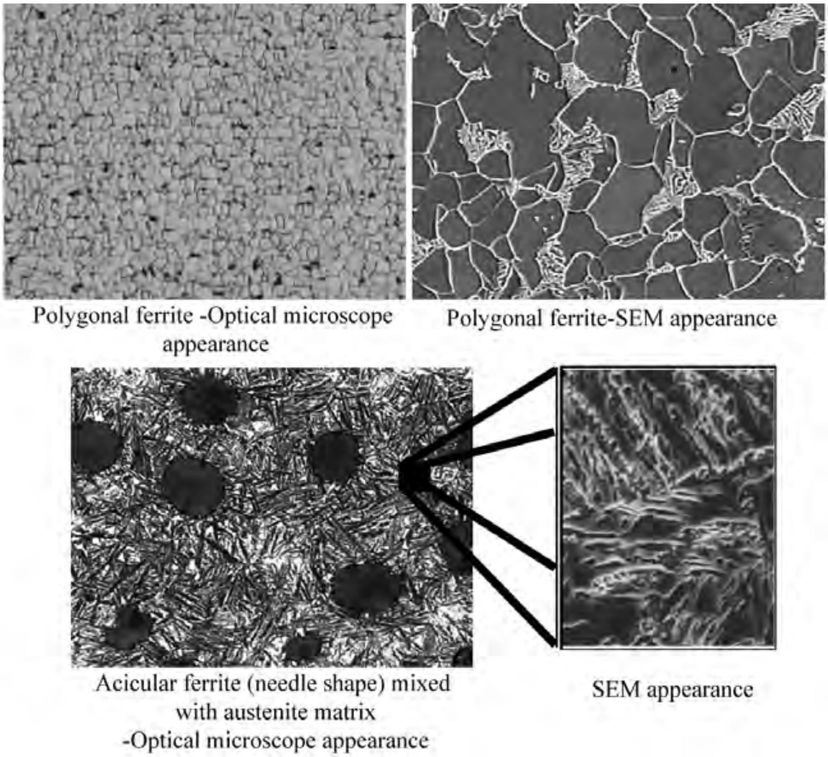

Figure 10.5 Typical appearance of ferrite structures.

tion will occur. When the temperature is decreased, more of the austenite transforms to martensite. Finally, when the martensite finish temperature (M_f) is reached, the transformation is complete. Martensite can also be formed by application of stress (this property is frequently used in toughened ceramics and special steels like TRIP steels (i.e. transformation induced plasticity steels)). Thus, martensite can be thermally induced or stress induced.

One of the differences between the two structures is that martensite has a body centered tetragonal (BCT) crystal structure, whereas austenite has a face centered cubic (FCC) structure. The transition between these two structures requires very little thermal activation energy because it is a diffusionless transformation, which results in the subtle but rapid rearrangement of atomic positions, and has been known to occur even at cryogenic temperatures. Martensite has a lower density than austenite, so that the martensitic transformation results in a relative change of volume.

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Chapter 11

Fundamental Concepts in Modeling with Finite Element

THE finite element method (FEM) or finite element analysis (FEA) is basically a discretization technique in mechanics. The basic concept in the physical interpretation of the FEM is the subdivision of the mathematical model into disjoint, non-overlapping, components of simple geometry, called *elements*. The response of each element is expressed in terms of a finite number of degrees of freedom characterized as the value of an unknown function(s) at a set of nodal points. The response of the mathematical model is then considered to be approximated by that of the discrete model obtained by assembling the collection of all elements. In simple terms, FEM is a method for dividing up a complicated problem into small elements that can be solved in relation to each other. It is a special case of the Galerkin method with polynomial approximation functions. The solution approach is based on eliminating the spatial derivatives from the partial differential equation (PDE). The sources for this chapter are published articles [162; 273; 299; 408] and also my unpublished personal notes and collections.

11.1 Brief History

FEM is originally the work of Hrennikoff and Courant. Hrennikoff's work discretizes the domain by using a lattice analogy, while Courant's approach divides the domain into finite triangular subregions to solve second order PDEs that arise from the problem of torsion of a cylinder [82; 161]. Courant's contribution was evolutionary, drawing on a large body of earlier results for PDEs developed by Rayleigh, Ritz, and Galerkin. FEM obtained its real debut when NASA sponsored the codes that is now known as NASTRAN. The term finite element itself was first coined by in 1960. In the early 1960s, engineers used the method for approximate solutions of Hrennikoff and Courant, which essentially FEM in various problems in stress analysis, fluid flow, heat transfer, and other areas. The first book using the title of FEM was that of Zienkiewicz's and Chung's, published in 1967.

Nowadays, so many commercial codes are available, Abaqus, Adina, Ansys, etc. Most those packages originated in the 1970s. Materials engineers and scientists can easily use them in their research. It is worth noting that evaluation must be done carefully since these programs allow an engineer to make mistakes at a rapid rate of speed. Errors caused by misunderstanding or oversight is not correctible by the use of a better commercial codes or more powerful computer.

Disadvantages of the FEM

Unlike analytical solution, FEM does not produce a general closed-form solution, which could permit one to examine system response to changes in various parameters. The FEM obtains only *approximate* solutions. Therefore, it has inherent errors. Mistakes by users can be serious, garbage in $\rightarrow$ garbage out. However, this statement should only be taken positively. It should not discourage the readers from using it. In fact, it is only encouraging the readers to use FEM with a full understanding.

11.2 Basic Concepts

The basic concept of FEM is to divide a complicated structure into simple geometries. A simple linear equation such as $F = kx$ is not valid on a large scale for a part with complex geometry but they can be valid for a small region of material within the complex part. However, if a complex physical object is broken down into finite number of small elements for which simple equations can be solved with acceptable accuracy, then reconnects elements at nodes as if nodes were pins or drops of glue

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reader's convenience. The discussion is also limited to the area of austenite seen in Figure 11.4.

Main Matrix, Solid Solution of the Austenite

The solid solution austenite is the main matrix of the structure. It is typically defined as one of the allotropes of iron or a solid solution of iron with carbon and other alloying elements diffused uniformly throughout the structure. The typical UTS (ultimate tensile strength) of this constituent typically ranges from 700 MPa to 850 MPa. Its yield strength is not commonly known. Only the engineering yield strength is usually known. The value of yield strength was assumed to be in the range of 290 MPa to 320 MPa. Its mechanical properties can usually be simulated as elasto-plastic. Depending on the researchers, the failure condition varies from simple von Mises yielding, to Tresca yielding to Johnson Cook's law. To accommodate the strain rate influence, many publications simulate it with the Johnson Cook's law. Several researchers have successfully implemented the modeling of the solid solution [65; 322].

Austenite Twin

The austenite twin is part of the austenite phase. Under the microscope, it usually appears as a straight texture within the main matrix. It is believed that the twin boundary is a mirror lattice symmetry. It is also known as a result of atomic displacements / crystallographic slip produced by shear forces (mechanical twins) or heat treatment (annealing twins). Austenite is believed to have the latter type. It contributes to increasing the strength of the austenite matrix. Twin variant, including twin plane and twin direction, have an influence on the texture of the austenite phase, which is one of the most crucial factor for determining strength and ductility. Research on this twin boundary and its variation on strain hardening rate, mechanical properties, and plastic strain are moderately available [245; 318]. In this simulation, the mechanical property of this constituent is assumed to be 1.02% of that of the solid solution. A failure law similar to that of the solid solution was applied for the simulation.

Grain Boundary

Strongly related to the two constituents above, the grain boundaries separate grains, which typically have the same crystal orientations. This interface is also known to have atomic mismatch and therefore traditionally is also known to be stronger than the matrix itself. When the mismatch is slight, by the order of few degrees, it is called small-angle grain boundary. It is also widely known that the grain boundaries are more chemically reactive than the grain. It is also a favorite location for the impurities to exist. Research on this is scarcely available [316; 318; 354]. For this research the grain boundary was assumed to have the mechanical property of 1.05% of that of the solid solution. A similar failure law was applied for the simulation.

Carbide

In austenite, (Cr) carbide often exists within the matrix as a Cr_2C, which shares the same crystal structure with the solid solution. Although other forms that are non-stoichiometric also exist, such as $Cr_{23}C_6$, Cr_3C, or Cr_7C_3. In austenitic stainless steel, the other commonly known form is Cr_3C_2, which has the crystal structure of orthorhombic. In any form, carbide is brittle and hard. Precipitation of the carbide at the grain boundaries, depleting the grain edges of chromium in austenitic stainless steel, is one of the causes for intergranular fracture. For the purpose of the modeling, the value of the mechanical properties are 518.7 GPa for Young's modulus, with the Poisson's ratio of 0.29. The failure mode is brittle cracking with strain type failure to follow typical hard materials [215].

Sigma (σ) phase

From the metallurgical point of view, the existence of sigma phase is seen as a detrimental. This phase is typically formed as a chromium or molybdenum inter-metallic compound formed during slow cooling or dwelling at high temperature (for stainless 304/316 stainless steel about 600^{o}C-1050^{o}C [355]). Sigma phase is also suspected to be transformed from the residual δ-ferrite at a similar range of temperature. Sigma phase typical morphology can be detrimental, as it tends to work like a stress concentrator, especially if it is perpendicular to the loading axis. Among the practitioner, the term sigma phase embrittlement is often used to describe its detrimental effect. Furthermore, this phase is also known to be brittle. In this research, this constituent is assumed to have the failure type of brittle failure.

Nitride

Similar to the chromium carbide, nitride exists within the austenite grain in the form of a hard and brittle substance. Its high lattice energy reflects the strong attraction of N_3^- for metal cations. The modeling in this case treated this constituent similar to carbide [244].

Delta (δ)-ferrite

δ-ferrite here refers to the residual δ-ferrite. It is a residual intermediate phase that typically transforms to austenite. The detrimental effect of this phase lies in the fact that under certain condition, it can transform into sigma phase that is brittle. In this modeling, the δ-ferrite is assumed to have mechanical properties that are slightly lower than that of the matrix. The failure mode is similar to that of matrix. Although from the mechanics point of view, this can be seen as a discontinuity, δ-ferrite worries practitioners more due to its possibility to change to other harder constituents, such as martensite [63; 403].

Alpha' (α') phase

The alpha$^{single'}$ phase usually refers to hcp martensite rather than the orthorombic (alpha$^{double'}$) martensite. This alpha$^{single'}$ phase is known to exist in austenitic stainless steels. Publications on this constituent are quite available [85; 92; 191; 259]. Although not as hard as the nitride or the carbide, this constituent is also thought to promote the brittleness. For the analysis here, the value of this is similar with that of non-tempered martensite and the failure mode is brittle failure with the failure strength at the level of 1800 MPa.

(MnS or NiS) Inclusion

Inclusions are commonly found in austenite either endogenous or exogenous. Endogenous inclusions, also known as indigenous, occur within the metal and are the result of chemical reactions. These products precipitate during cooling and are typically small. The second type, exogenous inclusions are caused by the entrapment of nonmetals, typically larger. They include oxides, sulfides, nitrides and phosphides. Similar to other hard constituents discussed above, inclusions are also considered detrimental. They disrupt the homogeneity of structure, so their influence on the mechanical and other properties is significant. Several studies on this subject are available [400]. For this analysis, brittle failure law is applied. A summary of the constituents adopted in this model is shown in Figure 11.5, while the rationales of the values usage is shown in Table 17.1. It is worth noting that here, the shape of the constituents also gives significant influence due to the continuum mechanics approach used. The influence of the strain rate for hard materials was neglected.

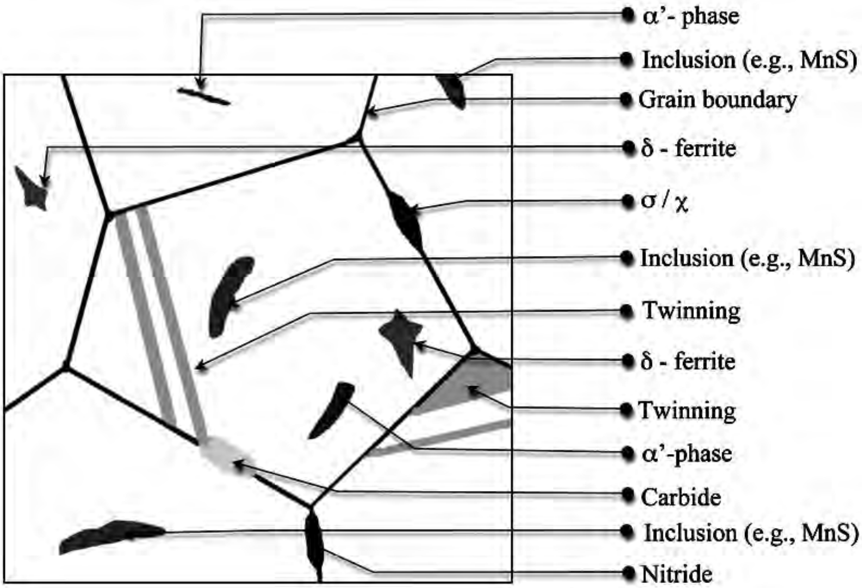

Figure 11.5 Major constituting phases in typical austenite grain that contributes to the load carrying capacity [220; 249; 311; 317].

11.4.3 Computational Approach

The computational approach was implemented with the commercial code $Abaqus^{TM}$ combined with OOF^{TM}, an open source computational tool developed by MIT with NIST. Two steps of modeling are employed: global model creation and local model creation. A similar concept was used in previous publications [284; 290]. Figure 11.6 illustrates the simplified concept. The global modeling enables us to apply the external loading and boundary conditions. This global model is then executed to obtain the stress and strain values near the area of interest. Using this strain result, the local model is then computed to obtain the final results. Unlike the traditional multi-level modeling, this method is not cumbersome. The basic microstructure is created by using the information of the austenite steel constituents that are simulated. This digitized micrograph is then meshed into finite element usable data. Using the strain result from the global model, the boundary condition for the local model is then set up. The modeling started with the global model creation. For this purpose, a two-dimensional CT (compact tension) specimen was made. For this simulation, a plain strain condition was chosen. A similar approach was used [272; 289]. This

Table 11.1 Main mechanical characteristics of austenite constituents.

Const.	**Main characteristics related to modeling**	**Ref.**
Matrix	UTS 700-850 MPa; can usually be simulated as elasto-plastic.	[65; 322].
γ-twin	Influencing texture of γ- phase; UTS is assumed to be 1.02% of that of γ- phase; same failure law.	[245; 318].
Boundary	Atomic mismatch; stronger than the matrix itself. UTS is assumed to be 1.05% of that of γ-phase; more chemically reactive than the grain. It is also a favorite location for the impurities to exist.	[316; 318; 354].
Cr_xC_y	exists as a Cr_2C, or in non-stoichiometric, such as $Cr_{23}C_6$, Cr_3C, or Cr_7C_3. Potential int. fract. Stiffness of 518.7 GPa, ν 0.29. The failure mode is brittle cracking with strain type failure	[215].
σ -phase	Cr or Mo inter-metallic comp. formed due to slow cooling or dwelling at high temp. (for SS 304/316 $\approx$ 600^{o}C-1050^{o}C); transf. from the res. δ-ferrite at a same temp.; failure type of brittle failure.	[355].
Nitride	Also brittle; high lattice energy reflects strong attraction of N_3^- for metal cat. Failure mode similar to carbide.	[244].
δ-ferrite	Slightly lower stiffness than that of the matrix; share similar failure law with that of matrix.	[63; 403].
α' -phase	HCP martensite, not orthorombic(α'') martensite; not as hard as the nitride or the carbide, similar with that of non-tempered mart.; failure mode is brittle failure with the failure strength of 1800 MPa.	[85; 92; 191; 259].
Inclusion	Disrupt the homogeneity; brittle failure law is applied.	[400].

approach is sufficient to mimic the failure condition well [272]. In this research, the size of the sample for the global model is 18.75 mm wide with the distance from pin to pin being 8.25 mm. A displacement of 5x10^{-2} mm is given to the upper pin, while the lower pin is held stationary. The analysis was performed under the *explicit* environment with the time of 0.1s. This condition simulates a speed of approximately 500μm/s or, 30mm/minute.

The result of the global model is then exported to the local model, which is created

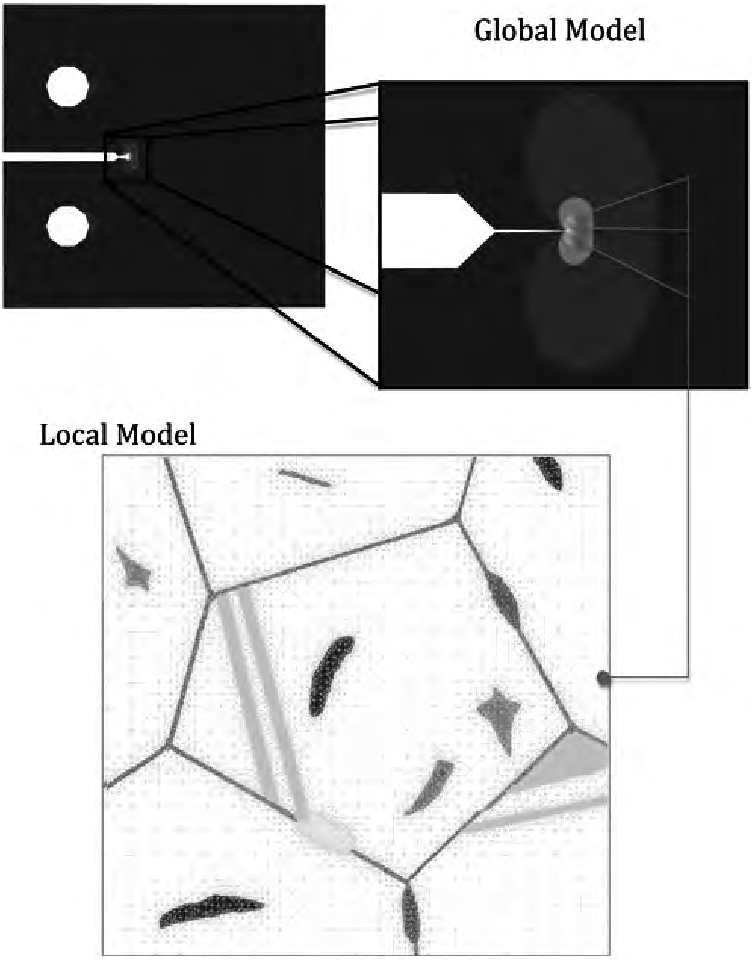

Figure 11.6 Procedure of the modeling. The local model is based on stainless steel with approximate grain size 6-7 ASTM GS. The square is 50μm x 50μm.

using the OOF^{TM}. Using the strain result from the global model as boundary conditions for the local model enabled us to simulate it efficiently. Further discussion on the modeling technique is can be found elsewhere [274; 289]. The end results are the stress distribution .

The failure mechanism of the model is designed based on the individual mechanisms. For the solid solution, twin boundary, grain boundary and δ ferrite, Johnson-

Cook model is used. Similar research has also been published [70; 280]. The damage accumulation ω is expressed as the summation of the plastic strain, expressed in Equations (11.38) and (11.39) [174; 175]:

$$\omega = \sum \left(\frac{\Delta \overline{\varepsilon}^{pl}}{\overline{\varepsilon}_f^{pl}} \right) \tag{11.38}$$

where the plastic strain is calculated as:

$$\overline{\varepsilon}_f^{pl} = \left[d_1 + d_2 \exp \left(d_3 \frac{p}{q} \right) \right] \left[1 + d_4 \ln \left(\frac{\dot{\overline{\varepsilon}}^{pl}}{\overline{\varepsilon_0}} \right) \right] \tag{11.39}$$

where p is the pressure stress and q is the von Mises stress. $d_1 - d_4$ are damage parameters, 0.13, 0.13, -1.5, and 0.011, respectively [70; 280]. For the brittle constituents, the rule of maximum stress/strain was employed.

$$\overline{\epsilon} = \overline{\epsilon}_{crit} \tag{11.40}$$

or

$$\overline{\sigma} = \overline{\sigma}_{crit} \tag{11.41}$$

It is also worth noting that the phase transformation is not considered in the model here.

11.4.4 Mechanics Point of View

The results of the global model are shown in Figure 11.7. This model is based on the assumption that the material is homogeneous. The figure shows the von Mises stress distribution when the model is run using an elastoplastic model. The classical *textbook style* plastic zone is obtained by running the model in a linear elastic approach. The shape of the plastic zone agrees with the theoretical prediction using the von Mises yielding condition, which typically appears in elementary fracture mechanics textbooks, e.g., [54; 274], which is essentially the solution to:

$$PZ = C \cdot \left(\frac{K}{\sigma_{YS}} \right)^2 \left(1 + \frac{3}{2} \sin^2 \theta + \cos \frac{\theta}{2} \right) \tag{11.42}$$

where the θ is the angle between the crack line and the location, and K is the SIF (stress intensity factor).

50 μm to the right of the crack tip, the local models are embedded. Figure 11.8 shows the results of the static analysis or the stress distribution when the sample undergoes slow and small loading, or a static condition, where stress does not cause any

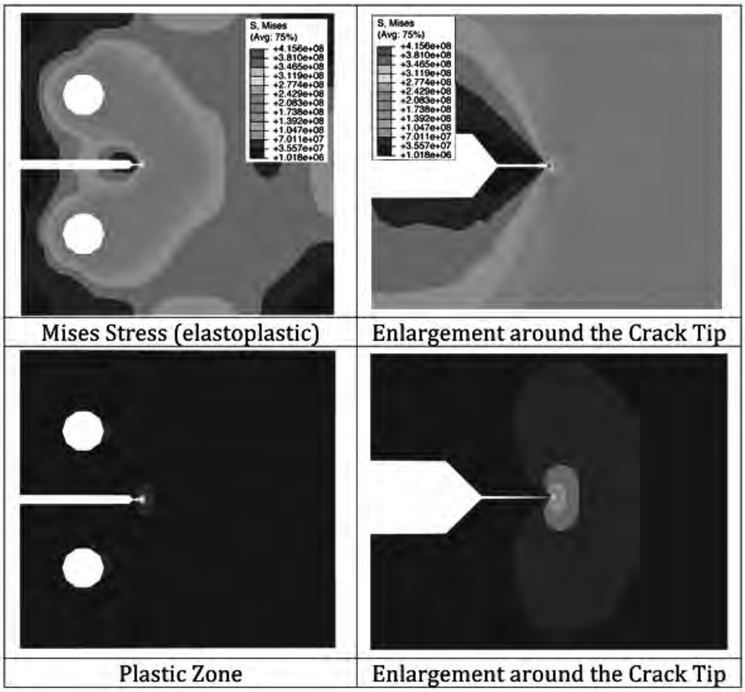

Figure 11.7 Main results of the global model.

damage. The figure shows that although the stresses do concentrate around the hard constituents, they are not detrimental at low stress level. In fact, they are beneficial in increasing the strength of the austenite. This statement generally applicable for all three conditions, in front of the crack tip, below it and above it. The analysis was continued with an *explicit* environment. This environment considered the speed of the loading. It simulates the more realistic phenomenon of cracking. The yield condition depends upon the strain rate. Figure 11.9 shows the implementation of this. The data was obtained from the global model. The figure shows one of the evaluation results, in which the condition is in front of a crack. The velocity here shows that the slower the velocity is, the lower the yield is, to follow JC equation [174; 175] :

$$\sigma^0 = [A + B(\varepsilon^p)^n] \cdot \left(1 + C \cdot \ln\left(\frac{\dot{\bar{\varepsilon}}^{pl}}{\dot{\bar{\varepsilon}}_0}\right)\right) \cdot \left(1 - \hat{T}^m\right) \tag{11.43}$$

where $\hat{T}^m$ is the homologous temperature. Cracking path predictions were obtained

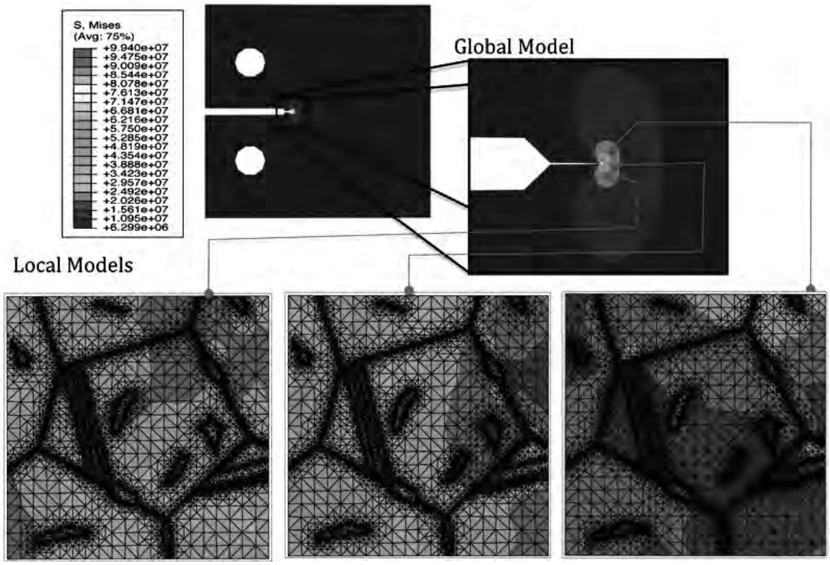

Figure 11.8 Stress distribution of the model at low stress; shown is the von Mises stress distribution. The local model simulates the condition 50μm in front of the crack tip, 50μm below it, and 50μm above it.

and shown in Figure 11.10. It is predicted based on the amount of the damage, ω. In general, from the mechanics point of view, in all locations, the cracking tends to initiate near the hard particles. In this case, from the left edges, through the solid solution nearby the grain boundary, and to the grain boundary where the carbides exist. It then continues to an area near the δ-ferrite. It is worth noting that in this situation, the nitride did not give a lot of influence due to the elongated shape that is parallel to the main loading axis. α' on the other hand gives some influence in generating high damage. However, it is not as large as the other hard constituents. Inclusions that are located parallel give less influence than the inclusions that are elongated perpendicular to the main loading axis. This fact agrees strongly with the basic principles of fracture mechanics. In short, three factors influencing the condition are: shape of the particles, strain rate, and failure law for the matrix.

Metallurgical Point of View

It has been known for long that microstructural variables influence the mechanical properties of materials, e.g., [209; 312]. These property variations and subsequently

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Chapter 12

Homogenization Concept Implemented with Finite Element

Several introductory variations of the homogenization theory are available, the simple one is presented here. This chapter is mainly based on the paper that the author wrote together with professor Aizawa from the University of Tokyo back in 2001 [6; 277; 285]. In this theory, the local constitutive structure is thought to have a locally specified periodic unit cell as shown in Figure 12.1. Hence, every physical variable field on this material support can be expressed by the combination of the averaged part with the local disturbance as depicted in part (b) of the figure. Assuming that the periodicity, ϵ, should be sufficiently small, every physical field $u(x,y)$ in total can be represented by the following asymptotic expansion in ϵ:

$$u(x,y) = u^0(x) + \epsilon\, u^1(x,y) + \frac{1}{2}\epsilon^2 u^2(x,y) + \ldots\ldots \text{ for } y \equiv x/\epsilon \tag{12.1}$$

or,

$$u(x,y) \simeq u^0(x) + \epsilon\, u^1(x,y) \tag{12.2}$$

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Chapter 13

Simple Analytical Examples

IN this chapter examples of classical analytical solid mechanics are discussed. The examples presented are not original of the author. They are extracted from various sources [55; 160; 164; 301]. They are presented here as examples for analytical research guidance.

13.1 Taking Advantage of Polar Coordinate

A polar coordinate system is a two-dimensional coordinate system in which each point on a plane is determined by a distance from a fixed point and an angle from a fixed direction. The fixed point (analogous to the origin of a Cartesian system) is called the pole, and the ray from the pole in the fixed direction is the polar axis. The distance from the pole is called the radial coordinate or radius, and the angle is the angular coordinate, polar angle, or azimuth [55]. Using $x = r\cos\theta$ and $y = r\sin\theta$, one can derive a relationship between derivatives in Cartesian and polar coordinates.

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either by comparing the complete expression for Δu_2 in Equation (13.25), or σ_{22} in Equation (13.24) to the analogous small r result, $\sigma_{22} = \frac{K_I}{\sqrt{2\sigma r}}$. For an edge crack penetrating by depth a into a half-space under the same remote tension, K_I is famously known to be 1.12 times that value, and for a circular crack of radius a in a large solid it is $2/\pi$ times that value. These values are usually known as a greek letter β. Readers interested in further discussion on this should refer to fracture mechanics books [108; 124; 264; 274].

The examples shown here are very easily implemented in the materials science research. The scale of the analysis here can directly be implemented in the mesomechanics scale.

made negative Poisson's ratio foam (also called anti-rubber, dilational material, or auxetic material).

- Measure the amount of permanent compression retained by the specimen by either measuring the new distance between the marks or by measuring the size of the transformed sample.
- Other kinds of moulds are possible and have been used successfully by others.

14.8 Concluding Remarks

This chapter shows example of how one can see certain topic purely from the mechanics point of view. Auxetic materials have a lot of potential applications from biomedical to automotive and defense industries. Also, these materials could potentially be used for completely new structures with special functions. However, more research work needs to be done for further understanding of these materials and their applications to real components. From the mechanical and computational point of view, it is predicted that research on this subject will be dominated by the unit cell concept, hierarchical, homogenization of both periodic/ordered and disordered cells. Until recently, almost all relevant papers have been based on ordered structures, which is convenient for the purpose of analysis. However, in the near future, the work presumably will be dominated by study of disordered structures since that analysis is closer to real material structures. The author believes that such materials, with little existing understanding of deformations in the presence of disorder, will require a newer theory and computational approach that could go beyond the currently available homogenization concept.

Chapter 15

Plastic Zone of Chiral Structure Material

This chapter summarizes the method of analytical formulation and computational approach of stress intensity factor and plastic zone calculation for auxetic materials, which have negative Poisson's ratio. A chiral structure based material is selected as an object of the study due to its popularity. The stress intensity factor is used in combination with the von Mises yielding condition to estimate the plastic zone's shape and size. The results show that macroscopically the shape of the plastic zone for auxetic material is the same with that of ordinary materials. However, its size is smaller due to the reduction in its Young's modulus from the solid material of which the auxetic material is made. Microscopically, an auxetic material has its plastic zone shape that is unique to its microstructure. Homogenization theory was convenient to use to bridge between the microscopic and macroscopic models.

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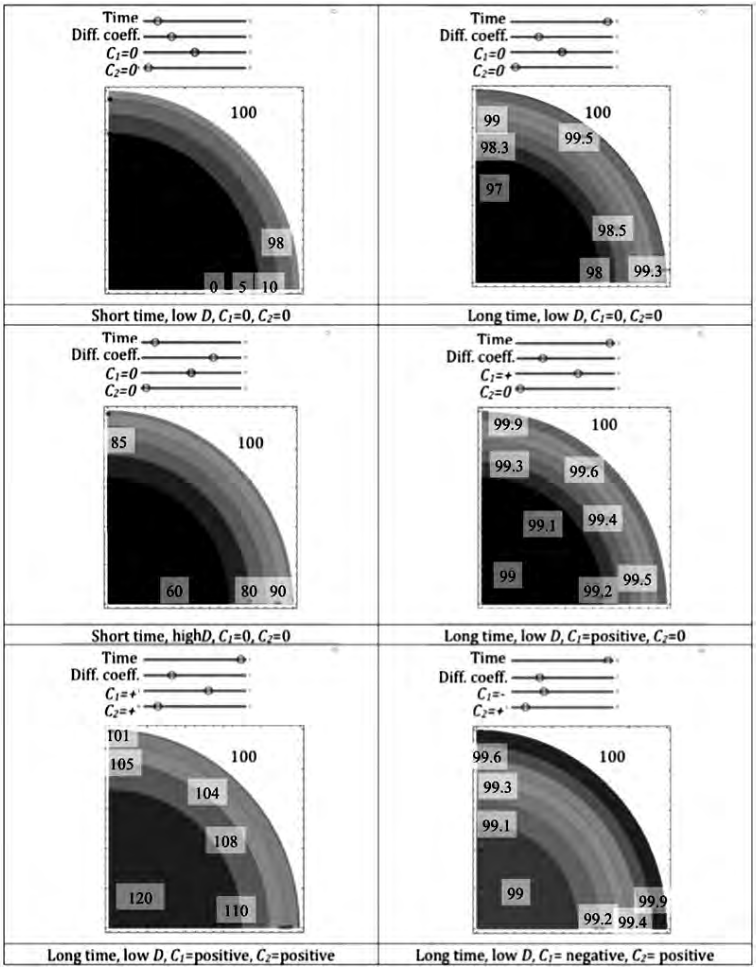

Figure 16.2 Numerical solution to cylindrical equation for our modified diffusion law. Constants are made adjustable with $Mathematica^{TM}$ to accommodate the variation of environments and types of surface engineering methods [276].

C_2, the condition becomes closer to the actual phenomena. In order to obtain the value that is closer to the experimental value, modeling in $Abaqus^{TM}$ is performed. It is shown in Figure 16.3. In the figure, all parts except the steel part follow the diffusion law. The main diffusion takes place through the channel that is assumed to be 1 μm located in between the steel and the coating. Other sources of diffusion include the coating itself. It is also worth noting that the direction of the diffusion is not necessarily inward. Based on the modified diffusion law and depending on the situation, the diffusion direction can be from underneath the coating (e.g. pretreatment) and outward through it. This concept is in agreement with the physical/experimental observation. The element types used are CPE3 (3-node linear element) and CPE4R

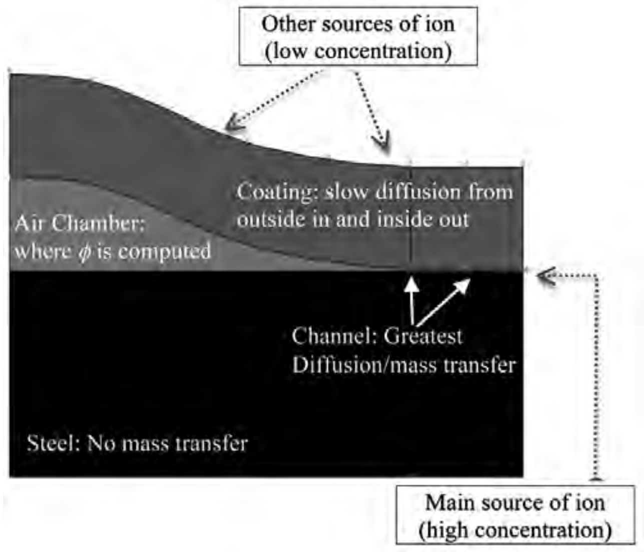

Figure 16.3 Basic modified diffusion modeling.

(4-node bilinear element, with reduced integration). The unit for computation is in μm. Coating thickness is 50 μm, all other units subsequently to follow this. Figure 16.4 illustrates the fundamental difference between the currently proposed equation with the conventional diffusion equation.

16.4 Discussion and Conclusions

In this chapter "*paper* and *pencil*" approach was used to integrate the mechanics concept into coating problem, the governing law for blister formation and development using modified Fourier solution for diffusion is developed. Implementation is performed using $Mathematica^{TM}$ and $Abaqus^{TM}$. The equation is proven capable of simulating the cathodic blistering closer to reality than those currently available.

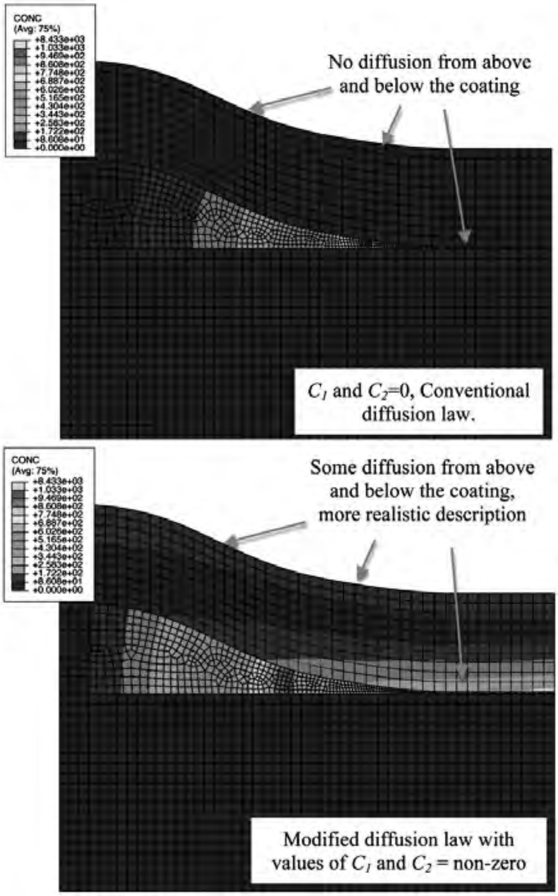

Figure 16.4 Computational results assuming C_1 and C_2 = 0 (conventional diffusion) and modified diffusion equation (C_1 and $C_2 \neq 0$).

It is capable of describing the continuously growing cathodic blistering occurring as natural phenomena or under laboratory conditions, while the conventional diffusion equation fails to do so. The result is beneficial for materials engineers and scientists working with coating or other surface engineering methods similar to coating.

Chapter 17

Rule of Mixture based on Homogenization

This chapter shows an example of the homogenization concept in microstructure research utilizing the mesomechanics approach [279]. It is one of the author's publications. The drawback of the traditional rule of mixture (ROM) is briefly discussed. The technique considers the effect of morphology based on classical continuum mechanics, taking the advantages of fracture mechanics. As an example, a model that simulates the possible configuration of constituting phases commonly found in austenite microstructure is chosen. The result is compared with traditional ROM. It is found that although similar, the result is better due to the stress amplification that is accommodated in the method, unlike the traditional ROM, which merely considers only the volumetric ratio.

17.1 Introduction

In many occasions, the need to homogenize physical properties of heterogeneous materials is unavoidable. The attempts to improve the method of averaging heterogeneous materials have been actively done over the past decades [186; 294; 296; 313; 319; 363]. There were also tendencies to incorporate the characteristics of the chemical compositions and microstructures while doing so [214; 230; 249; 378; 395]. However, to the knowledge of the authors, no article that discusses the incorporation of the shape of the constituent in the averaging process easily available. Most of the simple techniques available are basically similar to that of centroid concept, where almost all physical properties are averaged and treated like body mass, but the reality is different.

This short chapter highlights methods on how to incorporate the shape of the constituents in a simple manner. Classical continuum mechanics can then be applied and subsequently, better averaging method can be formulated. Although no new method is to be presented in this technical note, the idea of using the method for microstructure has not been done, let alone for austenite constituents.

The ausetenite is chosen due to its popularity. It is one of the common microstructural forms in steel. Researchers have been fascinated by the characteristics of austenite practically since its discovery and especially with the rise of stainless steels [220; 353]. Publications on the general characteristics of austenite and steel have flourished ranging from the point of view of purely metallurgy to mechanics [29; 100; 241; 348; 402]. At the same time research and understanding on the individual constituting phases have also been increasing both quantitatively and qualitatively, e.g., [303]. Among those published researches, several studies discuss the constituents that are known to contribute and influence the load carrying capacity [130; 220; 249; 311; 317]. The potential of tailoring the microstructure by means of metallurgical manipulation for particular usage is enormous [330; 354]. This is in parallel with the dynamic findings on the variation of microstructure stability and instability related to the facts that the austenite can change to other phases under specific conditions [198]. Although scarcely, research on the microscopic modeling of the stainless steel is also available [235]. This short note also aims to contribute to the advance of steel research by deepening the understanding of the characteristics of austenite by combining the mechanics and metallurgical point of views. Emphasis is put upon the load carrying capacity. Therefore, stiffness is chosen for the example in this averaging process. Although the computational modeling is based on 3xx stainless steel, the method should be applicable for other materials too.

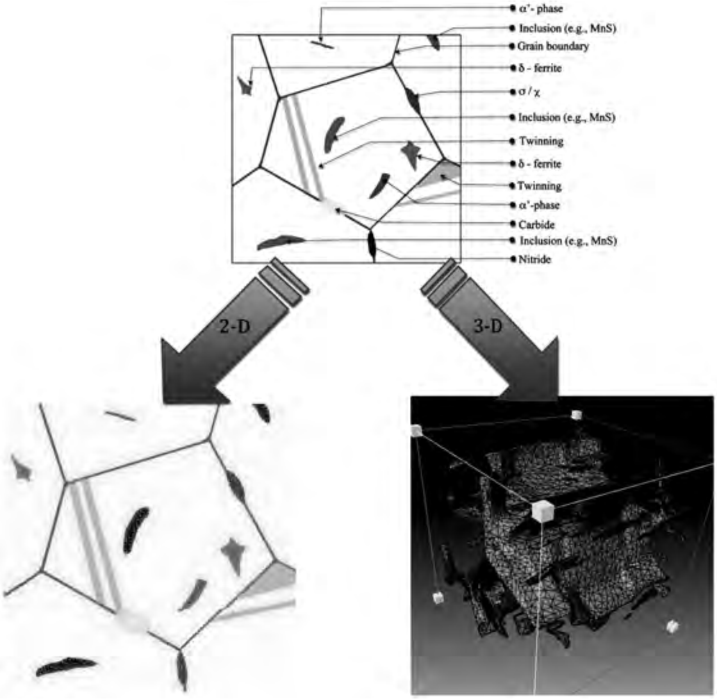

Figure 17.1 Constituting phases that are used for the basic of the model creation, partially from [286]. Note that the main matrix of austenite is intentionally not displayed on the 3D model due to visualization purpose.

17.2 Concept of Averaging

17.2.1 Rule of Mixture (ROM)

ROM is mathematical expressions which give some homogeneous property of the heterogeneous materials in terms of the properties, quantity and arrangement of its constituents. It is nothing but an operational tool that uses weighted volume average of the component properties in isolation to obtain the magnitude of the property for the heterogeneous materials. The simple mathematical expression is:

$$\bar{\rho} = \frac{1}{(\sum_{i=0}^{n} V_i)} \cdot \sum_{i=0}^{n} (\rho_i) \cdot (V_i) \tag{17.1}$$

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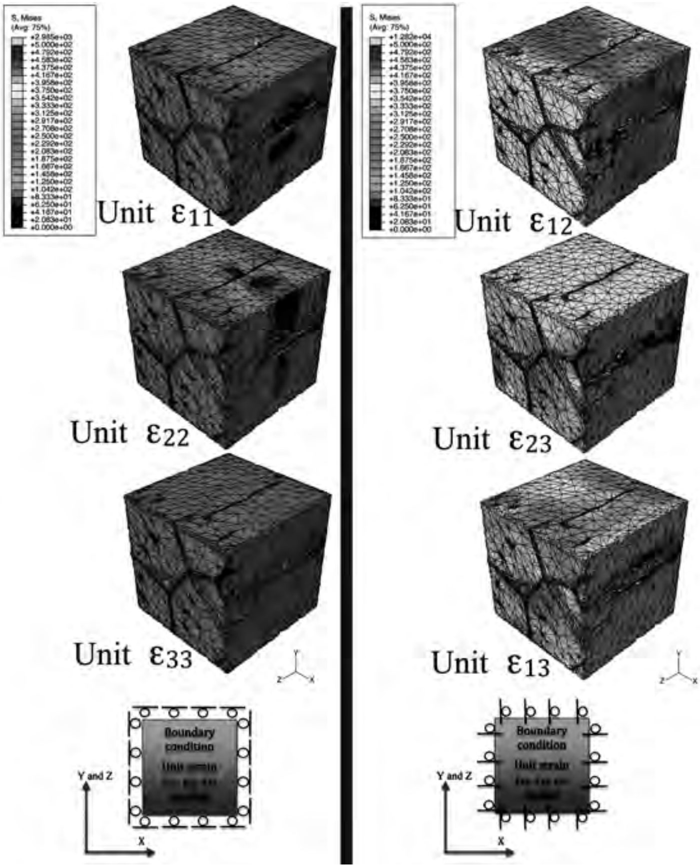

Figure 17.5 Stress distribution after unit strain application.

End of the Chapter

Part III

EXPERIMENTAL METHOD

Chapter 18

Critical View on A Standard Usage

AS the failures of orthopaedic devices due to stress corrosion cracking (SCC) have become more frequent nowadays, research on this area also has become popular. Many published articles show the basic characterizations and evaluations of the SCC performed based on ASTM standards by using the C-ring sample. This paper discusses stress redistribution during SCC testing. The results show that the stress versus displacement equation presented in the standard is erroneous as the specimen begins to crack. It is only true for a non-cracked specimen. As the crack propagates, the sharpness of the crack tip minimizes the validity of the equation, even when the thickness reduction is taken into account. Hence, the chapter here is presented as an easy method of integrating the mechanics concept into corrosion standard that has been used incorrectly. It is extracted from author's publication [278].

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Chapter 19

Stress Intensity Factor in Coating Life Prediction

UNLIKE metals, where failure analysis and life assessment methods are quite established, the failure analysis and life assessment of coatings are often underrated and disregarded. This research encourages failure analysts to be aware of the opportunity provided by an alternative approach. The authors use energy density mechanics concepts to develop a new parameter in coating blistering. A mixed mode stress intensity factor is used as a basis for the derivation. This new parameter will be useful for researchers and practitioners working with coating life assessment. It is proposed that the assessor combines field-determined adhesion strength values and blister evaluation, together with laboratory-derived strain energy density data, to quantitatively predict remaining coating life. This approach also provides a tool in failure analysis. This chapter is extracted from one of my publications [288] .

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Chapter 20

Ferrite Fraction

This chapter shows an example paper on the influence of a ferrite areal fraction within a martensite matrix on fatigue crack propagation is studied experimentally, part of my project compiled by one of my PhD students [167]. The variation of the areal fraction is achieved by means of intercritical thermal treatment, which specifically aims at optimizing the resistance to fatigue loading. Within the intercritical annealing temperature range, the areal fraction of ferrite increases with decreasing soaking temperature. Furthermore, the experiment also reveals that the highest fatigue strength was achieved when the ferrite areal fraction was approximately 65%, which in this particular test, corresponds to 748°C. It is concluded that appropriate thermal treatment can contribute to a significant improvement of fatigue properties and strength, which was also verified by computational modeling.

20.1 Introduction

Recent developments in the research of dual-phase materials has shown both the importance of multi-phase materials and the progress that has been achieved [3; 7; 32; 144; 150; 163; 185; 192; 205; 223; 227; 260; 272; 280; 349; 357]. While conventional steel always makes it impossible to obtain at the same time both good ductility and high strength, many engineering applications, especially in modern applications such as automobile industries, require economical high strength steel with good formability. Therefore, it would be ideal if multi-phase steels mostly containing ferrite and martensite phases could be obtained by a relatively simple thermal treatment process. This dream has inspired many researchers to put their effort and energy into this subject.

In general the paths to understanding the characteristics of multi-phase steels are multiple, e.g., microstructure, thermal treatment technique, chemical metallurgy, dislocation, etc. Below is a simple classifications of some recent papers:

- **Through observation of chemical metallurgy:** Researchers in this category study the effect of carbon content and an alloying element on fatigue strength. They typically find that the fatigue strength of dual-phase steels is significantly higher than that of as-received materials, due to the difference in its local chemical metallurgy [280; 357].
- **Through observation of dislocation:** In this category researchers investigate the relationship between mechanical properties and dislocation substructures. A significant improvement of the mechanical properties of dual-phase steel can be explained by the alteration in its dislocation density [3].
- **Through thermal treatment:** Researchers in this category usually focus on the method of achieving the optimum mechanical properties they intent to obtain. These steels can be produced by annealing plain and low-alloy steels in the $(\alpha - \gamma)$ region and cooling it below the martensite start temperature at a suitable rate [185; 272]. Several researchers claim to have obtained optimum results by intermediate quenching [32]. Others have obtained this by other thermal treatments, such as intercritical annealing [7; 150; 227; 289; 349]. The methods also vary from base metals to welding [144]. They are all convinced that better mechanical properties correspond to a more homogeneous and dense distribution of the fine martensite islands in the ferrite matrix obtained by thermal treatment [144]. They also agree that both the soft and ductile ferrite matrix and strong and tough martensite particles play an important role in determining the dual-phase properties, especially the continuous yielding behaviour of the steel [32; 144].
- **Through microstructure research with a focus on morphology:** The main finding in this category is that the volume fraction of proeutectoid ferrite and martensite can be controlled to influence the strength and ductility [223; 260]. Also, that the yield strength and the ultimate tensile strength increase with higher intercritical temperatures and cooling rates [163; 205]. They also report microstructural effects on the fatigue crack growth behavior of a micro-alloyed steel and these results allow correlating the tensile properties and crack growth

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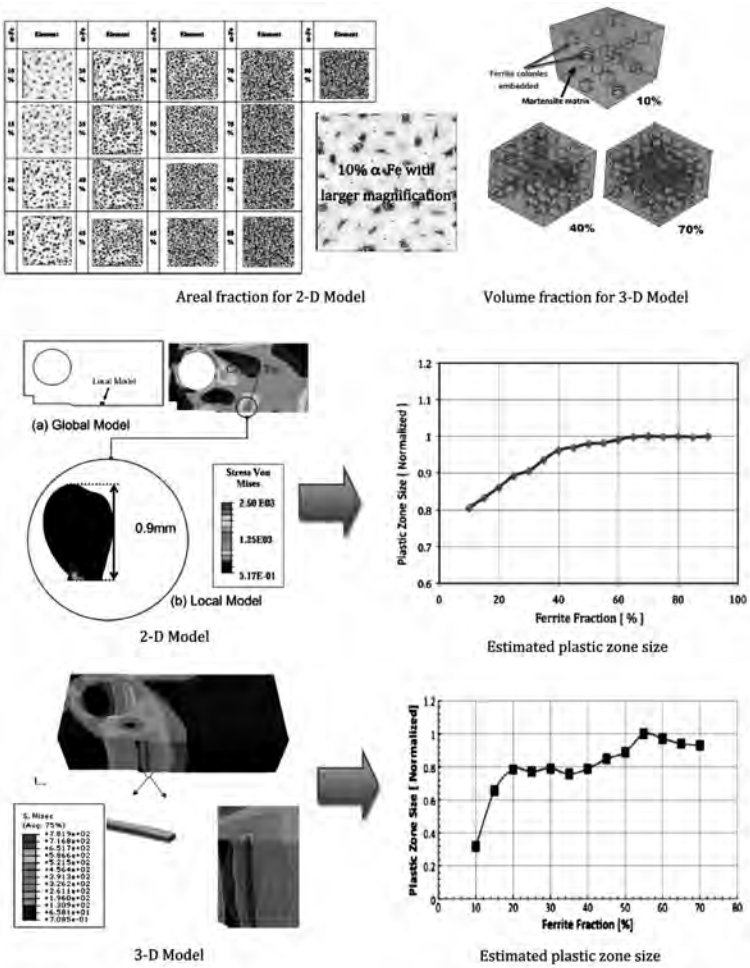

Figure 20.4 Summary of the computational models and their results [272; 289; 290].

20.4 Result and Discussion

20.4.1 Fatigue crack propagation test results

The rate of fatigue crack growth (FCG) was determined from the crack size versus the elapsed cycles data (a versus N) as shown in Figure 20.5. As can be seen in this graph, the crack grows gradually, initially at a slow rate and accelerates as the crack

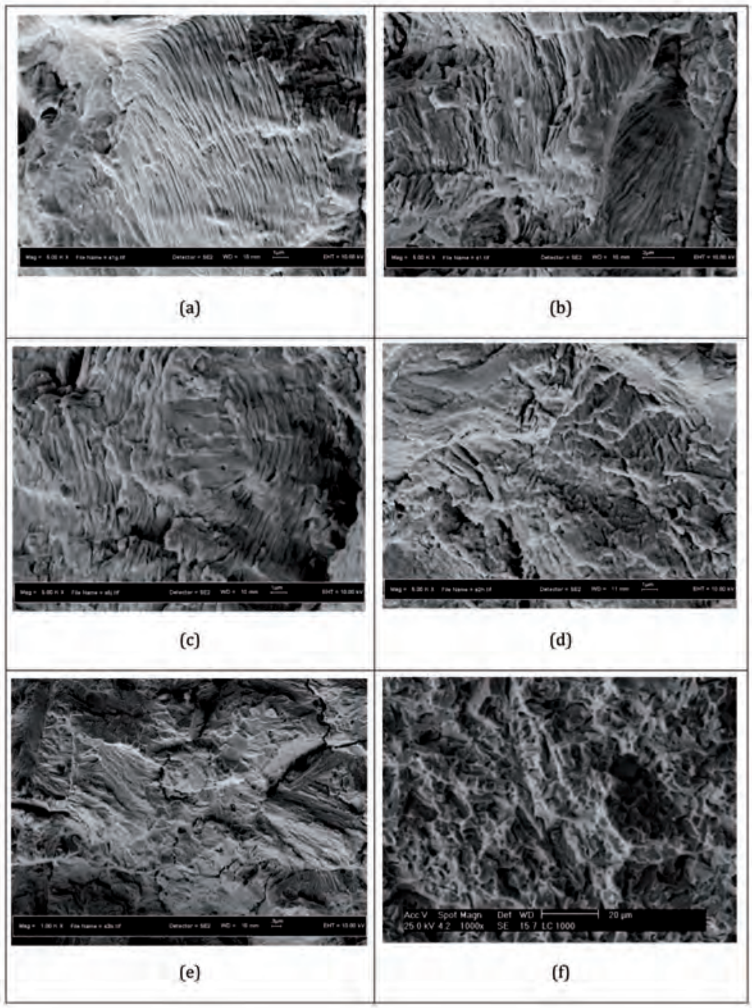

Figure 20.8 Representative fractographs, on which the striations were evaluated.

bands. Most of microcracks form slip bands adjacent to martensite-ferrite interfaces due to the side influence of the decreasing of ferrite fraction. Figure 20.8 (a) shows the striation due to fatigue. Figure 20.8 (b) shows microvoid coalescence (MVC) fracture, which is the mechanism of ductile transgranular fracture. Figure 20.8 (c) and (d) illustrates the ductile-to-brittle transition temperature in ferritic steels, and

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Chapter 21

Wire Rope Failure Modeling

THIS chapter presents an example on how to help designers and materials scientists to comprehend the mechanics of wire ropes under tension loading. It consists of simplified theory as well as computational, mechanical and metallurgical characterizations. The simple approach used enables one to comprehend the basic concept of wire rope and to utilize it in research, design and in field failure analysis. It is extracted from my published article [282].

21.1 Concept of Wire Rope

In general, wire rope is a heavy, tensile, strong, weather resistant hoisting cable made from many small metal filaments wrapped and braided together. Most often wire rope incorporates steel strands arranged in a collection around a central core. This design allows the entire wire to hold a lot of weight and still stay flexible. Performing failure analysis on the wire rope is completely different with that on other structures. The law of metallurgy, microscopically might be the same, but overall is different. The fracture mechanics law for wire rope is also different with the rest of the parts, which usually is continuum. Wire rope is used mainly due to its low bending moment

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Further, it was found that the wire ropes failure modes involved shearing in addition to regular necking.

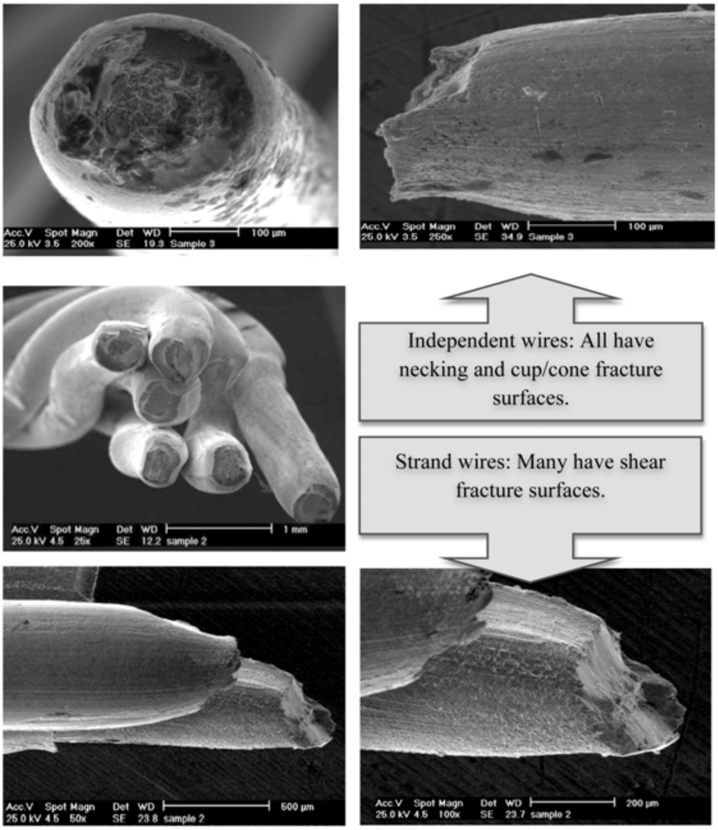

Figure 21.6 Failure modes of the wires failed both individually or as parts of wire rope.

End of the Chapter

Part IV

APPENDIX

Chapter 22

Vectors and Tensors

A vector is a quantity having both magnitude and a direction in space, such as displacement, velocity, force and acceleration. In general it is a mathematical structure formed by a collection of elements, which may be added together and multiplied scalars. A tensor is quantity that describes linear relations between vectors, scalars, and other tensors. Examples of such relations include the dot product and the cross product. *Vectors and scalars themselves are also tensors.* A tensor can be represented as a multi-dimensional array of numerical values. This chapter is extracted from various reading materials [34; 50; 338; 388]

A-1 Vector Algebra

A unit vector is a vector having magnitude of unity. If $\mathbf{a}$ is not a null vector then $\frac{\mathbf{a}}{|\mathbf{a}|}$ is a unit vector having the same direction as $\mathbf{a}$. The basic vector algebra includes operations defined for real numbers, with suitable definitions, capable of extension to an algebra of vectors. The following definitions are fundamental basic algebraic rules of vectors:

- Two vectors are equal if they have the same magnitude and direction regardless of the position of their initial point.

- A vector having direction opposite to a vector a but having the same magnitude **-a** is opposite of **a** .
- The resultant is the sum vectors **a** and **b** is a vector **c** formed by placing the initial point of **b** on the end point of **a** and then joining the initial point of **a** to the end point of **b** .
- The difference between two vectors, **a** and **b**, represented by **a-b** is the sum **a+(-b)** .
- The product of a vector **a** with a scalar n is a vector m **a** with magnitude n times the magnitude of **a**, with direction the same as or opposite to that of **a**, depending on wether m is positive or negative.

It also follows the basic algebraic laws, such as Commutative law for addition, Associate law for addition Associate law for multiplication, Distributive law, Commutative law for multiplication with scalar.

A-1.1 Scalar/Dot Product

The scalar product between two vectors, **a** and **b** is defined as:

$$a \cdot b = |a|\,|b| \cos\theta \tag{A-1}$$

where θ is the angle between **a** and **b** . The projection of a vector**a** on **b** is equal to **a** $\cdot$ $\mathbf{e}_b$, where $\mathbf{e}_b$ is the unit vector of **b**

A-1.2 Cross Product

The scalar product between two vectors, **a** and **b** is defined as:

$$a \times b = |a|\,|b| \sin\theta \;\; \mathrm{u} \tag{A-2}$$

where θ is the angle between **a** and **b** . **u** is a unit vector in the direction perpendicular to the plane of **a** and **b** to follow a right-handed system rule. For cross product, the following rules apply:

- **a** $\times$ **b** = **a** $\times$ **b** , a Cross product is not commutative.
- (**a** + **b**) $\times$ **c** = **a** $\times$ **c** + **b**) $\times$ **c** Distributive law.
- **a** $\times$ (**b**) + **c** = **a** $\times$ **b** + **a**) $\times$ **c** Distributive law.
- m (**a** $\times$ **b**) = (m **a**) $\times$ **b = a** $\times$ (m **b)** , m is a scalar.

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where $\underline{x} = (x_1, x_2, x_3)$. For each of the vector field $\mathbf{a}_i$=$\mathbf{T} \cdot \mathbf{e}_i$

$$\nabla \cdot \mathrm{T} = \sum_i (\nabla \cdot \mathrm{a}_i)\mathrm{e}_i \tag{A-51}$$

Curl

The Curl of a tensor field **T** is defined as

$$\begin{aligned} \mathrm{Curl(T)} &= \nabla \times \mathrm{T} \\ &= \sum_{mn} \epsilon_{imn} \partial_m T_{nj} \end{aligned} \tag{A-52}$$

For each of the vector field $\mathbf{a}_j$=$\mathbf{T} \cdot \mathbf{e}_j$

$$\nabla \times \mathrm{T} = \sum_j (\nabla \times \mathrm{a}_j)\mathrm{e}_j \tag{A-53}$$

A-2.6 Integral Theorems

Gauss Theorem

Gauss theorem says

$$\begin{aligned} \int_V (\sum_i \partial_i a_i) d\mathrm{V} &= \oint_S (\sum_i a_i n_i) dS \ \text{ Vector} \\ \int_V (\sum_i \partial_i T_{il}) d\mathrm{V} &= \oint_S (\sum_i T_{il} n_i) dS \ \text{ Tensor} \end{aligned} \tag{A-54}$$

Stokes Theorem

Stokes theorem for tensor is

$$\begin{aligned} \int_V (\sum_{ijk} \epsilon_{ijk} \partial_j a_k) n_i d\mathrm{S} &= \oint_C (\sum_i a_i) dx_i \ \text{ Vector} \\ \int_V (\sum_{ijk} \epsilon_{ijk} \partial_j T_{kl}) n_i d\mathrm{S} &= \oint_C (\sum_i T_{il}) dx_i \ \text{ Tensor} \end{aligned} \tag{A-55}$$

Chapter 23

Weight Function

THIS weight function is the one that the author originally developed back in 1999. The method is simple and can be applied to any shape of sample with any type of stress. The author originally developed it for converting the residual stress to residual stress intensity factor as part of his work within his PhD thesis.

B-1 Weight Function in LEFM

In here, the application of the weight function in fracture mechanics is briefly described. Further discussion is availabe elsewhere [274]. Bueckner and Rice [109; 110; 152; 274; 300] introduced the concept of the weight function (WF), which enable one to calculate the stress intensity factor (SIF) for certain loading system by using a reference SIF for different loading system. A WF exists for any crack problem specified by the geometry of the component and a crack type. If this function is known, the SIF can be obtained by simply multiplying this function by the stress distribution and integrating it along the crack length. **Basic Relations**: A crack of length $\boldsymbol{a}$ in a body may be loaded by tractions **T** acting normal to a curve Γ, see Figure B-1. The tractions are responsible for a stress field at the crack tip, which can be characterized by a SIF K^T, where the superscript ÒTÓ refers to the loading system.

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Chapter 24

Working with Commercial Codes

THIS chapter, part of appendix, presents the actual example on how to write the input file related to mechanics application in materials science. The readers are expected to know the basic usage of any simple analytical tools such as Mathematica^{TM}, MatLab, and any FEA program, such as Abaqus, Ansys, or Marc. In here Mathematica and Abaqus are used since most universities and research institutions have licenses of those two. The sources for this chapter are personal data and several public domain data [155; 199].

C-1 Mathematica

It is a computational software program used for analytical developed by Stephen Wolfram with his company Wolfram Research of Champaign, Illinois. It has several nice features that readers can utilize in their research. From simple elementary mathematical function library, matrix and data manipulation tools, 2D and 3D data and function visualization capability, until solvers for systems of equations, including PDEs. Here, source codes for the model used in Chapter 16 and Chapter 21 are

```
Manipulate[
 Module[{toplot, tosolve},

  (* YP_comment: equation solver part*)
  tosolve =
   NDSolve[
    {D[density[r, t], {t, 1}] ==
      coef (D[density[r, t], {r, 2}] + 1 / r D[density[r, t], {r, 1}])
       + cons1 D[density[r, t], {t, 1}] + cons2,
     density[r, 0] == 25 * (100 / 99.73557010035817)
       PDF[NormalDistribution[1, .1], r], density[1, t] == 100,
     (D[density[r, t], {r, 1}] /. r → 10^-8) == 0}, {density[r, t]},
    {t, 0, 10001}, {r, 10^-8, 1}];

  (* YP_comment: graphical depiction part*)
  toplot =
   Quiet[ContourPlot[density[r, t] /. tosolve /. t → time /. r → x^2 + y^2,
     {x, 0, 1}, {y, 0, 1}, RegionFunction → Function[{x, y}, 0 ≤ x^2 + y^2 ≤ 1],
     ColorFunction → "Rainbow", ContourLabels → Automatic,
     ColorFunctionScaling → True, Contours → 10, ImageSize → {500, 400}]]],

 (* YP_comment: button control part*)
 {{time, 1000., "time"}, 1., 10001., 1000., Appearance → "Labeled"},
 {{coef, 9.×10^-5, "ion diffusivity coefficient in m²/s"}, 6.0×10^-5,
  1.0×10^-4, 1.0×10^-5, Appearance → "Labeled"},
 {{cons1, 0, "1st. constant"}, -1, 1, .1, Appearance → "Labeled"},
 {{cons2, 0, "2nd. constant"}, 0, .01, .001, Appearance → "Labeled"},

 (* YP_comment: graphic appearance control part*)
 TrackedSymbols :→ {time, coef, cons1, cons2}, SynchronousUpdating → False]
```

Figure C-1 Source codes for diffusion model discussed in Chapter 16.

shown.

- Implementation of the diffusion using Mathematica. Figure C-1 shows the codes implemented with Mathematica. If this is implemented, the result would be that of Figure C-2, where the variable can be adjusted. This simple codes enables us to simulate the variable in the model in a simple manner. Recall that this models the situation describes in Figure C-3 discussed in Chapter 16.
- Implementation of the wire rope model using Mathematica. When the codes shown in Figure C-4 is implemented in Mathematica, the result would be that of Figure C-5, where the rope can be adjusted. This simple codes enables us to identify the friction in the model.

Above are two simple models that the readers can use to learn the analytical approach. Currently, there are at least three simple softwares available that are very easy to use, Matlab, Mathematica, Maple, etc.

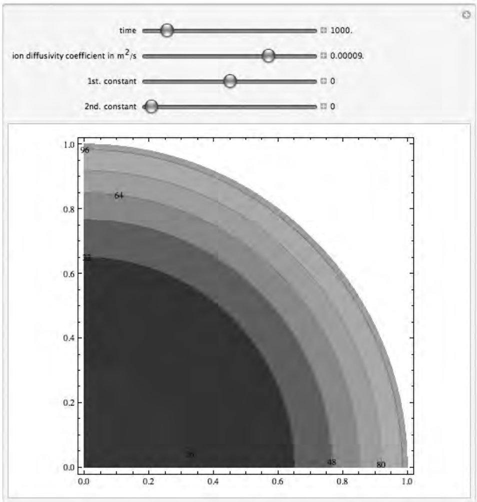

Figure C-2 Simple implementation of the diffusion model using Mathematica.

C-2 Abaqus

Nowadays, Abaqus became a software suite for finite element analysis and computer aided engineering, much different with what originally released back in 1978. Since the author is more familiar with the input file method than with the CAE method, here the example shown is based on input file. Younger generation typically prefer the CAE method and that is fine too. CAE method sure is more 'fancy'. In this particular example, since the model is to be used with materials science, the object is a three point bending on material with variation of microstructure, shown in Figure C-6. This example illustrates the modeling of crack length versus time to simulate crack propagation. and the use of crack opening displacement as a crack propagation criterion. For stable crack growth in ductile materials, experimental evidence indicates that the value of the crack opening displacement (COD) at a specified distance behind the crack tip associated with ongoing crack extension is usually a constant. Abaqus provides the critical crack opening displacement, at a specified distance behind the crack tip, as a crack propagation criterion. The other crack propagation model used in this example prescribed crack length versus time is usually used to verify the results obtained from experiments. Abaqus also provides the critical stress criterion for crack propagation in brittle materials.

In this example an edge crack in a three-point bend specimen is allowed to grow

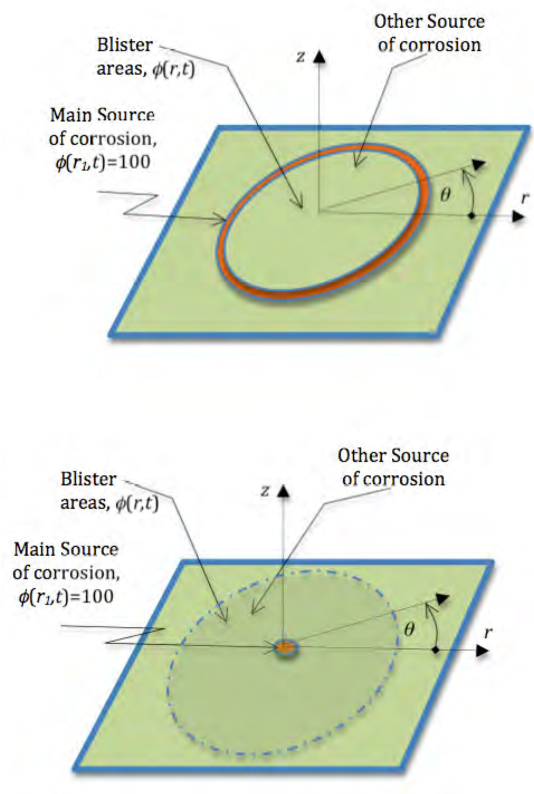

Figure C-3 The diffusion modeled using Mathematica.

based on the crack opening displacement criterion. Crack propagation is first modeled by giving the crack length as a function of time. The data for the crack length are taken from Kunecke, Klingbeil, and Schicker. The data for the crack propagation analysis using the COD criterion are taken from the first analysis. This example demonstrates how the COD criterion can be used in stable crack growth analysis.

Problem: An edge crack in a three-point bend specimen in plane strain, subjected to Mode I loading, is considered. The crack length to specimen width ratio is 0.2. The length of the specimen is 55 mm, and its width is 10 mm. The specimen is subjected to bending loads such that initially a well-contained plastic zone develops for the stationary crack. Subsequently, the crack is allowed to grow.

The analysis is carried out in two stages. The first stage consists of pushing the

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- 1.855e+11, 0.3125
- *Plastic, hardening=JOHNSON COOK
- 5.8e+08, 8.25e+08, 0.641, 0.076, 1540., 20.
- *Rate Dependent, type=JOHNSON COOK
- *Material, name=hammer
- *Density 1e+38,
- *Elastic 1e+12, 0.3
- *Surface Interaction, name=IntProp-1
- *Friction
- 0.,
- *Surface Behavior, no separation, pressure-overclosure=HARD
- **
- ** BOUNDARY CONDITIONS
- **
- ** Name: fixing sample Type: Displacement/Rotation
- *Boundary
- PickedSet31, 2, 2
- ** STEP: impacting
- * Step, name=impacting
- impacting
- *Dynamic, Explicit
- , 1.
- *Bulk Viscosity
- 0.06, 1.2
- *Boundary, amplitude=smooth pushing, type=VELOCITY
- PickedSet32, 2, 2, 5.
- ** Interaction: touching
- *Contact Pair, interaction=IntProp-1, mechanical constraint=PENALTY, cpset=touching
- PickedSurf21, PickedSurf37
- *Restart, write, number interval=1, time marks=NO
- *Output, field, variable=PRESELECT
- *End Step

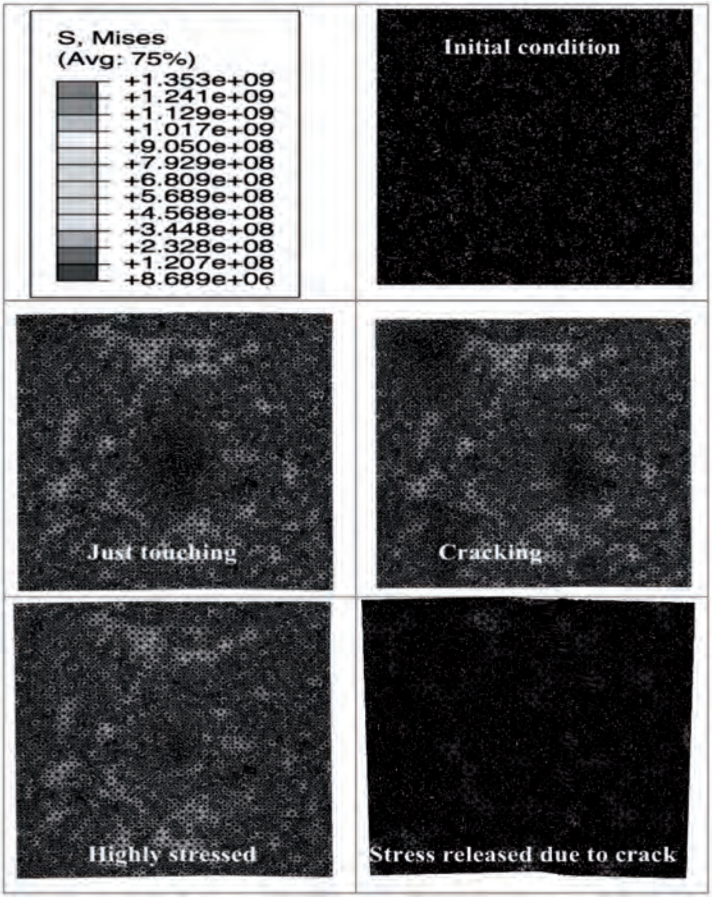

Figure C-9 Element knock down being employed in Abaqus.

After running this, safe the result and subsequently run the local model using the B.C from the Global model result. After running the global model, safe the odb file and run the following as local model. The software will give you a chance to input the name of the odb global file that you want to extract

- *Heading
- ** Job name: 15pct local Model name: 15pct
- *Preprint, echo=NO, model=NO, history=NO, contact=NO
- **

- ** PARTS
- **
- *Part, name=PART-1
- *Node
- *Submodel, type=NODE, exteriorTolerance=0.05
- LEFT,
- BOTTOM,
- RIGHT,
- TOP,
- *End Assembly
- *Amplitude, name=Amp-1, definition=EQUALLY SPACED, fixed interval=1.
- 0.5, 1.
- **
- ** MATERIALS
- **
- *Material, name=ferrite
- *Density
- 7800.,
- *Elastic
- 1.25e+11, 0.3125
- *Plastic, hardening=JOHNSON COOK
- 3.6e+08, 5.45e+08, 0.701, 0.091, 1540., 20.
- *Rate Dependent, type=JOHNSON COOK
- 0.01,1.
- *in here for element elimination: for constituent 1*
- *shear failure, type=JOHNSON COOK,
- *ELEMENT DELETION=YES
- *0.7,2,-1.58,0.0002,0.61
- *0.08, 2.1, 0.5, 0.0002, 0.61
- *tensile failure
- 2e8,
- **section control,NAME=Section-1-M1, ELEMENT
- DELETION=YES
- ***
- *Material, name=martensite
- *Density
- 8100.,
- *Elastic

- 2e+11, 0.3125
- *Plastic, hardening=JOHNSON COOK
- 6.8e+08, 9.13e+08, 0.463, 0.015, 1540., 20.
- *Rate Dependent, type=JOHNSON COOK
- 0.01,1.
- *in here for element elimination: for constituent 2*
- **shear failure, type=JOHNSON COOK,
- **ELEMENT DELETION=YES
- *0.7,2,-1.58,0.0002,0.61
- *0.08, 2.1, 0.5, 0.0002, 0.61
- *section control,NAME=Section-2-M2, ELEMENT DELETION=YES
- ***
- **
- ** BOUNDARY CONDITIONS

- *in here I used Abaqus Explicit*
- ** STEP: Step-1
- **
- *Step, name=Step-1
- *Dynamic, Explicit
- , 1.
- *Bulk Viscosity
- 0.06, 1.2
- **
- ** BOUNDARY CONDITIONS
- *Output, history, variable=PRESELECT
- *End Step

Chapter 25

Answers to Practice Problems

THIS chapter, part of appendix, consists of solutions to practice problems presented in the basic theory parts. To make the number of pages of the book to be minimal, only small number of questions and answers are presented. However, readers are encourage to find more questions themselves. Solving problems might not needed for some, but generally it helps us understand the concept easier.

D-1 Solution to Practice Problem for Chapter 2

To solve this problem, we need to develop the vector $\mathbf{r}_{CB}$. Subsequently, for each component the equilibrium condition can be applied both for the force and the moment.

$$\begin{aligned} \mathbf{r}_{CB} &= 0.9(\mathrm{i} + \mathrm{j} + 2\mathrm{k}) \\ \text{unit vector} &= \frac{0.9}{\sqrt{4.86}}(\mathrm{i} + \mathrm{j} + 2\mathrm{k}) \end{aligned} \tag{D-1}$$

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where the notation a_{mk} means the $\cos\phi_{mk}$. To obtain direction cosines (a_{ij}) shown

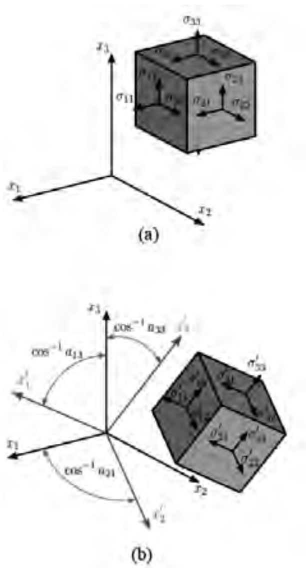

Figure D-1 (Redrawn of Figure 3.7) Three dimensional oordinate system transformation. The stress components acting on two different sets of coordinate systems; (a) original system, (b) system after rotation.

in Figure 3.7, we need each axis. Vectors **K, M** can be used to find them.

$$\begin{aligned}\mathbf{u}_1 &= \frac{1}{\sqrt{14}}(\mathrm{u}_1 + 2\mathrm{u}_2 + 3\mathrm{u}_3)\\ \mathbf{u}_2 &= \frac{1}{\sqrt{3}}(\mathrm{u}_1 + \mathrm{u}_2 - \mathrm{u}_3)\end{aligned} \tag{D-13}$$

the third axis can be obtained by cross product of the first axis and the second axis.

$$\mathbf{u}_3 = \frac{1}{\sqrt{42}}(-5\mathrm{u}_1 + 4\mathrm{u}_2 - \mathrm{u}_3) \tag{D-14}$$

Our transformed stress matrix is:

$$\begin{bmatrix} \frac{1}{\sqrt{14}} & \frac{2}{\sqrt{14}} & \frac{3}{\sqrt{14}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ -\frac{5}{\sqrt{42}} & \frac{4}{\sqrt{42}} & -\frac{1}{\sqrt{42}} \end{bmatrix} \begin{bmatrix} 1 & 5 & -5 \\ 5 & 0 & 0 \\ -5 & 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{14}} & \frac{2}{\sqrt{14}} & \frac{3}{\sqrt{14}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ -\frac{5}{\sqrt{42}} & \frac{4}{\sqrt{42}} & -\frac{1}{\sqrt{42}} \end{bmatrix} \tag{D-15}$$

The answer is therefore,

$$\begin{bmatrix} \sigma'_{11} & \sigma'_{12} & \sigma'_{13} \\ \sigma'_{21} & \sigma'_{22} & \sigma'_{23} \\ \sigma'_{31} & \sigma'_{32} & \sigma'_{33} \end{bmatrix} = \begin{bmatrix} -1.29 & 1.38 & 1.98 \\ 1.39 & 6.67 & -2.76 \\ 1.98 & -2.76 & -5.38 \end{bmatrix} \tag{D-16}$$

D-3 Solution to Practice Problem for Chapter 4

The Laplace equation given has the complete form of

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \frac{\partial^2 u}{\partial x_3^2} = 0 \tag{D-17}$$

for the two dimensional problems it reduce to

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} = 0 \tag{D-18}$$

for simplicity we write as

$$u_{xx} + u_{yy} = 0 \tag{D-19}$$

To solve this, we assume $u(x, y) = X(x)Y(y)$. Therefore, the above equation becomes:

$$\begin{aligned} u_{xx} + u_{yy} &= 0 \\ X''Y + XY'' &= 0 \\ \rightarrow \frac{X''}{X} + \frac{Y''}{Y} &= 0 \\ \rightarrow \frac{X''}{X} = -\frac{Y''}{Y} &= \mu \end{aligned} \tag{D-20}$$

Hence, we have two differential equation

$$\begin{aligned} X'' - \mu X &= 0 \\ Y'' + \mu Y &= 0 \end{aligned} \tag{D-21}$$

Recall the B.Cs.

$$\begin{aligned} u(0, y) &= X(0)Y(y) && = f(x) \\ u(L, y) &= X(L)Y(y) && = 0 \ \rightarrow X(L) = 0 \\ u(x, 0) &= X(x)Y(y) && = 0 \ \rightarrow Y(0) = 0 \\ u(x, M) &= X(x)Y(y) && = 0 \ \rightarrow Y(M) = 0 \end{aligned} \tag{D-22}$$

Illustrations

Tables

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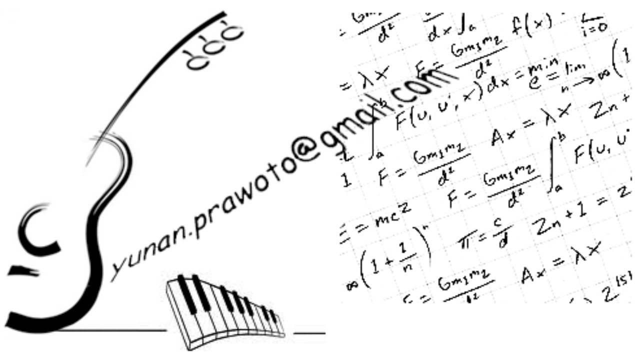

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