

Chapter 1

Introduction: Microstructural Features and Mechanics of Continua

1 Introduction

Materials of all kinds are routinely encountered in engineering applications. An ability to understand and to be able to quantify the deforming behavior of materials is often required of practicing engineers. This course aims to develop the fundamental bases of our understanding of the mechanical behavior of solid materials, including the required analytical and numerical methods for modeling and simulation of such behavior. The course also investigates the fundamental microstructural characteristics of engineering materials and the principles of structural mechanics employed in the design of mechanical engineering systems. In this first chapter the goal is to provide an introduction to the course by presenting an overall view of the contents. A second key objective is to familiarize students with the required analytical and computational tools to be used in the sequel.

1.1 Engineering Materials

Engineering systems and structures are composed of various types of materials. Reliability and life of such structures depends on the internal microstructural characteristics of the materials employed as well as on the structural design parameters. This section is devoted to a review of some basic characteristics of the materials commonly used in applications.

Ultimately, all matter is made of atomic size particles held together by interatomic forces. The mechanical response of matter to external loads is directly related to atomic cohesion. However, the specific, quantitative form of the relationship is complicated and has yet to be elucidated.

The disciplines of metallurgy and science of materials have achieved substantial progress in our understanding of the microstructural characteristics of materials and reasonably clear pictures of the atomic constitution of most engineering materials are now available.

Engineering Materials can be classified according to various criteria. If one considers the nature of atomic arrangements in the material, two main groups emerge; crystalline materials and amorphous materials. Crystalline materials are characterized by atomic arrangements of

great regularity with long range order. Atoms occupy well defined positions in a geometrically regular crystal lattice characterized by a high degree of pattern repetitiveness. In contrast, atoms in amorphous materials are located on rather more random locations and exhibit a lack of long range order. Examples of crystalline materials include metals and ceramics while glass and polymers are examples of amorphous materials. However, it is possible to produce metals with amorphous structures and polymers with crystalline arrangements as well as materials with various degrees of crystallinity.

A crystal structure is a regular three dimensional pattern of reticular locations. Crystals structures are thus characterized by a high degree of order, both short range (i.e. at the scale of a few atoms and long range (i.e. at the scale of macroscopic dimensions). The basic unit of repetition of the crystalline pattern is called the unit cell. The unit cells of all known crystals belong to one of the 14 Bravais space lattices.

Crystallographic directions are indicated using the vectors associated with them with the components enclosed in square brackets. Crystallographic planes are indicated by Miller indices which are produced by listing the reciprocal intersections of the plane with the coordinate axes in round parenthesis.

Most elements of periodic table are metals. A key characteristic of metallic materials is that they commonly possess a particular crystallographic structure. Most metals appear in three structures: face centered cubic (FCC) (e.g. copper), hexagonal close packed (HCP) (e.g. titanium) and body centered cubic (BCC)(e.g. iron). Often, metals can change structure as pressure or temperature are changed.

Ceramics are mainly ionic compounds and exist in many different structures, the most common being zinc blende, wurzite, perovskite, fluorite, sodium chloride, cesium chloride, spinel, corundum and cristobalite.

Combinations of carbon, nitrogen or boron with selected metals or semi metals (e.g. silicon carbide, titanium nitride) produce special types of ceramics known as cermets or hard metals. These have unique refractory characteristics that makes them desirable in high temperature applications.

Polymers are constituted by assemblies of large chain molecules with a distribution of molecular weights. Organic polymers are based on hydrocarbon chains. The chains can be linear, branched, cross linked or ladder type. Also, depending on the pattern along the chain one has homopolymers and copolymers. Organic polymers can also be classified according to their response to heat treatment as thermoplastics (e.g. polyethylene) or thermosets (e.g. epoxies). Further, by alignment of polymer chains polymers with various degrees of crystallinity can be produced.

Glasses are materials lacking long range order (e.g. silica). Their structure rather resembles that of a liquid in that although long range order is absent, there is significant short range order. Even metallic materials can be produced in this state. A common method for the production of metallic glasses is by cooling rapidly from the melt and thus preventing the formation of crystalline phases with long range order.

Composite materials consists of dispersions of multiple phases in intimate contact. Most

engineering materials are composites but the term is commonly used to refer to fiber reinforced materials. The properties of composites depend in a complex manner on the characteristics of the constituent phases and their interfaces.

Many structural materials have porous or cellular structures. Wood, bone and space shuttle tiles are good examples. The mechanical properties of these materials are complex functions of pore structure and characteristics as well as of the intrinsic properties of the matrix phase.

1.2 The Theoretical Strength of a Crystal

A fundamental problem in the mechanics of materials is that of determining the maximum load a given material can sustain without breaking. Orowan in the 1930's first proposed a model to estimate the intrinsic mechanical strength of a crystal. He envisioned a simple crystal of cross section A loaded in tension by a force F and failing at a certain critical value of the load, along a single crystal plane. He considered the atoms in the crystal as held together by interatomic forces due to electronic interactions. Using a simplified approximation for the cohesive strength of interatomic bonds he derived the following expression for the maximum theoretical strength

$$\sigma_{max} \approx \frac{E}{\pi}$$

where $\sigma_{max} = F/A$ is the maximum normal stress the material can bear and E is the elastic (Young's) modulus of the material.

A similar simple model was used to estimate the maximum strength under shear loading. In this case, the load F was applied parallel to the separating plane of area A . The corresponding expression is

$$\tau_{max} \approx \frac{G}{5}$$

where $\tau_{max} = F/A$ is the maximum tangential stress the material can bear and G is the shear modulus of the material.

The above formulae are first approximations to the expected strength of crystals and they are reference values well worth remembering. However, it was quickly recognized that they constitute upper bounds to the strength and are approximated in practice only under extreme circumstances. The reason being that in most real engineering materials (as opposed to the idealized crystal considered in Orowan's model) the crystal structure coexists with a large variety of crystallographic and microstructural defects. These include impurity and alloy atoms, vacant lattice sites, crystal dislocations, intercrystalline boundaries and interphase interfaces.

Crystallographic defects and microstructural features exert a powerful influence in the determination of the actual strength of a given piece of material. However, using special manufacturing methods, nearly perfect crystals can be produced with strengths approaching the theoretical values given by the above formulae.

1.3 Mechanics of Solid Materials

Solid mechanics was originally conceived and used as a continuum theory for the estimation of the mechanical response of materials subjected to loads. In continuum theory, the details of the atomistic structure of the material are neglected. Material response is expressed in terms of empirically determined constitutive equations of behavior. Much progress has been achieved in structural mechanics despite this assumption.

Nowadays, it is recognized that knowledge of materials science is a helpful tool for understanding the mechanical response of materials. This knowledge must necessarily be leveraged with insight obtained by studying classical constitutive models of material behavior. An ultimate goal of the discipline is the development of multi scale constitutive models of behavior linking atomic, defect, microstructural and macroscopic scales.

1.3.1 Linear Elasticity

Linear elasticity is the material deformation behavior described by Hooke's law which states that displacement is linearly proportional to the applied load, i.e. for a point inside a material subjected to external loads F_1, F_2, \dots, F_n , the displacement can be expressed as

$$u = \sum_{i=1}^n a_i F_i$$

where the coefficients a_i are independent of F_i . The simplest representation of linear elastic behavior is that of a spring subjected to small deflections.

A linear elastic material returns to the undeformed state once the loads are removed and the effects of multiple load systems can be computed by simple linear superposition. Moreover, the work done by the forces is calculated by multiplying the loads by the displacements. A linear elastic material under load also accumulates elastic strain energy U and one has Castigliano's theorem

$$\frac{\partial U}{\partial F_i} = u_i$$

and the associated principle of virtual work

$$\frac{\partial U}{\partial u_i} = F_i$$

The above relationships are extensively used as foundation for the quantitative analysis of the deformation behavior of linear elastic materials.

1.3.2 Viscoelasticity

A linear elastic solid that remembers its deformation history is called a viscoelastic material. Viscoelastic behavior can be represented by combinations of springs and dashpots (pistons

that move inside a viscous fluid). While linear springs instantaneously produce deformation proportional to the load, a dashpot produces a velocity proportional to the load at each instant. If a spring and a dashpot are placed in parallel one obtains Maxwell's viscoelastic model. If they are arranged in series, one has Voigt's model. Finally, a series/parallel arrangement yields Kelvin's model.

As an example, for the Voigt's model, the relationship among load F , displacement u and velocity du/dt is

$$F = \mu u + \eta \frac{du}{dt}$$

where μ is the spring constant and η the viscosity, and the displacement function resulting from a unit step force is a monotonic continuous function of time.

1.3.3 Plasticity

If the load applied to a piece of metal is increased from zero, the metal first deforms elastically according to Hooke's law but at some critical threshold load, it yields and continues deforming at stresses that are much smaller than those that would be required for continued elastic deformation. This behavior is known as plasticity. Two characteristic features of plasticity are that the material deforms instantaneously and it does not return to the undeformed state when unloaded. Another characteristic frequently found is that the material strain hardens.

1.3.4 Creep/Viscoplasticity

Materials at high temperatures exhibit time dependent deformation under constant load. Even very small loads may produce deformation and the body remains deformed after unloading. This behavior is known as creep or viscoplasticity.

1.3.5 Fracture of Materials

Fracture takes place when the applied load produces local stress concentrations that are enough to break interatomic bonds and thus lead to the nucleation of cracks or voids in the material. The resulting cracks grow to macroscopic dimensions and may eventually lead to complete structural failure of the component. Two main types of fracture failure are commonly encountered: brittle fracture and ductile fracture. Brittle fracture is characterized by the absence of any significant plastic deformation prior to failure, whereas in ductile fracture often very significant amounts of local plastic deformation precede failure. Fatigue failure is a type of fracture that results from cyclic loading. Fatigue may occur even at loads below the elastic limit because of local stress concentration at the site of microstructural defects.

1.4 Thermodynamics of Solids Materials

Materials often deform while subjected to non-homogenous temperature fields. In practice, the associated thermal problem must be solved together with the mechanical one. The thermal problem is formulated by stating the principle of conservation of energy. This is the subject matter of thermodynamics. Thermodynamic principles not only lead to the formal statement of energy conservation but they also place restrictions on the constitutive behavior of materials.

1.4.1 The First Law of Thermodynamics

The first law of thermodynamics states that the increase of internal energy of a material system is equal to the amount of heat absorbed by it minus the amount of work done, i.e.

$$\Delta U = Q - W$$

when the first law is expressed in rate form it becomes the principle of energy conservation.

1.4.2 The Second Law of Thermodynamics

The second law of thermodynamics requires the concepts of absolute temperature and entropy. Absolute temperature is an intensive quantity and a positive number associated with the notion of hotness. Entropy is an extensive property of the system that changes as a result of interaction with the external environment and also as a result of internal processes in the system. The second law states that the change in entropy resulting from internal processes is never negative, i.e.

$$dS_i \geq 0$$

1.5 Continuum Thermomechanics of Materials

Continuum thermomechanics investigates the deformation behavior of materials under mechanical and thermal loads. The discipline is founded on well established conservation principles of universal applicability. The conservation principles used in continuum thermomechanics are:

- Principle of Mass Conservation (Equation of Continuity)
- Principle of Conservation of Linear Momentum (Equation of Motion)
- Principle of Conservation of Angular Momentum (Equation of Moment of Momentum)
- Principle of Conservation of Energy (Energy Equation)
- Principle of Entropy Production (Clausius-Duhem Equation)

Ultimate predictions of material deformation require incorporating constitutive equations into the formulation. While the conservation principles apply to any material, constitutive relations specify individual material responses.

The mathematical formulation of problems in continuum thermomechanics invariably leads to initial-boundary problem for partial differential equations. The simplest problems can be solved analytically with very modest amount of effort and much insight can be gained from the obtained solutions. More complex problems typically require the use of numerical methods. Of these, the finite element method has been demonstrated particularly suitable in structural mechanics applications. In this course, insight about the deforming behavior of materials will be obtained by using analytical and numerical methods for the solution of selected problems.

2 Microstructural Features of Solid Materials

The deformation behavior of materials is intimately linked to the interatomic forces and to the microstructure of the material. Microstructure is the set of crystal structure, crystal imperfections, impurities, alloying elements, second phase particles and internal and external interfaces that characterizes real materials. This chapter contains a review of key concepts useful in the description of material microstructures and also provides a brief description of how the deformation behavior of particular materials is affected by the microstructure.

2.1 Crystal Structures

Crystal structures are three dimensional lattices generated by repetition of a simple pattern called the unit cell. The unit cell is described quantitatively by specifying its geometrical features. Crystal structure is the description of the atomic arrangement constituting the unit cell. Some of the simplest crystal structures are found in the metals and alloys commonly used in many engineering applications. Simple cubic (atoms at the vertices of a cube), body centered cubic (as in simple cubic but with an additional atom at the center of the cube), face centered cubic (as in simple cubic but with additional atoms at the center of each face of the cube) and hexagonal close packed (atoms on the vertices of an hexagonal prism with three additional atoms in the interior of the prism) are commonly observed structures in engineering metals and alloys. More complex structures are also observed, particularly in alloyed materials.

Crystallographic directions are readily specified in cubic systems by setting up a rectangular Cartesian system of coordinates and then using vector components to specify the direction. In the hexagonal system one uses a set of axes on the hexagonal plane with 120 degrees in between rather than the 90 degrees used in the cubic case. Crystallographic planes are described by Miller indices. These are simply the reciprocals of the intercepts the plane makes with the coordinate axes.

2.2 Crystal Defects

As mentioned before, simple models of material cohesion predict strengths many orders of magnitude higher than those commonly observed in engineering materials, although carefully produced specimens possess strengths approaching the theoretical predictions. In real materials the perfect crystalline arrangement implied by three dimensional repetition breaks down due to a broad variety of crystalline defects or imperfections. The reason for the much smaller observed strengths of engineering materials is the presence of these crystalline defects. The description of crystal and defect structure of a material is referred to as its microstructure.

Three main types of crystalline defects are encountered in many materials: point, line and surface defects. Point defects are isolated perturbations in the crystal lattice of the size of a single atom. Examples include empty lattice sites (vacancies), lodged-in (interstitial) atoms, and impurity (interstitial or substitutional) atoms. Line defects are perturbations of atomic size in two perpendicular directions and of macroscopic size along the third direction. The best known examples are the various types of dislocations (screw, edge, mixed, loops, partial and extended). Surface defects have atomic dimensions only in one direction and are of macroscopic size in the other two. Examples include the boundary separating two regions of the material containing unit cells with different orientations (grain boundaries) and boundaries separating different materials (interphase interfaces). Other types of imperfections are also encountered, particularly in non-metallic materials. Main features of these defects are described below. Emphasis is on crystal defects in crystalline materials and particularly in metals and alloys.

2.2.1 Point Defects

Point defects are perturbations in the crystalline arrangement with a size of the order of the atomic radius. There are three main types of these: Vacancies, Interstitial Atoms and Substitutional Atoms. Detailed studies of point defects have been carried out by simultaneous thermal expansion and lattice expansion measurements.

At any given temperature, there is an equilibrium concentration of point defects. Specifically, the equilibrium fraction of vacant lattice sites is simply given by

$$f = \exp\left(-\frac{G_f}{kT}\right)$$

where G_f is the energy required to form a vacancy and k is Boltzmann's constant. Typical values of f for engineering materials are of the order of 10^{-4} (i.e. $> 10^{12}$ vacancies/ m^3 .)

A point defect can be regarded as a center of contraction/dilation. It can be shown that the radial displacement at distance r associated with contraction/dilation u_0 at r_0 is given by

$$u(r) = u_0\left(\frac{r_0}{r}\right)^2$$

The strain energy associated with the above displacement is given by

$$U \approx \frac{16}{3}\pi Gr_0 u_0^2$$

where

$$u_0 \approx -\frac{3\gamma}{4G}$$

and where G is the shear modulus.

Point defects can be readily generated by rapidly quenching a material from a high temperature where a high concentration exists, thus freezing in the defects. They can also be generated by exposing the material to radiation with high energy particles.

Point defects affect the mechanical properties of a material. The use of solute atoms for strengthening purposes in alloys is a good example.

2.2.2 Line Defects

Dislocations are the most important line defects in metals. They represent boundaries between slipped and unslipped regions inside the crystal. The amount of slippage associated with a given dislocation is its Burgers vector \mathbf{b} . Dislocations are also characterized by their tangential vector \mathbf{t} . The crystallographic plane over which the dislocation slides is called the slip plane.

Various types of dislocations exist: Screw (\mathbf{t} and \mathbf{b} parallel), Edge (\mathbf{t} and \mathbf{b} perpendicular), Mixed, Loop, Partials, Extended. All have been observed in detail by high resolution electron microscopy. Large number of dislocations exist inside most engineering materials. Dislocation concentrations are described by specifying the number of dislocation lines that cut through a unit area of material. This is called the dislocation density ρ (units m^{-2}) and typical values encountered in real materials are at least of the order of 10^{12} dislocations/ m^2 . Dislocations consist of a small core region consisting of a few atoms (size r_0) where the distortion from the ideal crystallographic arrangement is most severe and a much larger surrounding region where atoms are only slightly displaced with respect to their unperturbed positions.

Since dislocations are perturbations of the crystal lattice, internal strain and stress fields are associated with their presence. Consider a rectangular Cartesian system of coordinates with axes x_1, x_2, x_3 . Let x_3 be aligned with the dislocation line and x_1 be the axis that together with x_3 constitutes the slip plane. Elasticity theory has been used to determine the displacement, strain and stress fields around dislocation lines and at some distance from the core.

Specifically, for a screw dislocation, the stress field is given by

$$\sigma_{13} = -\frac{Gb x_2}{2\pi(x_1^2 + x_2^2)}$$

$$\sigma_{23} = \frac{Gb x_1}{2\pi(x_1^2 + x_2^2)}$$

And for an edge dislocation the result is

$$\sigma_{11} = -\frac{Gb x_2(3x_1^2 + x_2^2)}{2\pi(1 - \nu)(x_1^2 + x_2^2)^2}$$

$$\sigma_{12} = \frac{Gb x_1(x_1^2 - x_2^2)}{2\pi(1 - \nu)(x_1^2 + x_2^2)^2}$$

$$\sigma_{22} = \frac{Gb x_2(x_1^2 - x_2^2)}{2\pi(1 - \nu)(x_1^2 + x_2^2)^2}$$

and

$$\sigma_{33} = -\frac{Gb \nu x_2}{\pi(1 - \nu)(x_1^2 + x_2^2)}$$

As before, G is the shear modulus and ν is Poisson's ratio.

The strain and stress fields of dislocations store elastic strain energy. Using elasticity theory one can show that the elastic strain energy per unit length of screw dislocation is given by

$$U_s = \frac{Gb^2}{8\pi^2(x_1^2 + x_2^2)} = \frac{Gb^2}{4\pi} \ln\left(\frac{R}{r_0}\right)$$

For an edge dislocation the corresponding result is

$$U_e = \frac{Gb^2}{4\pi(1 - \nu)} \ln\left(\frac{R}{r_0}\right)$$

where

$$R \approx \rho^{-\frac{1}{2}}$$

The total energy associated with a dislocation also includes a core components that can not be estimated using elasticity theory since they involve severe atomic distortions at the core of the dislocation. After adding an estimate for the core contribution, the total energy is

$$U_t = U_{core} + U_{strain} \approx \frac{Gb^2}{2}$$

An isolated curved dislocation inside an undisturbed crystal has a tendency to become straight. This effect is analogous to the surface tension that affects the shape of soap bubbles and is called the line tension. The line tension has units of energy per unit length and is numerically equal to the total energy of the dislocation as given above.

2.2.3 Interfaces

Interfaces separate regions of a material containing different crystallographic arrangement (homophase interfaces or grain boundaries) or composition (heterophase interfaces). Most engineering materials contain large amounts of internal interfaces.

Pure materials typically consist of assemblies of grains forming a polycrystal. Materials consisting of a single grain (single crystals) can be produced by carefully controlled crystal growth methods. Many engineering materials consist of multiple phases and are therefore polycrystalline polyphase materials.

If lattice planes are continuous on crossing a heterophase interface the interface is said to be coherent. When there is complete crystallographic disregistry between the two sides of the boundary one has an incoherent interface. Semicoherent interfaces, representing intermediate situations are commonly encountered.

Interfaces also exist that separate crystals that are either mirror reflections of each other or constitute a relative shift. These are called twin boundaries. Twin boundaries can form during deformation or on annealing of samples.

Internal interfaces in solids are readily investigated by microscopic examination of sectioned samples. The amount of grain boundary area per unit volume S_v in a given material can be readily determine by microscopy by simply measuring the mean lineal intercept distance l , i.e.

$$S_v = \frac{2}{l}$$

For a microstructure consisting of approximately spherical grains with average diameter D , $S_v = 3/D$.

By counting the number of grains per unit area N in a microstructural section one can readily determine the ASTM grain size number n from

$$n = \frac{\ln N}{\ln 2} + 1$$

A low angle grain boundary is obtained when two crystals meeting at the interface are slightly rotated with respect to each other about a common axis. Such boundary may actually consists of an array of interface edge dislocations with Burgers vector b and separated by distance D , such that

$$D \approx \frac{b}{\theta}$$

and is known as a tilt boundary. A twist boundary is similar except that the interface dislocations are of screw type.

Energy is stored inside a boundary. Specifically, for a tilt boundary, the energy is given by

$$U = \frac{Gb}{4\pi(1-\nu)}\theta(A - \ln \theta)$$

where A is a constant.

As the misorientation increases, complex grain boundary dislocation structures establish on the boundary and the energy of the boundary becomes more like a surface tension (values between 0.1 and 1 J/m^2).

2.3 Crystalline Defects and Deformation Behavior

A solid material may deform under load but regain its old shape once the load is removed. Such deformation is called elastic if there is no damping and viscoelastic if damping is observed. Elastic and viscoelastic deformations are the result of stretching interatomic bonds; atoms go back to their original positions once the load is removed. Permanent deformation and fracture involve atomic movements on a larger scale and atoms shift positions during deformation. Many engineering materials deform elastically under relatively small loads but begin to deform permanently once the load reaches some material-specific critical value called the yield strength. Deformation and failure mechanisms in crystalline materials and particularly in metals have been the subject of a great deal of study. These will be emphasized below.

When an external load is applied to a crystal containing a dislocation, there appears a force that pushes the dislocation. The force is given by (Peach-Koehler)

$$\mathbf{F} = \boldsymbol{\tau} \cdot \mathbf{b} \times \mathbf{t}$$

where $\boldsymbol{\tau}$ is the stress tensor (force per unit area) resulting from the applied load. As a result, dislocations contained inside a material move when loads are applied and the motion results in macroscopic permanent deformation of the material.

As mentioned before, dislocations are characterized by their Burgers vector and their direction of alignment. Burgers vectors can be integer multiples of the lattice parameter (perfect dislocations) or equal to a fraction of the parameter (partial dislocations). A given perfect dislocation can often dissociate into an equivalent pair of partials and these in turn can separate leaving a stacking fault between them. Partial dislocations and stacking faults play an important role in deformation mechanisms of engineering materials (e.g. nickel base superalloys).

Dislocations inside a material under load may be static or moving. When a collection of dislocations moving on the same slip plane encounter an obstacle (such as an interface) they may pileup thus developing a stress concentration region. Also, moving dislocations will often encounter transversal (forest) dislocations. By forming jogs and kinks the moving dislocation is able to cut through forest dislocations. These interactions play a strong role in hardening phenomena. Plastic deformation leads to the generation of many new dislocations. A well known mechanism for dislocation multiplication is the Frank-Read source.

Dislocation motion produces macroscopic deformation. The amount of deformation was first related to dislocation motion by Orowan as follows

$$\gamma = k\rho bL$$

where L is the average dislocation travel distance and k is a proportionality parameter.

Dislocation motion must overcome the mobility barrier posed by lattice periodicity. The Peierls-Nabarro stress is the stress required to overcome the barrier. Assuming a sinusoidal potential

$$\tau_{PN} = \frac{Gb}{2c} \exp(-\pi a/c) \sin(2\pi x/c)$$

Although elastic properties are only weakly dependent on temperature, the flow stress is a strong function of temperature. The drop in flow stress is larger for BCC than for FCC metals because the P-N stress is the main obstacle to motion in BCC metals and temperature effectively aids in overcoming this obstacle.

Grain boundaries and heterophase interfaces have important effects on the strength of materials. Specifically, it is well documented that the yield strength of a single phase polycrystal increases from some reference value σ_0 as the average grain diameter decreases as given by (Hall-Petch)

$$\sigma_y = \sigma_0 + \frac{k}{D^{\frac{1}{2}}}$$

The strengthening effect has been variously assumed due to (i) dislocation pileup resistance, (ii) inducement of dislocation multiplication across the grain boundary or (iii) the pumping of dislocations into neighboring grains. The strengthening effect of interfaces is dramatically illustrated by the behavior of nanocrystalline materials.

Voids, Inclusions and Second Phase Particles can coexist within a polycrystalline microstructure. These entities can have important effects on strength as they behave as obstacles to dislocation motion that must be surmounted for deformation to take place. An excellent example of the practical use of second phase particle strengthening is found in the γ/γ' system of nickel base superalloys used in the high temperature section of modern jet engines.

Defects, particularly macroscopic defect play an important role in the deformation and fracture behavior of non-metallic materials. Commonly used non-metallic materials include polymer plastics of all kinds, granular materials such as concrete and asphalt and cellular materials such as wood and natural and synthetic foams. Deformation and fracture mechanisms in these materials are very material specific and are often investigated on a case by case basis.

3 Stress, Strain, Virtual Power and Conservation Principles

Stress and strain are key concepts in the analytical characterization of the mechanical state of a solid body. While stress represents internal forces per unit area resulting from loads

applied to the body, strain is the resulting relative displacement of points in the body. This chapter formally introduces the notions of stress and strain tensors and it also shows how the mechanical equilibrium equations can be obtained directly from the application of the principle of virtual work. The chapter starts with a review of vectors and tensors.

3.1 Overview of Vectors and Tensors

Tensors are widely used in engineering analysis to denote physical quantities of interest. This section reviews basic notions of tensor analysis needed in continuum mechanics. Tensors are important in applications because governing equations which have general validity with respect to any frame of reference can be constructed by ensuring that every term in the equation has the same tensor characteristics. Thus tensor characteristic play a role analogous to that of dimensional analysis. Thus, once a physical quantity has been given the characteristic of a tensor then the components of the quantity can be transformed from one coordinate system to another according to the above rules.

3.1.1 Tensor Notation

In vector and tensor calculus, subscript and superscript index notation is used to denote collections of variables, for instance, the set x_1, x_2, \dots, x_n is denoted by $x_i, i = 1, 2, \dots, n$ or by $x^i, i = 1, 2, \dots, n$. Likewise, the set y^1, y^2, \dots, y^n is denoted as $y^j, j = 1, 2, \dots, n$. Note that the superscript is just an index, not a power. If a power is meant, the quantity will be enclosed in parenthesis.

The *summation convention* is used to simplify the writing of equations consisting of collection of similar looking terms. Whenever a sum involving two identically indexed variables appears one simply writes a single term using a dummy index and omits the summation sign. For instance

$$a_1x_1 + a_2x_2 + a_3x_3 = \sum_{i=1}^3 a_ix_i = a_ix_i$$

The summation convention also applies to derivatives, specifically, for a function $f(x_1, x_2, x_3)$ the total differential expressed in terms of the partial derivatives is

$$df = \frac{\partial f}{\partial x_1} dx_1 + \frac{\partial f}{\partial x_2} dx_2 + \frac{\partial f}{\partial x_3} dx_3 = \frac{\partial f}{\partial x_i} dx_i$$

A concrete example is provided by the unit vector \mathbf{u} in three dimensional Euclidean space in rectangular Cartesian coordinates. In tensor analysis, components are denoted by indices, so instead of writing x, y, z for the three coordinates in such space one writes $x_1, x_2, x_3 = x_i, i = 1, 2, 3$.

$$\mathbf{u} = u_1\mathbf{e}_1 + u_2\mathbf{e}_2 + u_3\mathbf{e}_3 = u_i\mathbf{e}_i$$

where u_i are the components of \mathbf{u} and $\mathbf{e}_i, i = 1, 2, 3$ are the unit coordinate vectors ($\mathbf{i}, \mathbf{j}, \mathbf{k}$ in rectangular Cartesian coordinates, respectively). The magnitude of \mathbf{u} , $u = |\mathbf{u}|$, is given by

$$u = \sqrt{u_i u_i} = \sqrt{u_i^2} = 1$$

Therefore, the dot product of two vectors \mathbf{a}, \mathbf{b} can be expressed as

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 = a_i b_i = \delta_{ij} a_i b_j$$

The quantity

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

is *Kronecker's delta*.

Another example is the differential arc or line element of a curve in space ds , this is

$$ds = \sqrt{\delta_{ij} dx_i dx_j}$$

where two summations are involved.

Another example is the determinant of a 3×3 matrix $|a_{ij}|$, this is given as

$$|a_{ij}| = e_{rst} a_{r1} a_{s2} a_{t3}$$

where e_{rst} is the *permutation symbol* defined as

$$e_{rst} = \begin{cases} 1 & \text{when subscripts permute like } 1, 2, 3 \\ 0 & \text{when any two indices coincide} \\ -1 & \text{otherwise} \end{cases}$$

The permutation symbol and Kronecker's delta are related by

$$e_{ijk} e_{rst} = \delta_{js} \delta_{kt} - \delta_{jt} \delta_{ks}$$

With the above, the vector product of two vectors can be simply expressed as

$$\mathbf{a} \times \mathbf{b} = e_{ijk} a_j b_k$$

3.1.2 Description of Geometrical Features using Tensor Notation

Consider now a system of rectangular coordinates x_1, x_2, x_3 . Consider also a new system of coordinates u_1, u_2, u_3 . The two systems being related by the expressions

$$x_i = x_i(u_1, u_2, u_3)$$

or

$$u_i = u_i(x_1, x_2, x_3)$$

so that to every triplet (x_1, x_2, x_3) there corresponds a triplet (u_1, u_2, u_3) .

In any system of coordinates, coordinate curves in space are generated by varying one coordinate while holding the other two constant. If the three coordinate curves resulting from the triplet (u_1, u_2, u_3) are mutually perpendicular at each point P , then the triplet constitutes a system of orthogonal curvilinear coordinates.

If a differential segment of an arbitrary curve in space is associated with differential displacements in the coordinates dx^1, dx^2, dx^3 then it can be expressed as The differential element of arc of a curve in coordinates x_i is

$$ds = \sqrt{\delta_{ij} dx^i dx^j} = \sqrt{dx^i dx^i}$$

But

$$dx^i = \frac{\partial x_i}{\partial u_k} du^k$$

therefore

$$(ds)^2 = dx^i dx^i = \frac{\partial x_i}{\partial u_k} \frac{\partial x_i}{\partial u_m} du^k du^m = g_{km} du^k du^m$$

where the functions

$$g_{km}(u_1, u_2, u_3) = g_{mk}(u_1, u_2, u_3) = \frac{\partial x_i}{\partial u_k} \frac{\partial x_i}{\partial u_m}$$

are the components of the *Euclidian metric tensor* in the coordinate system u_1, u_2, u_3 .

3.1.3 Scalars, Vectors and Tensors

Scalars, vectors and tensors are mathematical entities that are used in applications to represent meaningful physical quantities. Consider two systems of coordinates u^i and u^{i*} which are related by the coordinate transformation rules described above. Physical quantities of interest can be represented in any of these two systems. A *scalar* is an entity consisting of a single component and is represented in terms of u^i by the single component (number) ϕ and in terms of u_{i*} by ϕ^* . If the two numbers are one and the same

$$\phi(u^1, u^2, u^3) = \phi^*(u^{1*}, u^{2*}, u^{3*})$$

A scalar is also considered a tensor of rank or order zero.

If an entity has instead three components in each of the coordinate systems is called a *contravariant vector* or *contravariant tensor of order one* and individual components ξ^i and ξ^{i*} in the two systems are related by

$$\xi^{i*}(u^{1*}, u^{2*}, u^{3*}) = \xi^i(u^1, u^2, u^3) \frac{\partial u^{i*}}{\partial u^i}$$

The use of the index as superscript distinguishes contravariant vectors.

Likewise, if an entity has three components in each of the coordinate systems is called a *covariant vector* or *covariant tensor of rank or order one* and individual components ξ_i and ξ_{i*} in the two systems are related by

$$\xi_{i*}(u^{1*}, u^{2*}, u^{3*}) = \xi_i(u^1, u^2, u^3) \frac{\partial u^i}{\partial u^{i*}}$$

The use of the index as subscript distinguishes contravariant vectors. Covariant and contravariant components are identical in rectangular Cartesian systems of coordinates but they are not in curvilinear coordinates. By convention, only the subscript index notation is used to describe vectors in rectangular Cartesian systems of coordinates.

Now, if an entity has nine components one has *tensor of rank or order two*. There are also contravariant T^{ij} and covariant T_{ij} tensors which transform according to

$$T^{ij*}(u^{1*}, u^{2*}, u^{3*}) = T^{mn}(u^1, u^2, u^3) \frac{\partial u^m}{\partial u^{i*}} \frac{\partial u^n}{\partial u^{j*}}$$

and

$$T_{ij*}(u^{1*}, u^{2*}, u^{3*}) = T_{mn}(u^1, u^2, u^3) \frac{\partial u^{i*}}{\partial u^m} \frac{\partial u^{j*}}{\partial u^n}$$

respectively.

Mixed tensor fields of rank two T_j^i can also be defined as well as tensors of higher ranks.

Again, in rectangular Cartesian systems of coordinates, there is no distinction between contravariant and covariant tensors. By convention only the subscript index notation is used to describe tensors in rectangular Cartesian systems of coordinates.

The Kronecker delta defined before can be regarded as a component of a rank two tensor which turns out to be the Euclidian metric tensor (g^{ij}, g_{ij}, g_j^i) , while the permutation symbol can be regarded as a component of a rank three tensor called the *permutation tensor* or the *alternator* ϵ^{ijk} .

It should be noted that given a tensor, others can be generated from it by a process called *contraction* which consists of equating and summing a covariant and a contravariant index of a mixed tensor.

3.1.4 Algebraic Properties of Second Order Tensors

Recall that tensors, just as vectors can be added (each component of the resulting tensor is the sum of the corresponding components in the original tensors). They can also be multiplied according to the rule

$$C_{iklm} = A_{ik}B_{lm}$$

Also, tensors are symmetric if $A_{ij} = A_{ji}$ and antisymmetric if $A_{ij} = -A_{ji}$.

A vector B_i can be obtained from a tensor T_{ik} and an arbitrary vector A_k by multiplication as follows

$$B_i = T_{ik}A_k$$

The new vector \mathbf{B} has generally different magnitude and direction from \mathbf{A} . Now, if $B_i = \lambda A_i$, where λ is a scalar, it is called the *characteristic vector* of T_{ik} and the directions associated with it are called the *characteristic or principal directions* of T_{ik} . The axes determined by the principal directions are called the *principal axes* of T_{ik} . The problem of finding the principal axes of a tensor is called the *reduction of T_{ik} to principal axes*. The components of \mathbf{A} determining the principal axes of T_{ik} satisfy the system of equations

$$T_{ik}A_k - \lambda A_i = (T_{ik} - \lambda \delta_{ik})A_k = 0$$

This system has a nontrivial solution only when the determinant

$$\begin{vmatrix} T_{11} - \lambda & T_{12} & T_{13} \\ T_{21} & T_{22} - \lambda & T_{23} \\ T_{31} & T_{32} & T_{33} - \lambda \end{vmatrix} = \lambda^3 - \lambda^2 I_1 + \lambda I_2 - I_3 = 0$$

where the quantities

$$I_1 = T_{11} + T_{22} + T_{33} = T_{ii}$$

$$I_2 = \begin{vmatrix} T_{22} & T_{32} \\ T_{23} & T_{33} \end{vmatrix} + \begin{vmatrix} T_{11} & T_{21} \\ T_{12} & T_{22} \end{vmatrix} + \begin{vmatrix} T_{11} & T_{31} \\ T_{13} & T_{33} \end{vmatrix}$$

and

$$I_3 = \begin{vmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{vmatrix}$$

are called the *invariants* of the tensor T_{ik} .

The equation

$$\lambda^3 - \lambda^2 I_1 + \lambda I_2 - I_3 = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3) = 0$$

is called the *characteristic equation* for the determination of the eigenvalues of a tensor.

3.1.5 Partial Derivatives in Cartesian Coordinates

In Cartesian coordinates, the partial derivatives of any tensor field are the components of another tensor field. Consider two Cartesian systems of coordinates (x_1, x_2, x_3) and (x_1^*, x_2^*, x_3^*) related by the rule

$$x_i^* = a_{ij}x_j + b_i$$

where a_{ij} and b_i are constants. Let $\xi^{i*}(x_1^*, x_2^*, x_3^*)$ be a contravariant tensor so that

$$\xi^{i*}(x_1^*, x_2^*, x_3^*) = \xi^i(x_1, x_2, x_3) \frac{\partial x_i^*}{\partial x_\alpha}$$

then one has the relationship

$$\frac{\partial \xi^{i*}}{\partial x_j^*} = \frac{\partial \xi^\alpha}{\partial x_\beta} \frac{\partial x_\beta}{\partial x_j^*} \frac{\partial x_i^*}{\partial x_\alpha}$$

i.e. the partial derivatives of ξ transform as a rank two tensor in Cartesian coordinates. This is not the case in curvilinear coordinate systems.

The comma notation is often used to denote partial derivatives. For instance the tensors $\phi_{,i} = \partial\phi/\partial x_i$, $\xi_{i,j} = \partial\xi_i/\partial x_j$ and $\sigma_{ij,k} = \partial\sigma_{ij}/\partial x_k$ are of rank one, two and three, respectively assuming that ϕ , ξ_i and σ_{ij} are tensors of ranks zero, one and two, respectively.

Further, the covariant derivative of the covariant vector ξ_i is defined as

$$\xi_i|_\alpha = \frac{\partial \xi_i}{\partial x^\alpha} - \Gamma_{i\alpha}^\sigma \xi_\sigma$$

and they are the components of a covariant tensor of rank two. Here, the quantity

$$\Gamma_{\alpha\beta}^i = \frac{1}{2}g^{i\sigma} \left(\frac{\partial g_{\alpha\beta}}{\partial x^\sigma} + \frac{\partial g_{\alpha\sigma}}{\partial x^\beta} - \frac{\partial g_{\sigma\beta}}{\partial x^\alpha} \right)$$

is called the Euclidian Christoffel symbol.

3.1.6 Characteristics of Tensor Equations

The key property of tensor fields is that if all the components of a tensor vanish in a given coordinate system, they also vanish in all other systems obtainable from the first by admissible transformations. As a consequence, a tensor equation established in one coordinate system will also hold in any other system obtainable from the first by admissible transformations.

For instance, the mass contained inside a given volume V is

$$M = \int \int \int_V \rho_0(x_1, x_2, x_3) dx_1 dx_2 dx_3 = \int \int \int_V \rho_0 \left| \frac{\partial x_i}{\partial x_j^*} \right| dx_1^* dx_2^* dx_3^*$$

Also the total volume contained inside a closed surface is

$$V = \int \int \int_V dx_1 dx_2 dx_3 = \int \int \int_V \left| \frac{\partial x_i}{\partial x_j^*} \right| dx_1^* dx_2^* dx_3^* = \int \int \int_V \sqrt{g} dx_1^* dx_2^* dx_3^*$$

3.1.7 Geometric Interpretation of Tensor Components

Recall that the set of unit vectors or base vectors, \mathbf{i}_r for $r = 1, 2, 3$ in Euclidean space is a set of linearly independent vectors such that any vector in the space can be generated from them by simple linear combination. Consider an infinitesimal vector $d\mathbf{r} = dx^r \mathbf{i}_r = dx_r \mathbf{i}^r$ connecting two closely space points in space referred to a Cartesian coordinate system. In a new and arbitrary coordinate system $u^i = u^i(x_1, x_2, x_3)$, the same vector is represented as

$$d\mathbf{r} = \mathbf{g}_r du^r = \mathbf{g}^r du_r$$

where $\mathbf{g}_r = (\partial x^s / \partial u^r) \mathbf{i}_s$ is the covariant base vector and \mathbf{g}^r is the contravariant base vector. Moreover,

$$\mathbf{g}_i = \frac{\partial \mathbf{r}}{\partial u^i}$$

so that \mathbf{g}_i represents the change in the position vector \mathbf{r} with u^i and points along the tangent to the coordinate curve.

It can be shown that $\mathbf{g}_r \cdot \mathbf{g}_s = g_{rs}$, $\mathbf{g}^r \cdot \mathbf{g}^s = g^{rs}$ and $\mathbf{g}^r \cdot \mathbf{g}_s = g_s^r = \delta_s^r$.

A vector \mathbf{v} can then be expressed

$$\mathbf{v} = v^r \mathbf{g}_r = v_s \mathbf{g}^s$$

and the contravariant components v^r of \mathbf{v} are the components in the direction of the covariant base vectors and vice versa.

Consider two coordinate systems. The associated base vectors are $\mathbf{g}_i, \mathbf{g}^i$ and $\mathbf{g}_i^*, \mathbf{g}^{i*}$. Then, the transformation laws for a vector are

$$v^{i*} = \mathbf{g}^i \cdot \mathbf{g}_m v^m$$

and

$$v^j = \mathbf{g}_i^* \cdot \mathbf{g}^j v^i$$

Likewise, in the case of tensors of rank two the transformation laws are

$$A^{rs*} = \mathbf{g}^{r*} \cdot \mathbf{g}_m \mathbf{g}^{s*} \cdot \mathbf{g}_n A^{mn}$$

and

$$A^{mn} = \mathbf{g}_r^* \cdot \mathbf{g}^m \mathbf{g}_s^* \cdot \mathbf{g}^n A^{mn*}$$

3.2 Analysis of Stress, the Laws of Motion and the Equilibrium Equations

When external loads are applied to a solid body, forces are transmitted through body's interior. Stress is a concept used to represent the mechanical interaction across imaginary surfaces in the interior of solid bodies.

3.2.1 Concept of Stress

Consider a closed surface enclosing an interior region of a solid body. The surface can be characterized by its outward pointing normal vector ν . The material outside the surface exerts a force \mathbf{F} over the adjacent material on the other side of the surface. The *stress vector* \mathbf{T} is the force per unit area and is defined as

$$\mathbf{T} = \frac{d\mathbf{F}}{dS}$$

In a rectangular Cartesian system of coordinates \mathbf{T} has three components, $T_i, i = 1, 2, 3$. Cauchy first pointed out that the force exerted by the material behind the surface on the material outside the surface is equal in magnitude and opposite in sign.

If the region enclosed by the surface has the shape of a cube and a rectangular Cartesian system of coordinates is introduced such that the cube faces are normal to the coordinate axes, there are three components of \mathbf{T} on each of the three positive faces of the cube. These nine numbers are the *stresses* τ_{ij} where the subscript i indicates the plane on which the force acts and the subscript j denotes the direction of action. If $i = j$ one has *normal stresses* and if $i \neq j$ one has shearing stresses. With the above, the stress vector components are expressed as

$$T_i = \nu_j \tau_{ji}$$

Because of Cauchy's idea, the nine components of stress above are necessary and sufficient to characterize the state of stress in a body.

The stresses can be readily represented on a second (primed) rectangular Cartesian system of coordinates according to the following transformation rule

$$\tau'_{km} = \tau_{ji} \frac{\partial x'_k}{\partial x_j} \frac{\partial x'_m}{\partial x_i}$$

3.2.2 The Laws of Motion and the Equilibrium Equations

As load is applied on a body of volume V , the particles that make up the body are displaced. For any given particle, its position vector is \mathbf{r} and its velocity is \mathbf{v} .

The linear momentum of the body is defined as

$$\mathbf{P} = \int_V \mathbf{v} \rho dV$$

and its moment of momentum is defined as

$$\mathbf{H} = \int_V \mathbf{r} \times \mathbf{v} \rho dV$$

where B is the space occupied by the body.

If the total force applied on the body is \mathbf{F}_T and the total applied torque is \mathbf{L}_T the laws of motion are

$$\frac{d\mathbf{P}}{dt} = \mathbf{F}_T$$

and

$$\frac{d\mathbf{H}}{dt} = \mathbf{L}_T$$

The forces applied on bodies are of two types: body forces and surface forces. Body forces \mathbf{X} act in the interior of the body while surface forces \mathbf{T} act on surface elements. Gravity is a good example of a body force while stress is an example of surface force. Therefore,

$$\mathbf{F} = \int_V \mathbf{X}dV + \oint_S \mathbf{T}dS$$

The equations of equilibrium are simply the statements that no net force and no moment act on a body in a state of mechanical equilibrium. They are easily obtained by carrying out force and moment balances on the cube shaped volume element mentioned above and then taking the limit as the size goes to zero. The results are

$$\frac{\partial\tau_{ij}}{\partial x_j} + X_i = \tau_{ij,j} + X_i = 0$$

for the force equation, and

$$\tau_{ij} = \tau_{ji}$$

for the moment equation.

3.2.3 Concept of Principal Stresses

There are always three perpendicular directions at any point inside a loaded body where the shear stresses vanish. These are called *principal directions* and the planes normal to them are the *principal planes*. The three principal stresses be $\sigma_1, \sigma_2, \sigma_3$ and are the roots of the equation

$$\sigma^3 - I_1\sigma^2 + I_2\sigma + I_3 = 0$$

where I_1, I_2, I_3 are the *stress tensor invariants* given by

$$I_1 = \tau_{ii}$$

$$I_2 = \frac{1}{2}(\tau_{ii}\tau_{jj} - \tau_{ij}\tau_{ji})$$

$$I_3 = \det \tau_{ij}$$

At a point in a loaded body, the mean stress σ_0 is defined as

$$\sigma_0 = \frac{1}{3} \tau_{ii}$$

and the *stress deviation tensor* τ'_{ij} is defined as

$$\tau'_{ij} = \tau_{ij} - \sigma_0 \delta_{ij}$$

The invariants of the stress deviation tensor are

$$J_1 = 0$$

$$J_2 = \frac{1}{2} \tau'_{ij} \tau'_{ij} = 3\sigma_0^2 - I_2 = \frac{3}{2} \tau_0^2$$

$$J_3 = \frac{1}{3} \tau'_{ij} \tau'_{jk} \tau'_{ki} = I_3 + J_2 \sigma_0 - \sigma_0^3$$

where τ_0 is the *octahedral stress*.

A useful graphical representation of the state of stress at a point can be obtained by drawing the stress Mohr circle.

3.3 Analysis of Strain

As loads are applied to a body, individual material particles are displaced from their positions. Let the point coordinates before deformation be a^i and x^i after it. An infinitesimal element of arc connecting two adjacent points in the body ds_0 distorts to ds . The difference between the squares of the length elements is given by

$$ds^2 - ds_0^2 = 2E_{ij} da^i da^j$$

or

$$ds^2 - ds_0^2 = 2e_{ij} dx^i dx^j$$

where

$$E_{ij} = \frac{1}{2} (g_{\alpha\beta} \frac{\partial x_\alpha}{\partial a_i} \frac{\partial x_\beta}{\partial a_j} - a_{ij})$$

is the Green-St. Venant (or Lagrangian) strain tensor and

$$e_{ij} = \frac{1}{2} (g_{ij} - a_{\alpha\beta} \frac{\partial a_\alpha}{\partial x_i} \frac{\partial a_\beta}{\partial x_j})$$

is the Almansi (or Eulerian) strain tensor.

One can show, that the necessary and sufficient condition for rigid body motion is the vanishing of the strain tensor.

Since the strain tensors are tensors, they exhibit similar properties to those of the stress tensor. Specifically, one can define strain invariants (the first one, for instance is $e_{ii} = \Delta V/V$ and is called the *dilatation*. Strain deviation tensors can also be defined.

Note that if rectangular Cartesian coordinates are used to describe the deformation $g_{ij} = a_{ij} = \delta_{ij}$. In this case, defining components of the *displacement vector* \mathbf{u} as

$$u_i = x_i - a_i$$

yields

$$E_{ij} = \frac{1}{2} \left[\frac{\partial u_j}{\partial a_i} + \frac{\partial u_i}{\partial a_j} + \frac{\partial u_\alpha}{\partial a_i} \frac{\partial u_\alpha}{\partial a_j} \right]$$

and

$$e_{ij} = \frac{1}{2} \left[\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{\partial u_\alpha}{\partial x_i} \frac{\partial u_\alpha}{\partial x_j} \right]$$

For the important case of *small deformations* (i.e. infinitesimal displacements) the product terms are negligible and one obtains

$$e_{ij} = \epsilon_{ij} = \frac{1}{2} \left[\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right]$$

I.e. for the case of small deformations the Lagrangian and Eulerian strains are the same.

Note that if an element of a body is stretched in the x -direction by an amount dx ,

$$ds^2 - ds_0^2 = 2e_{xx}(dx)^2$$

i.e. e_{xx} represents an *extension* (change of length per unit length). If instead the element is sheared in the $x - y$ plane, the *shear* is e_{xy} . Therefore e_{ii} are called normal strains and e_{ij} are shearing strains (although engineers sometimes use this name for the quantity $2e_{ij}$). Furthermore, the quantity

$$\omega_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right)$$

is called the *rotation*.

Deformation is assumed to take place without the formation of cracks or voids or interpenetration of materials particles. This requirement is expressed by the *equations of compatibility*. These equations must be fulfilled by the strain components of any admissible deformation field. They are

$$e_{ij,kl} + e_{kl,ij} - e_{ij,jl} - e_{jl,ik} = 0$$

Although the above represent 81 equations, only six turn out to be essential.

A useful graphical representation of the state of strain at a point can be obtained by drawing the strain Mohr circle.

3.4 Concept of Virtual Power

Virtual motions are useful concepts in mechanics of material. They are used both in the analytical formulation of problems and also constitute the foundation of the finite element methodology. Virtual motions are imaginary movements of material points and the method of virtual power consists of determining the associated work or power involved. If the virtual motion of point M is described by the vector \mathbf{v} , the associated power is $P(\mathbf{v}(M))$. In this section we show how the static equilibrium equation is readily obtained by applying the principle of virtual power.

The virtual motion can be described with reference to the coordinates of the initial location of point M , M_0 (Lagrangian description) or in terms of the current coordinates of M (Eulerian description). The total time rate of change of \mathbf{v} in Lagrangian variables is simply $\gamma = d\mathbf{v}/dt = \partial\mathbf{v}/\partial t$ while in the Eulerian description one has

$$\gamma = \frac{d\mathbf{v}}{dt} = \frac{\partial\mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla\mathbf{v} = \frac{dv_i}{dt} = \frac{\partial v_i}{\partial t} + v_{i,j}v_j$$

where $\nabla\mathbf{v}$ is an important second order tensor, the velocity gradient tensor which can be expressed as

$$\nabla\mathbf{v} = \Omega + \mathbf{D} = \frac{1}{2}(v_{i,j} - v_{j,i}) + \frac{1}{2}(v_{i,j} + v_{j,i})$$

where $\mathbf{D} = D_{ij}$ is the rate of deformation tensor and $\Omega = \Omega_{ij}$ is the rate of rotation tensor.

The fundamental laws of dynamics are embodied in the principle of virtual power. According to it, for a body in mechanical equilibrium, for any virtual motion the virtual power associated with rigid body movement is zero and the virtual power of inertia forces equals the sum of the virtual powers of all internal and external forces.

Consider a material body of volume V and surface S which is subjected to a body force density X_i . Further, let the internal stress field be τ_{ij} and the surface density of cohesive forces T_i . The principle of virtual power is expressed as

$$-\int_V \tau_{ij} D_{ij} dV + \int_V X_i v_i dV + \oint_S T_i v_i dS = \int_V \gamma_i v_i \rho dV$$

Since $T_i = \tau_{ij} n_j$, integration by parts yields

$$\int_V (\tau_{ij,j} + X_i - \rho\gamma_i) v_i dV = 0$$

Since the integrand must vanish, for the special but important case of zero inertia forces one obtains the static equilibrium equation

$$\tau_{ij,j} + X_i = 0$$

As mentioned before, analysis is simpler if the assumption of small displacements and strains can be used. If this is not the case, finite deformation theory must be used to describe the geometry of the deformation.

3.5 Summary of Conservation Principles

Conservation principles are balance statements for physical quantities the amounts of which are conserved in physical processes. Conservation principles are valid regardless the material constitution of the medium in which they apply, therefore, they have a universal character. Mathematical expressions for these conservation principles in the form of differential equations are readily obtained by performing balances of the conserved quantities over differential volume elements and then taking the limit as the volume shrinks down to zero. In the thermomechanics of solids and fluids the conservation principles most frequently invoked are:

The principle of mass conservation, or equation of continuity, i.e.

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_j}{\partial x_j} = 0$$

where ρ is the local density (mass per unit volume), v_j is the local velocity, x_j are the local Eulerian coordinates and

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \rho v_j \frac{\partial}{\partial x_j}$$

is the material or substantial derivative.

The principle of conservation of linear momentum, or equation of motion, i.e.

$$\rho \frac{Dv_i}{Dt} = \frac{\partial \sigma_{ij}}{\partial x_j} + X_i$$

where σ_{ij} is the stress tensor and X_i is the body force vector. Note this become the standard equilibrium equation under static conditions (i.e. $v_i = 0$).

The principle of balance of angular momentum, or stress tensor symmetry equation, i.e.

$$\sigma_{ij} = \sigma_{ji}$$

The principle of conservation of energy, or first law of thermodynamics, i.e.

$$\rho \frac{Du}{Dt} = -\frac{\partial q_i}{\partial x_i} + r + \sigma_{ij} \frac{\partial v_i}{\partial x_j}$$

where u is the specific internal energy per unit mass, q_i is the heat flux vector, r is the distributed rate of internal energy generation and the last term on the right hand side represents the rate of irreversible degradation of mechanical to thermal energy.

The principle of entropy production or second law of thermodynamics, i.e.

$$\rho \frac{D\eta}{Dt} = -\frac{\partial (q_i/T)}{\partial x_i} + \rho \frac{D\eta_{int}}{Dt}$$

where η is the specific entropy per unit mass, q_i/T is the entropy flux vector (with T being the absolute temperature) and η_{int} is the internal entropy production per unit mass. The last term above equals zero for reversible processes, is greater than zero for irreversible ones and there are no processes in nature for which it is negative. Because of the nature of this last term, the entropy equation is not directly useful in the determination of the various fields but rather acts as a constraint condition that must be fulfilled by all solutions of the other conservation equations.

All the above balance equations can be represented by a single expression by introducing the generic conserved quantity ψ , its internal supply per unit mass s and the influx of ψ per unit area $-j_i n_i$ where n_i is the normal vector. With the above, the generic conservation equation becomes

$$\rho \frac{D\psi}{Dt} = \rho s - \frac{\partial j_i}{\partial x_i}$$

In the case of a single component system, the equations of continuity, motion and energy constitute a set of five scalar equations involving the unknowns, velocity (three components), temperature, density, stress (six components), energy, heat flux (three components) and entropy; a total of sixteen unknowns. Clearly, the balance equations of thermomechanics constitute a severely underdetermined system and additional equations are required in order to be able to produce well posed problems that can be solved by standard mathematical methods.

The additional equations that must be incorporated in order to solve actual technical problems consist of mathematical descriptions of individual material response or behavior. Such equations are called constitutive equations. These equations, in contrast with the conservation principles, do not have a universal character but rather describe in detail individual material behavior. Fortunately, constitutive equations are available for whole groups of material behavior, namely, elastic, viscoelastic, plastic, creep and viscoplastic and others. In formulating problems in solid mechanics one then proceeds by identifying the appropriate constitutive equations to use, then combines these equations with the balance equations, applies boundary conditions and proceeds to solve the resulting system of equations using analytical or more commonly, numerical solution techniques such as finite element methods.