4 Continuum Mechanics Foundations

Chapter Outline

Mechanics of Solid Polymers.
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4.1 Introduction

Continuum mechanics is a subject that unifies solid mechanics, fluid mechanics, thermodynamics, and heat transfer, all of which are core subjects of mechanical engineering. The approach taken in this text is to use continuum mechanics as a universal tool in which to formulate the polymer mechanics theories that will be presented in the following chapters. In some undergraduate textbooks, the polymer mechanics frameworks are often presented using a traditional small-strain solid mechanics approach in an effort to make the theory less abstract. Here, a different approach is taken. Polymer components, due to their mechanical characteristics, are often both able and designed to undergo large deformations, and it is therefore important for the polymer mechanist to know that it is not sufficient to simply talk about *stress* and *strain* when working with polymers, but that there are in fact different types of stress and strain that can be used, and hence it is important to specify and correctly use the different types of stress and strain that are available.

The most logical approach for presenting these concepts is to use a continuum mechanics approach, specifically tailored to solid polymers. The approach taken here has been to reduce some of the abstraction, while at the same time keep the direct tensor notation due to its simplicity. The content presented in this chapter is meant to be self-sufficient, and has been given a somewhat condensed representation in order to fit into one chapter. There are many excellent references that present a more comprehensive treatment of the subject [1–8]. The chapter starts with a discussion about the small-strain definitions of stress and strain followed by a brief review of tensor algebra, and then introduces the different topics in a logical order.

4.2 Classical Definitions of Stress and Strain

The classical approach to define stress and strain is based on the assumption of small deformations. As will be discussed below, this means that the functional dependence of the displacement of each material point[1] is assumed to be linear. The implications of this linearized theory for uniaxial loading is presented in Section 4.2.1, and for multiaxial loading in Section 4.2.2.

4.2.1 Uniaxial Loading

The classical approach to define stress and strain in uniaxial deformation is given in Figure 4.1.

This figure shows a cylinder with an initial length L_0 and initial cross-sectional area A_0 that is uniaxially loaded with a force F. The bottom of the cylinder is held fixed, and the top is displaced a distance u as a result of the applied force F.

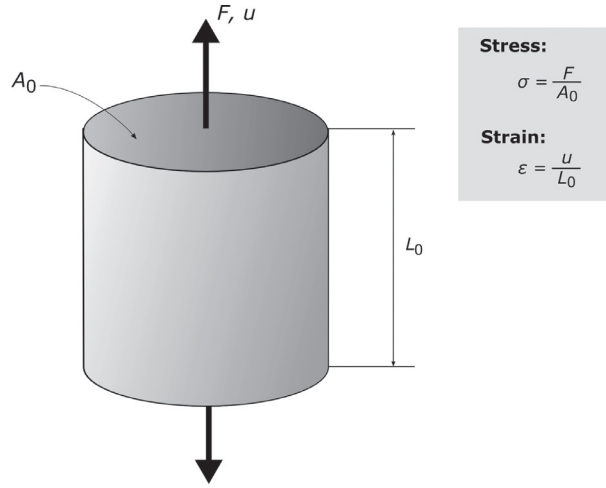


Figure 4.1 Classical definition of stress and strain for uniaxial loading with small deformations.

[1] *A* material point *is a location that is fixed in a body and moves with the material during deformations.*

In general, the length of the cylinder L can be a nonlinear function of the applied force: $L = \hat{L}(F)$. This functional relationship can be represented as a Taylor series expansion:

$$L = L_0 + \frac{\mathrm{d}\hat{L}(F)}{\mathrm{d}F}F + \cdots . \tag{4.1}$$

In the small-strain theory, only the linear term (first derivative of $\hat{L}(F)$) is included. By defining $u = L - L_0$ and $k = \mathrm{d}F/\mathrm{d}L$, the force-displacement relationship becomes the classical linear elastic spring equation:

$$F = ku. \tag{4.2}$$

The mechanical stress is defined as the force intensity, that is, stress = force/area. One important question is what area should be used in the calculation of the stress. When a tensile force is applied on the cylindrical specimen it will not only get longer, but it will also typically[2] reduce its cross-sectional area. Let us start by defining the radius of the cylinder at a given applied force to be r, the initial (undeformed) radius to be r_0, and the change in radius to be Δr, then $r = r_0 + \Delta r$. In the small deformation approach, the change in radius is assumed to be much smaller than the initial radius: $\Delta r \ll r_0$. The cross-sectional area in a deformed state can then be calculated from:

$$A = \pi r^2 = \pi(r_0 + \Delta r)^2 = \pi(r_0^2 + 2\Delta r r_0 + \Delta r^2) \approx \pi r_0^2. \tag{4.3}$$

This means that for small deformations the cross-sectional area is constant and the stress is simply given by $\sigma = F/A_0 = F/A$.

As mentioned, the strain is given by the normalized displacement $\varepsilon = u/L_0$. With these definitions the stress is proportional to the applied force and inversely proportional to the cross-sectional area, and the strain is given by the normalized displacement. Note that the stress can take any value, but the strain has be to be larger than -1.

[2] *The amount of reduction of the cross-sectional area is determined by the Poisson's ratio. Almost all materials have a positive Poisson's ratio.*

The small-strain classical theory is based on the assumption that the geometric changes that occur during the loading are so small that they can be represented using a first-order linear representation. Within this theory there is only one stress and one strain measure to consider.

4.2.2 Multiaxial Loading

A small deformation multiaxial loading situation is shown in Figure 4.2.

In the multiaxial case, the stress and strain at each point of the sample are characterized by six values: $\sigma_{11}, \sigma_{12}, \sigma_{13}, \sigma_{22}, \sigma_{23}, \sigma_{33}$ and $\varepsilon_{11}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{22}, \varepsilon_{23}, \varepsilon_{33}$. These values are often arranged into symmetric 3×3 matrices:

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix}, \tag{4.4}$$

$$\varepsilon_{ij} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix}. \tag{4.5}$$

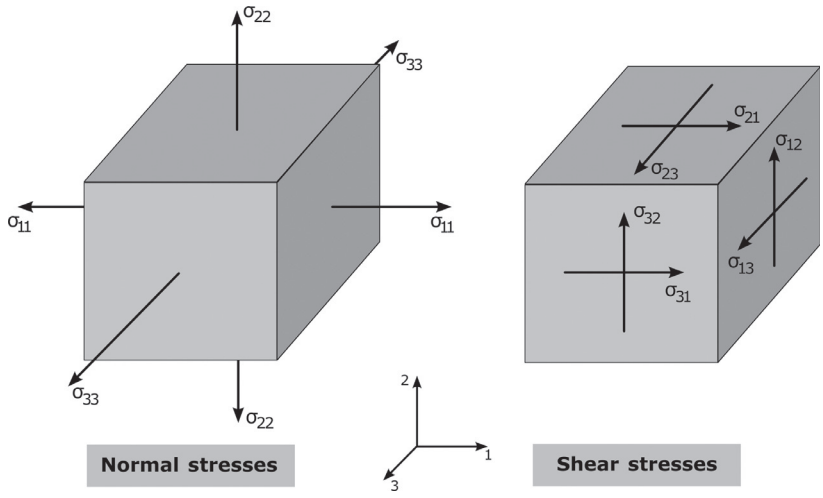


Figure 4.2 Classical definition of multiaxial stresses. The strain components are defined analogously.

In the multiaxial case, the stress and strain at each point can be represented by normal and shear stresses on a small cube-shaped volume element, as shown in Figure 4.2. The first subscript of a stress or strain quantity represents the normal direction of the face and the second subscript represents the direction of the stress or strain quantity.[3] Each face contains one normal stress and two shear stresses. To satisfy force equilibrium, the shear stress matrix is symmetric, that is, $\sigma_{12} = \sigma_{21}$, $\sigma_{13} = \sigma_{31}$, and $\sigma_{23} = \sigma_{32}$.

The strain in the multiaxial case can be calculated in a similar way to the uniaxial case. Start by defining a displacement vector $\mathbf{U} = [U_1, U_2, U_3]$ that varies with the position in the material specified by $\mathbf{X} = [X_1, X_2, X_3]$:

$$\mathbf{U}(\mathbf{X}) = \mathbf{x}(\mathbf{X}) - \mathbf{X}. \tag{4.6}$$

In this equation, (uppercase) $\mathbf{X}$ is the initial location of the material point that in the deformed state is at location (lowercase) $\mathbf{x}$. The partial derivative of the displacement vector with respect to the initial position is the gradient of the displacements:

$$\text{Grad } \mathbf{U}(\mathbf{X}) = \frac{\partial \mathbf{U}(\mathbf{X})}{\partial \mathbf{X}} = \frac{\partial U_i}{\partial X_j} = \begin{bmatrix} \frac{\partial U_1}{\partial X_1} & \frac{\partial U_1}{\partial X_2} & \frac{\partial U_1}{\partial X_3} \\ \frac{\partial U_2}{\partial X_1} & \frac{\partial U_2}{\partial X_2} & \frac{\partial U_2}{\partial X_3} \\ \frac{\partial U_3}{\partial X_1} & \frac{\partial U_3}{\partial X_2} & \frac{\partial U_3}{\partial X_3} \end{bmatrix}. \tag{4.7}$$

The strain matrix is defined as the symmetric part of Equation (4.7):

$$\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i}\right] \tag{4.8}$$

$$= \begin{bmatrix} \frac{\partial U_1}{\partial X_1} & \frac{1}{2}\left(\frac{\partial U_1}{\partial X_2} + \frac{\partial U_2}{\partial X_1}\right) & \frac{1}{2}\left(\frac{\partial U_1}{\partial X_3} + \frac{\partial U_3}{\partial X_1}\right) \\ \frac{1}{2}\left(\frac{\partial U_2}{\partial X_1} + \frac{\partial U_1}{\partial X_2}\right) & \frac{\partial U_2}{\partial X_2} & \frac{1}{2}\left(\frac{\partial U_2}{\partial X_3} + \frac{\partial U_3}{\partial X_2}\right) \\ \frac{1}{2}\left(\frac{\partial U_3}{\partial X_1} + \frac{\partial U_1}{\partial X_3}\right) & \frac{1}{2}\left(\frac{\partial U_3}{\partial X_2} + \frac{\partial U_2}{\partial X_3}\right) & \frac{\partial U_3}{\partial X_3} \end{bmatrix}.$$

[3] *In some textbooks, the interpretation of the two subscripts is reversed. Since the stress and strain matrices are symmetric, this does not have a significant influence.*

These definitions of stress and strain are sufficient for analyzing problems involving small deformations. The situation, however, becomes more complicated if the applied deformations become sufficient large such that the shape or size of the specimen becomes significantly different during the applied deformation. In these cases, a more general description of stress and strain is in order. The next section presents an extension of the theory suitable for large deformations.

Example
To demonstrate the short comings of the small-strain approach consider a situation in which the cylinder in Figure 4.1 is made from a flexible rubber and a large force is applied. In this case, the change in both the specimen length and cross-section area can be significant. In the small-strain theory, the stress is calculated from $\sigma = F/A$, but one obvious complication here is that the cross-sectional area is changing during the deformation. In the small-strain case, A is assumed to be constant, but in the large strain case that assumption is not valid. In fact, if we use the initial area A_0 in the calculation of the stress we get the engineering stress: $\sigma_{\text{eng}} = F/A_0$, and if we use the current (actual) area we get the true stress: $\sigma_{\text{true}} = F/A$.

Note: *There is no hard rule for when the small-strain theory is sufficient, but a general rule is that the strain magnitude has to be less than 1%. If an effective strain is larger than that magnitude it is usually better to switch to large strain theory.*

In Abaqus, you can switch on large-deformation theory by setting `NLGEOM=yes` *on the* `*STEP` *command.*

In ANSYS, you can switch on large-deformation theory by setting `nlgeom,on`.

4.3 Large Strain Kinematics

Polymer mechanics, and solid mechanics in general, are topics concerned with the evolution of stresses and strains when a component is exposed to external loads in the form of forces,

displacements, and temperatures. One of the key foundations of this topic is related to the kinematics of the deformation, that is how to mathematically express the displacements of different parts of a body of interest.

To study this topic, we will start by considering a body that initially (at time 0) has a configuration (shape and location) Ω_0 and then at a later time t has another configuration Ω_c, see Figure 4.3.

The body can be considered to consist of a collection of small volume elements that collectively make up the body. Each of these infinitesimal volume elements is referred to as a material point. Kinematics is a topic that describes the movement of material points during a deformation event. As was discussed earlier, in the small-strain theory, the displacements are assumed to be so small that the configuration of the body does not significantly change during a loading event. This is one of the key factors that make small-strain theory easy to understand and work with.

When the deformations are finite, the shape and location of a body can undergo large changes during a loading event. The following example illustrates two different ways to keep track of the motion of a deforming body.

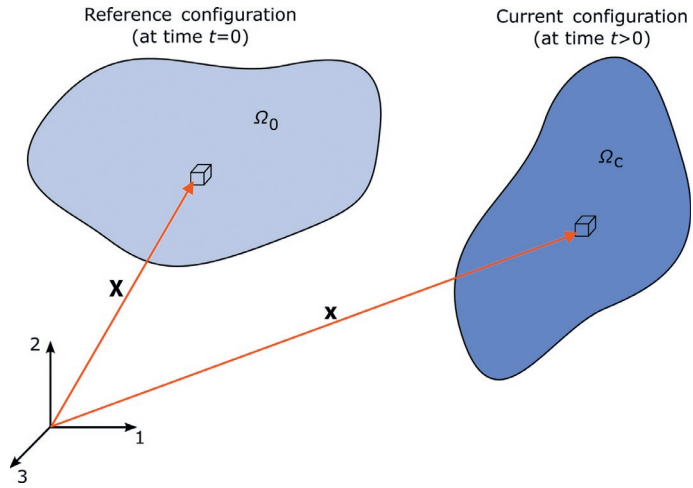


Figure 4.3 Schematic figure showing a body that move and change shape as a function of time.

Example: Lagrangian and Eulerian Formulations.
To illustrate the use of different kinematic formulations we will consider a rubber band that is axially stretched by a time-varying force $\mathbf{f}(t)$, see Figure 4.4. In this example, one material point on the rubber band has been marked with a $\times$.

One way to keep track of the stresses and strains in the rubber band is to focus on one material point at a time (e.g., the location on the rubber band with the $\times$). If we specify the location of the $\times$ in the unloaded configuration we can then uniquely express the stress and strain of that material point as a function of time. This approach where we focus on each material point labeled by its position in the reference configuration is called a *Lagrangian formulation*.

An alternative approach to specify the stresses and strains in the rubber band is to superimpose a fixed grid (coordinate system), as is shown in Figure 4.5, and then use the spatial coordinates to specify the stresses and strains in the rubber band during the loading event.

This way we can keep track of the rubber band in terms of its current spatial coordinates. This way to describe the motion is called an *Eulerian formulation*.

We can mathematically formalize the previous example by considering a material point that is initially located at $\mathbf{X}$ and at time t located at $\mathbf{x}(t)$. The motion of the material point can be described by the mapping:

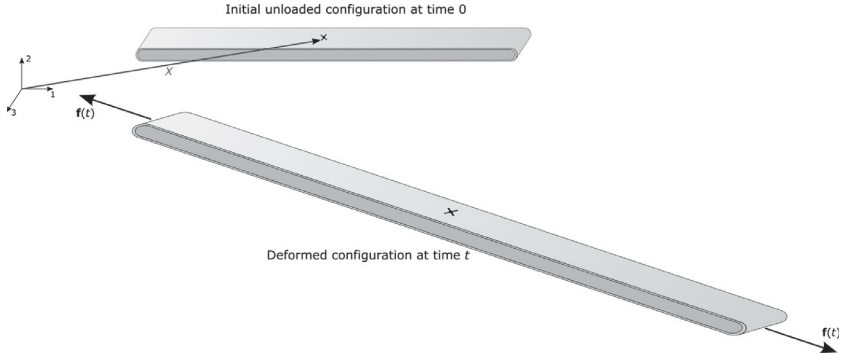


Figure 4.4 Example of a Lagrangian representation of a deformation.

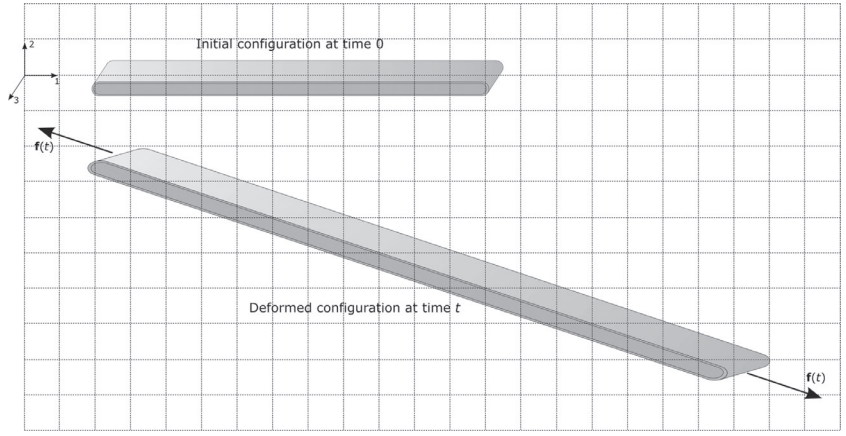


Figure 4.5 Example of an Eulerian representation of a deformation.

$$\mathbf{x} = \mathcal{X}(\mathbf{X}, t), \tag{4.9}$$

where $\mathcal{X}(\cdot)$ is a vector function that as input takes an initial position vector and a time, and as an output gives the position of that material point at the specified time. The vector $\mathbf{X}$ is called the *reference* (or *material*) location, and the vector $\mathbf{x}$ is called the *current* (or *spatial*) location of the material point.

When studying continuum quantities it is often necessary to follow and keep track of a certain region of a body. As discussed in the example above, there are two ways to do this. One is to label each point of the region of interest based on the its initial reference location. This way we can make statements such as: "the material point that at time 0 was at the location $\mathbf{X}$ is having a velocity of $\mathbf{V}$ at time t." This formulation, where everything is referred back to the initial configuration, is called a *Lagrangian formulation*.

The other way to keep track of the motion of a body is to utilize the current configuration to label the material points. This way we can make statements as: "the material point which at time t is at $\mathbf{x}$ has a velocity of $\mathbf{v}$." This formulation, where everything is referred to in the current configuration is called an *Eulerian formulation*.

The nomenclature in this text closely follows recent continuum mechanics texts (e.g., Holzapfel [2]). Specifically, quantities that are expressed in the reference configuration are denoted with

uppercase letters, and quantities that are expressed in the current configuration are denoted with lowercase letters.

The following discussion will utilize tensor notation and tensor algebra. In order to fully understand the continuum mechanics theory, it is important to have a good understanding of what tensors are and how they can be manipulated. The following section presents a brief summary of this topic.

4.4 Vector and Tensor Algebra

It can be shown that, in a mathematical sense, both stress and strain are second-order tensors [2, 4, 7], hence the rules of tensor algebra are of importance in polymer mechanics. For the novice, second-order tensors can at first appear to be complicated and abstract. This conception is fueled by the many different ways tensor notation have been written in different books. The approach taken here is to limit the discussion to results that are commonly used in polymer mechanics, and not to place too much emphasis of mathematical proofs. For the interested reader there are numerous resources [1–4, 9] that focus on the mathematical details.

The three types of variables that are of importance in polymer mechanics are scalars (e.g., temperature, density), vectors (e.g., force, velocity), and second-order tensors (e.g., stress, strain). In some texts, scalars are referred to as zeroth-order tensors, and vectors as first-order tensors. Here, we will not use those terms, and the second-order tensors will simply be called tensors.

4.4.1 Vector Operations

A vector represents a direction and a magnitude in three-dimensional (3D) space. In the following, a vector is represented by a bold-face letter, or by letters with indices, for example:

$$\mathbf{v} = v_1\hat{\mathbf{e}}_1 + v_2\hat{\mathbf{e}}_2 + v_3\hat{\mathbf{e}}_3 = v_i\hat{\mathbf{e}}_i. \tag{4.10}$$

In this example, $[\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3]$ is a set of orthogonal basis vectors. Here, and in the following, vectors with unit length are denoted

with a superscript hat; for example, $\hat{\mathbf{e}}_1$. The last term in Equation (4.10) illustrates the use of the Einstein repeated indexes summation convention: if exactly two variables in a term have the same subscript then that subscript is to be repeated with the values 1, 2, and 3. For example:

$$\begin{aligned} u_i u_i &= u_1 u_1 + u_2 u_2 + u_3 u_3 = |\mathbf{u}|^2, \\ A_{jj} &= A_{11} + A_{22} + A_{33}, \\ A_{i1} u_i &= A_{11} u_1 + A_{21} u_2 + A_{31} u_3. \end{aligned}$$

When working with vectors there are a number of operations that are commonly used. The following is a short summary of the most common vector functions and operations.

The length of a vector, also called the norm, is defined by:

$$|\mathbf{u}| = \sqrt{\mathbf{u} \cdot \mathbf{u}} = \sqrt{u_i u_i} = \sqrt{u_1^2 + u_2^2 + u_3^2}. \tag{4.11}$$

Two vectors can be added or subtracted by adding or subtracting the components of the vectors:

$$\mathbf{u} + \mathbf{v} = \sum_{i=1}^{3} (u_i + v_i) \hat{\mathbf{e}}_i, \tag{4.12}$$

$$\mathbf{u} - \mathbf{v} = \sum_{i=1}^{3} (u_i - v_i) \hat{\mathbf{e}}_i. \tag{4.13}$$

A scalar and a vector can be multiplied by multiplying the scalar with each of the components of the vector:

$$a\mathbf{u} = (a u_i) \hat{\mathbf{e}}_i. \tag{4.14}$$

There are different ways to multiply two vectors. A first way is through the dot-product which is defined by:

$$\mathbf{u} \cdot \mathbf{v} = u_i v_j = u_1 v_1 + u_2 v_2 + u_3 v_3 = |\mathbf{u}| \cdot |\mathbf{v}| \cdot \cos\theta, \tag{4.15}$$

where θ is the angle between the two arbitrary vectors $\mathbf{u}$ and $\mathbf{v}$. Note that the dot-product of two vectors becomes a scalar. A second way to multiply two vectors is through the cross-product which is defined by:

$$\mathbf{u} \times \mathbf{v} = \begin{bmatrix} \hat{\mathbf{e}}_1 & \hat{\mathbf{e}}_2 & \hat{\mathbf{e}}_3 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{bmatrix} = u_i v_j \epsilon_{ijk} \hat{\mathbf{e}}_k, \tag{4.16}$$

where ϵ_{ijk} is the *permutation symbol* defined by

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) = (1,2,3) \text{ or } (2,3,1) \text{ or } (3,1,2) \\ -1 & \text{if } (i,j,k) = (1,3,2) \text{ or } (3,2,1) \text{ or } (2,1,3) \\ 0 & \text{for any other combination of } i,j,k \end{cases}. \tag{4.17}$$

The cross-product of two vectors is a vector quantity that is orthogonal to the two initial vectors.

4.4.2 The Dyadic Product

A third way to multiply two vectors **a** and **b** is through the *dyad* (or tensor product) denoted by $\mathbf{a} \otimes \mathbf{b}$. The dyad is a second-order tensor, which will be discussed in more detail in the next section, and that can be defined by how it operates on an arbitrary vector **x**:

$$(\mathbf{a} \otimes \mathbf{b})\, \mathbf{x} = (\mathbf{b} \cdot \mathbf{x})\, \mathbf{a}. \tag{4.18}$$

The dyad between two vectors can also more intuitively be written as a 3×3 matrix:

$$\mathbf{a} \otimes \mathbf{b} = \begin{bmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{bmatrix}. \tag{4.19}$$

In general, any general tensor can be written as a sum of nine dyad terms (also called a dyadic):

$$\mathbf{A} = A_{ij} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \quad \text{(summation implied)}. \tag{4.20}$$

For example, the identity tensor can be written as the sum of three dyads:

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \sum_{i=1}^{3} \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_i = \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_i. \tag{4.21}$$

The following pre- and post-multiplications between a dyad and a vector or second-order tensor ($\mathbf{A}$) are commonly used:

$$(\mathbf{a} \otimes \mathbf{b})(\mathbf{c} \otimes \mathbf{d}) = (\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \otimes \mathbf{d}), \tag{4.22}$$

$$(\mathbf{a} \otimes \mathbf{b})\mathbf{A} = \mathbf{a} \otimes (\mathbf{A}^{\top}\mathbf{b}), \tag{4.23}$$

$$\mathbf{A}(\mathbf{a} \otimes \mathbf{b}) = (\mathbf{A}\mathbf{a}) \otimes \mathbf{b}. \tag{4.24}$$

The proof of these relations are discussed in various text books [1–3, 10] and are here left as exercises.

4.4.3 Tensor Operations

A (second-order) tensor represents a quantity that contain more information than a vector: it assigns a value and direction for each value and direction, and can hence be thought of as a mapping from one vector to another. In index-form, a second-order tensor can be written as $\mathbf{A} = A_{ij}$.

There are different ways to interpret a second-order tensor. For example, as mentioned, a second-order tensor can be thought of as a linear operator $\mathbf{A}$ that acts on a vector $\mathbf{u}$ generating another vector $\mathbf{v} = \mathbf{A}\mathbf{u}$. In the context of this text, it is often sufficient to simply consider a second-order tensor as a 3×3 matrix.

When working with tensors there are also numerous operations that are important. The following are definitions of the most common operations:

- Two tensors can be added (or subtracted) by adding (or subtracting) their indices:

$$(\mathbf{A} + \mathbf{B})_{ij} = A_{ij} + B_{ij} \tag{4.25}$$

$$(\mathbf{A} - \mathbf{B})_{ij} = A_{ij} - B_{ij}. \tag{4.26}$$

- A tensor can be operated on a vector creating another vector using the following multiplication and summation:

$$\mathbf{A}\mathbf{u} = A_{ij}u_j\hat{\mathbf{e}}_j = A_{11}u_1\hat{\mathbf{e}}_1 + A_{12}u_2\hat{\mathbf{e}}_2 + A_{13}u_3\hat{\mathbf{e}}_3. \tag{4.27}$$

- Two tensors can be multiplied, giving a new tensor, using the following multiplication and summation:

$$(\mathbf{AB})_{ij} = A_{ik}B_{kj} = A_{i1}B_{1j} + A_{i2}B_{2k} + A_{i3}B_{3k}. \quad (4.28)$$

- The *inner product* of two tensors (also called the *dot-product* or the *contraction*) is a scalar defined by

$$\mathbf{A} : \mathbf{B} = \mathrm{tr}[\mathbf{AB}^\top] = A_{ij}B_{ij}. \quad (4.29)$$

- The *transpose* of a tensor $\mathbf{A}$ is defined by

$$\mathbf{Au} \cdot \mathbf{v} = \mathbf{u} \cdot \mathbf{A}^\top\mathbf{v}, \qquad \text{for all vectors } \mathbf{u}, \mathbf{v}. \quad (4.30)$$

  The transpose of a tensor can also be written in index notation

$$(A_{ij})^\top = A_{ji}. \quad (4.31)$$

  which also gives the following useful equation

$$(\mathbf{AB})^\top = \mathbf{B}^\top\mathbf{A}^\top. \quad (4.32)$$

- The *trace* of a tensor is a scalar quantity that is given by the sum of the diagonal terms:

$$\mathrm{tr}[\mathbf{A}] = A_{ii} = A_{11} + A_{22} + A_{33}. \quad (4.33)$$

- The *determinant* of a tensor can be calculated the same way as it is calculated for a 3×3 matrix:

$$\det[\mathbf{A}] = \det \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}. \quad (4.34)$$

- A tensor can be uniquely decomposed into *deviatoric* and *volumetric* parts:

$$\mathbf{A} = \mathrm{dev}[\mathbf{A}] + \mathrm{vol}[\mathbf{A}], \quad (4.35)$$

  where

$$\mathrm{dev}[\mathbf{A}] = \mathbf{A} - \frac{1}{3}\mathrm{tr}[\mathbf{A}]\mathbf{I}, \quad (4.36)$$

$$\text{vol}[\mathbf{A}] = \frac{1}{3}\,\text{tr}[\mathbf{A}]\mathbf{I}. \tag{4.37}$$

A deviatoric tensor has a trace of zero. This decomposition is useful when working with the deformation gradient, as will be discussed in later chapters.

- A tensor can also be decomposed into a product of *distortional* and *dilatational* parts:

$$\mathbf{A} = \text{distortional}[\mathbf{A}]\ \text{dilatational}[\mathbf{A}], \tag{4.38}$$

where

$$\text{distortional}[\mathbf{A}] = \det[\mathbf{A}]^{-1/3}\,\mathbf{A}, \tag{4.39}$$

$$\text{dilatational}[\mathbf{A}] = (\det[\mathbf{A}])^{1/3}\,\mathbf{I}. \tag{4.40}$$

A distortional tensor has a determinant of zero. This deformation gradient is useful when working with the deformation gradient, as will be discussed in later chapters.

- An *orthogonal* tensor $\mathbf{Q}$ is a tensor with the following properties:

$$\mathbf{Q}^{\top} = \mathbf{Q}^{-1} \tag{4.41}$$

$$\det \mathbf{Q} = \mathbf{1}. \tag{4.42}$$

- A *diagonal* tensor is a tensor with zero off-diagonal terms:

$$A_{ij} = 0, \quad \text{if } i \neq j. \tag{4.43}$$

- The components of a tensor A_{ij} can be determined from the unit vectors $\hat{\mathbf{e}}_i$ and $\hat{\mathbf{e}}_j$ as follows:

$$A_{ij} = \mathbf{A}\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j. \tag{4.44}$$

- It is often useful to calculate functions of a tensor, such as $\exp(\mathbf{A})$. One way to calculate these functions is to write the tensor $\mathbf{A}$ in its spectral representation (see Section 4.5.1) and then apply the function on the principal values of the tensor:

$$f(\mathbf{F}) = \sum_{i=1}^{3} f(\lambda_i)\hat{\mathbf{n}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.45}$$

This theorem is discussed in more detail in linear algebra texts [11, 12].

From the discussion above it is clear that direct notation is more compact and often easier to understand than index notation. For these reasons direct notation will be used almost exclusively in the following.

4.4.4 Derivatives of Scalar, Vector, and Tensor Fields

When formulating and integrating certain advanced constitutive theories it is important to incorporate time and spacial derivatives of scalar, vector, and tensor fields. This section summarizes the most commonly used approach to perform these derivatives.

First consider a scalar function $a(\mathbf{x}, t)$ that is expressed in the spatial configuration. The *spatial time derivative of the spatial field* $a(\mathbf{x}, t)$ is given by the partial derivative of a with respect to t holding $\mathbf{x}$ constant:

$$\frac{\partial a(\mathbf{x}, t)}{\partial t}. \tag{4.46}$$

Another commonly used time derivative is the *material time derivative of the spatial field* $a(\mathbf{x}, t)$. This time derivative is defined by the partial derivative of a with respect to t holding $\mathbf{X}$ constant:

$$\frac{\partial a(\mathbf{x}, t)}{\partial t} = \frac{\partial a(\mathbf{x}, t)}{\partial t} + \frac{\partial a(\mathbf{x}, t)}{\partial \mathbf{x}} \cdot \frac{\partial \mathcal{X}(\mathbf{X}, t)}{\partial t}, \tag{4.47}$$

giving

$$\frac{\mathrm{D}a(\mathbf{x}, t)}{\mathrm{D}t} = \dot{a}(\mathbf{x}, t) = \frac{\partial a(\mathbf{x}, t)}{\partial t} + (\operatorname{grad} a(\mathbf{x}, t)) \cdot \mathbf{v}(\mathbf{x}, t). \tag{4.48}$$

This can be written as a total derivative

$$\frac{\mathrm{D}}{\mathrm{D}t} a(\mathbf{x}, t) = \dot{a}(\mathbf{x}, t) = \left[\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} \right] a(\mathbf{x}, t). \tag{4.49}$$

Spacial derivatives are commonly used in addition to time derivatives. The gradient of a scalar and a vector field is defined as follows:

$$\operatorname{grad}\phi(\mathbf{x}) = \frac{\partial \phi}{\partial x_i}\hat{\mathbf{e}}_i, \tag{4.50}$$

$$\operatorname{grad}\mathbf{u}(\mathbf{x}) = \frac{\partial u_i}{\partial x_j}\hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j. \tag{4.51}$$

The divergence of a vector field $\mathbf{u}(\mathbf{x})$ and a tensor field $\mathbf{A}(\mathbf{x})$ is defined by

$$\operatorname{div}\mathbf{u} = \frac{\partial u_i}{\partial x_i}. \tag{4.52}$$

$$\operatorname{div}\mathbf{A} = \frac{\partial A_{ij}}{\partial x_j}\hat{\mathbf{e}}_i. \tag{4.53}$$

The divergence theorem is commonly used in theoretical polymer mechanics and will be extensively used in the following sections. As shown in Figure 4.6, let $\mathbf{u}(\mathbf{x})$ be a vector field defined on a domain Ω_c with the boundary $\partial\Omega_c$.

The divergence theorem [1, 2, 10] then states that the surface integral of a vector field can be related to the volume integral of the divergence of the same vector field as follows:

$$\int_{\partial\Omega_c} \mathbf{u}\cdot\hat{\mathbf{n}}\,ds = \int_{\Omega_c} \operatorname{div}\mathbf{u}\,dv, \tag{4.54}$$

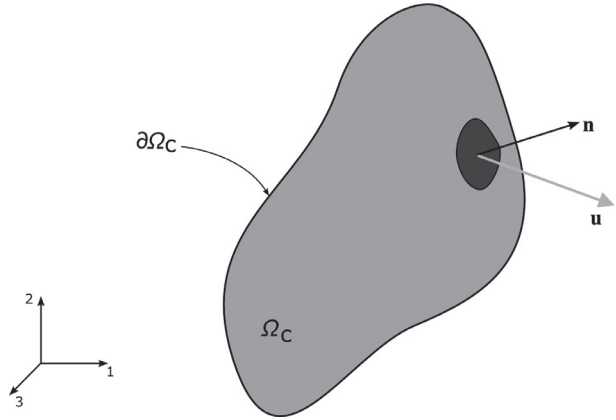


Figure 4.6 Definition of the domain Ω_c that is studied in the divergence theorem.

where $\hat{\mathbf{n}}$ is the surface normal, ds is a surface area element, and dv is a volume element.

There are other more general forms of the divergence theorem, and other integral theorems such as the Stokes theorem. These theorems and the proof of Equation (4.54) are discussed in introductory vector algebra books [10]. For the topics of this book it is sufficient to only cover the divergence theorem as presented in Equation (4.54).

4.4.5 Coordinate Transformations

In polymer mechanics analysis, it is often necessary to perform coordinate transformations. To illustrate how to perform these transformations we will consider two coordinate systems $\hat{\mathbf{e}}'_i$ and $\hat{\mathbf{e}}_i$ that are related by a rotation $\mathbf{Q}$

$$\hat{\mathbf{e}}'_i = \mathbf{Q}^\top \hat{\mathbf{e}}_i, \tag{4.55}$$

where $\mathbf{Q}$ is an orthogonal tensor. Now consider one component of $\mathbf{Q}$:

$$Q_{ij} = \mathbf{Q}\hat{\mathbf{e}}_j \cdot \hat{\mathbf{e}}_i \tag{4.56}$$

$$= \hat{\mathbf{e}}_j \cdot \mathbf{Q}^\top \hat{\mathbf{e}}_i \hat{\mathbf{e}}_j \cdot \hat{\mathbf{e}}'_i \tag{4.57}$$

$$= \cos(\text{angle between } \hat{\mathbf{e}}'_i \text{ and } \hat{\mathbf{e}}_j). \tag{4.58}$$

Hence, each component of $\mathbf{Q}$ is given by the dot-product of the corresponding unit vectors. Since an arbitrary vector can be written $\mathbf{x} = x_i \hat{\mathbf{e}}_i$, we see that the coordinate transformation implies the vector transformation:

$$\mathbf{x}' = \mathbf{Q}\mathbf{x}. \tag{4.59}$$

Similarly, as will be shown in Section 4.12, a second-order tensor is transformed according to:

$$\mathbf{A}' = \mathbf{Q}\mathbf{A}\mathbf{Q}^\top, \tag{4.60}$$

where Q_{ij} is equal to cosine between the basis vectors $\hat{\mathbf{e}}'_i$ and $\hat{\mathbf{e}}_i$.

4.4.6 Invariants

The invariants of a tensor are very important for many polymer mechanics constitutive theories. A second-order tensor has three invariants that are related to the eigenvalues defined by:

$$\mathbf{A}\hat{\mathbf{n}}_i = \lambda_i \hat{\mathbf{n}}_i, \tag{4.61}$$

which can also be written

$$(\mathbf{A} - \lambda_i \mathbf{I}) = 0. \tag{4.62}$$

This equation only has nontrivial solutions if

$$\det(\mathbf{A} - \lambda_i \mathbf{I}) = 0, \tag{4.63}$$

where

$$\det(\mathbf{A} - \lambda_i \mathbf{I}) = -\lambda_i^3 + I_1 \lambda_i^2 - I_2 \lambda_i + I_3 = 0. \tag{4.64}$$

This cubic polynomial in λ_i is called the *characteristic polynomial*. The scalar values I_1, I_2, and I_3 are the principal invariants of $\mathbf{A}$ and are given by:

$$I_1(\mathbf{A}) = \operatorname{tr}\mathbf{A} = \lambda_1 + \lambda_2 + \lambda_3, \tag{4.65}$$

$$I_2(\mathbf{A}) = \frac{1}{2}\left[(\operatorname{tr}\mathbf{A})^2 - \operatorname{tr}\left(\mathbf{A}^2\right)\right] = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1, \tag{4.66}$$

$$I_3(\mathbf{A}) = \det\mathbf{A} = \lambda_1\lambda_2\lambda_3. \tag{4.67}$$

As will be discussed in Chapter 5, the invariants of the deformation gradient are used to formulate hyperelastic constitutive models. What the deformation gradient is and how it can be used is the topic of the next section.

4.5 Deformation Gradient

One of the most important goals of polymer mechanics is to determine the stress state as a function of applied displacements and loads. The stress at a given material point is determined by how stretched and distorted the material is at that point relative to its initial undeformed configuration. One convenient way to express the local stretch state is to use the deformation gradient $\mathbf{F}$ defined by:

$$\mathbf{F} = \frac{\partial \mathcal{X}(\mathbf{X}, t)}{\partial \mathbf{X}}, \tag{4.68}$$

which in index notation can be written $F_{ij} = \partial x_i / \partial X_j$. The deformation gradient is a very important descriptor of the applied deformation state and is extensively used in both theoretical and computational works. In fact, it can be said that: *deformation gradients rule theoretical polymer mechanics.*

The following examples illustrate the definition and use of the deformation gradient $\mathbf{F}$.

Example: Deformation Gradient in the Undeformed State.
If a specimen is undeformed, then the current state is equal to the reference state and the deformation gradient is equal to the identity tensor

$$\mathbf{F} = \mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Example: Uniaxial Tension.
Consider a cube that is uniaxially stretched in the one-direction by a stretch ratio $\lambda = L/L_0$. Further assume that the contraction in the two- and three-directions are equal and that the total volume is conserved. In this case, the coordinates of a material point in the current configuration is given by

$$x_1 = \lambda \cdot X_1 \tag{4.69}$$

$$x_2 = \frac{1}{\sqrt{\lambda}} \cdot X_2 \tag{4.70}$$

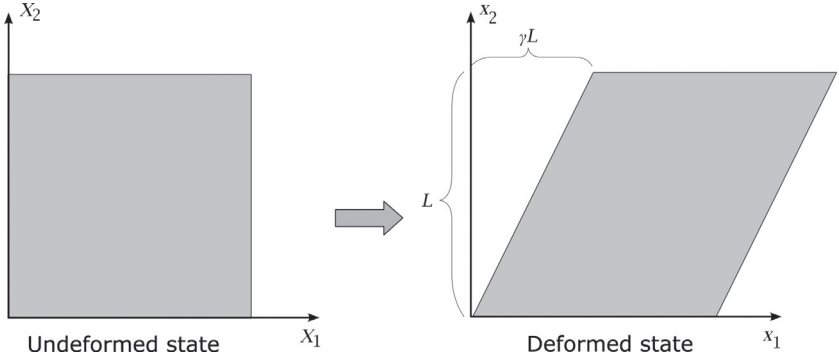
$$x_2 = \frac{1}{\sqrt{\lambda}} \cdot X_3. \tag{4.71}$$

The deformation gradient in this case can be directly obtained from the definition (4.68)

$$\mathbf{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}. \tag{4.72}$$

Example: Simple Shear.
Consider a specimen that is deformed in simple shear. In this case, the coordinates of a material point in the current configuration are given by

$$x_1 = X_1 + \gamma X_2, \tag{4.73}$$
$$x_2 = X_2, \tag{4.74}$$
$$x_3 = X_3. \tag{4.75}$$



Note that we have assumed that there is no deformation in the three-direction. The deformation gradient in this case is given by:

$$\mathbf{F} = \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{4.76}$$

illustrating that $\mathbf{F}$ in general is not symmetrical.

From the definition of the deformation gradient we can also write $\mathbf{F}$ as a mapping or linear transformation:

$$d\mathbf{x} = \mathbf{F}(\mathbf{X})\, d\mathbf{X}. \tag{4.77}$$

That is, by operating $\mathbf{F}$ on a vector $d\mathbf{X}$ in the reference configuration we get the location of that vector in the current configuration. This is a general result: operating a second-order tensor (such as $\mathbf{F}$) on a vector creates another vector that is the linear transformation of the second-order tensor ($\mathbf{F}$). This can also be expressed in matrix terminology: multiplying a 3×3 matrix (such as $\mathbf{F}$) with a 3×1 vector gives another 3×1 vector.

Since the deformation gradient $\mathbf{F}$ is a linear transformation from the reference configuration to the current configuration, the inverse of the deformation gradient $\mathbf{F}^{-1}$ must also exist and is the transformation from the current configuration to the reference configuration:

$$\mathrm{d}\mathbf{X} = \mathbf{F}^{-1}\,\mathrm{d}\mathbf{x}. \tag{4.78}$$

Furthermore, if we first operate with $\mathbf{F}$ and then with $\mathbf{F}^{-1}$ (or first with $\mathbf{F}^{-1}$ and then with $\mathbf{F}$), then we get back the original configuration, that is $\mathbf{F}^{-1}\mathbf{F} = \mathbf{F}\mathbf{F}^{-1} = \mathbf{I}$, giving $\mathbf{X} = \mathbf{F}^{-1}\mathbf{F}\mathbf{X}$.

Example: Volumetric Deformation.
One important use of the deformation gradient is that it specifies how the volume is changed during a transformation. If $\mathrm{d}V$ is a small volume element in the reference configuration, then that volume element is transformed into the volume element

$$\mathrm{d}v = \det(\mathbf{F})\,\mathrm{d}V \tag{4.79}$$

in the current configuration. The quantity $\det(\mathbf{F})$ is commonly referred to as J (the Jacobian determinant)

$$J = \det \mathbf{F}. \tag{4.80}$$

The proof of this theorem is given in different text books [2, 10] and is here left as an exercise.

The deformation of a body can be divided into different classes depending on the structure of the deformation gradient:

- If $\mathbf{F}$ does not vary from location to location in a body then the deformation is said to be *homogeneous*.
- If $\mathbf{F}(\mathbf{X})$ is a function of the position then the deformation is said to be *inhomogeneous*.
- If $J = \det \mathbf{F} = 1$ then the deformation is said to be *isochoric*.

4.5.1 Eigenvalue and Spectral Decompositions

As is known from linear algebra [12], any symmetric tensor $\mathbf{A}$ can be characterized by its eigenvalues $(\lambda_1, \lambda_2, \lambda_3)$ and its eigenvectors $(\hat{\mathbf{n}}_1, \hat{\mathbf{n}}_2, \hat{\mathbf{n}}_3)$ by:

$$\mathbf{A}\hat{\mathbf{n}}_i = \lambda_i \hat{\mathbf{n}}_i \quad \text{(for } i\text{=1, 2, 3; no summation implied).} \tag{4.61-repeat}$$

In this equation, and in the following, unit vectors are distinguished from other vector quantities by a superimposed hat-sign; for example, $\hat{\mathbf{n}}$. For a symmetric tensor $\mathbf{A}$, the eigenvalues (λ_i) are real and the eigenvectors $(\hat{\mathbf{n}}_i)$ form a mutually orthogonal basis of unit vectors. The tensor $\mathbf{A}$ can in this case be written in its *eigenvalue representation* as:

$$\mathbf{A} = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i. \tag{4.81}$$

This eigenvalue representation is based on the dyadic product that was defined and discussed in Section 4.4.2.

Another way of writing the eigenvalue decomposition of a symmetric tensor $\mathbf{A}$ is:

$$\mathbf{A} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{\top}, \tag{4.82}$$

where $\mathbf{Q}$ is orthogonal $(\mathbf{Q}^{\top} = \mathbf{Q}^{-1})$, and $\boldsymbol{\Lambda}$ is diagonal $(\boldsymbol{\Lambda} = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_i)$. Hence, $\mathbf{A}$ can also be written

$$\mathbf{A} = \mathbf{Q}\left[\sum_{i=1}^{3} \lambda_i \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_i\right]\mathbf{Q}^{\top} = \sum_{i=1}^{3} \lambda_i (\mathbf{Q}\hat{\mathbf{e}}_i) \otimes (\mathbf{Q}\hat{\mathbf{e}}_i) = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i, \tag{4.81-repeat}$$

which is another way of writing the eigenvalue representation of $\mathbf{A}$.

The focus of this section is on the deformation gradient $\mathbf{F}$, which in general is nonsymmetric and hence does not have real eigenvalues [12]. Instead of using the eigenvalue decomposition, the deformation gradient $\mathbf{F}$ is often decomposed using the *singular value decomposition*:

$$\mathbf{F} = \mathbf{Q}_1 \mathbf{\Lambda} \mathbf{Q}_2, \tag{4.83}$$

where $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are two different orthogonal tensors (rotations), and $\mathbf{\Lambda}$ is diagonal. Hence, the singular value decomposition of $\mathbf{F}$ can also be expressed as follows:

$$\mathbf{F} = \mathbf{Q}_1 \left[\sum_{i=1}^{3} \lambda_i \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_i \right] \mathbf{Q}_2^\top \tag{4.84}$$

$$\mathbf{F} = \sum_{i=1}^{3} \lambda_i (\mathbf{Q}_1 \hat{\mathbf{e}}_i) \otimes (\mathbf{Q}_2 \hat{\mathbf{e}}_i) \tag{4.85}$$

$$\mathbf{F} = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.86}$$

In these equations, λ_i is the *principal stretches* of the deformation, $\hat{\mathbf{n}}_i$ and $\hat{\mathbf{N}}$ are the basis vectors of the deformation gradient. This way of writing a tensor as a sum of the dyadic product of its eigenvectors is called the *spectral representation*.

The following two examples illustrate how the deformation gradient can be used to transform line and area elements.

Example: Transformation of Line Elements.
Consider a vector $\mathrm{d}\mathbf{X} = \mathrm{d}S\hat{\mathbf{N}}$ in the reference configuration, where $\mathrm{d}S$ is the length of the vector and $\hat{\mathbf{N}}$ is a unit vector in the direction of the vector $\mathrm{d}\mathbf{X}$.

If we operate with $\mathbf{F}$ on $\mathrm{d}\mathbf{X}$ we get

$$\mathrm{d}\mathbf{x} = \mathbf{F}\,\mathrm{d}\mathbf{X}. \tag{4.77-repeat}$$

The length of $\mathrm{d}\mathbf{x}$ is

$$|\mathrm{d}\mathbf{x}| \equiv \mathrm{d}s = \left| \mathbf{F} \left(\mathrm{d}S\hat{\mathbf{N}} \right) \right| = \mathrm{d}S \left| \mathbf{F}\hat{\mathbf{N}} \right|. \tag{4.87}$$

Hence, the length of a vector in the current configuration is equal to the length of that vector in the reference configuration times $|\mathbf{F}\hat{\mathbf{N}}|$.

Example: Transformation of Area Elements (Nanson's Formula).
Let $d\mathbf{S}$ be an area element in the reference configuration with a unit normal vector $\hat{\mathbf{N}}$, and let $d\mathbf{s}$ be the corresponding area element in the current configuration with a unit normal $\hat{\mathbf{n}}$.

In this case, the corresponding volume element dv in the current configuration can be written

$$dv = d\mathbf{s} \cdot d\mathbf{x} = J d\mathbf{S} \cdot d\mathbf{X}, \tag{4.88}$$

but $d\mathbf{x} = \mathbf{F} d\mathbf{X}$ giving

$$d\mathbf{s} \cdot (\mathbf{F} d\mathbf{X}) - J d\mathbf{S} \cdot d\mathbf{X} = 0 \tag{4.89}$$

$$\mathbf{F}^{\top} d\mathbf{s} = J d\mathbf{S} \tag{4.90}$$

$$d\mathbf{s} = J\mathbf{F}^{-T} d\mathbf{S}. \tag{4.91}$$

This relation between area elements is often called the Nanson's formula and is useful when defining different stress measures.

When working with continuum mechanics formulations it is often necessary to consider the gradient and the divergence of scalar and vector fields. The following two examples illustrate how to perform these operations in the reference and the current configurations.

Example: Gradient of a Scalar Field.
Consider a scalar field that is $a(\mathbf{x}, t)$ in spatial coordinates and $A(\mathbf{x}, t)$ in reference (material) coordinates. The gradient of this field in the reference frame is then the space derivative of $A(\mathbf{X}, t)$ and can be written

$$\frac{\partial A(\mathbf{X}, t)}{\partial X_i} = \frac{\partial a(\mathbf{x}, t)}{\partial x_k} \frac{\partial x_k}{\partial X_i}, \tag{4.92}$$

which is equivalent to

$$\operatorname{Grad} A = \mathbf{F}^{\top} \operatorname{grad} a. \tag{4.93}$$

In this equation, and in the following, we will use Grad to represent the gradient in the reference configuration and grad to represent the gradient with respect to the spatial coordinates.

Example: Divergence of a Vector Field.
The divergence of a reference vector field $\mathbf{U}(\mathbf{X}, t)$ can be written

$$\operatorname{Div}\mathbf{U}(\mathbf{X},t) = \frac{\partial U_i(\mathbf{X},t)}{\partial X_i} = \frac{\partial u_i(\mathbf{x},t)}{\partial x_k}\frac{\partial x_k}{\partial X_i} = \operatorname{grad}\mathbf{U}(\mathbf{X},t) : \mathbf{F}^\top. \tag{4.94}$$

Similarly, the divergence of a spatial vector field $\mathbf{u}(\mathbf{x}, t)$ can be written

$$\operatorname{div}\mathbf{u}(\mathbf{x},t) = \frac{\partial u_i(\mathbf{x},t)}{\partial x_i}. \tag{4.95}$$

In these equations, and in the following, we will use Div to represent the gradient in the reference configuration and div to represent the gradient with respect to the spatial coordinates.

4.6 Strain, Stretch, and Rotation

From the polar decomposition theorem [2, 10] it is known that any general deformation can be uniquely decomposed into a rotation followed by a stretch component, or a stretch component followed by a rotation:

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{v}\mathbf{R}, \tag{4.96}$$

where

- $\mathbf{F}$ is the deformation gradient,
- $\mathbf{R}$ is the *rotation tensor*, which is orthogonal, ($\mathbf{R}^{-1} = \mathbf{R}^\top$) and volume conserving ($\det\mathbf{R} = 1$),
- $\mathbf{U}$ is the *right stretch tensor*, which is positive definite and symmetric ($\mathbf{U} = \mathbf{U}^\top$),
- $\mathbf{v}$ is the *left stretch tensor*, which is positive definite and symmetric ($\mathbf{v} = \mathbf{v}^\top$).

Note that if $\mathbf{U} = \mathbf{v} = \mathbf{I}$, then $\mathbf{F} = \mathbf{R}$ is a *rigid body rotation*. Similarly, if $\mathbf{R} = \mathbf{I}$ then $\mathbf{F} = \mathbf{U} = \mathbf{v}$ is a *pure stretch*.

From Equation (4.96) we know that the right stretch tensor $\mathbf{U}$ is symmetric, hence it can be written in a spectral representation as

$$\mathbf{U} = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.97}$$

In this equation, λ_i is the principal stretches and $\hat{\mathbf{N}}_i$ is the corresponding eigenvectors of the tensor $\mathbf{U}$. Similarly the left stretch tensor can be written

$$\mathbf{v} = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i. \tag{4.98}$$

Note that $\mathbf{U}$ and $\mathbf{v}$ have the same principal stretches but different principal directions (basis vectors) since they are expressed in different reference frames. The eigenvectors of $\mathbf{v}$ can be related to the eigenvectors of $\mathbf{U}$ by solving for $\mathbf{v}$ in Equation (4.96):

$$\mathbf{v} = \mathbf{R}\mathbf{U}\mathbf{R}^{\top} = \sum_{i=1}^{3} \lambda_i \left(\mathbf{R}\hat{\mathbf{N}}_i\right) \otimes \left(\mathbf{R}\hat{\mathbf{N}}_i\right). \tag{4.99}$$

Hence, the eigenvectors of $\mathbf{U}$ and $\mathbf{v}$ are related by

$$\hat{\mathbf{n}}_i = \mathbf{R}\hat{\mathbf{N}}_i \tag{4.100}$$

and

$$\hat{\mathbf{N}}_i = \mathbf{R}^{\top}\hat{\mathbf{n}}_i. \tag{4.101}$$

The deformation gradient can also be expressed in spectral form by $\mathbf{F} = \mathbf{R}\mathbf{U}$ giving

$$\mathbf{F} = \mathbf{R}\sum_{i=1}^{3} \lambda_i \hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i = \sum_{i=1}^{3} \lambda_i \left(\mathbf{R}\hat{\mathbf{N}}_i\right) \otimes \hat{\mathbf{N}}_i = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{N}}_i, \tag{4.102}$$

which is the same result that was presented in Equation (4.86). Since the basis vectors of $\mathbf{F}$ contain both $\hat{\mathbf{n}}_i$ and $\hat{\mathbf{N}}_i$, $\mathbf{F}$ is called a *two-point tensor*.

The rotation tensor $\mathbf{R}$ can by written as

$$\mathbf{R} = \mathbf{R}\mathbf{I} = \mathbf{R}\sum_{i=1}^{3} \hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i, \tag{4.103}$$

giving

$$\mathbf{R} = \sum_{i=1}^{3} \hat{\mathbf{n}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.104}$$

There are a number of other important and useful tensor quantities that are defined from the polar decomposition of $\mathbf{F}$:

- $\mathbf{C} = \mathbf{F}^\top\mathbf{F}$ is the *right Cauchy-Green tensor*. Since $\mathbf{F} = \mathbf{RU}$, we get $\mathbf{C} = \mathbf{U}^\top\mathbf{R}^\top\mathbf{RU} = \mathbf{U}^2$. Hence, $\mathbf{C}$ can also be written

$$\mathbf{C} = \mathbf{F}^\top\mathbf{F} = \sum_{i=1}^{3} \lambda_i^2 \hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.105}$$

- $\mathbf{b} = \mathbf{FF}^\top$ is the *left Cauchy-Green tensor*.[4] From Equation (4.96) the tensor $\mathbf{b}$ can also be written

$$\mathbf{b} = \mathbf{FF}^\top = \mathbf{vRR}^\top\mathbf{v}^\top = \mathbf{v}^2. \tag{4.106}$$

  Hence, $\mathbf{b}$ is also given by

$$\mathbf{b} = \sum_{i=1}^{3} \lambda_i^2 \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i. \tag{4.107}$$

Example: How to Calculate the Polar Decomposition of a Tensor.
One of the easiest ways to calculate the polar decomposition of a tensor $\mathbf{F} = \mathbf{RU}$ is to recall that $\mathbf{C} = \mathbf{F}^\top\mathbf{F} = \mathbf{U}^2$. This allows $\mathbf{U}$ to be determined from $\mathbf{U} = \sqrt{\mathbf{FF}^\top}$. One way to perform the square root operation is to write $\mathbf{U}^2$ in its spectral representation by calculating the eigenvalues and eigenvectors of $\mathbf{U}^2$:

$$\mathbf{U}^2 = \sum_{i=1}^{3} \lambda_i^2 \hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.108}$$

The tensor $\mathbf{U}$ can then be calculated from

$$\mathbf{U} = \sum_{i=1}^{3} \lambda_i \hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i. \tag{4.109}$$

[4] *The left versus right terms in the definitions of the Cauchy-Green tensors is determined by which side* $\mathbf{F}$ *is compared to* $\mathbf{F}^\top$.

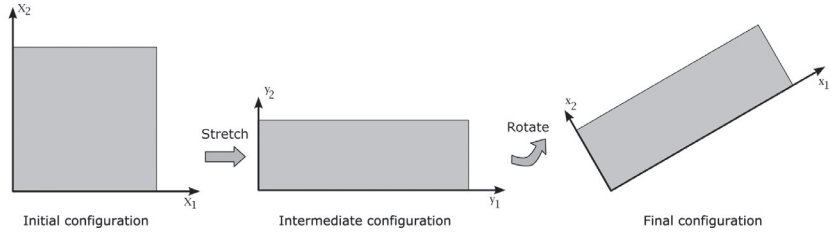
Once $\mathbf{U}$ has been determined, the tensor $\mathbf{R}$ can be calculated from

$$\mathbf{R} = \mathbf{F}\mathbf{U}^{-1} \tag{4.110}$$

and $\mathbf{v}$ from

$$\mathbf{v} = \mathbf{F}\mathbf{R}^{\top}. \tag{4.111}$$

Example: Determination of the Deformation Gradient for a Case of Stretch and Rotation.
Consider a deformation that is performed in two steps: first, the material is stretched by a factor of two in the one-direction, and then rotated 45° around the three-direction, see the figure below.



The stretch deformation is given by:

$$\begin{cases} y_1 &= 2X_1 \\ y_2 &= 0.5X_2 \\ y_3 &= X_3 \end{cases} \tag{4.112}$$

giving the right stretch tensor:

$$\mathbf{U} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{4.113}$$

The components of the rotation can be written

$$\begin{cases} x_1 &= \cos\theta y_1 + \sin\theta y_2 \\ x_2 &= -\sin\theta y_1 + \cos\theta y_2 \\ x_3 &= y_3 \end{cases} \tag{4.114}$$

giving the rotation tensor

$$\mathbf{R} = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{4.115}$$

In this case, $\theta = 45°$ giving the deformation gradient $\mathbf{F} = \mathbf{RU}$:

$$\mathbf{F} = \begin{bmatrix} 1.41 & 0.35 & 0 \\ -1.41 & 0.35 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{4.116}$$

Example: Numerical Calculation of the Deformation Gradient for a Case of Stretch and Rotation.
The polar decomposition is straightforward to calculate using a high-level math application or language. For example, Matlab [13], Mathematica [14], and Python [15] are all suitable tools. Many of the examples in this book are based on Python with NumPy and SciPy. Since these tools are very mature, powerful, and free, it is an excellent choice for numerical calculations.

In this example, we will start with the deformation gradient in Equation (4.116) and then calculate the **U** and **R** tensors. The Python code for this calculation is shown below.

Python code:

```
from pylab import *
from scipy.linalg import sqrtm, inv

# initialize U
U = array([[2,0,0], [0,0.5,0], [0,0,1]])
print('U=', U)

# initialize R
v = 45.0 * pi/180.0
c = cos(v)
s = sin(v)
R = array([[c,s,0], [-s,c,0], [0,0,1]])
print('R=', R)

# calculate F
F = dot(R,U)
print('F=RU=', F)

# calculate U from F
U = real(sqrtm(dot(F.T, F)))
print('U=', U)

# calculate R from F and U
R = dot(F, inv(U))
print('R=', R)

# if RU=F then it worked
print('R*U-F=', dot(R,U)-F)
```

Output:

```
U= [[ 2.   0.   0. ]
    [ 0.   0.5  0. ]
    [ 0.   0.   1. ]]

R= [[ 0.70710678  0.70710678  0.        ]
    [-0.70710678  0.70710678  0.        ]
    [ 0.          0.          1.        ]]

F=RU= [[ 1.41421356  0.35355339  0.        ]
       [-1.41421356  0.35355339  0.        ]
       [ 0.          0.          1.        ]]

U= [[ 2.   0.   0. ]
    [ 0.   0.5  0. ]
    [ 0.   0.   1. ]]

R= [[ 0.70710678  0.70710678  0.        ]
    [-0.70710678  0.70710678  0.        ]
    [ 0.          0.          1.        ]]

R*U-F= [[ 0.  0.  0.]
        [ 0.  0.  0.]
        [ 0.  0.  0.]]
```

The strain at a material point, by definition, should not be influenced by rigid body rotations. This means that the strain tensor cannot directly depend on the deformation gradient **F**, since **F** also depends on rotations. Instead the strain tensor has to depend on the right or left stretch tensors. If the right stretch tensor (**U**) is used to define the strains then the strain will be expressed in the reference configuration, and if the left stretch tensor (**v**) is used, the strain will be expressed in the current configuration.

The strain tensor in the reference configuration can most generally be written as a function of **U**:

$$\mathbf{E} = \hat{\mathbf{E}}(\mathbf{U}). \tag{4.117}$$

This tensorial dependence can be expressed in the spectral representation

$$\mathbf{E} = \mathbf{E}(\mathbf{U}) = \sum_{i=1}^{3} f(\lambda_i)\hat{\mathbf{N}}_i \otimes \hat{\mathbf{N}}_i, \tag{4.118}$$

where $f(\lambda_i)$ is a scalar function of the principal stretches. Hence, **E** will be coaxial[5] with **U** but have different eigenvalues. The function $f(\lambda_i)$ need to fulfill three requirements for **E** to become a valid strain tensor:

1. The strain has to be zero in the undeformed state, hence $f(1) = 0$.
2. At small deformations the strain should become equal to the classical strain defined in Section 4.2, hence $f'(1) = 1$.
3. The strain has to increase monotonically with the applied deformation, that is $f(\lambda)$ has to monotonically increase with increasing λ.

[5] *Two tensors are said to be coaxial if they have the same basis vectors.*

The following are commonly used strain measures expressed in the reference configuration. These strains are also called Lagrangian strains.

- The *Green-Lagrange strain*, which corresponds to $f(\lambda_i) = \frac{1}{2}(\lambda_i^2 - 1)$, can be written

$$\mathbf{E} = \frac{1}{2}\left[\mathbf{U}^2 - \mathbf{I}\right]. \tag{4.119}$$

- The *Hencky strain* (also called the *true strain*, or the *logarithmic strain*), which corresponds to $f(\lambda_i) = \ln \lambda_i$, can be written

$$\mathbf{E} = \ln \mathbf{U}. \tag{4.120}$$

- The *Biot strain*, corresponding to $f(\lambda_i) = \lambda_i - 1$, can be written

$$\mathbf{E} = \mathbf{U} - \mathbf{I}. \tag{4.121}$$

- The *Almansi strain*, corresponding to $f(\lambda_i) = \frac{1}{2}(1 - \lambda_i^{-2})$, can also be written

$$\mathbf{E} = \frac{1}{2}\left[\mathbf{I} - \mathbf{U}^{-2}\right]. \tag{4.122}$$

It is also possible to formulate the strain in the current (spatial) configuration:

$$\mathbf{e} = \mathbf{e}(\mathbf{v}), \tag{4.123}$$

which can also be expressed in its spectral representation

$$\mathbf{e} = \sum_{i=1}^{3} f(\lambda_i)\hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i. \tag{4.124}$$

The following are commonly used strain measures expressed in the current configuration. These strains are also called Eulerian strains.

- The *nominal strain*, corresponding to $f(\lambda_i) = \lambda_i - 1$, can be written

$$\mathbf{e} = \mathbf{v} - \mathbf{I}. \tag{4.125}$$

- The *Hencky strain* (also called the *true strain* or the *logarithmic strain*), which corresponds to $f(\lambda_i) = \ln(\lambda_i)$, can be written

$$\mathbf{e} = \ln \mathbf{v}. \tag{4.126}$$

- The *Euler-Almansi strain*, corresponding to $f(\lambda_i) = \frac{1}{2}(1 - \lambda_i^{-2})$, can also be written

$$\mathbf{e} = \frac{1}{2}\left[\mathbf{I} - \mathbf{b}^{-1}\right]. \tag{4.127}$$

Note: *Most FE programs, for example Abaqus and ANSYS, can create contour plots of the Eulerian nominal (engineering) strain, and the Eulerian logarithmic (true) strain. These strains are often simply called the "engineering strain" and the "true strain," respectively.*

4.7 Rates of Deformation

Many advanced constitutive theories for polymers includes considerations of the inherent viscoelasticity and viscoplasticity of the material. To incorporate these effects into a model it is necessary to consider the time derivative of the deformation gradient

$$\dot{\mathbf{F}} = \frac{\partial}{\partial t}\frac{\partial x_i}{\partial X_j} = \frac{\partial}{\partial X_j}\frac{\partial x_i}{\partial t} = \frac{\partial \mathbf{v}}{\partial \mathbf{X}} = \operatorname{Grad} \mathbf{v}. \tag{4.128}$$

From this equation we can also write the time derivative of $\mathbf{F}$ as

$$\dot{\mathbf{F}} = \frac{\partial v_i}{\partial X_j} = \frac{\partial v_i}{\partial x_k}\frac{\partial x_k}{\partial X_j} = \mathbf{l}\mathbf{F}, \tag{4.129}$$

where $\mathbf{l}$ is a tensor quantity called the *spatial velocity gradient*:

$$\mathbf{l} \equiv \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \operatorname{grad} \mathbf{v}. \tag{4.130}$$

It is often useful to decompose the spatial velocity gradient into a symmetric ($\mathbf{d} = \mathbf{d}^\top$) and an anti-symmetric ($\mathbf{w} = -\mathbf{w}^\top$) part:

$$\mathbf{l} = \mathbf{d} + \mathbf{w}, \tag{4.131}$$

where

$$\mathbf{d} = \frac{1}{2}\left(\mathbf{l} + \mathbf{l}^\top\right), \tag{4.132}$$

$$\mathbf{w} = \frac{1}{2}\left(\mathbf{l} - \mathbf{l}^\top\right). \tag{4.133}$$

The tensor $\mathbf{d}$ is called the *rate of deformation tensor* and $\mathbf{w}$ is called the *spin tensor*. Note that $\mathbf{d}$ captures rates of deformation and $\mathbf{w}$ captures rates of rotation. All three of $\mathbf{l}$, $\mathbf{d}$, and $\mathbf{w}$ are spatial fields.

The spatial velocity gradient can also be used to determine the time rate of change of a vector in the current configuration:

$$\mathbf{l}\,\mathrm{d}\mathbf{x} = \mathbf{l}\mathbf{F}\mathrm{d}\mathbf{X} = \dot{\mathbf{F}}\mathrm{d}\mathbf{X} = \frac{\mathrm{D}}{\mathrm{D}t}(\mathrm{d}\mathbf{x}). \tag{4.134}$$

Another useful relationship is the time derivative of $J = \det \mathbf{F}$:

$$\frac{\mathrm{D}J}{\mathrm{D}t} = \dot{J} = J \operatorname{tr} \mathbf{l} = J \operatorname{div} \mathbf{v}. \tag{4.135}$$

4.8 Stress Tensors

In order to answer real-life polymer mechanics questions, such as: how much will a polymer component deform when subjected to an external load field, it is necessary to introduce the concept of mechanical stress. To do this we will consider a general body exposed to external forces on its surface as illustrated in Figure 4.7. This figure shows the configuration and acting forces on the body at time t. Now let us perform a virtual cut along a plane through the body, see Figure 4.8. In order to satisfy force equilibrium for each of the two parts of the body there must be internal surface forces on the cut plane. The magnitude of the internal surface forces will depend on the direction of the cut surface (specified by the normal $\mathbf{n}$ to the surface) and the location $\mathbf{x}$ of the force:

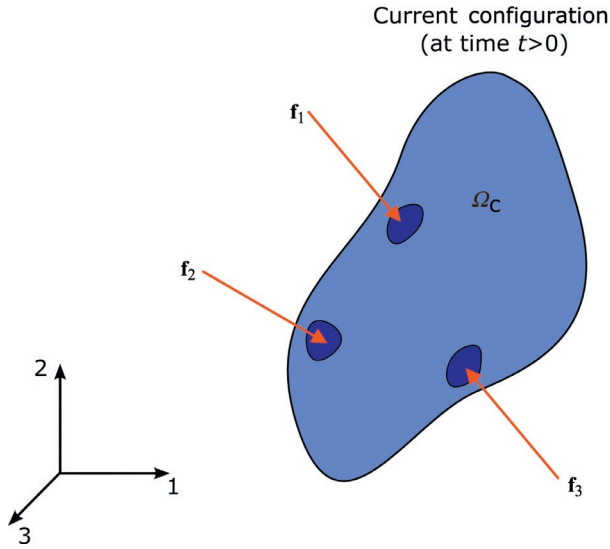


Figure 4.7 Schematic figure showing a body in its deformed configuration Ω_c loaded by external forces, here exemplified by forces distributed over an area.

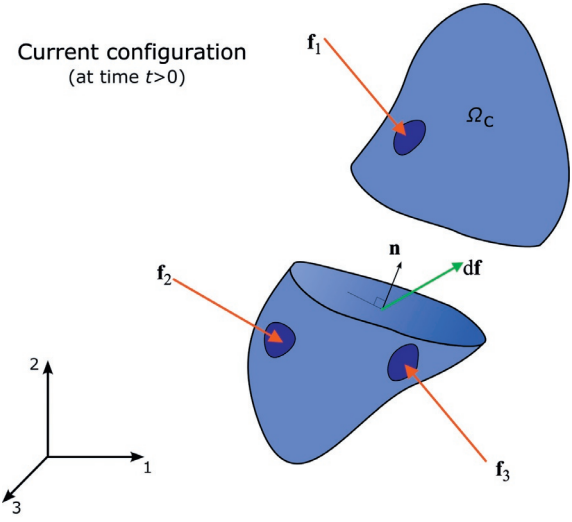


Figure 4.8 Schematic figure of a body in its deformed configuration showing that internal forces d**f** are need to keep the body in equilibrium when a virtual cut is made.

$$\mathrm{d}\mathbf{f} = \mathrm{d}\mathbf{f}(\mathbf{x}, \mathbf{n}). \tag{4.136}$$

These surface forces can be represented as tractions $\mathbf{t}$ (i.e., force per unit area):

$$\mathrm{d}\mathbf{f}(\mathbf{x}, \mathbf{n}) = \mathbf{t}(\mathbf{x}, \mathbf{n})\, \mathrm{d}s, \tag{4.137}$$

which is the force acting on the surface element $\mathrm{d}s$. The force at each material point can be related to a stress field by the Cauchy stress theorem [2, 3] which states that there exists a unique tensorial stress field $\boldsymbol{\sigma}(\mathbf{x})$ that is independent of the direction of the virtual cut (specified by the normal $\mathbf{n}$) and is defined by:

$$\mathbf{t}(\mathbf{x}, \mathbf{n}) = \boldsymbol{\sigma}(\mathbf{x})\mathbf{n}. \tag{4.138}$$

In this equation, $\mathbf{t}(\mathbf{x}, \mathbf{n})$ is the Cauchy (true) surface traction, and

$$\boldsymbol{\sigma} = \sum_{i=1}^{3} \sigma_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_i \tag{4.139}$$

is the Cauchy stress tensor.

The traction vector and the stress tensor in Equation (4.138) can also be written in the reference configuration as

$$\mathbf{T}(\mathbf{X}, \mathbf{N}) = \mathbf{P}(\mathbf{X})\mathbf{N}, \tag{4.140}$$

where $\mathbf{T}$ is the *nominal traction vector* (also called the *first Piola-Kirchhoff traction* vector), and $\mathbf{P}(\mathbf{X})$ is the *nominal stress tensor* (also called the *first Piola-Kirchhoff stress tensor*) which can be written

$$\mathbf{P} = \sum_{i=1}^{3} P_i \hat{\mathbf{n}}_i \otimes \hat{\mathbf{N}}_i, \tag{4.141}$$

illustrating that $\mathbf{P}$ is a two-point tensor.

The force vector in the reference and the current configurations have to be equal:

$$\mathbf{T}(\mathbf{X}, \mathbf{N})\, \mathrm{d}S = \mathbf{t}(\mathbf{x}, \mathbf{n})\, \mathrm{d}s \tag{4.142}$$

giving

$$\mathbf{P}(\mathbf{X})\mathbf{N}\, \mathrm{d}S = \boldsymbol{\sigma}(\mathbf{x})\mathbf{n}\, \mathrm{d}s. \tag{4.143}$$

From Nanson's formula $\mathrm{d}\mathbf{s} = J\mathbf{F}^{-1}\mathrm{d}\mathbf{S}$ we get the following relationship between the Cauchy stress tensor and the first Piola-Kirchhoff stress tensor:

$$\mathbf{P}(\mathbf{X}) = J\boldsymbol{\sigma}\mathbf{F}^{-\top}, \tag{4.144}$$

or when solved for the Cauchy stress

$$\boldsymbol{\sigma} = J^{-1}\mathbf{P}\mathbf{F}^{\top}, \tag{4.145}$$

showing that the first Piola-Kirchhoff stress tensor is not symmetric.

There are numerous other stress tensors that have been defined and used in the literature. One common stress is the Kirchhoff stress defined by:

$$\boldsymbol{\tau} = J\boldsymbol{\sigma}. \tag{4.146}$$

Another common stress is the second Piola-Kirchhoff stress $\mathbf{S}$. If we apply $\mathbf{F}^{-1}$ on the Cauchy surface traction vector we get a traction vector in the reference configuration denoted by $\tilde{\mathbf{T}}$:

$$\tilde{\mathbf{T}} = \mathbf{F}^{-1}\mathbf{t} = \mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{n}. \tag{4.147}$$

The traction vector $\tilde{\mathbf{T}}$ is obtained from the second Piola-Kirchhoff stress:

$$\tilde{\mathbf{T}} = \mathbf{S}\mathbf{N}. \tag{4.148}$$

The force vector in the reference and the current configurations have to be the same:

$$\mathbf{S}\mathbf{N}\mathrm{d}S = \mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{n}\mathrm{d}s. \tag{4.149}$$

From Nanson's formula (Equation (4.91)) we get

$$\mathbf{S} = J\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-T} = \mathbf{F}^{-1}\mathbf{P}. \tag{4.150}$$

Example: Uniaxial Loading.
To illustrate the different stress measures let us consider a uniaxial tension case in which the deformation gradient is

$$\mathbf{F} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0.7 & 0.7 \\ 0 & 0 & 0.7 \end{bmatrix}$$

and the Cauchy stress is given by

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

In this case, the first Piola-Kirchhoff stress is given by Equation (4.144):

$$\mathbf{P} = \begin{bmatrix} 0.49\sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and the second Piola-Kirchhoff stress is given by Equation (4.150):

$$\mathbf{S} = \begin{bmatrix} 0.245\sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and the Kirchhoff stress is given by Equation (4.146):

$$\boldsymbol{\tau} = \begin{bmatrix} 0.985\sigma_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

This example shows that the magnitude of the different stress measures can be quite different for a finite deformation load case.

4.8.1 Stress Invariants

Since a stress tensor contains six or nine different components (depending on whether it is symmetric or not) it is often convenient to consider a single scalar quantity that characterizes certain aspects of the stress tensor. These scalar values are often characteristic values or invariants of the stress tensor. Since multiplying or adding two invariants leads to another invariant, there are infinitely many invariants that can be defined and used.

The perhaps easiest invariants to define, interpret, and use are the principal values of the stress tensor. As was shown in

Equation (4.83), any tensor can be uniquely decomposed into a singular value decomposition:

$$\mathbf{A} = \mathbf{Q}_1 \mathbf{\Lambda} \mathbf{Q}_2, \tag{4.151}$$

where $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are orthogonal tensors that specify rotations, and $\mathbf{\Lambda}$ is a diagonal tensor with three principal values. If the stress tensor is symmetric (such as the Cauchy stress and the second Piola-Kirchhoff stress), the singular value decomposition becomes the same as the eigenvalue decomposition, and the principal values coincide with the eigenvalues of the stress tensor. The principal stresses are often referred to as $\sigma_1 > \sigma_2 > \sigma_3$.

From Equation (4.151) it is clear that the diagonal stress matrix $\mathbf{\Lambda}$ is given by:

$$\mathbf{\Lambda} = \mathbf{Q}_1^\top \mathbf{A} \mathbf{Q}_2^\top. \tag{4.152}$$

Hence, by premultiplying a stress tensor with a suitable rotation $\mathbf{Q}_1^\top$ and then postmultiplying with another rotation $\mathbf{Q}_2^\top$ the stress tensor can be transformed into diagonal form, corresponding to a purely axial stress state with only normal stresses and no shear stresses. This means that σ_1 corresponds to the largest tensile stress, and σ_3 corresponds to the smallest tensile stress (i.e., the largest compressive stress).

There are two other invariants of the stress tensor that are commonly used when describing the magnitude of shear stress at a point: the Mises stress and the Tresca stress. The Mises stress is defined by:

$$\sigma_{\mathrm{M}} = \sqrt{\frac{1}{2}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]} \tag{4.153}$$

and the Tresca stress is defined by:

$$\sigma_{\mathrm{T}} = \sigma_1 - \sigma_3. \tag{4.154}$$

As will be discussed in more detail in a later chapter, the maximum principal stress (σ_1) is the driving force for crack nucleation and growth, and the Mises and Tresca stresses are driving viscoplastic flow.

4.9 Balance Laws and Field Equations

When developing constitutive equations for a material, or when solving continuum mechanics problems, it is important to obey important physical principles such as: conservation of mass, conservation of linear momentum, conservation of angular momentum, conservation of energy, and the first and second laws of thermodynamics. These principles apply to all materials and loading conditions, and give rise to balance laws and field equations that need to be satisfied.

In this context, a *balance law* is a physical rule expressed in terms of a given volume of material, and a *field equation* is a physical rule expressed at a material point.

The following sections present these physical principles in the context of continuum mechanics. Field variables that are needed for this discussion, and have not been defined yet, are listed in Table 4.1. A summary of all variables that are used in this chapter is given in Section 4.14.

To facilitate the upcoming discussion of the balance laws and field equations it is useful to establish the following transport theorem expressing the time derivative of a quantity inside a volume:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_\mathrm{c}} \phi \,\mathrm{d}v = \int_{\Omega_\mathrm{c}} \left(\dot{\phi} + \phi \,\mathrm{tr}\,\mathbf{l}\right) \mathrm{d}v. \tag{4.155}$$

In this equation, $\phi(\mathbf{x}, t)$ is any spatial scalar field, Ω_c is the volume of the studied region at time t, and $\mathbf{l}$ is the spatial velocity gradient. The transport theorem can be proved by the help of Equations (4.79) and (4.135) as follows:

$$\begin{aligned}\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_\mathrm{c}} \phi(\mathbf{x}, t) \,\mathrm{d}v &= \frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_0} \phi J \,\mathrm{d}V \\ &= \int_{\Omega_0} \frac{\mathrm{D}}{\mathrm{D}t}\left[\phi J\right] \mathrm{d}V \\ &= \int_{\Omega_0} \left(J\dot{\phi} + \phi\dot{J}\right) \mathrm{d}V\end{aligned}$$

$$= \int_{\Omega_c} \left(\dot{\phi} + \phi \frac{\dot{J}}{J} \right) \, \mathrm{d}v$$
$$= \int_{\Omega_c} \left(\dot{\phi} + \phi \, \mathrm{div}\, \mathbf{v} \right) \, \mathrm{d}v.$$

The transport theorem and its derivation is discussed in more detail in the next section.

Table 4.1 Field Variables Used in the Balance Laws and Field Equations

Specific mass (density)	
ρ_c	Mass density in the current configuration
ρ_0	Mass density in the reference configuration
Temperature	
θ_c	Temperature in the current configuration
θ_0	Temperature in the reference configuration
Specific internal energy	
e_c	Internal energy per unit current volume
e_0	Internal energy per unit reference volume
Specific Helmholtz free energy	
ψ	Helmholtz free energy per unit current volume
Ψ	Helmholtz free energy per unit reference volume
Specific internal entropy	
η_c	Entropy per unit current volume
η_0	Entropy per unit reference volume
Specific heat flux	
$\mathbf{q}$	Heat flux per unit current surface area
$\mathbf{Q}$	Heat flux per unit reference surface area
Specific heat supply	
r	Rate of heat supply per unit current volume
R	Rate of heat supply per unit reference volume
Specific body force	
$\mathbf{b}_f$	Body force per unit reference volume
$\mathbf{B}_f$	Body force per unit current volume

4.9.1 Conservation of Mass

This section presents the principle of mass conservation and how it applies to mechanics of continuous media. The discussion presented here is based on the simple fact that the mass of a body is given by the sum of its parts. As before, we are focusing on a body that does not exchange material with its surroundings.

Let Ω_c be the configuration of the body at time t, as illustrated in Figure 4.9. Since no material is entering or leaving the body, the total mass must be constant and the time derivative of the total mass has to be zero:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_c}\rho_c(\mathbf{x},t)\,\mathrm{d}v = 0, \tag{4.156}$$

which when expressed in the reference configuration can be written

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_0}\rho_0(\mathbf{X},t)\,\mathrm{d}V = 0, \tag{4.157}$$

where Ω_0 is the configuration of the body at the initial time. These equations integrate the density over the volume of the body to get the total mass. Equations (4.156) and (4.157) are the *balance*

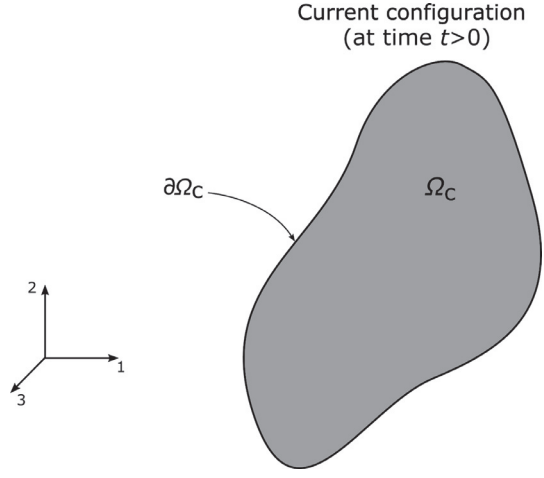


Figure 4.9 Schematic figure showing the configuration of the body at time t is Ω_c. The boundary of the body is denoted by $\partial\Omega_c$.

laws for mass conservation. The balance laws, which govern the response of a finite domain, can be converted to field equations that are valid at each point of the body. Let us first focus on Equation (4.157) that expresses the time rate of change of mass in the reference configuration. In this equation, the domain Ω_0 is not dependent on time and we can therefore move the time derivative operator inside the integral sign:

$$\int_{\Omega_0} \frac{\mathrm{D}}{\mathrm{D}t}\big[\rho_0(\mathbf{X},t)\big]\,\mathrm{d}V = 0. \tag{4.158}$$

This equation has to be valid also for an arbitrary subdomain of Ω_0, and hence the integrand has to be identically zero for the equation to always hold. Hence

$$\dot{\rho}_0(\mathbf{X},t) = 0 \tag{4.159}$$

is the field equation for mass concentration in the reference configuration.

The field equation for mass conservation in the current (spatial) configuration can in a similar way be derived from Equation (4.156). In this case, the volume integral is over Ω_c which is changing with time. We therefore cannot directly move the time-derivative operator inside the integral. To simplify the equation we will instead first perform a variable substitution to bring the integral back to the reference configuration. Specifically, from Equations (4.9) and (4.79), we chose the variable substitution $\mathbf{x} = \mathcal{X}(\mathbf{X},t)$, giving $\mathrm{d}v = J\,\mathrm{d}V$ and the integration domain is transformed from Ω_c to Ω_0:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_0} \rho_\mathrm{c}(\mathcal{X}(\mathbf{X},t))\,J\mathrm{d}V. \tag{4.160}$$

We can now move the time-derivative operator inside the integral giving

$$\int_{\Omega_0} \frac{\mathrm{D}}{\mathrm{D}t}\left[\rho_\mathrm{c}(\mathcal{X}(\mathbf{X},t))J\right]\,\mathrm{d}V. \tag{4.161}$$

Since this equation also has to be valid for an arbitrary subdomain of Ω_0, the integrand has to be identically zero giving the useful equation:

$$\frac{\mathrm{D}}{\mathrm{D}t}\left[\rho_{\mathrm{c}}(\mathbf{X},t)J\right]=0. \tag{4.162}$$

The field equation for mass conservation expressed in the current configuration can be obtained by applying the chain-rule on Equation (4.161):

$$\int_{\Omega_0}\left[\dot{\rho}_{\mathrm{c}}\left(\mathcal{X}(\mathbf{X},t)\right)J+\rho_{\mathrm{c}}\left(\mathcal{X}(\mathbf{X},t)\right)\dot{J}\right]\mathrm{d}V=0. \tag{4.163}$$

By applying the reverse variable substitution, $\mathbf{X}=\mathcal{X}^{-1}(\mathbf{x},t)$, this equation can be converted back to the current configuration:

$$\int_{\Omega_{\mathrm{c}}}\left[\dot{\rho}_{\mathrm{c}}(\mathbf{x},t)+\rho_{\mathrm{c}}(\mathbf{x},t)\frac{\dot{J}}{J}\right]\mathrm{d}v=0. \tag{4.164}$$

From Equation (4.135) we know that $\dot{J}/J=\operatorname{div}\mathbf{x}$, giving the field equation for mass conservation as

$$\dot{\rho}_{\mathrm{c}}(\mathbf{x},t)+\rho_{\mathrm{c}}(\mathbf{x},t)\operatorname{div}\mathbf{v}=0. \tag{4.165}$$

From Equations (4.158) and (4.161) we also get the interesting result that

$$\rho_0(\mathbf{X})=J\rho_{\mathrm{c}}(\mathbf{x}). \tag{4.166}$$

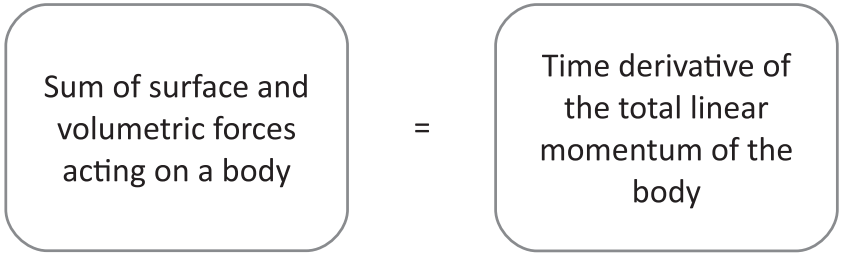
To summarize, a balance equation expresses the time derivative of an extensive quantity contained in a volume in terms of its fluxes through the boundary and the internal source of the quantity. In this case, as is commonly done for solids, we have limited our interest to closed systems where no mass can pass through the boundary, hence the mass fluxes are zero. When studying fluids, on the other hand, it is often convenient to use an open system in which material can enter and leave through the boundary of the domain of interest [16].

4.9.2 Balance of Linear Momentum

From the theory of rigid body dynamics we know that Newton's law of motion can be expressed as [17]:

> *The force on a body is equal to the time-derivative of its linear momentum.*

In this text, we are focusing on deformable bodies undergoing large deformations, for which the balance of linear momentum can be written in the following form:



This principle can be written as a balance law expressed in the current configuration:

$$\int_{\partial\Omega_c} \mathbf{t}\, ds + \int_{\Omega_c} \mathbf{b}_f\, dv = \frac{D}{Dt}\int_{\Omega_c} \mathbf{v}\, \rho_c\, dv, \tag{4.167}$$

where $\mathbf{t}$ is the distribution of Cauchy surface tractions on the boundary of the current configuration, ds is a surface area element in the current configuration, $\partial\Omega_c$ is the surface of the body in the current configuration, $\mathbf{v}$ is the velocity field, and $\mathbf{b}_f$ is the vector field of body forces per unit current volume. The forces used in this equation are defined and illustrated in Figure 4.10.

To convert Equation (4.167) to a field equation we will start by first applying the Cauchy stress theorem (Equation (4.138)): $\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$, giving

$$\int_{\partial\Omega_c} \boldsymbol{\sigma}\mathbf{n}\, ds + \int_{\Omega_c} \mathbf{b}_f\, dv = \frac{D}{Dt}\int_{\Omega_c} \mathbf{v}\rho_c\, dv. \tag{4.168}$$

Applying the divergence theorem (Equation (4.54)) on the first term in Equation (4.168) gives

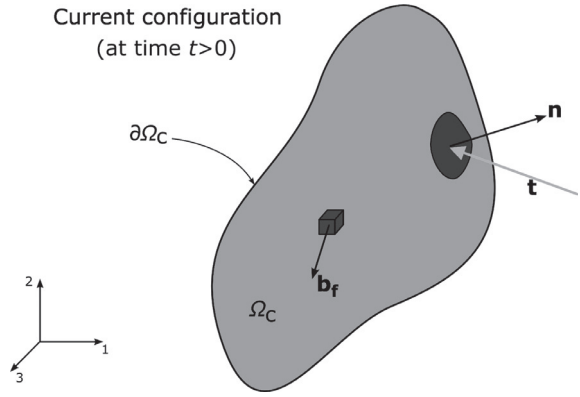


Figure 4.10 Schematic figure illustrating the definition of forces used in the balance of linear momentum.

$$\int_{\partial\Omega_c} \boldsymbol{\sigma}\mathbf{n}\mathrm{d}s = \int_{\Omega_c} \mathrm{div}\,\boldsymbol{\sigma}\,\mathrm{d}v. \tag{4.169}$$

The time-derivative of the linear momentum can be simplified further by using the same variable substitution that was used in the derivation of the field equation for mass conservation $\mathbf{x} = \mathcal{X}(\mathbf{X}, t)$:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_c} \mathbf{v}(\mathbf{x},t)\rho_c(\mathbf{x},t)\,\mathrm{d}v = \frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_0} \mathbf{v}(\mathbf{X},t)\rho_c(\mathbf{X},t)J\,\mathrm{d}V \tag{4.170}$$

$$= \int_{\Omega_0}\left[\dot{\mathbf{v}}(\mathbf{X},t)\rho_c(\mathbf{X},t)J + \mathbf{v}(\mathbf{X},t)\frac{\mathrm{D}}{\mathrm{D}t}(\rho_c(\mathbf{X},t)J)\right]\mathrm{d}V. \tag{4.171}$$

From mass conservation (Equation (4.162)) the term $\mathrm{D}(\rho_c J)/\mathrm{D}t = 0$, giving

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_c} \mathbf{v}\rho_c\,\mathrm{d}v = \int_{\Omega_0} \dot{\mathbf{v}}(\mathbf{X},t)\rho_c(\mathbf{X},t)J\,\mathrm{d}V = \int_{\Omega_c} \dot{\mathbf{v}}\rho_c\,\mathrm{d}v. \tag{4.172}$$

The balance of linear momentum can therefore be obtained from Equations (4.168), (4.169), and (4.172) as

$$\int_{\Omega_c} [\mathrm{div}\,\boldsymbol{\sigma} + \mathbf{b}_f - \rho_c\dot{\mathbf{v}}]\,\mathrm{d}v = 0. \tag{4.173}$$

This equation has to be valid also for an arbitrary sub-domain of Ω_c, hence the integrand has to be identically zero giving the following field equation representation of the balance of linear momentum:

$$\operatorname{div} \boldsymbol{\sigma} + \mathbf{b}_f = \rho_c \dot{\mathbf{v}}. \tag{4.174}$$

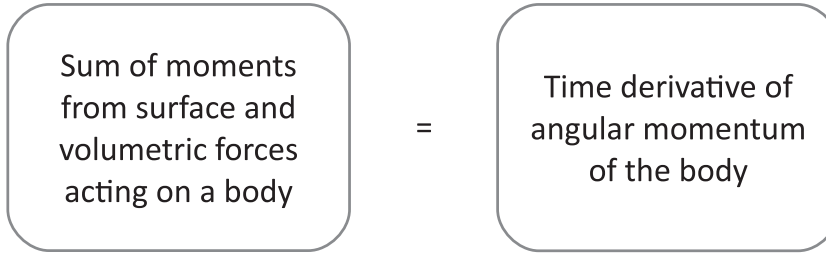
The derivation presented above can be repeated in the reference configuration. The details of the derivation are left as an exercise, the final field equation for the balance of linear momentum is:

$$\operatorname{Div} \mathbf{P} + \mathbf{B}_f = \rho_0 \dot{\mathbf{V}}. \tag{4.175}$$

4.9.3 Balance of Angular Momentum

The balance of angular momentum principle states that the moment that is applied on a body is equal to the time-derivative of the angular momentum. This principle is directly obtained from the linear momentum equation by taking the cross-product of both the force and the linear momentum with the position vector [17]. It is therefore to be expected that the balance of angular momentum will provide similar results to the balance of linear momentum.

For a deformable body undergoing large deformations the balance of angular momentum can be written as follows:



This can be written as a balance law expressed in the current configuration:

$$\int_{\partial\Omega_c} \mathbf{x} \times \mathbf{t}\, \mathrm{d}s + \int_{\Omega_c} \mathbf{x} \times \mathbf{b}_f\, \mathrm{d}v = \frac{\mathrm{D}}{\mathrm{D}t} \int_{\Omega_c} \mathbf{x} \times \mathbf{v}\, \rho_c\, \mathrm{d}v. \tag{4.176}$$

This equation can be simplified using the Cauchy stress theorem (Equation (4.138)), $\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$, and converting it to index form. From Equation (4.16) the index form becomes

$$\int_{\partial\Omega_c} \epsilon_{ijk} x_j \sigma_{kl} n_l \mathrm{d}s + \int_{\Omega_c} \epsilon_{ijk} x_j b_{fk} \,\mathrm{d}v = \frac{\mathrm{D}}{\mathrm{D}t} \int_{\Omega c} \epsilon_{ijk} x_j v_k \rho_c \,\mathrm{d}v, \tag{4.177}$$

where b_{fk} is the kth component of the body force vector $\mathbf{b}_f$. The first term on the left-hand side can be simplified by applying the divergence theorem:

$$\int_{\partial\Omega_c} \epsilon_{ijk} x_j \sigma_{kl} n_l \mathrm{d}s = \int_{\Omega_c} \epsilon_{ijk} \frac{\partial}{\partial x_l} \left[x_j \sigma_{kl} \right] \mathrm{d}v \tag{4.178}$$

$$= \int_{\Omega_c} \left[\epsilon_{ijk} \sigma_{kj} + \epsilon_{ijk} x_j \frac{\partial \sigma_{kl}}{\partial x_l} \right] \mathrm{d}v. \tag{4.179}$$

The term on the right-hand size can be simplified by transforming the integration from the current to the reference configuration by the variable substitution $\mathbf{x} = \mathcal{X}(\mathbf{X})$:

$$\begin{aligned} \frac{\mathrm{D}}{\mathrm{D}t} \int_{\Omega_c} \epsilon_{ijk} x_j v_k \rho_c \,\mathrm{d}v &= \frac{\mathrm{D}}{\mathrm{D}t} \int_{\Omega_0} \epsilon_{ijk} X_j V_k \rho_c J \,\mathrm{d}V \\ &= \int_{\Omega_0} \left[\epsilon_{ijk} V_j V_k \rho_c J + \epsilon_{ijk} X_j \dot{V}_k \rho_c J + \epsilon_{ijk} X_j V_k \frac{\mathrm{D}}{\mathrm{D}t} (\rho_c J) \right] \mathrm{d}V \\ &= \int_{\Omega_c} \epsilon_{ijk} x_j \dot{v}_k \rho_c \,\mathrm{d}v. \end{aligned} \tag{4.180}$$

Inserting Equations (4.180) and (4.179) into Equation (4.177) gives

$$\int_{\Omega_c} \left\{ \epsilon_{ijk} \sigma_{kj} + \epsilon_{ijk} x_j \left[\frac{\partial \sigma_{kl}}{\partial x_l} + b_{fk} - \dot{v}_k \rho_c \right] \right\} \mathrm{d}v. \tag{4.181}$$

This equation has to be valid also for an arbitrary sub-domain of Ω_c, hence the integrand has to be identically zero. Furthermore, the expression within the square bracket is also zero from the balance of linear momentum (Equation (4.172)).

By expanding the terms in $\epsilon_{ijk}\sigma_{kj} = 0$, we get the equivalent condition

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^\top. \tag{4.182}$$

Hence, the balance of angular momentum is satisfied if the balance of linear momentum is satisfied and the Cauchy stress is symmetrical.

The balance of angular momentum can also be expressed in the reference configuration using a similar derivation. The details are left as an exercise, the final field equation is:

$$\mathbf{P}\mathbf{F}^{\top} = \mathbf{F}\mathbf{P}^{\top}, \tag{4.183}$$

where $\mathbf{P}$ is the first Piola-Kirchhoff stress and $\mathbf{F}$ is the deformation gradient.

4.9.4 First Law of Thermodynamics

In this section, we will introduce the concept of energy conservation, specifically the first law of thermodynamics which has far reaching consequences in many fields of mechanical engineering.

The system we are studying is a closed system that can perform work and exchange heat with its surroundings, but that cannot transfer material through its boundary, see Figure 4.11. The body has internal volumetric heat generation (r) and heat flux ($\mathbf{q}$) through its boundary to the surroundings. The body is also exposed to external surface tractions ($\mathbf{t}$) and a volumetric body force ($\mathbf{b}_{\mathrm{f}}$).

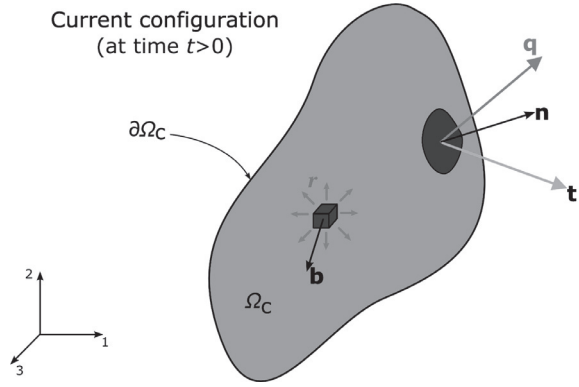
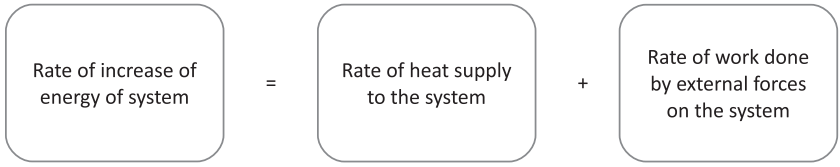


Figure 4.11 Schematic figure illustrating the definition of thermodynamic quantities in the current configuration.

The first law of thermodynamics states that [18, 19]:



This can be written as a balance law in the current configuration:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_\mathrm{c}}\left(e_\mathrm{c}+\frac{\rho_\mathrm{c}}{2}\mathbf{v}\cdot\mathbf{v}\right)\mathrm{d}v=\left\{\int_{\partial\Omega_\mathrm{c}}-\mathbf{q}\cdot\mathbf{n}\mathrm{d}s+\int_{\Omega_\mathrm{c}}r\,\mathrm{d}v\right\}+\left\{\int_{\partial\Omega_\mathrm{c}}\mathbf{t}\cdot\mathbf{v}\mathrm{d}s+\int_{\Omega_\mathrm{c}}\mathbf{b}_\mathrm{f}\cdot\mathbf{v}\,\mathrm{d}v\right\}, \tag{4.184}$$

or as a balance law in the reference configuration:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_0}\left(e_0+\frac{\rho_0}{2}\mathbf{V}\cdot\mathbf{V}\right)\mathrm{d}V=\left\{\int_{\partial\Omega_0}-\mathbf{Q}\cdot\mathbf{N}\,\mathrm{d}S+\int_{\Omega_0}R\,\mathrm{d}V\right\}+\left\{\int_{\partial\Omega_0}\mathbf{T}\cdot\mathbf{V}\,\mathrm{d}S+\int_{\Omega_0}\mathbf{B}_\mathrm{f}\cdot\mathbf{V}\,\mathrm{d}V\right\}. \tag{4.185}$$

In the following, we will focus on the expression for the current configuration. The first term on the left-hand side in Equation (4.184) expresses the time derivative of the internal and kinetic energies. This term can be simplified by introducing the variable substitution, $\mathbf{x}(x)=\mathcal{X}(\mathbf{X},t)$, transforming the integration to the reference configuration:

$$\begin{aligned}\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_\mathrm{c}}\left(e_\mathrm{c}+\frac{\rho_\mathrm{c}}{2}v^2\right)\mathrm{d}v&=\int_{\Omega_0}\frac{\mathrm{D}}{\mathrm{D}t}\left(e_\mathrm{c}J+\frac{\rho_\mathrm{c}}{2}v^2J\right)\mathrm{d}V\\&=\int_{\Omega_0}\left(\dot{e}_\mathrm{c}J+e_\mathrm{c}\dot{J}+\frac{1}{2}\frac{\mathrm{D}}{\mathrm{D}t}\left(\rho_\mathrm{c}+J\right)v^2+\dot{\mathbf{v}}\cdot\mathbf{v}J\right)\mathrm{d}V.\end{aligned} \tag{4.186}$$

From Equation (4.162) we know that $\mathrm{D}/\mathrm{D}t(\rho_c J) = 0$, giving

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_c}\left(e_c + \frac{\rho_c}{2}v^2\right)\,\mathrm{d}v = \int_{\Omega_c}\left[\dot{e}_c + e_c\,\mathrm{div}\,\mathbf{v} + \rho_c\dot{\mathbf{v}}\cdot\mathbf{v}\right]\,\mathrm{d}v. \tag{4.187}$$

The rate of heat supply to the system is given by

$$\int_{\partial\Omega_c} -\mathbf{q}\cdot\mathbf{n}\mathrm{d}s + \int_{\Omega_c} r\,\mathrm{d}v = \int_{\Omega_c}\left[-\,\mathrm{div}\,\mathbf{q} + r\right]\,\mathrm{d}v. \tag{4.188}$$

By using the divergence theorem (Equation (4.54)), the rate of work down by external surface forces on the system can be written

$$\begin{aligned}\int_{\partial\Omega_c}\mathbf{t}\cdot\mathbf{v}\mathrm{d}s &= \int_{\partial\Omega_c}(\boldsymbol{\sigma}\,\mathbf{n})\cdot\mathbf{v}\mathrm{d}s = \int_{\partial\Omega_c}\sigma_{ij}n_j n_i\mathrm{d}s\\ &= \int_{\Omega_c}\frac{\partial(\sigma_{ij}v_i)}{\partial x_j}\\ &= \int_{\Omega_c}\left(\frac{\partial\sigma_{ij}}{\partial x_j}v_i + \sigma_{ij}\frac{\partial v_i}{\partial x_j}\right)\,\mathrm{d}v\\ &= \int_{\Omega_c}(\mathrm{div}\,\boldsymbol{\sigma}\cdot\mathbf{v} + \boldsymbol{\sigma}:\mathbf{d})\,\mathrm{d}v.\end{aligned} \tag{4.189}$$

By inserting Equations (4.187), (4.188), and (4.189) into Equation (4.184) we get the following expression

$$\begin{aligned}\int_{\Omega_c}(\boldsymbol{\sigma}:\mathbf{d} - \mathrm{div}\,\mathbf{q} + r - [\mathrm{div}\,\boldsymbol{\sigma} + \mathbf{b}_f - \rho_c\dot{\mathbf{v}}]\cdot\mathbf{v}\\ - \dot{e}_c - e_c\,\mathrm{div}\,\mathbf{v})\,\mathrm{d}v.\end{aligned} \tag{4.190}$$

From the balance of linear momentum (Equation (4.174)), this equation gives the field equation for energy conservation in the current configuration:

$$\boldsymbol{\sigma}:\mathbf{d} - \mathrm{div}\,\mathbf{q} + r = \dot{e}_c + e_c\,\mathrm{div}\,\mathbf{v}. \tag{4.191}$$

Using a similar derivation the corresponding field equation for energy conservation in the reference configuration can be written:

$$\mathbf{P}:\dot{\mathbf{F}} - \mathrm{Div}\,\mathbf{Q} + R = \dot{e}_0. \tag{4.192}$$

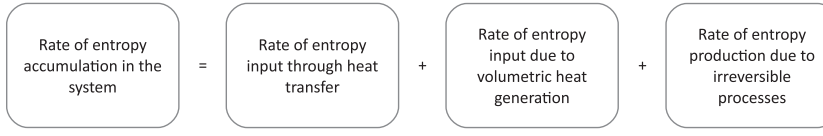
4.9.5 Second Law of Thermodynamics

The second law of thermodynamics applies to all systems and can be written in many different forms. One form suitable for the discussion in this section is that [18, 19]:

> *The entropy of a thermally isolated macroscopic system never decreases.*

Entropy is a measure of the amount of energy in a system that cannot be converted to work. The unit of entropy is J/K. Through the field of statistical mechanics it be shown that entropy is also be a measure of the disorder in the system [20]. As is taught in introductory thermodynamics [21], if a system is undergoing a reversible process during which a given amount of heat is applied at a known temperature, then the change in entropy of the system is given by the heat divided by the temperature.

For a deformable body the second law of thermodynamics can for a closed system be written as the following balance law, see Figure 4.12.



By using the nomenclature presented in Table 4.1, we can write the second law of thermodynamics as the following balance law in the current configuration:

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_\mathrm{c}} \eta_\mathrm{c}\,\mathrm{d}v = \int_{\partial\Omega_\mathrm{c}} -\frac{\mathbf{q}\cdot\mathbf{n}}{\theta_\mathrm{c}}\mathrm{d}s + \int_{\Omega_\mathrm{c}} \frac{r}{\theta_\mathrm{c}}\,\mathrm{d}v + \Gamma, \tag{4.193}$$

or when expressed in the reference configuration

$$\frac{\mathrm{D}}{\mathrm{D}t}\int_{\Omega_0} \eta_0\,\mathrm{d}V = \int_{\partial\Omega_0} -\frac{\mathbf{Q}\cdot\mathbf{N}}{\theta_0}\,\mathrm{d}S + \int_{\Omega_0} \frac{R}{\theta_0}\,\mathrm{d}V + \Gamma. \tag{4.194}$$

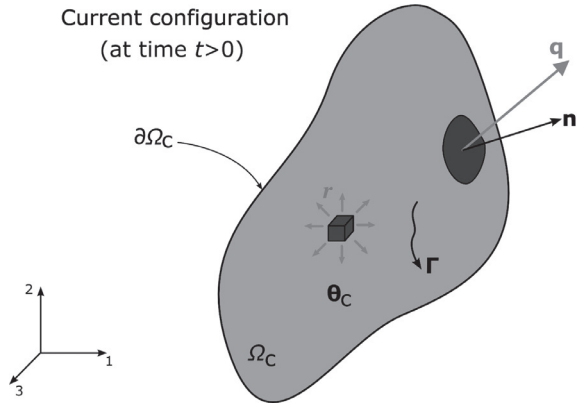


Figure 4.12 Schematic figure showing the definition of thermodynamic quantities in the current configuration.

In these equations, $\Gamma \geq 0$ is the entropy generation rate due to irreversible mechanisms. These equations are often referred to as the Clausius-Duhem equation.

By using the divergence theorem (Equation (4.54)), the field equation in the current configuration becomes:

$$\dot{\eta}_c + \eta_c \operatorname{div} \mathbf{v} \geq -\operatorname{div}\left(\frac{\mathbf{q}}{\theta_c}\right) + \frac{r}{\theta_c}. \tag{4.195}$$

and in the reference configuration:

$$\dot{\eta}_0 \geq -\operatorname{Div}\left(\frac{\mathbf{Q}}{\theta_0}\right) + \frac{R}{\theta_0}. \tag{4.196}$$

These equations are very useful when developing constitutive equations as will be discussed in Section 4.11.

4.10 Energy Balance and Stress Power

The balance of mechanical effect is introduced in this section, and it is shown how that leads to the definition of stress power. To start, define the rate of work done by external forces on a body in configuration Ω_c:

$$\mathcal{P}_{\text{ext}} = \int_{\partial\Omega_c} \mathbf{t} \cdot \mathbf{v}\, ds + \int_{\Omega_c} \mathbf{b}_f \cdot \mathbf{v}\, dv, \tag{4.197}$$

where $\mathbf{t}$ is a surface traction, $\mathbf{b}_\mathrm{f}$ is the body force, and $\mathbf{v}$ is the velocity field, all of which are expressed in the current configuration. By using the Cauchy stress theorem (Equation (4.138)) and the divergence theorem (Equation (4.54)), this equation can be written

$$\mathcal{P}_\mathrm{ext} = \int_{\Omega_\mathrm{c}} [\mathrm{div}(\boldsymbol{\sigma}\mathbf{v}) + \mathbf{b}_\mathrm{f} \cdot \mathbf{v}] \, \mathrm{d}v \tag{4.198}$$

$$= \int_{\Omega_\mathrm{c}} [\boldsymbol{\sigma} : \mathbf{l} + (\mathrm{div}\,\boldsymbol{\sigma}) \cdot \mathbf{v} + \mathbf{b}_\mathrm{f} \cdot \mathbf{v}] \, \mathrm{d}v \tag{4.199}$$

$$= \int_{\Omega_\mathrm{c}} \boldsymbol{\sigma} : \mathbf{d} \, \mathrm{d}v + \int_{\Omega_\mathrm{c}} \rho_\mathrm{c} \dot{\mathbf{v}} \cdot \mathbf{v} \, \mathrm{d}v \tag{4.200}$$

$$= \int_{\Omega_\mathrm{c}} \boldsymbol{\sigma} : \mathbf{d} \, \mathrm{d}v + \frac{\mathrm{D}}{\mathrm{D}t} \int_{\Omega_\mathrm{c}} \frac{1}{2} \rho_\mathrm{c} \mathbf{v}^2 \, \mathrm{d}v \tag{4.201}$$

$$= \mathcal{P}_\mathrm{int} + \frac{\mathrm{D}}{\mathrm{D}t} \mathcal{K}. \tag{4.202}$$

Hence, the rate of external work ($\mathcal{P}_\mathrm{ext}$) is equal to the rate of internal mechanical work (also called the stress-power $\mathcal{P}_\mathrm{int}$) plus the time derivative of the kinetic energy ($\mathrm{D}\mathcal{K}/\mathrm{D}t$).

From this equation we see that the stress power per unit current volume is $\boldsymbol{\sigma} : \mathbf{d}$, which can be converted to reference volume by Equation (4.79) giving:

$$J\boldsymbol{\sigma} : \mathbf{d}, \tag{4.203}$$

where $J\boldsymbol{\sigma}$ is the Kirchhoff stress $\boldsymbol{\tau}$. From this equation, we say that $\boldsymbol{\tau}$ and $\mathbf{d}$ are *work conjugate* stress and deformation rate measures.

The expression for stress power can be converted to other stress measures. First, recall from Equation (4.150) that $J\boldsymbol{\sigma} = \mathbf{P}\mathbf{F}^T$, inserting this into Equation (4.203) gives

$$\begin{aligned} J\boldsymbol{\sigma} : \mathbf{d} &= \mathbf{P}\mathbf{F}^T : \mathbf{d} \\ &= \mathbf{P}\mathbf{F}^T : \mathbf{l} \\ &= \mathbf{P} : \mathbf{l}\mathbf{F} \\ &= \mathbf{P} : \dot{\mathbf{F}}, \end{aligned} \tag{4.204}$$

illustrating that the first Piola-Kirchhoff stress is work conjugate to the time derivative of the deformation gradient.

The stress power per unit reference volume can also be expressed in terms of the second Piola-Kirchhoff stress **S**. Recall from Equation (4.150) that $\boldsymbol{\sigma} = \mathbf{F}\mathbf{S}\mathbf{F}^T/J$, giving

$$\begin{aligned} J\boldsymbol{\sigma} : \mathbf{d} &= \mathbf{F}\mathbf{S}\mathbf{F}^T : \mathbf{d} \\ &= \mathbf{S} : \mathbf{F}^T\mathbf{d}\mathbf{F}. \end{aligned} \tag{4.205}$$

The term $\mathbf{F}^\top\mathbf{d}\mathbf{F}$ can be simplified by inserting $\mathbf{F} = \mathbf{R}\mathbf{U}$, $\mathbf{d} = \mathbf{l} - \mathbf{w}$, $\dot{\mathbf{F}} = \dot{\mathbf{R}}\mathbf{U} + \mathbf{R}\dot{\mathbf{U}}$, and $\dot{\mathbf{R}} = \mathbf{w}\mathbf{R}$, giving

$$\mathbf{F}^\top\mathbf{d}\mathbf{F} = \dot{\mathbf{U}}\mathbf{U} = \dot{\mathbf{E}}^G, \tag{4.206}$$

where the Green strain (Equation (4.119)) is defined by: $\mathbf{E}^G = \frac{1}{2}\left[\mathbf{U}^2 - \mathbf{I}\right]$, giving

$$J\boldsymbol{\sigma} : \mathbf{d} = \mathbf{S} : \dot{\mathbf{E}}^G. \tag{4.207}$$

Hence, the second Piola-Kirchhoff stress is work conjugate to the time derivative of the Green strain.

When developing constitutive equations it is important to use work conjugate stress and strain measures. The following table summarizes the three most commonly used pairs of stress and strain measures:

Table 4.2 Work Conjugate Stress and Deformation Rate Measures

Stress Measure	Work Conjugate Deformation Rate Measure
Kirchhoff stress $J\boldsymbol{\sigma} \equiv \boldsymbol{\tau}$	Stress rate tensor $\mathbf{d}$
First Piola-Kirchhoff stress $\mathbf{P}$	Time derivative of deformation gradient $\dot{\mathbf{F}}$
Second Piola-Kirchhoff stress $\mathbf{S}$	Time derivative of Green strain $\dot{\mathbf{E}}^G$

4.11 Constitutive Equations

A constitutive equation (sometimes also called a *material model* or *constitutive model*) is a relationship that describes how a material behaves, for example, the stress response for a given strain, or the heat transfer for a given temperature gradient. The constitutive equations are what distinguish the response of different materials. Everything presented so far in this chapter is valid for all materials. Next, we will discuss how the continuum mechanics framework that we have developed can be used to formulate the constitutive equations for a material. The presentation will focus on general relations that all constitutive equations need to fulfill. The following chapters of this book will demonstrate how these results can be used to develop specific material models for polymers.

There are different classes of constitutive models that can be developed and used. For example, a nonlinear elastic model is based on a stress function that only depend on the applied deformation:

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}\left(\mathbf{F}\right). \tag{4.208}$$

In this equation, we have indicated that the Cauchy stress $\hat{\boldsymbol{\sigma}}(\mathbf{F})$ is a function of the deformation gradient. Note that this and other constitutive models can equally well be written also in terms of other stress measures, for example

$$\mathbf{P} = \hat{\mathbf{P}}(\mathbf{F}), \tag{4.209}$$

$$\mathbf{S} = \hat{\mathbf{S}}(\mathbf{F}). \tag{4.210}$$

For simplicity we will in the following focus mostly on the Cauchy stress in the derivations.

As a second example of a constitutive equation, consider a more common polymeric material characterized by a rate-dependent response (i.e., a material with a slight memory of past deformation). For this material the stress depends on both the current deformation state ($\mathbf{F}$) and the rate of deformation ($\dot{\mathbf{F}}$):

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}\left(\mathbf{F}, \dot{\mathbf{F}}\right). \tag{4.211}$$

In general, to specify the response of a material that is exposed to thermal and mechanical loads it is necessary to specify how the stress ($\boldsymbol{\sigma}$), internal energy (ϵ), heat flux ($\mathbf{q}$), and entropy (η) depend on the applied fields. To completely know the state of the material it is necessary to know the following field variables at each point:

- the velocity $\mathbf{v}$,
- the stress tensor $\boldsymbol{\sigma}$,
- the mass density ρ,
- the internal energy per unit current volume ϵ_c,
- the temperature θ,
- the heat flux vector $\mathbf{q}$, and
- the entropy η.

In total, by using the symmetry of $\boldsymbol{\sigma}$, there are therefore 16 unknown field variable that need to be determined. The following equations are needed to solve for the field variables:

Governing Field Equations	**Number of Equations**
Conservation of mass	1
Conservation of linear momentum	3
Conservation of angular momentum	0 (already used)
First law of thermodynamics	1
Second law of thermodynamics	0 (only an inequality)

Total of 5 equations

Since there are only 5 governing field equations and there are 16 unknown field variables, more equations are needed. The missing equations are the constitutive equations which provide the following relationships.

Constitutive Equation	Number of Equations
Stress $\boldsymbol{\sigma}(\cdot)$	6
Internal energy $\epsilon_c(\cdot)$	1
Heat flux per unit volume $\mathbf{q}(\cdot)$	3
Entropy per unit volume $\eta_c(\cdot)$	1
	Total of 11 equations

In summary, by combining the constitutive equations with the field equations we get 16 governing equations to solve for the 16 unknown field variables.

As mentioned, there are many different classes of constitutive equations that can be used to describe the behavior of a solid material. One of the most basic approaches is to model the material as thermoelastic and specifying constitutive equations that depend on the deformation gradient ($\mathbf{F}$), the temperature (θ_c), and the gradient of the temperature ($\operatorname{grad}\theta_c$). This case is discussed in more detail in the next section.

4.11.1 Constitutive Equations for a Thermoelastic Material

A thermoelastic material is characterized by having the heat flux vector ($\mathbf{q}$), Cauchy stress ($\boldsymbol{\sigma}$), internal energy per unit current volume (ϵ_c), and entropy per unit current volume (η_c) all depend on the deformation gradient, temperature, and temperature gradient:

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F}, \theta_c, \operatorname{grad}\theta_c), \tag{4.212}$$

$$\mathbf{q} = \hat{\mathbf{q}}(\mathbf{F}, \theta_c, \operatorname{grad}\theta_c), \tag{4.213}$$

$$\epsilon_c = \hat{\epsilon}_c(\mathbf{F}, \theta_c, \operatorname{grad}\theta_c), \tag{4.214}$$

$$\eta_c = \hat{\eta}_c(\mathbf{F}, \theta_c, \operatorname{grad}\theta_c). \tag{4.215}$$

The requirements on these constitutive equations for a thermoelastic material can be further specified by using an approach that was originally developed by Truesdell et al. [7]. To derive the governing equations we will start by listing the balance laws in the reference configuration:

- linear momentum

$$\operatorname{Div}\mathbf{P} + \mathbf{B}_{\mathrm{f}} = \rho_0 \dot{\mathbf{V}}, \qquad \text{(4.175-repeat)}$$

- angular momentum

$$\mathbf{P}\mathbf{F}^{\top} = \mathbf{F}\mathbf{P}^{\top}, \qquad \text{(4.183-repeat)}$$

- first law of thermodynamics

$$\mathbf{P} : \dot{\mathbf{F}} - \operatorname{Div}\mathbf{Q} + R = \dot{e}_0, \qquad \text{(4.192-repeat)}$$

- second law of thermodynamics

$$\dot{\eta}_0 \geq -\operatorname{Div}\left(\frac{\mathbf{Q}}{\theta_0}\right) + \frac{R}{\theta_0}. \qquad \text{(4.196-repeat)}$$

The constitutive functions in Equations (4.212)–(4.215) need to satisfy all of these governing equations in order to be valid. These requirements can be simplified by first solve for R/θ_0 in Equation (4.196) and then inserting the result into Equation (4.196):

$$-\operatorname{Div}\left(\frac{\mathbf{Q}}{\theta_0}\right) + \frac{\dot{e}_0}{\theta_0} - \frac{\mathbf{P} : \dot{\mathbf{F}}}{\theta_0} + \frac{\operatorname{Div}\mathbf{Q}}{\theta_0} \geq \dot{\eta}_0. \qquad (4.216)$$

The term $-\operatorname{Div}(\mathbf{Q}/\theta_0)$ can be simplified by expanding the divergence operator:

$$\begin{aligned} -\operatorname{Div}\left(\frac{\mathbf{Q}}{\theta_0}\right) &= -\frac{\partial}{\partial X_i}\left(\frac{Q_i}{\theta_0}\right) \\ &= -\frac{1}{\theta_0}\frac{\partial Q_i}{\partial X_i} + \frac{Q_i}{\theta_0^2}\frac{\partial \theta_0}{\partial X_i} \\ &= -\frac{1}{\theta_0}\operatorname{Div}\mathbf{Q} + \frac{\mathbf{Q}\cdot\operatorname{Grad}\theta_0}{\theta_0^2}, \end{aligned} \qquad (4.217)$$

which when inserted into Equation (4.216) give

$$\frac{\mathbf{Q}\cdot\operatorname{Grad}\theta_0}{\theta_0^2}+\frac{\dot{e}_0}{\theta_0}-\frac{\mathbf{P}:\dot{\mathbf{F}}}{\theta_0}\geq\dot{\eta}_0. \tag{4.218}$$

When working with thermoelastic materials it is often more convenient to work with the Helmholtz free energy (Ψ) instead of the internal energy (e_c). The Helmholtz free energy per unit reference volume is defined by:

$$\Psi=e_0-\theta_0\eta_0. \tag{4.219}$$

From the definition of Ψ we can solve for $\dot{e}_0$:

$$\dot{e}_0=\dot{\Psi}+\dot{\theta}_0\eta_0+\theta_0\dot{\eta}_0. \tag{4.220}$$

Inserting Equation (4.220) into Equation (4.218) gives

$$\dot{\Psi}+\eta_0\dot{\theta}_0-\mathbf{P}:\dot{\mathbf{F}}+\frac{\mathbf{Q}\cdot\operatorname{Grad}\theta_0}{\theta_0}\geq 0. \tag{4.221}$$

As shown in Equations (4.212)–(4.215), the constitutive equations for a thermoelastic material are given by the following functional forms

$$\mathbf{P}=\hat{\mathbf{P}}(\mathbf{F},\theta_0,\operatorname{Grad}\theta_0), \tag{4.222}$$

$$\mathbf{Q}=\hat{\mathbf{Q}}(\mathbf{F},\theta_0,\operatorname{Grad}\theta_0), \tag{4.223}$$

$$\Psi=\hat{\Psi}(\mathbf{F},\theta_0,\operatorname{Grad}\theta_0), \tag{4.224}$$

$$\eta_0=\hat{\eta}_0(\mathbf{F},\theta_0,\operatorname{Grad}\theta_0). \tag{4.225}$$

Inserting Equation (4.224) into Equation (4.221) gives:

$$\left\{\frac{\partial\hat{\Psi}}{\partial\mathbf{F}}:\dot{\mathbf{F}}+\frac{\partial\hat{\Psi}}{\partial\theta_0}\dot{\theta}_0+\frac{\partial\hat{\Psi}}{\partial(\operatorname{Grad}\theta_0)}\cdot\left(\frac{\mathrm{d}(\operatorname{Grad}\theta_0)}{\mathrm{d}t}\right)\right\}$$
$$+\hat{\eta}_0\dot{\theta}_0-\hat{\mathbf{P}}:\dot{\mathbf{F}}+\frac{1}{\theta_0}\hat{\mathbf{Q}}\cdot(\operatorname{Grad}\theta_0)\geq 0, \tag{4.226}$$

which also can be written:

$$\left\{\frac{\partial\hat{\Psi}}{\partial\mathbf{F}}-\hat{\mathbf{P}}\right\}:\dot{\mathbf{F}}+\left\{\frac{\partial\hat{\Psi}}{\partial\theta_0}+\hat{\eta}_0\right\}\dot{\theta}_0+\left\{\frac{\partial\hat{\Psi}}{\partial(\mathrm{Grad}\,\theta_0)}\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{Grad}\,\theta_0)\right\}+\frac{1}{\theta_0}\hat{\mathbf{Q}}\cdot(\mathrm{Grad}\,\theta_0)\geq 0. \tag{4.227}$$

This equation has to be valid for all processes, hence for all possible values and histories of $\mathbf{F}$, $\dot{\mathbf{F}}$, θ, $\dot{\theta}$, $\mathrm{Grad}\,\theta_0$, and $\mathrm{d}(\mathrm{Grad}\,\theta_0)/\mathrm{d}t$.

If we consider a process in which $\dot{\theta}_0 = 0$ and $\mathrm{d}(\mathrm{Grad}\,\theta_0)/\mathrm{d}t = 0$, then the entropy inequality (Equation (4.226)) becomes:

$$\left\{\frac{\partial\hat{\Psi}}{\partial\mathbf{F}}-\hat{\mathbf{P}}\right\}:\dot{\mathbf{F}}+\frac{1}{\theta_0}\hat{\mathbf{Q}}\cdot(\mathrm{Grad}\,\theta_0)\geq 0. \tag{4.228}$$

This equation has to be true for all $\dot{\mathbf{F}}$, hence the first Piola-Kirchhoff stress has to be equal to the partial derivative of the Helmholtz free energy with respect to the deformation gradient:

$$\hat{\mathbf{P}}(\mathbf{F},\theta_0)=\frac{\partial\hat{\Psi}}{\partial\mathbf{F}}. \tag{4.229}$$

If we instead consider a process in which $\dot{\mathbf{F}} = 0$ and $\mathrm{d}(\mathrm{Grad}\,\theta_0)/\mathrm{d}t = 0$, then the entropy inequality (Equation (4.226)) becomes:

$$\left\{\frac{\partial\hat{\Psi}}{\partial\theta_0}+\hat{\eta}_0\right\}\dot{\theta}_0+\frac{1}{\theta_0}\hat{\mathbf{Q}}\cdot(\mathrm{Grad}\,\theta_0)\geq 0. \tag{4.230}$$

This equation has to be true for all $\dot{\theta}_0$, hence the entropy per unit reference volume has to be given by the partial derivative of the Helmholtz free energy with respect to the temperature:

$$\hat{\eta}_0(\mathbf{F},\theta)=-\frac{\partial\hat{\Psi}}{\partial\theta_0}. \tag{4.231}$$

Finally, if we consider a process in which $\dot{\mathbf{F}} = 0$ and $\dot{\theta}_0 = 0$, the entropy inequality (Equation (4.226)) becomes:

$$\left\{\frac{\partial\hat{\Psi}}{\partial(\mathrm{Grad}\,\theta_0)}\right\}\cdot\left(\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{Grad}\,\theta_0\right)+\frac{1}{\theta_0}\hat{\mathbf{Q}}\cdot(\mathrm{Grad}\,\theta_0)\geq 0. \tag{4.232}$$

For this to hold for any value of $\mathrm{d}(\mathrm{Grad}\,\theta_0)/\mathrm{d}t$, it is clear that $\hat{\Psi}$ cannot depend on $\mathrm{Grad}\,\theta_0$, that is

$$\frac{\partial \hat{\Psi}}{\partial (\mathrm{Grad}\,\theta_0)} = 0. \tag{4.233}$$

By inserting Equations (4.228), (4.230), and (4.232) into Equation (4.226) we finally get the entropy inequality as:

$$\hat{\mathbf{Q}} \cdot (\mathrm{Grad}\,\theta_0) \geq 0, \tag{4.234}$$

which simply states that the heat has to flow in the same direction as the temperature gradient. In summary, the constitutive behavior of a thermoelastic material is completely specified by the two functions $\hat{\Psi}(\mathbf{F}, \theta_0)$ and $\hat{\mathbf{Q}}(\mathbf{F}, \theta_0)$. The remaining field variables can be determined from these two functions:

$$\hat{\mathbf{P}}(\mathbf{F}, \theta_0) = \frac{\partial \hat{\Psi}(\mathbf{F}, \theta_0)}{\partial \mathbf{F}} \tag{4.228-repeat}$$

$$\hat{\eta}_0(\mathbf{F}, \theta_0) = \frac{\partial \hat{\Psi}(\mathbf{F}, \theta_0)}{\partial \mathbf{F}}. \tag{4.230-repeat}$$

From these equations, we can also determine expressions for other stress measures. For example, from Equation (4.145), we get that the Cauchy stress can be determined from the Helmholtz free energy by

$$\boldsymbol{\sigma}(\mathbf{F}, \theta_0) = \frac{1}{J} \frac{\partial \hat{\Psi}(\mathbf{F}, \theta_0)}{\partial \mathbf{F}} \mathbf{F}^{\top}. \tag{4.235}$$

For many materials, the rate of heat flow $\mathbf{Q}$ is often modeled using Fourier's equation of heat conduction [18]:

$$\mathbf{Q} = \mathbf{K}(\mathbf{F}, \theta_0)(\mathrm{Grad}\,\theta_0). \tag{4.236}$$

If the heat conductivity tensor $\mathbf{K}$ is positive definite then the entropy inequality (Equation (4.233)) is always satisfied.

The are many other classes of material models that can be defined and used. The following two examples present two simple cases. More advanced models are discussed in the following chapters.

Example
An adiabatic thermoelastic material is defined by having no heat flux ($\mathbf{q} = 0$), and having the Cauchy stress ($\boldsymbol{\sigma}$), internal energy per unit volume (e_c), and entropy per unit volume (η_c) only depend on the deformation gradient and the temperature

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F}, \theta), \tag{4.237}$$

$$e_c = \hat{e}_c(\mathbf{F}, \theta), \tag{4.238}$$

$$\eta_c = \hat{\eta}_c(\mathbf{F}, \theta). \tag{4.239}$$

For this material, the second law of thermodynamics is satisfied if

$$\hat{\mathbf{P}}(\mathbf{F}, \theta) = \frac{\partial \Psi(\mathbf{F}, \theta)}{\partial \mathbf{F}}, \tag{4.240}$$

$$\hat{\eta}_0(\mathbf{F}, \theta) = -\frac{\Psi(\mathbf{F}, \theta)}{\theta_0}. \tag{4.241}$$

That is, for this material, only one thermoelastic function is needed.

Example
An isothermal thermoelastic material is defined by zero heat flux and entropy generation, and having Cauchy stress ($\boldsymbol{\sigma}(\mathbf{F})$), internal energy ($e_c$) only depend on $\mathbf{F}$. For this material, the second law of thermodynamics is satisfied if

$$\hat{\mathbf{P}}(\mathbf{F}) = \frac{\partial \Psi(\mathbf{F})}{\partial \mathbf{F}} = \frac{\partial e_c(\mathbf{F})}{\partial \mathbf{F}}. \tag{4.242}$$

In this case, the Helmholtz free energy and the internal energy become equal.

4.12 Observer Transformation

The functions $\hat{\boldsymbol{\sigma}}(\cdot)$, $\hat{\mathbf{q}}(\cdot)$, $\hat{e}_c(\cdot)$, and $\hat{\eta}_c(\cdot)$ cannot take arbitrary forms. One of the requirements on the constitutive functions is that they satisfy *material frame indifference*. That is, if we first

apply a deformation field specified by $\mathbf{F}$ and then apply a rotation $\mathbf{Q}$, then the combined deformation

$$\mathbf{x}^* \equiv \mathbf{QFX} = \mathbf{Qx} \tag{4.243}$$

should not change the specific internal energy or the specific entropy:

$$\hat{e}_c(\mathbf{QF}) = \hat{e}_c(\mathbf{F}), \tag{4.244}$$

$$\hat{\eta}_c(\mathbf{QF}) = \hat{\eta}_c(\mathbf{F}). \tag{4.245}$$

These equations must hold for all nonsingular deformation gradients $\mathbf{F}$ and for all proper orthogonal rotations $\mathbf{Q}$. If we chose $\mathbf{Q} = \mathbf{R}^\top$ then we get the following necessary condition on $\hat{e}_c(\cdot)$ and $\hat{\eta}_c(\cdot)$:

$$\hat{e}_c(\mathbf{R}^\top\mathbf{F}) = \hat{e}_c(\mathbf{U}) = \hat{\epsilon}_c(\mathbf{F}), \tag{4.246}$$

$$\hat{\eta}_c(\mathbf{R}^\top\mathbf{F}) = \hat{\eta}_c(\mathbf{U}) = \hat{\eta}_c(\mathbf{F}). \tag{4.247}$$

Now if we instead insert $\mathbf{F} = \mathbf{RU}$ into Equations (4.246) and (4.247) we get the both necessary and sufficient conditions:

$$\hat{e}_c(\mathbf{F}) = \hat{e}_c(\mathbf{U}), \tag{4.248}$$

$$\hat{\eta}_c(\mathbf{F}) = \hat{\eta}_c(\mathbf{U}). \tag{4.249}$$

Hence, to fulfill frame-indifference the functions $\hat{e}_c(\cdot)$ and $\hat{\eta}_c(\cdot)$ cannot depend directly on $\mathbf{F}$ but only on $\mathbf{U}$.

If we, as before, after deforming the body apply a proper rotation $\mathbf{Q}$, then the resulting surface traction vector and the heat flux vectors need to be rotated as well:

$$\mathbf{t}^* \equiv \hat{\mathbf{t}}(\mathbf{QF}) = \mathbf{Q}\hat{\mathbf{t}}(\mathbf{F}), \tag{4.250}$$

$$\mathbf{q}^* \equiv \hat{\mathbf{q}}(\mathbf{QF}) = \mathbf{Q}\hat{\mathbf{q}}(\mathbf{F}). \tag{4.251}$$

Recall from the Cauchy stress theorem (Equation (4.138)) that $\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$, which here gives

$$\mathbf{t}^* = \boldsymbol{\sigma}^*\mathbf{n}^* = \mathbf{Qt} = \mathbf{Q}\boldsymbol{\sigma}\mathbf{n}, \tag{4.252}$$

but $\mathbf{n}^* = \mathbf{Qn}$ giving

$$\mathbf{t}^* = \boldsymbol{\sigma}^*\mathbf{Qn} = \mathbf{Q}\boldsymbol{\sigma}\mathbf{n}. \tag{4.253}$$

This has to hold for any vector $\mathbf{n}$, hence

$$\boldsymbol{\sigma}^* = \mathbf{Q}\boldsymbol{\sigma}\mathbf{Q}^\top. \tag{4.254}$$

In summary, to satisfy the requirement of frame indifference the stress and heat flux need to have the following forms

$$\hat{\boldsymbol{\sigma}}(\mathbf{QF}) = \mathbf{Q}\hat{\boldsymbol{\sigma}}(\mathbf{F})\mathbf{Q}^\top, \tag{4.255}$$

$$\hat{\mathbf{q}}(\mathbf{QF}) = \mathbf{Q}\hat{\mathbf{q}}(\mathbf{F}). \tag{4.256}$$

These equations have to be valid for any arbitrary proper orthogonal $\mathbf{Q}$. If we chose $\mathbf{Q} = \mathbf{R}^\top$ then we get a necessary condition for Equations (4.255) and (4.256) to be true:

$$\hat{\boldsymbol{\sigma}}(\mathbf{R}^\top\mathbf{F}) = \hat{\boldsymbol{\sigma}}(\mathbf{U}) = \mathbf{R}^\top\hat{\boldsymbol{\sigma}}(\mathbf{F})\mathbf{R}, \tag{4.257}$$

$$\hat{\mathbf{q}}(\mathbf{R}^\top\mathbf{F}) = \hat{\mathbf{q}}(\mathbf{U}) = \mathbf{R}^\top\hat{\mathbf{q}}(\mathbf{F}). \tag{4.258}$$

By inserting $\mathbf{F} = \mathbf{RU}$ into Equations (4.255) and (4.256) we get the both necessary and sufficient conditions:

$$\hat{\boldsymbol{\sigma}}(\mathbf{QRU}) = \mathbf{Q}\hat{\boldsymbol{\sigma}}(\mathbf{RU})\mathbf{Q}^\top \tag{4.259}$$

$$\Rightarrow \quad \mathbf{QR}\hat{\boldsymbol{\sigma}}(\mathbf{U})\mathbf{R}^\top\mathbf{Q}^\top = \mathbf{Q}\hat{\boldsymbol{\sigma}}(\mathbf{F})\mathbf{Q}^\top \tag{4.260}$$

$$\Rightarrow \quad \hat{\boldsymbol{\sigma}}(\mathbf{F}) = \mathbf{R}\hat{\boldsymbol{\sigma}}(\mathbf{U})\mathbf{R}^\top \tag{4.261}$$

and

$$\hat{\mathbf{q}}(\mathbf{QRU}) = \mathbf{Q}\hat{\mathbf{q}}(\mathbf{RU}) \tag{4.262}$$

$$\Rightarrow \quad \mathbf{QR}\hat{\mathbf{q}}(\mathbf{U}) = \mathbf{Q}\hat{\mathbf{q}}(\mathbf{F}) \tag{4.263}$$

$$\Rightarrow \quad \hat{\mathbf{q}}(\mathbf{F}) = \mathbf{R}\hat{\mathbf{q}}(\mathbf{U}). \tag{4.264}$$

That is, the Cauchy stress cannot directly depend on $\mathbf{F}$, but has to have the following form

$$\hat{\boldsymbol{\sigma}}(\mathbf{F}) = \mathbf{R}\hat{\boldsymbol{\sigma}}(\mathbf{U})\mathbf{R}^\top \tag{4.265}$$

to satisfy material frame indifference. Similarly, the heat flux vector has to be given by

$$\hat{\mathbf{q}}(\mathbf{F}) = \mathbf{R}\hat{\mathbf{q}}(\mathbf{U}). \tag{4.266}$$

These restrictions on the constitutive response can be formulated in a more general observer transformation. If we have two observers inspecting a mechanical experiment or deformation event then the measured distances between points should not depend on the locations of the observers. The two observers can be specified by their coordinate systems which are related by:

$$\mathbf{x}' = \mathbf{c} + \mathbf{Q}\mathbf{x}, \tag{4.267}$$

where $\mathbf{c}$ is a displacement and $\mathbf{Q}$ is a proper orthogonal tensor (a rotation).

If one observer determines that the deformation gradient is $\mathbf{F}$ at one specific location, then the second observer should see the deformation gradient $\mathbf{QF}$ at the same location. If we now consider a scalar field that is ϕ when referred to by the first observer, and as ϕ' when referred to by the second observer then

$$\phi'(\mathbf{x}) = \phi(\mathbf{x}). \tag{4.268}$$

If we have a vector field that the first observer refers to as $\mathbf{u}$ and the second observer refers to as $\mathbf{u}'$ then

$$\mathbf{u}'(\mathbf{x}') = \mathbf{Q}\mathbf{u}(\mathbf{x}). \tag{4.269}$$

Finally, if we have a tensor field that the first observer refers to as $\mathbf{A}$ and the second observer refers to as $\mathbf{A}'$, and if $\mathbf{n}$ and $\mathbf{n}'$ are the representations of an arbitrary vector from the two observers, then

$$\mathbf{A}'\mathbf{n}' = \mathbf{Q}(\mathbf{A}\mathbf{n}), \tag{4.270}$$

but since $\mathbf{n}' = \mathbf{Q}\mathbf{n}$ we also get

$$\mathbf{A}'\mathbf{Q}\mathbf{n} = \mathbf{Q}\mathbf{A}\mathbf{n}. \tag{4.271}$$

This must hold for any $\mathbf{n}$, hence $\mathbf{A}'\mathbf{Q} = \mathbf{Q}\mathbf{A}$ which is equivalent to

$$\mathbf{A}' = \mathbf{Q}\mathbf{A}\mathbf{Q}^{\top}. \tag{4.272}$$

If the scalar, vector, or tensor field satisfies these conditions then they are said to be *objective*, or invariant to observer transformation.

4.12.1 Objective Rates

To demonstrate the time-derivative of second-order tensors consider a case where the basis vectors in the current spatial configuration rotate as a function of time with respect to the reference configuration:

$$\hat{\mathbf{n}}_i = \mathbf{Q}(t)\hat{\mathbf{N}}_i. \tag{4.273}$$

Then $\dot{\hat{\mathbf{n}}}_i = \dot{\mathbf{Q}}\hat{\mathbf{N}}_i = \dot{\mathbf{Q}}\mathbf{Q}^\top\hat{\mathbf{n}}_i \equiv \boldsymbol{\Omega}\hat{\mathbf{n}}_i$. Consider a tensor $\boldsymbol{\sigma} = \sigma_{ij}\hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_j$. From the chain rule, the time derivative of this tensor can be written

$$\dot{\boldsymbol{\sigma}} = \dot{\sigma}_{ij}\hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_j + \sigma_{ij}\dot{\hat{\mathbf{n}}}_i \otimes \hat{\mathbf{n}}_j + \sigma_{ij}\hat{\mathbf{n}}_i \otimes \dot{\hat{\mathbf{n}}}_i. \tag{4.274}$$

Define $\mathring{\boldsymbol{\sigma}} \equiv \dot{\sigma}_{ij}\hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_j$ to be the co-rotational rate, giving

$$\dot{\boldsymbol{\sigma}} = \mathring{\boldsymbol{\sigma}} + \sigma_{ij}\boldsymbol{\Omega}\hat{\mathbf{n}}_i \otimes \hat{\mathbf{n}}_j + \sigma_{ij}\hat{\mathbf{n}}_i \otimes (\boldsymbol{\Omega}\hat{\mathbf{n}}_i), \tag{4.275}$$

which also can be written

$$\dot{\boldsymbol{\sigma}} = \mathring{\boldsymbol{\sigma}} + \boldsymbol{\Omega}\boldsymbol{\sigma} + \boldsymbol{\sigma}\boldsymbol{\Omega}^\top. \tag{4.276}$$

If we are spinning with the material ($\boldsymbol{\Omega} = \mathbf{W}$) this becomes:

$$\dot{\boldsymbol{\sigma}} = \mathring{\boldsymbol{\sigma}} + \mathbf{W}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}^\top, \tag{4.277}$$

where

$$\mathring{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} - \mathbf{W}\boldsymbol{\sigma} - \boldsymbol{\sigma}\mathbf{W}^\top \tag{4.278}$$

is a commonly used rate definition called the Jaumann rate.

4.13 Material Symmetry

Consider a case in which a body is exposed to a given deformation $\mathbf{F}$ resulting in a stress state $\boldsymbol{\sigma}$. Now, consider another body that is identical to the first except that it has been rotated 90° before the deformation was applied, as is shown in Figure 4.13. For some materials, the initial 90° prerotation (i.e., change of reference configuration) does not influence the final stress state $\boldsymbol{\sigma}$.

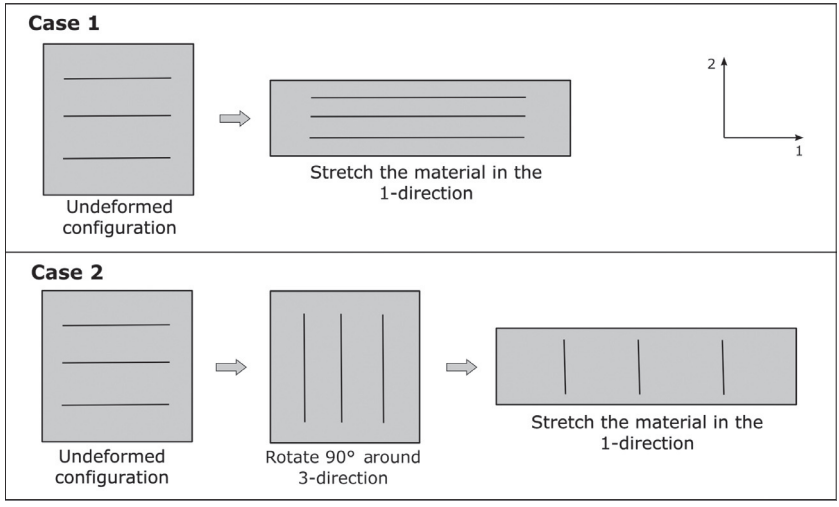


Figure 4.13 Example of material symmetry during deformation.

These materials are said to have material symmetry with respect to 90° rotation.

If the material response is invariant to any rotation then the material is said to be *isotropic*. A material that is not invariant to arbitrary rotations will have different properties in different directions and is called *anisotropic*.

In mathematical terms, if $\mathbf{P}$ is the mapping from the initial configuration to an alternative configuration, $\mathbf{F}$ is the deformation gradient, and the stress is independent of the initial mapping:

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F}) = \hat{\boldsymbol{\sigma}}(\mathbf{FP}), \tag{4.279}$$

then the mapping $\mathbf{P}$ is said to be a *symmetry group* of the material. The use of symmetry groups is discussed in more detail in Chapter 5.

4.14 List of Symbols

The following is a list of the variables that are used in this chapter and the rest of the book. The nomenclature is similar to various recent text books, particular [2]. Direct notation is used throughout, with the same conventions as in [1, 3, 7].

Symbol	Description	Definition
$\mathbf{b}_{\mathrm{f}}$	Body force per unit current volume	–
$\mathbf{B}_{\mathrm{f}}$	Body force per unit reference volume	–
$\mathbf{b}$	Left Cauchy-Green tensor (spatial configuration)	$\mathbf{b} = \mathbf{F}\mathbf{F}^{\top}$
$\mathbf{C}$	Right Cauchy-Green tensor (reference configuration)	$\mathbf{C} = \mathbf{F}^{\top}\mathbf{F}$
$\mathbf{d}$	Rate of deformation tensor (spatial configuration)	$\mathbf{l} = \mathbf{d} + \mathbf{w}$
$\mathbf{e}$	Strain tensor (spatial configuration)	$\mathbf{e} = \hat{\mathbf{e}}(\mathbf{v})$
e_0	Internal energy per unit reference volume	–
e_{c}	Internal energy per unit current volume	–
η_{c}	Entropy per unit current volume	–
η_0	Entropy per unit reference volume	–
$\mathbf{E}$	Strain tensor (reference configuration)	$\mathbf{E} = \hat{\mathbf{E}}(\mathbf{U})$
$\mathbf{f}$	Force vector (spatial configuration)	$\mathrm{d}\mathbf{f} = \mathbf{t}\mathrm{d}s$
$\mathbf{F}$	Force vector (reference configuration)	$\mathrm{d}\mathbf{F} = \mathbf{T}\,\mathrm{d}S$
$\mathbf{F}$	Deformation Gradient (two-point tensor)	$\frac{\partial \mathbf{x}}{\partial \mathbf{X}}$
J	Jacobian determinant	–
$\mathcal{K}$	Kinetic energy of the body	–
$\mathbf{l}$	Spatial velocity gradient (spatial configuration)	$\mathbf{l} = \operatorname{grad}\mathbf{v}$
$\mathbf{n}_i$	Eigenvectors of $\mathbf{v}$ (spatial configuration)	–
$\mathbf{N}_i$	Eigenvectors of $\mathbf{U}$ (reference configuration)	–
Ω_0	Volume of body in reference configuration	–

Ω_c	Volume of body in spatial configuration	–
$\partial\Omega_0$	Surface area of body in reference configuration	–
$\partial\Omega_c$	Surface area of body in the current configuration	–
$\mathbf{P}$	First Piola-Kirchhoff stress (two-point tensor)	$\mathbf{T} = \mathbf{PN}$
$\mathcal{P}_{ext}$	External work done on the body	–
$\mathcal{P}_{int}$	Internal work done on the body	–
Ψ	Helmholtz free energy per unit current volume	$\Psi = e_0 - \theta_0\eta_0$
ψ	Helmholtz free energy per unit reference volume	–
$\mathbf{q}$	Heat flux vector per unit current area	–
q_n	Heat flux per unit current surface area	–
$\mathbf{Q}$	Heat flux vector per unit reference area	–
Q_n	Heat flux per unit reference surface area	–
ρ_0	Mass density in reference configuration	–
ρ_c	Mass density in spatial configuration	–
r	Rate of heat supply per unit current volume	–
R	Rate of heat supply per unit reference volume	–
$\mathbf{R}$	Rotation tensor (two-point tensor)	$\mathbf{F} = \mathbf{RU} = \mathbf{vR}$
$\boldsymbol{\sigma}$	Cauchy stress in spatial configuration	–
s	Area element in spatial configuration	–
	Area element in reference configuration	–
$\mathbf{S}$	Second Piola-Kirchhoff stress (reference configuration)	$\mathbf{S} = F^{-1}\boldsymbol{\sigma}\mathbf{F}^{-\top}$
σ_i	Principal Cauchy stresses (spatial configuration)	–

σ_{M}	Mises stress	–
σ_{T}	Tresca stress	–
θ_0	Temperature (reference configuration)	–
θ_{c}	Temperature (spatial configuration)	–
$\mathbf{t}$	Cauchy surface traction (spatial configuration)	$\mathbf{t} = \boldsymbol{\sigma}\mathbf{n}$
$\mathbf{T}$	Nominal surface traction (reference configuration)	$\mathbf{T} = \mathbf{P}\mathbf{N}$
$\boldsymbol{\tau}$	Kirchhoff stress (spatial configuration)	$\boldsymbol{\tau} = J\boldsymbol{\sigma}$
$\mathbf{U}$	Right stretch tensor (reference configuration)	$\mathbf{F} = \mathbf{R}\mathbf{U}$
$\mathbf{v}$	Left stretch tensor (spatial configuration)	$\mathbf{F} = \mathbf{v}\mathbf{R}$
$\mathbf{v}$	Velocity of a material point in the current configuration	$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}$
$\mathbf{V}$	Velocity of a material point in the reference configuration)	$\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t}$
v	Volume element in spatial configuration	–
V	Volume element in reference configuration	–
$\mathbf{w}$	Spin tensor (spatial configuration)	$\mathbf{l} = \mathbf{d} + \mathbf{w}$
$\mathbf{x}$	Position vector in spatial configuration	–
$\mathbf{X}$	Position vector in reference configuration	–

4.15 Exercises

1. What is the difference between a Lagrangian and an Eulerian reference frame?
2. How many different stress and strain measures can be defined? Which stress and strain measure is your favorite?
3. Use an applied math software to calculate the singular value decomposition of the following matrix:

$$\mathbf{F} = \begin{bmatrix} 1.6 & 0.15 & 0 \\ 0.1 & 1.1 & 0.1 \\ 0.3 & 0.05 & 0.8 \end{bmatrix}.$$

4. Use the definition of a dyad (Equation (4.18)) to prove the following equations:

$$(\mathbf{a} \otimes \mathbf{b})(\mathbf{c} \otimes \mathbf{d}) = (\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \otimes \mathbf{d}), \qquad \text{(4.22-repeat)}$$
$$(\mathbf{a} \otimes \mathbf{b})\mathbf{A} = \mathbf{a} \otimes (\mathbf{A}^{\top}\mathbf{b}), \qquad \text{(4.23-repeat)}$$
$$\mathbf{A}(\mathbf{a} \otimes \mathbf{b}) = (\mathbf{A}\mathbf{a}) \otimes \mathbf{b}. \qquad \text{(4.24-repeat)}$$

5. Calculate the trace, determinant, invariants (I_1, I_2, I_3), deviatoric, volumetric, distortional, and dilatational parts of the following tensor:

$$\mathbf{F} = \begin{bmatrix} 1.3 & 0.25 & 0 \\ 0.2 & 1.1 & 0.1 \\ 0 & 0.05 & 1.1 \end{bmatrix}.$$

6. Typically a second-order tensor is said to have the invariants I_1, I_2, and I_3. Is it possible to define other invariants of a second-order tensor?
7. What deformation gradients have the same left and right Cauchy-Green tensors?
8. Calculate the natural logarithm of the following deformation gradient using Equation (4.45):

$$\mathbf{F} = \begin{bmatrix} 2.1 & 0.25 & 0 \\ 0.25 & 1.1 & 0.1 \\ 0 & 0.1 & 0.9 \end{bmatrix}.$$

9. A material point in a body is exposed to the following deformation gradient:

$$\mathbf{F} = \begin{bmatrix} 2.6 & 0.15 & 0 \\ 0.10 & 1.1 & 0.1 \\ 0 & 0.1 & 0.9 \end{bmatrix}.$$

   (a) Calculate the rotation tensor $\mathbf{R}$, the right stretch tensor $\mathbf{U}$, the left stretch tensor $\mathbf{v}$, the right

Cauchy-green tensor **C**, the left Cauchy-Green tensor **b**, and the spectral representation of **F**.

(b) Calculate the following Lagrangian strain: the Green strain, the Hencky strain, the Biot strain, and the Almansi strain.

(c) Calculate the following Eulerian strains: the Euler-Almansi strain and the Hencky strain.

10. Consider two coordinate systems defined by:

$$\begin{cases} \hat{\mathbf{e}}_1 &= \frac{1}{\sqrt{2}}\left[1.0\hat{\mathbf{e}}_x + 1.0\hat{\mathbf{e}}_y\right] \\ \hat{\mathbf{e}}_2 &= \frac{1}{\sqrt{2}}\left[1.0\hat{\mathbf{e}}_y + 1.0\hat{\mathbf{e}}_z\right] \\ \hat{\mathbf{e}}_3 &= \frac{1}{\sqrt{3}}\left[1.0\hat{\mathbf{e}}_x - 1.0\hat{\mathbf{e}}_y + 1.0\hat{\mathbf{e}}_z\right] \end{cases}$$

and

$$\begin{cases} \hat{\mathbf{e}}'_1 &= \frac{1}{\sqrt{2}}\left[2.0\hat{\mathbf{e}}_x - 1.0\hat{\mathbf{e}}_y\right] \\ \hat{\mathbf{e}}'_2 &= \frac{1}{\sqrt{2}}\left[-1.0\hat{\mathbf{e}}_y + 1.0\hat{\mathbf{e}}_z\right] \\ \hat{\mathbf{e}}'_3 &= \frac{1}{3}\left[-1.0\hat{\mathbf{e}}_x - 2.0\hat{\mathbf{e}}_y - 2.0\hat{\mathbf{e}}_z\right] \end{cases}.$$

Calculate the rotation tensor **Q** defined in Equation (4.55).

11. A polymer melt is exposed to the following deformation history for times $t \in [0, 1]$:

$$\begin{cases} x_1 = X_1 \mathrm{e}^t, \\ x_2 = X_2 t, \\ x_3 = X_3. \end{cases}$$

Determine:

(a) the deformation gradient **F**,

(b) the velocity gradient **l**,

(c) the components of the velocity of a material point at time t,

(d) Grad **v** and grad **v**, and

(e) Div **v** and div **v**.

12. A test sample is deformed in simple shear:

$$\begin{cases} x_1 = X_1 + ktX_2 \\ x_2 = X_2 \\ x_3 = X_3 \end{cases}.$$

Calculate:
(a) the strain tensor $\mathbf{E} = \ln \mathbf{U}$,
(b) the strain-rate tensor $\dot{\mathbf{E}}$, and
(c) the co-rotational strain-rate tensor $\mathring{\mathbf{E}}$:

$$\mathring{\mathbf{E}} = \dot{\mathbf{E}} - \mathbf{W}\mathbf{E} - \mathbf{E}\mathbf{W}^{\top}.$$

13. In simple shear defined by

$$\mathbf{F} = \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

show that $\mathbf{U}$ is given by:

$$\mathbf{U} = \frac{1}{\sqrt{4+\gamma^2}} \begin{bmatrix} 2 & \gamma & 0 \\ \gamma & 2+\gamma^2 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

show that $\mathbf{v}$ is given by:

$$\mathbf{v} = \frac{1}{\sqrt{4+\gamma^2}} \begin{bmatrix} 2+\gamma^2 & \gamma & 0 \\ \gamma & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

show that $\mathbf{R}$ is given by:

$$\mathbf{R} = \frac{1}{\sqrt{4+\gamma^2}} \begin{bmatrix} 2 & \gamma & 0 \\ -\gamma & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

and finally show that the engineering shear strain ε_{12} (that is used by most FE software) is given by

$$\varepsilon_{12} = \frac{\gamma}{\sqrt{1+\gamma^2/4}}.$$

14. Show that the largest engineering shear strain `NE12` that Abaqus will predict for simple shear is 2.0.

15. Two symmetric tensors are *coaxial* if they have the same principal axes. Prove that Cauchy stress tensor $\boldsymbol{\sigma}$ and the left Cauchy-Green tensor $\mathbf{b} = \mathbf{F}\mathbf{F}^{\top}$ are coaxial.
16. How can you check if the first law of thermodynamic is satisfied in an FE simulation?
17. What deformation rate measure is work conjugate to the Kirchhoff stress?
18. What deformation rate measure is work conjugate to the Cauchy stress?
19. How many governing field equations can be formulated from the conservation laws? How many unknown field variables are there? and What are the missing equations?

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