

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

For a solid under finite strain conditions, Hooke's law, valid for infinitesimal deformations, does not hold, and the fundamental definitions for stress and strain must be revisited.

1.3.6.2. Lagrangian and Eulerian description

Finite elastic strains may be treated from two different viewpoints using either the *Lagrangian (material)* or the *Eulerian (spatial)* descriptions.

Let us consider a fixed rectangular Cartesian coordinate system with axes x_i ($i = 1, 2, 3$). Any particular position vector \mathbf{r} of components (x_1, x_2, x_3) denotes a point in space. A point that always moves with the material is called a particle or *material point*. Let every particle be identified by its coordinates at some reference time t_0 . These reference coordinates, referred to the same Cartesian system, will be denoted by (a_1, a_2, a_3) and the corresponding position vector \mathbf{a} . A particular vector \mathbf{a} can serve as a name for the particle located at that position at the reference time t_0 .

The vectors \mathbf{r} and \mathbf{a} both specify a position in a fixed Cartesian frame of reference. At any time, we associate each \mathbf{r} with an \mathbf{a} by the rule that \mathbf{r} is the present position vector of the particle initially at \mathbf{a} . This connection between \mathbf{r} and \mathbf{a} is written symbolically as

$$\mathbf{r} = \mathbf{r}(t, \mathbf{a}) \quad \text{or} \quad x_i = x_i(t, a_1, a_2, a_3), \quad (1.3.6.1)$$

where

$$\mathbf{a} = \mathbf{r}(t_0, \mathbf{a}) \quad \text{or} \quad a_i = x_i(t_0, a_1, a_2, a_3). \quad (1.3.6.2)$$

The coordinates a_i that identify the particles are called *material coordinates*. A description that, like (1.3.6.1), uses (t, a_1, a_2, a_3) as independent variables is called a *material* or *Lagrangian* description.

The converse of (1.3.6.1) and (1.3.6.2) may be written

$$\mathbf{a} = \mathbf{a}(t, \mathbf{r}) \quad \text{or} \quad a_i = a_i(t, x_1, x_2, x_3), \quad (1.3.6.3)$$

where

$$\mathbf{r} = \mathbf{a}(t_0, \mathbf{r}) \quad \text{or} \quad x_i = a_i(t_0, x_1, x_2, x_3). \quad (1.3.6.4)$$

A spatial description or *Eulerian* description uses the independent variables (t, x_1, x_2, x_3) , the x_i being called *spatial coordinates*.

Now, for the sake of simplicity, we shall work with the Lagrangian formulation exclusively. For more details see, for instance, Thurston (1964) and Wallace (1970, 1972).

1.3.6.3. Strain and stress tensors

The displacement vector from the reference position of a particle to its new position has as components

$$u_i = x_i - a_i. \quad (1.3.6.5)$$

The term strain refers to a change in the relative positions of the material points in a body. Let a final configuration be described in terms of the reference configuration by setting t equal to a constant in (1.3.6.1). Then t no longer appears as a variable and (1.3.6.1) can be written

$$x_i = x_i(a_1, a_2, a_3),$$

where the a_i are the independent variables. It follows that

$$dx_j = \frac{\partial x_j}{\partial a_i} da_i = \left(\frac{\partial u_j}{\partial a_i} + \delta_{ij} \right) da_i. \quad (1.3.6.6)$$

Let now the particle initially at (a_1, a_2, a_3) move to (x_1, x_2, x_3) . The square of the initial distance to a neighbouring particle whose initial coordinates were $a_j + da_j$ is

$$ds^2 = da_j da_j.$$

The square of the final distance to the same neighbouring particle is

$$ds^2 = dx_j dx_j.$$

In a material description, the strain components S_{ik} are defined by the following equations:

$$dx_j dx_j - da_j da_j = 2S_{ik} da_i da_k. \quad (1.3.6.7)$$

Substituting (1.3.6.6) into (1.3.6.7), it follows that

$$\left(\frac{\partial u_j}{\partial a_i} + \delta_{ji} \right) \left(\frac{\partial u_j}{\partial a_k} + \delta_{jk} \right) da_i da_k - da_j da_j = 2S_{ik} da_i da_k.$$

Hence

$$S_{ik} = \frac{1}{2} \left(\frac{\partial u_k}{\partial a_i} + \frac{\partial u_i}{\partial a_k} + \frac{\partial u_j}{\partial a_i} \frac{\partial u_j}{\partial a_k} \right).$$

If the products and squares of the displacement derivatives are neglected, the strain components reduce to the usual form of 'infinitesimal elasticity' [see equation (1.3.1.8)]:

$$S_{ik} = \frac{1}{2} \left(\frac{\partial u_i}{\partial a_k} + \frac{\partial u_k}{\partial a_i} \right).$$

It is often useful to introduce the Jacobian matrix associated with the transformation (\mathbf{a}, \mathbf{x}) . The components of this matrix are

$$J = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix},$$

where

$$\alpha_{ik} = \frac{\partial x_i}{\partial a_k} = \frac{\partial u_j}{\partial a_k} + \delta_{jk}.$$

From the definition of matrix J , one has

$$d\mathbf{x} = J d\mathbf{a}$$

and

$$dx^2 - da^2 = (d\mathbf{x})^T d\mathbf{x} - (d\mathbf{a})^T d\mathbf{a} = (d\mathbf{a})^T (J^T J - \delta) d\mathbf{a},$$

where $(d\mathbf{a})^T$, $(d\mathbf{x})^T$ and J^T are the transpose matrices of $d\mathbf{a}$, $d\mathbf{x}$ and J , respectively, and δ is the Kronecker matrix.

The Lagrangian strain matrix S may then be written symbolically:

$$S = \frac{1}{2} (J^T J - \delta). \quad (1.3.6.8)$$

When finite strains are concerned, we have to distinguish three states of the medium: the natural state, the initial state and the final or present state: The *natural* state is a state free of stress. The *initial* state is deduced from the natural state by a homogeneous strain. The *final* state is deduced from the initial state by an arbitrary strain.

Concerning the stress tensor, as pointed out by Thurston (1964), the stress-deformation relation is complicated in nonlinear elasticity because 'the strain is often referred to a natural unstressed state, whereas the stress T_{ij} is defined per unit area of the deformed body'. For this reason, the differential of work done by the stress is not equal to the stress components times the differentials of the corresponding strain components. So, following Truesdell & Toupin (1960), we shall introduce a *thermodynamic tension tensor* t_{ij} defined as the first derivative of the energy with respect to strain. If the internal energy U per unit

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mass is considered, the *thermodynamic tension* refers to an isentropic process. Then

$$t_{ij}^{\sigma} = \rho_0 \left(\frac{\partial U}{\partial S_{ij}} \right)_{\sigma},$$

where σ is the entropy and ρ_0 the volumic mass in the initial state.

If the Helmholtz free energy F is considered, the thermodynamic tension refers to an isothermal process. Then

$$t_{ij}^{\Theta} = \rho_0 \left(\frac{\partial U}{\partial S_{ij}} \right)_{\Theta},$$

where Θ is the temperature. It will be shown in Section 1.3.7.2 that

$$T_{ij} = (1/J) \alpha_{ik} \alpha_{jl} t_{kl}.$$

1.3.6.4. Second-order and higher-order elastic stiffnesses

Following Brugger (1964), the strain-energy density, or strain energy per unit volume Φ , is assumed to be a polynomial in the strain:

$$\Phi = \Phi_0 + c_{ij} S_{ij} + \frac{1}{2!} c_{ijkl} S_{ij} S_{kl} + \frac{1}{3!} c_{ijklmn} S_{ij} S_{kl} S_{mn}, \quad (1.3.6.9)$$

where $\Phi = \rho_0 U(X, S_{ij})$, $\Phi_0 = \rho_0 U(X, 0)$, X denotes the configuration of the initial state and the S_{ij} 's are the Lagrangian finite strain-tensor components.

If the initial energy and the deformation of the body are both zero, the first two terms in (1.3.6.9) are zero. Note that c_{ij} is a stress and not an intrinsic characteristic of the material. In this expression, the elastic stiffnesses c_{ijkl} and c_{ijklmn} are the second- and third-order stiffnesses, respectively. Since the strain tensor is symmetric, pairs of subscripts can be interchanged [see equation (1.3.3.4)]:

$$\begin{aligned} c_{ijkl} &= c_{jikl} = c_{ijlk} = c_{jilk}, \\ c_{ijklmn} &= c_{jiklmn} = c_{ijlkmn} = c_{jilkmn} = c_{ijklnm} \\ &= c_{jiklnm} = c_{ijlknm} = c_{jilknm}. \end{aligned}$$

More accurately, the isentropic and the isothermal elastic stiffnesses are defined as the n th partial derivatives of the internal energy and the Helmholtz free energy, respectively. For example, the third-order isentropic and isothermal stiffnesses are, respectively,

$$\begin{aligned} c_{ijklmn}^{\sigma} &= \rho_0 \frac{\partial^3 U}{\partial S_{ij} \partial S_{kl} \partial S_{mn}}, \\ c_{ijklmn}^{\Theta} &= \rho_0 \frac{\partial^3 F}{\partial S_{ij} \partial S_{kl} \partial S_{mn}}, \end{aligned}$$

where the internal energy, U , is a function of X , S_{ij} and σ , and the Helmholtz free energy, F , is a function of X , S_{ij} and Θ .

From these definitions, it follows that the Brugger stiffness coefficients depend on the initial state. *When no additional information is given, the initial state is the natural state.*

The third-order stiffnesses form a sixth-rank tensor containing $3^6 = 729$ components, of which 56 are independent for a triclinic crystal and 3 for isotropic materials (the independent components of a sixth-rank tensor can be obtained for any point group using the accompanying software to this volume). The three independent constants for isotropic materials are often taken as c_{123} , c_{144} and c_{456} and denoted respectively by ν_1 , ν_2 , ν_3 , the 'third-order Lamé constants'.

The 'third-order Murnaghan constants' (Murnaghan, 1951), denoted by l , m , n , are given in terms of the Brugger constants by the relations

$$l = \frac{1}{2} c_{112}; \quad m = c_{155}; \quad n = 4c_{456}.$$

Similarly, the fourth-order stiffnesses form an eighth-rank tensor containing $3^8 = 6561$ components, 126 of which are independent for a triclinic crystal and 11 for isotropic materials (the independent components of a sixth-rank tensor can be obtained for any point group using the accompanying software to this volume).

For a solid under finite strain conditions, the definition of the elastic compliance tensor has to be reconsidered. In linear elasticity, the second-order elastic compliances s_{ijkl} were defined through the relations (1.3.3.2):

$$S_{ij} = s_{ijkl} T_{kl} \quad \text{or} \quad s_{ijkl} = \frac{\partial S_{ij}}{\partial T_{kl}},$$

while, in nonlinear elasticity, one has

$$s_{ijkl} = \frac{\partial S_{ij}}{\partial t_{kl}},$$

where

$$t_{kl} = \rho_0 \frac{\partial U}{\partial S_{kl}}.$$

1.3.6.5. Expansion of elastic constants for small initial stress

In most experiments, the initial stress is small compared with the second-order elastic constants (for example, 1 GPa hydrostatic pressure compared with the usual value $c_{ijkl} = 100$ GPa). Consequently, the deformation between the initial (stressed) state and the natural (unstressed) state is small compared with 1. For this reason, it is convenient to expand the elastic constants in the initial state as a power series in the strain about the natural state. *To avoid confusion, we introduce new notations:* \bar{X} now represents the coordinates in the *natural* or unstressed state; X represents the coordinates in the *initial* or homogeneously strained state; $u_i = x_i - X_i$ are the components of displacement. All letters with superscript bar refer to the natural state; for example, \bar{S}_{ij} denotes the Lagrangian strain in the natural state; $\bar{U} = U(\bar{X}, \bar{S}_{ij})$.

Now, in order to relate the properties at X to those at \bar{X} , we need to specify the strain from \bar{X} to X . Let

$$a_{ij} = \frac{\partial X_i}{\partial \bar{X}_j} = \bar{\alpha}_{ij}.$$

Consequently,

$$\frac{\partial \bar{S}_{ij}}{\partial S_{mn}} = a_{mi} a_{nj}.$$

The second-order elastic constants at X can be expressed in terms of the second- and third-order elastic constants at \bar{X} :

$$c_{ijkl} = \rho_0 \frac{\partial^2 U}{\partial S_{ij} \partial S_{kl}} = \rho_0 \frac{\partial^2 \bar{U}}{\partial \bar{S}_{mn} \partial \bar{S}_{pq}} a_{im} a_{jn} a_{kp} a_{lq}$$

or

$$c_{ijkl} = \frac{\rho_0}{\rho_0} \left(\bar{c}_{mnpq} + \bar{c}_{mnpqrs} S_{rs} + \frac{1}{2!} \bar{c}_{mnpqrst} S_{rs} S_{tu} + \dots \right) a_{im} a_{jn} a_{kp} a_{lq}.$$

This expression holds for both isentropic and isothermal elastic constants.