

A Diverse Collection of
**FORMULAS,
DEFINITIONS AND
DERIVATIONS**

in the Realm of Mechanical Engineering

©Jörgen S. Bergström

A DIVERSE COLLECTION OF FORMULAS, DEFINITIONS,
AND DERIVATIONS IN THE REALM OF MECHANICAL ENGINEERING.

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1	Mathematical Foundation	1
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1.1 Gradient, divergence and curl in subscript notation

gradient	$\nabla\phi = \phi_{,i}$
divergence	$\nabla \cdot \mathbf{A} = A_{i,i}$
curl	$\nabla \times \mathbf{A} = e_{ijk}A_{k,j}$

Note, $\mathbf{C} = \mathbf{A} \times \mathbf{B}$ can be written as $C_i = e_{ijk}A_jB_k$.

1.2 The divergence theorem (Gauss's theorem)

$$\int_V B_{i,i}dV = \oint_S B_in_idS,$$

where B_i is a vector field, note $B_{i,i}$ corresponds physically to source strength per unit volume and B_in_i is the flux. In vector notation we get

$$\int_V \nabla \cdot \mathbf{B} dV = \oint_S \mathbf{B} \cdot d\mathbf{S}$$

$$\int_V \nabla \mathbf{B} dV = \oint_S \mathbf{B} \otimes d\mathbf{S}$$

1.3 Stoke's Theorem

$$\int_S e_{ijk}B_{k,j}n_idS = \oint_C B_idx_i,$$

where dx_i is the elemental vector of the contour C . In vector notation the equation can be written

$$\int_S (\nabla \times \mathbf{B}) \cdot d\mathbf{S} = \oint_C \mathbf{B} \cdot d\mathbf{r}.$$

1.4 The correlation between e_{ijk} and δ_{ij}

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

According to Pearson: 'The only formula in vector algebra which needs memorization.'

2.1 Definition of rectilinear base vectors

Three linearly independent vectors whose directions are fixed in space when used to represent any arbitrary vector, are called *rectilinear base vectors*. If they have unit magnitudes, they are named *rectilinear unit base vectors*.

2.2 Definition of orthogonal base vectors

When the base vectors are mutually orthogonal they are called *orthogonal base vectors*.

2.3 Physical meaning of the vector triple product

The product $\mathbf{a} \times \mathbf{b} \cdot \mathbf{c}$ is numerically equal to the volume of a parallelepiped having \mathbf{a} , \mathbf{b} , \mathbf{c} , as concurrent edges.

2.4 Definition of reciprocal base vectors

Two sets of base vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ and $\mathbf{e}^1, \mathbf{e}^2, \mathbf{e}^3$ are called *reciprocal* if

$$\mathbf{e}_i \cdot \mathbf{e}^j = \delta_{.i}^j$$

2.5 Definition of self-reciprocal bases

When a set of base vectors and their reciprocals are identical, we say that the bases are *self-reciprocal*. A set of base vectors are self-reciprocal if and only if they are mutually orthogonal unit vectors.

2.6 Definition of contravariant and covariant vectors

Components of a vector with respect to base vectors \mathbf{e}_i are called *contravariant*, and with respect to reciprocal basis \mathbf{e}^i are called *covariant*. We write

$$\mathbf{a} = a^i \mathbf{e}_i \text{ and } \mathbf{a} = a_i \mathbf{e}^i.$$

Note that this leads to

$$a^i = \mathbf{a} \cdot \mathbf{e}^i \text{ and } a_i = \mathbf{a} \cdot \mathbf{e}_i.$$

2.7 Definition of covariant and contravariant tensors

Covariant g_{ij} , contravariant g^{ij} and mixed g_i^j components of the Euclidean metric tensor are defined by

$$\begin{aligned} g_{ij} &= \mathbf{e}_i \cdot \mathbf{e}_j \\ g^{ij} &= \mathbf{e}^i \cdot \mathbf{e}^j \\ g_i^j &= \delta_i^j = \mathbf{e}_i \cdot \mathbf{e}^j \end{aligned}$$

Note, components of the Euclidean metric tensor are symmetric.

2.8 Ways to calculate the scalar product of \mathbf{a} and \mathbf{b}

The scalar product of \mathbf{a} and \mathbf{b} in rectilinear coordinates may be calculated by any one of the following formulas

$$\mathbf{a} \cdot \mathbf{b} = a^i b_i = a_i b^i = g_{ij} a^i b^j = g^{ij} a_i b_j$$

2.9 Relation between the covariant and contravariant components of \mathbf{a}

\mathbf{a} are related to each other by

$$a_i = g_{ij}a^j \quad a^i = g^{ij}a_j$$

2.10 Curvilinear coordinates

Let z^k ($k = 1, 2, 3$) be rectangular coordinates of a geometrical point, and x^i ($i = 1, 2, 3$) be three variables. If between z^k and x^i we can establish a correspondence, then we say that there exists a coordinate transformation between z^k and x^i . It can be shown that a unique inverse to this transformation exists in some neighborhood of z^k if the Jacobian

$$J = \det \left(\frac{\partial z^k}{\partial x^l} \right) \neq 0.$$

Base vectors $\bar{g}_k(x^i)$ are defined by

$$\bar{g}_k = \frac{\partial \bar{p}}{\partial x^k} = \frac{\partial z^m}{\partial x^k} \bar{i}_m.$$

The metric tensor is defined by

$$g_{kl} \equiv \bar{g}_k \cdot \bar{g}_l = \frac{\partial z^m}{\partial x^k} \frac{\partial z^n}{\partial x^l} \delta_{mn}.$$

This name is justified through the fact that when g_{kl} is known we can calculate the length of any vector and the angle between two vectors. Note that vanishing g_{kl} ($k \neq l$) is necessary and sufficient for orthogonality of the curvilinear coordinates.

2.11 Contravariant and covariant components of a vector

The quantities $A^k(\bar{x})$ and $A_k(\bar{x})$ are called, respectively contravariant and covariant components of a vector if, upon a transformation of coordinates, they transform respectively according to the rules

$$A'^k(\bar{x}') = A^m(\bar{x}) \frac{\partial x'^k}{\partial x^m} \quad \text{contravariant}$$

$$A'_k(\bar{x}') = A^m(\bar{x}) \frac{\partial x^m}{\partial x'^k} \quad \text{covariant}$$

Higher order tensors are similarly defined.

2.12 Partial derivatives of a vector in curvilinear coordinates

The partial derivatives of a vector in curvilinear coordinates becomes

$$\frac{\partial \bar{u}}{\partial x^l} = \frac{\partial (u^k \bar{g}_k)}{\partial x^l} = \frac{\partial u^k}{\partial x^l} \bar{g}_k + u^k \frac{\partial \bar{g}_k}{\partial x^l}$$

But

$$\frac{\partial \bar{g}_k}{\partial x^l} = \frac{\partial}{\partial x^l} \left(\frac{\partial z^n}{\partial x^k} \bar{i}_n \right) = \frac{\partial^2 z^n}{\partial x^k \partial x^l} \bar{i}_n$$

which becomes

$$\frac{\partial \bar{g}_k}{\partial x^l} = \left\{ \begin{matrix} m \\ kl \end{matrix} \right\} \bar{g}_m$$

where

$$\left\{ \begin{matrix} m \\ kl \end{matrix} \right\} \equiv \frac{\partial^2 z^n}{\partial x^k \partial x^l} \frac{\partial x^m}{\partial z^n}$$

are known as the Christoffel symbols of the second kind. The Christoffel symbols of the first kind are also of frequent occurrence; they are defined by

$$[kl, m] \equiv g_{mn} \left\{ \begin{matrix} n \\ kl \end{matrix} \right\}$$

2.13 Definition of a dyad

The tensor $\mathbf{a} \otimes \mathbf{b}$ is called a dyad and is defined by

$$(\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{c} = \mathbf{a}(\mathbf{b} \cdot \mathbf{c}).$$

The components of the dyad are given by

$$(\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j.$$

2.14 Pre- and post-multiplication of a tensor and a vector

The components of the dot product of a tensor and a vector are given by

$$(\mathbf{T} \cdot \mathbf{v})_k = T_{ki} v_i.$$

The pre-multiplication is defined by

$$(\mathbf{a} \cdot \mathbf{T}) \cdot \mathbf{c} = \mathbf{a} \cdot (\mathbf{T} \cdot \mathbf{c}), \quad \forall \mathbf{c}.$$

Furthermore, the component $(\mathbf{a} \cdot \mathbf{T})_i$ is given by $a_k T_{ki}$.

2.15 The inner product of two tensors – contraction

The inner product of two tensors is defined by

$$(\mathbf{S} \cdot \mathbf{T}) \cdot \mathbf{v} = \mathbf{S} \cdot (\mathbf{T} \cdot \mathbf{v}) \quad \forall \mathbf{v}.$$

Which in results in the following expression for the components

$$(\mathbf{S} \cdot \mathbf{T})_{ik} = S_{im} T_{mk}.$$

The double inner product of two tensors is defined by

$$\mathbf{S} : \mathbf{T} = \text{Tr}(\mathbf{S} \cdot \mathbf{T}) = S_{im} T_{mi}.$$

3	Energy Principles	3
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3.1 *Different types of work and energy quantities used in solid mechanics*

- W_i total internal work
- W_e total external work
- U_i total potential energy (strain energy) of the internal forces
- U_e potential energy of the external forces
- U_0 strain energy density
- U_0^* complementary strain energy
- W_e^* total complementary external work
- Π total potential energy
- Π^* total complementary potential energy

3.2 *Fundamental definitions of work and energy*

- Energy is defined as a quantity representing the ability to perform work. We say a structural system *possesses* energy, whereas the forces in the system may *perform* work.
- The amount of work performed is proportional to the change in energy of the structural system.
- The potential energy is the capacity of a conservative force system to perform work by virtue of its position with respect to a reference level.
- Work is defined as the product of a force and the displacement of its point of application in the direction of the force.
- For a conservative system: work done by the applied forces is equal to the strain energy stored in the solid.

3.3 *Work and potential energy of internal forces*

Consider a one-dimensional bar of length L and cross-sectional area A . Suppose that the left-hand side end of the bar is fully built in and that the right-hand side end of the bar is subjected to an axial tensile force N . Now, consider an infinitesimal volume element ($dx A$) located at position x . Assume no body forces. Find the net work done by the forces acting on the element when the applied load undergoes an infinitesimal change to $(N + dN)$. (Or equivalently, find the net work when the applied strain undergoes a small change.) The change in the loading conditions result in a change in the internal stress $\sigma(x)$ and the displacement $u(x)$, furthermore, let $\Delta u(x) \equiv u(x, N + dN) - u(x, N)$.

The work done by the forces on the volume element during the change in state is given by

$$d(\text{work}) \cdot A dx = \sigma(x + dx) A \Delta u(x + dx) - \sigma(x) A \Delta u(x).$$

Taylor expanding the first term on the right hand side and keeping only the linear terms yields

$$d(\text{work}) \cdot dx = \frac{d}{dx}(\sigma \Delta u) dx$$

which can be written as

$$d(\text{work}) = \sigma \Delta \epsilon.$$

Now notice that during this strain increment, *the work done by the internal forces in this differential element will be the negative of that performed by the stresses acting upon it.* (The acting stresses

tries to elongate the bar, whereas the internal forces tries to prevent this elongation.) Thus the total internal work of the bar as the strains increase from zero to their final value is

$$W_i = - \int_0^L \int_0^{\varepsilon_f} \sigma(\varepsilon) d\varepsilon Adx.$$

For a general three-dimensional case, the total internal work can in a similar fashion be shown to be given by

$$W_i = - \int_V \int_0^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij} dV. \quad (1)$$

If the strained solid were permitted to return slowly to its unstrained state, the solid would be capable of returning the work performed by the external forces. This capacity of the internal forces to do work in a strained solid is due to the *strain energy* or the internal energy stored in the body. If the work performed is independent of path, a potential function may be associated with the work. To find the potential energy of the internal forces consider the expression for the specific internal work

$$dW_i = - \int_0^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij}. \quad (2)$$

If the internal forces are conservative, then $\sigma_{ij} d\varepsilon_{ij}$ must be a perfect differential $d(dW_i)$. Furthermore, let this be the differential of some functional dU_i . Equation (2) can now be written

$$dW_i(\varepsilon_{ij}) = - \int_0^{\varepsilon_{ij}} d(dU_i) = -dU_i(\varepsilon_{ij}),$$

assuming the potential energy to be zero at the lower limit. The total potential energy therefore becomes

$$U_i = -W_i = \int_V \int_0^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij} dV. \quad (3)$$

We also note from (3) that the total strain energy is always positive. The identity $W_i = -U_i$ states that the decrease in the potential energy U_i in moving from the final state to the reference level is equal to the work done by the internal forces. Conversely, the increase in potential energy in moving from the reference level to the final state is equal to the work done against the conservative force field.

The strain energy density can be defined by

$$U_0 = \int_0^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij}.$$

By integrating this equation by parts, we can get a quantity called the complimentary strain energy density

$$U_0^* = \int_0^{\sigma_{ij}} \varepsilon_{ij} d\sigma_{ij} = \sigma_{ij} \varepsilon_{ij} - \int_0^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij}.$$

If during loading and unloading U_0 and U_0^* are independent of the path of deformation, the differentials dU_0 and dU_0^* will be exact differentials, and U_0 and U_0^* are then potential functions. From the definition of a differential and the expression for dU_0 and dU_0^* we see that

$$\sigma_{ij} = \frac{\partial U_0}{\partial \varepsilon_{ij}},$$

$$\varepsilon_{ij} = \frac{\partial U_0^*}{\partial \varepsilon_{ij}}.$$

3.4 Work and potential energy of the external forces applied on a solid

The external work done by prescribed external forces can be expressed as

$$W_e = \int_{S_T} \int_0^{u_i} T_i du_i dS + \int_V \int_0^{u_i} F_i du_i dV.$$

If the solid is linear in its response, then

$$W_e = \frac{1}{2} \int_{S_T} T_i u_i dS + \frac{1}{2} \int_V F_i u_i dV$$

where T_i and F_i are the final values. If the work performed by the applied loads is independent of path, then dW_e is an exact differential of the potential function U_e . By the same argument as for the internal work, we conclude that

$$W_e = -U_e.$$

Furthermore, the quantity *complementary external work* can be established in a similar fashion.

$$W_e^* = \int_{S_T} \int_0^{T_i} u_i dT_i dS$$

3.5 Principle of virtual work

The principle of virtual work for a solid can be derived from the equations of equilibrium and vice versa. They are, in a sense, equivalent because the principle of virtual work is a global (integral) form of the conditions of equilibrium and static boundary conditions. If the local equilibrium equations are integrated the following form can be obtained:

$$- \int_V (\sigma_{ji,j} + \bar{F}_i) \delta u_i dV + \int_{S_T} (T_i - \bar{T}_i) \delta u_i dS = 0 \quad (1)$$

where both integrals are zero, the signs have been chosen for later convenience and where a bar denotes a prescribed value. Now consider the following integral in more detail

$$\begin{aligned} \int_{S_T} T_i \delta u_i dS &= \int_S T_i \delta u_i dS - \int_{S_u} T_i \delta u_i dS \\ &= \int_V (\sigma_{ji} \delta u_i)_{,j} dV - \int_{S_u} T_i \delta u_i dS \\ &= \int_V \sigma_{ji,j} \delta u_i dV + \int_V \sigma_{ji} \delta u_{i,j} dV - \int_{S_u} T_i \delta u_i dS. \end{aligned} \quad (2)$$

Inserting (2) into (1) yields

$$\int_V \sigma_{ji} \delta u_{i,j} dV - \int_V \bar{F}_i \delta u_i dV - \int_{S_T} \bar{T}_i \delta u_i dS - \int_{S_u} T_i \delta u_i dS = 0.$$

But $\delta u_i = 0$ on S_u and $\sigma_{ij} \delta u_{i,j} = \sigma_{ij} \delta \varepsilon_{ij}$ giving

$$\int_V \sigma_{ij} \delta \varepsilon_{ij} dV - \int_V \bar{F}_i \delta u_i dV - \int_{S_T} \bar{T}_i \delta u_i dS = 0$$

which can be written

$$\delta W = \delta(W_i + W_e) = 0$$

where $\delta W_i = -\int_V \sigma_{ij} \delta \varepsilon_{ij} dV$ is the internal virtual work and $\delta W_e = \int_{S_T} \bar{T}_i \delta u_i dS + \int_V \bar{F}_i \delta u_i dV$ is the external virtual work. The principle of virtual work can be stated as follows:

A deformable system is in equilibrium if the sum of the external virtual work and the internal virtual work is zero for virtual displacements that are kinematically admissible. (The fundamental unknowns are the displacements.)

3.6 Principle of stationary potential energy

The principle of virtual work can be written

$$\delta W_i + \delta W_e = 0.$$

But for systems for which a potential exist for both the internal and external forces, this equation can be written as

$$\delta U_i + \delta U_e = 0$$

or $\delta \Pi = 0$ where $\Pi = U_i + U_e$. Or in other words:

Of all kinematically admissible deformations, the actual deformations are the ones for which the total energy assumes a stationary value.

3.7 Principle of complementary virtual work

The first kinematic condition can be stated in the following form

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \text{ in } V$$

and the second kinematic condition is as follows

$$u_i = \bar{u}_i, \text{ on } S_u$$

Can now form the following equation

$$\int_V \left[\varepsilon_{ij} - \frac{1}{2}(u_{i,j} + u_{j,i}) \right] \delta \sigma_{ij} dV - \int_{S_u} (\bar{u}_i - u_i) \delta T_i dS = 0. \quad (1)$$

Now consider the second integral

$$\begin{aligned} \int_V u_{i,j} \delta \sigma_{ij} dV &= \int_V (u_i \delta \sigma_{ij})_{,j} dV - \int_V u_i \delta \sigma_{i,j} dV \\ &= \int_S u_i \delta \sigma_{ij} n_j dS, \end{aligned}$$

we see that the second and the fourth integrals cancel out. Equation (1) can therefore be written as $\delta(W_i^* + W_e^*) = 0$ where $\delta W_i^* = -\int_V \varepsilon_{ij} \delta \sigma_{ij} dV$ and $\delta W_e^* = \int_{S_u} \bar{u}_i \delta T_i dS$. This principle can accordingly be stated as follows:

A deformable system satisfies all kinematic requirements if the sum of the external complementary virtual work and the internal complementary virtual work is zero for all statically admissible virtual stresses $\delta \sigma_{ij}$. (The fundamental unknowns are the stresses.)

3.8 Principle of stationary complementary energy

The principle of complementary virtual work gives

$$\delta W^* = \delta(W_i^* + W_e^*) = \delta(-U_i^* - U_e^*) = -\delta\Pi^* = 0$$

3.9 Generalized variational principles

The classical variational principles can be considered as single field principles involving either displacements or forces as unknowns, the generalized principles may involve both these fields simultaneously. To derive a generalized variational principle we will use the following relations:

$$\begin{aligned} \sigma_{ji,j} + F_i &= 0 && \text{in } V \\ T_i &= \bar{T}_i && \text{on } S_T \\ \varepsilon_{ij} &= \frac{1}{2} [u_{i,j} + u_{j,i}] && \text{in } V \\ u_i &= \bar{u}_i && \text{on } S_u \end{aligned}$$

By multiplying by virtual stresses or displacements and integrating the following fundamental equation can readily be obtained

$$\begin{aligned} - \int_V (\sigma_{ji,j} + F_i) \delta u_i dV + \int_V (u_{i,j} - \varepsilon_{ij}) \delta \sigma_{ij} dV \\ + \int_{S_T} (T_i - \bar{T}_i) \delta u_i dS - \int_{S_u} (u_i - \bar{u}_i) \delta T_i dS = 0. \end{aligned}$$

3.10 Castigliano's first theorem

Consider a general three-dimensional solid subjected to a system of external forces (or moments) \bar{P}_i with corresponding displacements u_i . The term u_k is the displacement of \bar{P}_k in the direction of \bar{P}_k . The total potential energy is given by

$$\Pi = U_i + U_e = U_i(u_k) - \sum_{k=1}^n \bar{P}_k u_k.$$

If the solid is in equilibrium then $\delta\Pi = 0$ giving

$$\frac{\partial U_i}{\partial u_k} \delta u_k - \bar{P}_k \delta u_k = 0,$$

hence,

$$\frac{\partial U_i}{\partial u_k} = \bar{P}_k.$$

3.11 The unit displacement method

Apply a virtual displacement, say δu_k , in the direction of a particular force \bar{P}_k . Then the principle of virtual work gives

$$\delta u_k \bar{P}_k = \int_V \sigma_{ij} \delta \varepsilon_{ij} dV.$$

The virtual displacement δu_k is arbitrary, and for simplicity, set equal to unity. Then

$$\bar{P}_k = \int_V \sigma_{ij} \delta \varepsilon_{ij} dV,$$

where $\delta \varepsilon_{ij}$ are the strains due to a unit displacement applied in the direction of \bar{P}_k .

3.12 Castigliano's second theorem

Consider a general three-dimensional solid acted on by a system of forces P_k with corresponding displacements \bar{u}_k . Here, the forces can be regarded as reactions generated by prescribed displacements \bar{u}_k . The total complementary potential energy can be expressed as

$$\Pi^* = U_i^* + U_e^* = U_i^*(P_k) - \sum_{k=1}^N P_k u_k.$$

According to the principle of stationary complementary energy

$$\delta \Pi^* = 0 = \frac{\partial U_i^*}{\partial P_k} \delta P_k - u_k \delta P_k,$$

giving

$$\frac{\partial U_i^*}{\partial P_k} = u_k$$

3.13 The reciprocal theorem of Betti

Consider a linear elastic body subjected only to surface forces. Suppose the body is first subjected to $\bar{T}_i^{(1)}$ and then, at the same locations as $\bar{T}_i^{(1)}$ and in the same directions, is subjected to applied forces $\bar{T}_i^{(2)}$. Denote the external work done by $\bar{T}_i^{(1)}$ by

$$W_{e11} = \frac{1}{2} \int_{S_T} \bar{T}_i^{(1)} u_i^{(1)} dS$$

where $u_i^{(1)}$ is the displacement resulting from $T_i^{(1)}$. Now let additional tractions $T_i^{(2)}$ be applied, causing displacements $u_i^{(2)}$, while force set $T_i^{(1)}$ is still constant. The work of $T_i^{(2)}$ moving through $u_i^{(2)}$ is

$$W_{e22} = \frac{1}{2} \int_{S_T} T_i^{(2)} u_i^{(2)} dS.$$

An additional increment of work will be done by the first tractions $T_i^{(1)}$ moving through the displacements $u_i^{(2)}$ giving

$$W_{e12} = \int_{S_T} T_i^{(1)} u_i^{(2)} dS.$$

Thus, the total work performed by the two sets of forces is

$$W_e = W_{e11} + W_{e22} + W_{e12}.$$

Now, remove the loads and apply them again, but this time in reverse order. For this second case, the total work will be

$$W_e = W_{e11} + W_{e22} + W_{e12}$$

where

$$W_{e21} = \int_{S_T} T_i^{(2)} u_i^{(1)} dS.$$

Since the total work of the applied forces must be independent of the order of application of the loading it follows that

$$W_{e12} = W_{e21}.$$

3.14 Betti's theorem for linear elastic bodies

Consider a linear elastic body that is first subjected to $T_i^{(1)}$ and then at the same locations is subjected to $T_i^{(2)}$. Consider the following integral

$$\begin{aligned} \int_V \sigma_{ij}^{(1)} \varepsilon_{ij}^{(2)} dV &= \int_V \sigma_{ij}^{(1)} u_{i,j}^{(2)} dV \\ &= \int_V \left(\sigma_{ij}^{(1)} u_j^{(2)} \right)_{,j} dV - \int_V \sigma_{ij,j}^{(1)} u_i^{(2)} dV \\ &= \int_S \sigma_{ij}^{(1)} u_j^{(2)} n_i^{(1)} dS - \int_V \sigma_{ij,j}^{(1)} u_i^{(2)} dV \\ &= \int_S T_j^{(1)} u_j^{(2)} dS + \int_V F_i^{(1)} u_i^{(2)} dV \end{aligned} \quad (1)$$

Now consider $\sigma_{ij}^{(1)} \varepsilon_{ij}^{(2)}$. Note that this is a scalar quantity, hence

$$\begin{aligned} \boldsymbol{\sigma}^T \boldsymbol{\varepsilon}^* &= (\boldsymbol{\sigma}^T \boldsymbol{\varepsilon}^*)^T = \boldsymbol{\varepsilon}^{*T} \boldsymbol{\sigma} = \boldsymbol{\varepsilon}^{*T} \mathbf{E} \boldsymbol{\varepsilon} \\ &= \boldsymbol{\varepsilon}^{*T} \mathbf{E}^T \boldsymbol{\varepsilon} = (\mathbf{E} \boldsymbol{\varepsilon}^*)^T \boldsymbol{\varepsilon} = \boldsymbol{\sigma}^{*T} \boldsymbol{\varepsilon}. \end{aligned}$$

This means that

$$\int_V \sigma_{ij}^{(1)} \varepsilon_{ij}^{(2)} dV = \int_V \sigma_{ij}^{(2)} \varepsilon_{ij}^{(1)} dV. \quad (2)$$

Equation (1) and (2) gives

$$\int_V F_i^{(1)} u_i^{(2)} dV + \int_S T_i^{(1)} u_i^{(2)} dS = \int_V F_i^{(2)} u_i^{(1)} dV + \int_S T_i^{(2)} u_i^{(1)} dS$$

which is referred to as Betti's theorem for linear elastic problems.

3.15 Maxwell's reciprocal theorem

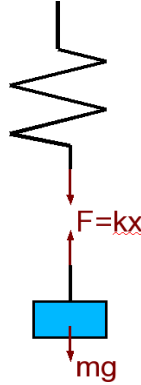
Start with Betti's theorem

$$\int_{S_T} T_i^{(1)} u_i^{(2)} dS = \int_{S_T} T_i^{(2)} u_i^{(1)} dS.$$

Suppose that for our linearly elastic body, each force system contains only a single non-zero force. Then we directly conclude:

For a linearly elastic body subjected to two forces equal in magnitude, the displacement of the location (and the direction of) the first force caused by the second force is equal to the displacement at the location of the second force which is due to the first force. If f_{ij} are the flexibility coefficients then $f_{ij} = f_{ji}$.

4.1 Harmonic Vibrations of a Spring



Force equilibrium in the vertical direction:

$$\ddot{x} + \frac{k}{m}x = g$$

The ODE has the following solution:

$$x = A \sin\left(\sqrt{\frac{k}{m}}t\right) + B \cos\left(\sqrt{\frac{k}{m}}t\right) + \frac{mg}{k}.$$

The natural frequency is $\omega = \sqrt{k/m}$, and the time to complete one cycle is $2\pi\sqrt{m/k}$.

4.2 Work and kinetic energy of a particle

Start with Newton's law of motion

$$\mathbf{F} = m\ddot{\mathbf{r}},$$

then take the line integral of each side of the equation over a given path from A to B .

$$\int_A^B \mathbf{F} \cdot d\mathbf{r} = \int_A^B m\ddot{\mathbf{r}} \cdot d\mathbf{r}.$$

But

$$\ddot{\mathbf{r}} \cdot d\mathbf{r} = \frac{1}{2}d(\dot{\mathbf{r}} \cdot \dot{\mathbf{r}}) = \frac{1}{2}d(v^2)$$

Thus

$$W = \int_A^B \mathbf{F} \cdot d\mathbf{r} = \frac{m}{2}(v_B^2 - v_A^2) = T_B - T_A$$

If \mathbf{F} is conservative ($\mathbf{F} = -\nabla V$), then $W = V_A - V_B$ giving

$$E = V_A + T_A = V_B + T_B.$$

4.3 Moment equilibrium for a particle

Start with Newton's law of motion

$$\mathbf{F} = m\ddot{\mathbf{r}}.$$

Take the cross product of each side of the equation with the position vector \mathbf{r}

$$\mathbf{r} \times \mathbf{F} = \mathbf{r} \times m\ddot{\mathbf{r}}.$$

Which is equal to

$$\mathbf{M} = \frac{d}{dt}(\mathbf{r} \times m\mathbf{v}) = \frac{d}{dt}(\mathbf{r} \times \mathbf{p}) = \dot{\mathbf{H}}$$

where \mathbf{H} is the angular momentum.

4.4 König's Theorem

The total kinetic energy is equal to that due to the total mass moving with the velocity of the center of mass plus that due to the motion relative to the center of mass.

4.5 Moment of inertia and angular momentum of a rigid body

The angular momentum for a rigid body rotating about a reference point P is

$$\mathbf{H}_p = \int_V \mathbf{r} \times \rho \dot{\mathbf{r}} dV. \quad (1)$$

Assume P is fixed in the body, then

$$\dot{\mathbf{r}} = \boldsymbol{\omega} \times \mathbf{r}$$

this gives

$$\mathbf{H}_p = \int_V \rho \mathbf{r} \times (\boldsymbol{\omega} \times \mathbf{r}) dV.$$

Assume

$$\begin{aligned} \mathbf{r} &= x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z \\ \boldsymbol{\omega} &= \omega_x\mathbf{e}_x + \omega_y\mathbf{e}_y + \omega_z\mathbf{e}_z. \end{aligned}$$

And define

$$\begin{aligned} I_{xx} &= \int_V \rho (y^2 + z^2) dV \quad ; \text{cycl.} \\ I_{xy} &= - \int_V \rho xy dV \quad ; \text{cycl.} \end{aligned}$$

Then (1) can be written as

$$\mathbf{H} = I_{ij}\omega_j\mathbf{e}_i.$$

4.6 Rotational kinetic energy of a rigid body

$$\begin{aligned} T_{rot} &= \frac{1}{2} \int_V \rho \dot{\mathbf{r}}^2 dV \\ &= \frac{1}{2} \int_V \rho \dot{\mathbf{r}} \cdot \boldsymbol{\omega} \times \mathbf{r} dV \\ &= \frac{1}{2} \int_V \rho \boldsymbol{\omega} \cdot \mathbf{r} \times \dot{\mathbf{r}} dV \\ &= \frac{1}{2} \boldsymbol{\omega} \cdot \mathbf{H} \end{aligned}$$

4.7 Holonomic, Scleronomic, and Rheonomic constrains

Holonomic constrains can be written in the following form:

$$\phi_j(q_1, q_2, \dots, q_n, t) = 0, \quad (j = 1, 2, \dots, m)$$

Scleronomic constraint: *no* explicit time dependence

Rheonomic constrain: explicit time dependence

4.8 Derive Lagrange's equations from Newton's law of motion

Define the generalized momentum by

$$p_i = \frac{\partial T}{\partial \dot{q}_i} \quad (1)$$

where q_i are the generalized coordinates defined by

$$x_i = f_i(q_1, q_2, \dots, q_n, t) \quad (2)$$

and T is the kinetic energy. For a system of N particles the total kinetic energy is

$$T = \frac{1}{2} \sum_{j=1}^{3N} m_j \dot{x}_j^2. \quad (3)$$

Inserting (3) into (1) gives

$$p_i = \sum_{j=1}^N m_j \dot{x}_j \frac{\partial \dot{x}_j}{\partial \dot{q}_i}, \quad (4)$$

but from (2) we find that

$$\dot{x}_j = \sum_{i=1}^N \frac{\partial x_j}{\partial q_i} \dot{q}_i + \frac{\partial x_j}{\partial t}. \quad (5)$$

Hence

$$\frac{\partial \dot{x}_j}{\partial \dot{q}_i} = \frac{\partial x_j}{\partial q_i}. \quad (6)$$

Eqs. (4) and (6) yield

$$p_i = \sum_{j=1}^{3N} m_j \dot{x}_j \frac{\partial x_j}{\partial q_i}. \quad (7)$$

Find the time rate of change of the generalized momentum

$$\frac{dp_i}{dt} = \sum_{j=1}^{3N} m_j \ddot{x}_j \frac{\partial x_j}{\partial q_i} + \sum_{j=1}^{3N} m_j \dot{x}_j \frac{d}{dt} \left(\frac{\partial x_j}{\partial q_i} \right). \quad (8)$$

But

$$\frac{d}{dt} \left(\frac{x_j}{q_i} \right) = \sum_{k=1}^n \frac{\partial^2 x_j}{\partial q_i \partial q_k} \dot{q}_k + \frac{\partial^2 x_j}{\partial q_i \partial t} = \{\text{Eq. (5)}\} = \frac{\partial \dot{x}_j}{\partial q_i}. \quad (9)$$

Next, use (3) to get

$$\frac{\partial T}{\partial q_i} = \sum_{j=1}^{3N} m_j \dot{x}_j \frac{\partial \dot{x}_j}{\partial q_i} \quad (10)$$

From Eqs. (8)–(10), we see that

$$\frac{dp_i}{dt} = \sum_{j=1}^{3N} m_j \ddot{x}_j \frac{\partial x_j}{\partial q_i} + \frac{\partial T}{\partial q_i}. \quad (11)$$

Newton's law of motion states $m_j \ddot{x}_j = F_j + R_j$, where R_j is the total force from the workless constraints, and F_i includes all other forces. Eq. (11) can therefore be written as

$$\frac{dp_i}{dt} = \sum_{j=1}^{3N} F_j \frac{\partial x_j}{\partial q_i} + \sum_{j=1}^{3N} R_j \frac{\partial x_j}{\partial q_i} + \frac{\partial T}{\partial q_i}. \quad (12)$$

But the generalized force Q_i is given by

$$Q_i = \sum_{j=1}^{3N} F_j \frac{\partial x_j}{\partial q_i}. \quad (13)$$

In a similar fashion, the second term in (12) is a generalized force resulting from the workless constraint forces. Consider the virtual work of these forces

$$\delta W = \sum_{i=1}^n \sum_{j=1}^{3N} R_j \frac{\partial x_j}{\partial q_i} \delta q_i = 0. \quad (14)$$

If the δq 's can be chosen independently, then the coefficient of each δq_i must be zero. We can now simplify (12) to the form

$$\frac{dp_i}{dt} = Q_i + \frac{\partial T}{\partial q_i} \quad (15)$$

or equivalent

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_i} \right) - \frac{\partial T}{\partial q_i} = Q_i, \quad (i = 1, 2, \dots, n). \quad (16)$$

These n equations are known as the fundamental form of Lagrange's equation. If all the Q_i 's are derivable from a potential function $V = V(q, t)$ as follows:

$$Q_i = -\frac{\partial V}{\partial q_i},$$

then (16) can be written as

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0, \quad (i = 1, 2, \dots, n) \quad (17)$$

where $L = T - V$ is the Lagrangian function.

5.1 Definition of material system, adiabatic system, isolated system

- A *material system* is any fixed quantity of matter contained in a defined region of space. A system can exchange energy in the form of work or heat, with its environment, but it cannot exchange matter.
 - An *adiabatic system* is thermally insulated from its environment, and can exchange energy in the form of work only.
 - An *isolated system* is a system that cannot exchange energy with its environment.
-

5.2 Thermodynamic equilibrium

A system is in thermodynamic equilibrium if its thermodynamic properties do not change spontaneously in a finite time period when the system is isolated from its environment.

5.3 Definition of Enthalpy

$$H = E + PV$$

where E is the internal energy

5.4 Definition of Helmholtz free energy

$$A = E - TS$$

where S is the entropy

5.5 Definition of Gibbs free energy

$$G = H - TS = A + PV = E + PV - TS$$

Gibbs free energy can be thought of as a thermodynamic potential the negative gradient of which can be considered as a thermodynamic force for the change in state of the system.

5.6 The ideal gas law

$$PV = nRT$$

where n is the number of moles of gas and R is the gas constant, $R = 8.314 \text{ J}/(\text{mole K})$

5.7 Two basic tendencies of nature

1. Tendency to minimize the energy of a system.
2. Tendency toward random mixing.

5.8 The zeroth law of thermodynamics

Two systems that are in thermal equilibrium with a third system, are also in thermal equilibrium with each other.

5.9 The first law of thermodynamics

The first law of thermodynamics simply advocates the energy conservation law, which for a quasi-static process can be written as

$$dE = dQ - dW$$

where dE is the increase in internal energy, dQ is the heat absorbed, and dW is the work done by the system. For a hydrostatic system $dW = pdV$, and for a solid $dW = -\sigma_{ij}d\varepsilon_{ij}$.

5.10 The second law of thermodynamics

A system operating in a cycle cannot convert into work all the heat supplied to it since some energy is always rejected as heat to a lower temperature sink. A decrease in entropy can only be temporal and local, with a greater increase incurred elsewhere. Entropy always increases for an isolated system.

5.11 The third law of thermodynamics

The entropy of a pure substance in its most stable state approaches zero as the temperature approaches zero.

5.12 Isentropic process

A reversible adiabatic process produces no change in entropy and is said to be isentropic. An isentropic process, therefore, is one in which no heat exchange occurs with the environment, and also no heat arises internally from the dissipation of kinetic energy by viscous effects.

5.13 Conduction

Heat can cross the boundary by means of conduction, in which molecules from the system and the environment meet and exchange energy at the stationary boundary. Heat conducts at a rate directly proportional to the temperature gradient causing the heat flow, as indicated by Fourier's law

$$\frac{dQ}{dt} = -k_T A \frac{dT}{dx}$$

where A is the cross-sectional area of the heat flow, x the distance between hot and cold surface areas, k_T the thermal conductivity.

5.14 Heat capacity at constant pressure

The heat capacity is the amount of heat required to raise the temperature of a material by one degree.

$$C_p = \left(\frac{\partial Q}{\partial T} \right)_P = \left\{ \begin{array}{l} \text{definition of} \\ \text{enthalpy} \end{array} \right\} = \frac{\partial H}{\partial T}$$

5.15 The classical definition of entropy

For a system in contact with a heat reservoir, the entropy increases when the system absorbs heat:

$$dS = \frac{dQ}{T} \text{ for a reversible reaction}$$

$$dS > \frac{dQ}{T} \text{ for an irreversible reaction}$$

5.16 *The statistical mechanics definition of entropy*

$$S = k \ln \Omega$$

where k is Boltzmann's constant, and Ω is the number of distinguishable states in which the system may be found.

5.17 *Physical meaning of the minimum value of Gibbs free energy*

Any system held at constant temperature and pressure comes to equilibrium when Gibbs free energy reaches a minimum. The proof is as follows:

$$G \equiv E + PV - TS$$

Consider a small change in the system

$$\Delta G = \Delta E + P\Delta V - T\Delta S$$

The first law of thermodynamics, $\Delta E + P\Delta V = \Delta Q$, gives

$$\Delta G = \Delta Q - T\Delta S$$

The second law of thermodynamics: $\Delta S \geq \Delta Q/T$ gives

$$\Delta G \leq 0$$

\therefore Any spontaneous process in the system will reduce G . Equilibrium is reached when no spontaneous changes will occur.

5.18 *Physical significance of Helmholtz free energy*

Any system held at constant temperature and volume will reach equilibrium when Helmholtz free energy has a minimum.

5.19 *Derive the equilibrium vacancy concentration in a crystal lattice*

Let G_0 be the free energy in a crystal without any vacancies. Then introduce n_v vacancies; to create one vacancy requires the energy $\Delta E_v \approx \Delta H_v$. But creating vacancies also contributes configuration entropy. Thus

$$G = G_0 + n_v \Delta H_v - TS_{conf}$$

where

$$S_{conf} = k \ln \Omega = k \ln \binom{N}{n_v} = k \ln \frac{N!}{n_v!(N - n_v)!}$$

where N is the number of atom sites in the crystal. At equilibrium the Gibbs free energy is at minimum with respect to n_v , hence

$$\frac{\partial G}{\partial n_v} = 0 \Rightarrow \Delta H_v - T \frac{\partial S_{conf}}{\partial n_v} = 0.$$

To evaluate the partial derivative, use Stirling's approximation: $\ln N! = N \ln N - N$. This gives

$$\frac{\partial S_{conf}}{\partial n_v} = k \ln \left| \frac{N - n_v}{n_v} \right| \approx k \ln \frac{N}{n_v}$$

giving

$$\Delta H_v = kT \ln \frac{N}{n_v}$$

and finally

$$n_v = N e^{-\frac{\Delta H_v}{kT}}.$$

5.20 Non-hydrostatic thermodynamics

First, we will make two assumptions: the deformation gradient is independent of position, and more importantly, the state of the homogeneous phase can be uniquely specified by a set of independent thermodynamic variables. That is, we are assuming the state of the phase is independent of the previous history of processes.

From the first law of thermodynamics we can infer the existence of an internal energy function for an elastic phase. The internal energy U of a state is measured by the work done under adiabatic conditions in going from a standard state to the state in question. The second law of thermodynamics leads to the introduction of another function of the state, i.e. the entropy, and also to the introduction of the absolute temperature scale.

In non-hydrostatics it is convenient to express extensive quantities such as U and S as densities referred to the reference volume v . The first and second laws of thermodynamics can for an elastic homogeneous phase subjected to a quasistatic reversible process be combined to yield

$$du = Tds + \sigma_i d\varepsilon_i, \quad \{i; i \in [1, 6]\}.$$

Here we regard u as a function of seven variables, s and the six ε_i . Using Legendre transformations, other functions of state may be formed from¹ u and s . For instance, a , the Helmholtz free energy per unit reference volume is defined by

$$a = u - Ts,$$

giving $da = \sigma_i d\varepsilon_i - s dT$. And, on taking the differential of this equation we obtain

$$s = - \left(\frac{\partial a}{\partial T} \right)_\varepsilon, \quad \sigma_i = \left(\frac{\partial a}{\partial \varepsilon_i} \right)_T.$$

We can also define another function, which we shall call g by analogy to the Gibbs free energy in hydrostatics, as follows

$$g = u - \sigma_i \varepsilon_i - Ts, \quad \{i; i \in [1, 6]\}.$$

Which upon differentiation yields

$$dg = -s dT - \varepsilon_i d\sigma_i,$$

giving

$$s = - \left(\frac{\partial g}{\partial T} \right)_\sigma, \quad \varepsilon_i = \left(\frac{\partial g}{\partial \sigma_i} \right)_T.$$

¹See, e.g. Goldstein, 1950, Classical Mechanics.

6.1 Definition of viscosity

Newton's definition of (dynamic) viscosity

$$\sigma_{12} = \eta \frac{dv_1}{dx_2}$$

Kinematic viscosity

$$\nu = \frac{\eta}{\rho}$$

6.2 Variation of pressure with position in a fluid in equilibrium

Consider the equilibrium equation

$$\sigma_{ji,j} + F_i = 0. \quad (1)$$

F_i is the body force per unit volume and is here assumed to be given by the gravitational force; i.e. $F_i = -\rho g_i$, where the minus sign indicates that the gravitational force acts in the negative direction of x_i . Furthermore, in a fluid in rest, σ_{ij} is given by the fluid pressure:

$$\sigma_{ij} = -p\delta_{ij}.$$

Eq. (1) therefore becomes

$$-\frac{\partial p}{\partial x_i} - \rho g_i = 0,$$

which can be written

$$\nabla p = -\rho \mathbf{g}$$

6.3 Material derivative

The material derivative is given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla,$$

where \mathbf{u} is the velocity vector.

6.4 Conservation of mass for a fluid

$$\int_A \rho \mathbf{u} \cdot \mathbf{n} dS + \int_V \frac{\partial \rho}{\partial t} dV = 0$$

The divergence theorem gives

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

or alternatively

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0$$

which for incompressible fluids becomes

$$\nabla \cdot \mathbf{u} = 0.$$

6.5 Conservation of momentum for a fluid

The linear momentum of a control system at time t is

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

where ρ and \mathbf{v} are the mass density and the absolute velocity, respectively, of the material within the volume element dV . Now, if we evaluate the same integral at time $t + \Delta t$, we find that a slightly different set of particles is within the control volume. So, in order to follow the original set of particles, we calculate the momentum of all particles within the control volume at $t + \Delta t$, and then we must add the momentum of all the “native” particles that left the control volume during Δt , and subtract the momentum of all the “foreign” particles that entered during the same interval. Therefore, at time $t + \Delta t$, the momentum of the original set of particles is

$$\left[\int_V \rho \mathbf{v} dV \right]_{t+\Delta t} + \Delta t \int_A \rho \mathbf{v} (\mathbf{v}_r \cdot d\mathbf{A}).$$

The vector \mathbf{v}_r is the velocity, *relative to the surface*, of the particles that are entering or leaving. Thus, by Newton’s law of motion, the change in linear momentum as $\Delta t \rightarrow 0$ is equal to the total external force applied to the mass within the control volume. Therefore we see that

$$\mathbf{F} = \frac{d}{dt} \int_V \rho \mathbf{v} dV + \int_A \rho \mathbf{v} (\mathbf{v}_r \cdot d\mathbf{A}).$$

6.6 Euler’s equation for a perfect fluid

Newton’s law of motion can be expressed in the form of the equilibrium equation

$$\sigma_{ji,j} + F_i = \rho \frac{Dv_i}{Dt}.$$

For a non-viscous flow these stress components are given by

$$\sigma_{ij} = -p\delta_{ij}.$$

Hence the equations of motion for a perfect fluid are

$$-\frac{\partial p}{\partial x_i} + F_i = \rho \frac{Dv_i}{Dt}$$

6.7 Bernoulli’s equation

For a frictionless fluid of constant density when the flow is steady and along a single stream line (or everywhere if the flow is irrotational) the following relation is true:

$$\frac{p}{\rho} + \frac{u^2}{2} + gz = \text{constant}.$$

The first term p/ρ represents the potential energy associated with internal forces, $u^2/2$ is the kinetic energy per unit mass, and gz represents the potential energy due to the gravitational force. Bernoulli’s equation therefore has the simple physical interpretation that the total energy constant. The term p/ρ can be ‘derived’ in the following manner. The net force (due to the pressure) acting on an infinitesimal element is $A\delta p$ in the direction of motion. The work done by this force is therefore $-A dp ds$. But the mass of the element is $\rho A ds$, giving the work per unit mass $-dp/\rho$. If the element

moves from a point where the pressure is 0 to one where the pressure is p , then the work done by the 'pressure forces' per unit mass fluid is $\int_0^p (-dp/\rho) = p/\rho$.

6.8 Irrotational incompressible flow in three dimensions

$$\text{Irrotational flow} \Rightarrow \nabla \times \mathbf{v} = 0 \quad (1)$$

$$\text{Vector identity } \nabla \times (\nabla \phi) = 0 \Rightarrow \mathbf{v} = -\nabla \phi \quad (2)$$

$$\text{Incompressibility} \Rightarrow \nabla \cdot \mathbf{v} = 0 \quad (3)$$

Combining (2) and (3) yields Laplace's equation

$$\nabla^2 \phi = 0$$

where ϕ is called the velocity potential.

6.9 Potential flow in two dimensions

The incompressibility condition becomes

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0.$$

From this equation one infers that the following is a perfect differential

$$d\psi = v_y dx - v_x dy = \frac{\partial \psi}{\partial x} dx + \frac{\partial \psi}{\partial y} dy. \quad (1)$$

The function ψ is called the stream function, $\psi = \text{constant}$ is called a stream line. Now assume irrotational flow, $\nabla \times \mathbf{v} = 0$, giving

$$\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y} = 0.$$

Inserting the expressions for v_x and v_y from (2) yields

$$\nabla^2 \psi = 0.$$

But irrotational flow also implies $\mathbf{v} = -\nabla \phi$

$$v_x = -\frac{\partial \phi}{\partial x}, \quad v_y = -\frac{\partial \phi}{\partial y}. \quad (2)$$

Equations (1) and (2) give

$$\frac{\partial \psi}{\partial y} = \frac{\partial \phi}{\partial x}, \quad \frac{\partial \psi}{\partial x} = -\frac{\partial \phi}{\partial y}.$$

These equations are automatically fulfilled if a complex potential is defined by

$$\Omega(z) = \phi + i\psi$$

6.10 Derive Navier-Stokes equation

Start with the equilibrium equation

$$\sigma_{ji,j} + F_i = \rho \frac{Dv_i}{Dt}. \quad (1)$$

For a real fluid σ_{ij} is given by

$$\sigma_{ij} = -p\delta_{ij} + \Pi_{ij}$$

where Π_{ij} represent the viscosity stress tensor. Now introduce the velocity gradient tensor

$$v_{ij} = \frac{1}{2} [v_{i,j} + v_{j,i}]. \quad (2)$$

Since fluids are isotropic, we can relate Π_{ij} and v_{ij} by

$$\Pi_{ij} = 2\eta v_{ij} + \eta' v_{kk} \delta_{ij}.$$

Here, η and η' are known as the first and second coefficients of viscosity (and take the place of Lamé's constants). Can now rewrite (1)

$$F_i - \frac{\partial p}{\partial x_i} + \Pi_{j,i,j} = \rho \frac{Dv_i}{Dt}$$

which reduces to

$$F_i - \frac{\partial p}{\partial x_i} + \eta' \frac{\partial}{\partial x_i} \nabla \cdot \mathbf{v} + 2\eta v_{j,i,j} = \rho \frac{Dv_i}{Dt}.$$

Introducing (2) gives

$$F_i - \frac{\partial p}{\partial x_i} + (\eta + \eta') \frac{\partial}{\partial x_i} \nabla \cdot \mathbf{v} + \eta \nabla^2 v_i = \rho \frac{Dv_i}{Dt}$$

which in vector notation becomes

$$\mathbf{F} - \nabla p + (\eta + \eta') \nabla (\nabla \cdot \mathbf{v}) + \eta \nabla^2 \mathbf{v} = \rho \frac{D\mathbf{v}}{Dt} \quad (3)$$

or if we utilize

$$\frac{D\mathbf{v}}{Dt} = \frac{\partial \mathbf{v}}{\partial t} + \frac{1}{2} \text{grad } \mathbf{v}^2 - \mathbf{v} \times \text{curl } \mathbf{v}$$

then (3) becomes

$$\mathbf{F} - \text{grad } p - \frac{\rho}{2} \text{grad } \mathbf{v}^2 + \rho (\mathbf{v} \times \text{curl } \mathbf{v}) + (\eta + \eta') \text{grad } \text{div } \mathbf{v} + \eta \nabla^2 \mathbf{v} = \rho \frac{\partial \mathbf{v}}{\partial t}$$

6.11 Reynold's number and the condition for turbulent flow

$$\text{Re} = \frac{\rho L u}{\eta}$$

where η is the dynamic viscosity. The flow becomes turbulent approximately when $\text{Re} > 2300$.

7.1 Hooke's law for an isotropic material, infinitesimal displacements

Hooke's law can be written:

$$\begin{aligned}\varepsilon_{11} &= \frac{1}{E} [\sigma_{11} - \nu (\sigma_{22} + \sigma_{33})] \quad ; \text{cycl.} \\ \varepsilon_{12} &= \frac{\sigma_{12}}{2\mu} \quad ; \text{cycl.}\end{aligned}$$

where E is Young's modulus, and μ is the shear modulus.

7.2 Hooke's law in tensor form

$$\varepsilon_{ij} = \frac{1 + \nu}{E} \sigma_{ij} - \frac{\nu}{E} \sigma_{kk} \delta_{ij}$$

7.3 Hooke's law solved for the stresses

$$\begin{aligned}\sigma_{ij} &= 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij}, \\ \lambda &= \frac{2\mu\nu}{1 - 2\nu},\end{aligned}$$

where μ and λ are Lamé's constants, and ν is the Poisson's ratio.

7.4 Conversion of Elastic Constants

Known	E	ν	μ	κ
μ, κ	$\frac{9\kappa\mu}{3\kappa + \mu}$	$\frac{3\kappa - 2\mu}{6\kappa + 2\mu}$	μ	κ

7.5 Compatibility Equations

The physical meaning of the compatibility equations is

$$\oint \frac{\partial \mathbf{u}}{\partial s} ds = 0$$

which in index form becomes

$$\begin{aligned}\varepsilon_{11,22} + \varepsilon_{22,11} &= 2\varepsilon_{12,12}, \\ \varepsilon_{11,23} + \varepsilon_{23,11} &= \varepsilon_{31,12} + \varepsilon_{12,13}.\end{aligned}$$

7.6 Rules for Mohr's circle

- An angle of θ on the physical element is replaced by 2θ on Mohr's circle.
- A shear stress causing a clockwise rotation about any point in the physical element is plotted above the horizontal axis of the Mohr's circle.

7.7 Transformation of the stress tensor

$$\sigma_{i'j'} = a_{i'k}a_{j'l}\sigma_{kl}$$

7.8 Strain energy density, in general and for a linear elastic material

$$\begin{aligned} dW &= \sigma_{ij}d\varepsilon_{ij} \\ W &= \frac{1}{2}\sigma_{ij}\varepsilon_{ij} = \frac{1}{2}\boldsymbol{\sigma} : \boldsymbol{\varepsilon} \end{aligned}$$

7.9 Bulk modulus

$$K = \frac{\sigma_{ii}}{3\varepsilon_{jj}}$$

7.10 Generalized Hooke's law

$$\begin{aligned} \varepsilon_{ij} &= S_{ijkl}\sigma_{kl} \text{ where } S_{ijkl} \text{ is the compliance tensor.} \\ \sigma_{ij} &= C_{ijkl}\varepsilon_{kl} \text{ where } C_{ijkl} \text{ is the stiffness tensor.} \end{aligned}$$

7.11 Definition of true strain

$$\varepsilon = \int_{L_0}^{L_f} \frac{dL}{L} = \ln \frac{L_f}{L_0} = \ln \lambda$$

7.12 Relative displacement tensor (assuming infinitesimal displacements)

$$d_{ij} = u_{i,j} \equiv \frac{\partial u_i}{\partial x_j}$$

7.13 Strain tensor and rotational tensor in terms of the displacement vector (assuming infinitesimal displacements)

The rotational tensor is given by $\omega_{ij} = \frac{1}{2}[u_{i,j} - u_{j,i}]$ or the rotation vector $\frac{1}{2}\nabla \times \mathbf{u}$.
The strain tensor is given by $\varepsilon_{ij} = \frac{1}{2}[u_{i,j} + u_{j,i}]$, furthermore $d_{ij} = \varepsilon_{ij} + \omega_{ij}$.

7.14 Fractional volume change in terms of the strains and displacements

$$\varepsilon_{ii} = \text{div } \mathbf{u} = \nabla \cdot \mathbf{u} = u_{i,i}$$

7.15 Correspondence between a stress tensor and a traction vector specified by its normal n_i .

$$T_i = \sigma_{ji}n_j$$

7.16 Force equilibrium of a solid

Newton's law yields

$$\int_V F_i dV + \int_S T_i dS = \int_V \rho a_i dV.$$

Gauss's theorem gives

$$\int_V (F_i + \sigma_{ji,j} - \rho a_i) dV = 0.$$

This must hold for any volume, hence

$$\sigma_{ji,j} + F_i = \rho a_i = \rho \frac{Dv_i}{Dt}.$$

7.17 Moment equilibrium of a solid

If body moments are neglected, the moment equation ($\mathbf{M} = \mathbf{r} \times \mathbf{F}$) becomes

$$\int_V e_{ijk} x_j F_k dV + \int_S e_{ijk} x_j T_k dS = \int_V e_{ijk} x_j a_k \rho dV.$$

By utilizing the divergence theorem and the force equilibrium equation we get

$$e_{ijk} \sigma_{jk} = 0,$$

which reduces to

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

7.18 Lagrangian, Eulerian variables, and material derivatives

In the Lagrangian system, all quantities are expressed in terms of the initial position coordinates of each particle and time; in the Eulerian system, the independent variables are x_i and t , where x_i are the position coordinates at the time of interest.

As a particle moves, it will observe a change in ϕ ; the rate at which an observer attached to the particle would see ϕ alter is called the *material derivative* of ϕ and is denoted by $d\phi/dt$.

$$\begin{aligned} \frac{d\phi(a_i, t)}{dt} &= \frac{\partial \phi}{\partial t} \\ \frac{d\phi(x_i, t)}{dt} &= \frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial x_j} \frac{dx_j}{dt} \end{aligned}$$

7.19 Derivation of the Airy stress function for plane problems

Equilibrium Equations:

$$\begin{aligned} \sigma_{xx,x} + \sigma_{xy,y} &= 0 \\ \sigma_{yy,y} + \sigma_{xy,x} &= 0 \end{aligned}$$

The equilibrium equations are automatically satisfied if

$$\sigma_{xx} = \frac{\partial^2 \psi}{\partial y^2}; \quad \sigma_{yy} = \frac{\partial^2 \psi}{\partial x^2}; \quad \sigma_{xy} = -\frac{\partial^2 \psi}{\partial x \partial y}.$$

The only non-trivial compatibility equation is

$$\frac{\partial^2 \varepsilon_{xx}}{\partial y^2} + \frac{\partial^2 \varepsilon_{yy}}{\partial x^2} = 2 \frac{\partial^2 \varepsilon_{xy}}{\partial x \partial y}$$

which is for an isotropic elastic material is fulfilled when

$$\nabla^4 \psi = 0.$$

7.20 Show that the general solution of an elasticity problem is unique. Assume linear elasticity (infinitesimal displacements), finite region with no singularities

Assume that there are two solutions to the problem, each denoted by the superscripts (1) and (2) respectively. Define

$$\begin{aligned} u_i &= u_i^{(1)} - u_i^{(2)}, \\ \varepsilon_{ij} &= \frac{1}{2} (u_{i,j} + u_{j,i}) = \varepsilon_{ij}^{(1)} - \varepsilon_{ij}^{(2)}, \\ \sigma_{ij} &= \sigma_{ij}^{(1)} - \sigma_{ij}^{(2)}, \end{aligned}$$

and note that

$$\sigma_{ij,j} = -F_i + F_i = 0.$$

The strain energy density is positive definite, and if σ_{ij} is considered as a function of ε_{ij} , then the total strain energy of the body only vanishes if $\varepsilon_{ij} = 0$. Expanding,

$$\begin{aligned} \int_V \varepsilon_{ij} \sigma_{ij} dV &= \int_V \frac{1}{2} (u_{i,j} + u_{j,i}) \sigma_{ij} dV \\ &= \int_V u_{i,j} \sigma_{ij} dV \\ &= \int_V (u_i \sigma_{ij})_{,j} dV - \int_V u_i \sigma_{ij,j} dV \\ &= \int_S u_i \sigma_{ij} n_j dS \\ &= \int_S (u_i^{(1)} - u_i^{(2)}) (T_i^{(1)} - T_i^{(2)}) dS \end{aligned}$$

and, if the prescribed boundary conditions are such that this last integral vanishes, then this will imply that $\varepsilon_{ij} = 0$ and so that the only difference between solutions (1) and (2) is a rigid-body motion (and if the displacement is known on part of the boundary, there can not even be a difference in rigid-body motion between the solutions).

7.21 Relation between strain energy density and applied loads for a linearly elastic material in equilibrium

$$\begin{aligned} U &= \frac{1}{2} \int_V \sigma_{ij} u_{i,j} dV \\ &= \frac{1}{2} \int_V (\sigma_{ij} u_i)_{,j} dV - \frac{1}{2} \int_V \sigma_{ij,j} u_i dV \\ &= \frac{1}{2} \int_S T_i u_i dS + \frac{1}{2} \int_V F_i u_i dV \end{aligned}$$

7.22 Connection between the full and the contracted notation for the elastic constants in a general anisotropic material

For the most general linear elastic material the connection between stress and strain is given by

$$\varepsilon_{ij} = S_{ijkl} \sigma_{kl}, \tag{1}$$

where S_{ijkl} is a fourth order tensor. But since both ε_{ij} and σ_{kl} are symmetric, most of the terms in (1) are not independent, hence it is convenient to work with a contracted notation. In general, the most contracted notation of (1) is

$$\varepsilon_i = S_{ij}\sigma_j, \quad \{i, j \in [1, 6]\}. \quad (2)$$

It can furthermore be shown that S_{ij} is symmetric, and consequently, there are 21 independent elastic constants at most. If the stresses and strains in the contracted notation are given by

$$\begin{array}{ll} \varepsilon_1 \equiv \varepsilon_{11} & \sigma_1 = \sigma_{11} \\ \varepsilon_2 \equiv \varepsilon_{22} & \sigma_2 = \sigma_{22} \\ \varepsilon_3 \equiv \varepsilon_{33} & \sigma_3 = \sigma_{33} \\ \varepsilon_4 \equiv \gamma_{23} = 2\varepsilon_{23} & \sigma_4 = \sigma_{23} \\ \varepsilon_5 \equiv \gamma_{13} = 2\varepsilon_{13} & \sigma_5 = \sigma_{13} \\ \varepsilon_6 \equiv \gamma_{12} = 2\varepsilon_{12} & \sigma_6 = \sigma_{12}. \end{array}$$

Then we get the following relation between the elastic constants

$$\begin{array}{ll} S_{ijkl} = S_{mn} & \text{when } m \text{ and } n \in [1, 2, 3] \\ 2S_{ijkl} = S_{mn} & \text{when } m \text{ or } n \in [4, 5, 6] \\ 4S_{ijkl} = S_{mn} & \text{when } m \text{ and } n \in [4, 5, 6] \end{array}$$

7.23 Universal binding energy relation

The Helmholtz free energy is related to ε , where ε is the uniaxial strain with lateral confinement or uniaxial strain without lateral confinement or dilatational strain

$$F(\varepsilon) = -(1 - \alpha\varepsilon)F_0e^{-\alpha\varepsilon}.$$

Furthermore, $F = E - TS$, which leads to

$$dF = dE - SdT - TdS.$$

The first and second laws of thermodynamics give

$$dE = TdS + \sigma_{ij}d\varepsilon_{ij}$$

for a reversible quasi-static reversible process. The differential of Helmholtz free energy can now be written

$$dF = \sigma_{ij}d\varepsilon_{ij} - SdT.$$

Consequently, for a uniaxial isothermal process

$$\frac{\partial F}{\partial \varepsilon} = \sigma = F_0\alpha^2\varepsilon e^{-\alpha\varepsilon}.$$

Young's modulus as a function of the strain is given by

$$E(\varepsilon) = \frac{\partial \sigma}{\partial \varepsilon} = \frac{\partial^2 F}{\partial \varepsilon^2} = F_0\alpha^2(1 - \alpha\varepsilon)e^{-\alpha\varepsilon}.$$

The initial Young's modulus is

$$E_0 = E(0) = F_0\alpha^2,$$

and the cohesive strength is given by

$$\frac{\partial \sigma}{\partial \varepsilon} = 0 \Rightarrow \varepsilon_c = \frac{1}{\alpha}.$$

Also, the binding energy per unit volume

$$F_0 = \frac{2\chi}{b} = \int_0^\infty \sigma d\varepsilon = \frac{E_0}{\alpha^2} \Rightarrow \varepsilon_c = \sqrt{\frac{2\chi}{bE_0}}$$

where χ is the surface energy. The universal binding relation can therefore be written in terms of the macroscopic terms as

$$F(\varepsilon) = - \left(\frac{2\chi}{b} \right) \left(1 + \frac{\varepsilon}{\varepsilon_c} \right) \exp \left[\frac{-\varepsilon}{\varepsilon_c} \right].$$

7.24 Upper bound for the elastic constants for an inhomogeneous solid

We consider first determining the bulk modulus of the composite, K_c . For this we impose an external dilatation σ and assume in our approximate solution that this dilatation is uniform in all components. Thus, we satisfy compatibility trivially. Then the elastic strain energy of this approximate solution is E_ε where ε indicates that a dilatation is imposed.

$$\frac{2U_\varepsilon}{V} = \sigma_c \varepsilon - \frac{1}{V} \sum_{i=1}^n \varepsilon \sigma_i V_i = \sum_i^n K_i \varepsilon^2 c_i$$

giving

$$K_\varepsilon = \sum_i^n K_i c_i.$$

But since $U_\varepsilon > U_c$, where U_c is the energy of the exact solution, we get

$$\sum_{i=1}^n K_i c_i > K_c.$$

Similarly, by considering that the shear strain is uniform in all components we obtain

$$\sum_{i=1}^n \mu_i c_i > \mu_c.$$

Thus, a solution that satisfies compatibility gives an over estimate of the elastic properties. It furnishes an upper bound.

7.25 Lower bound for the elastic constants of an inhomogeneous solid

By imposing on a heterogeneous material a mean normal stress σ and assume that the stress is uniform in all components satisfying equilibrium. Then

$$\frac{2U_\sigma}{V} = \sigma \varepsilon_c = \frac{1}{V} \sum_{i=1}^n \sigma \varepsilon_i V_i = \sum_{i=1}^n \frac{\sigma^2}{K_i} c_i,$$

giving

$$K_c > \frac{1}{\sum_{i=1}^n \left(\frac{c_i}{K_i} \right)}.$$

Similarly, considering the application of a shear stress τ which is assumed to be uniform in all components we obtain

$$\mu_c > \frac{1}{\sum_{i=1}^n \left(\frac{c_i}{\mu_i} \right)}.$$

Thus, the solution for a uniform shear which satisfies equilibrium only gives an underestimate of the actual modulus and therefore, furnishes a lower bound. Finally, since statistical randomness should assure isotropy we can derive from these expressions the Young's modulus and Poisson's ratios to obtain

$$E_c = \frac{9K_c}{1 + 3\frac{K_c}{\mu_c}}$$
$$\nu_c = \frac{1 - 2\frac{\mu_c}{3K_c}}{2 + 2\frac{\mu_c}{3K_c}}$$

For heterogeneous material with components of very different individual properties these bounds can be quite far apart and would not give satisfactory results. Therefore, other techniques would be desirable to have.

8 Engineering Beam Theory 8

8.1 Euler-Bernoulli Beam Theory

Consider pure bending of a linear elastic beam.

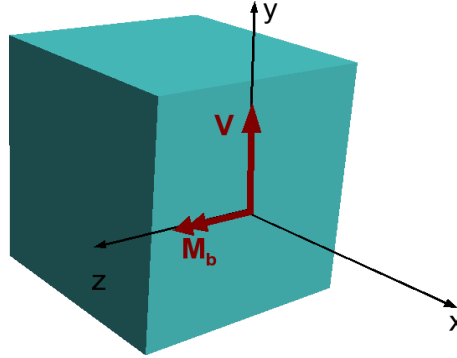


Fig. 1. Pure bending of a beam.

Let the xyz -coordinate system be located at the center of mass (CM) of the cross section of the beam. Furthermore, let the x -axis be aligned along the centerline and the y -axis be parallel to the deflection v . Then the equilibrium equations become:

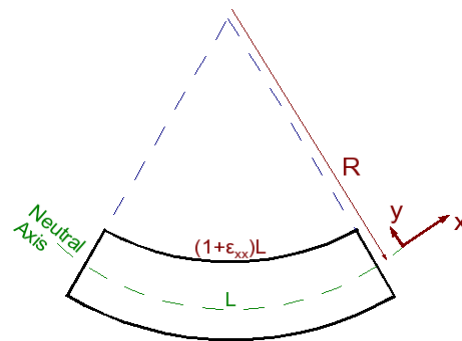
$$\int_A \sigma_{xx} dA = 0, \tag{1}$$

$$\int_A \sigma_{xx}(-y) dA = M_b, \tag{2}$$

$$\int_A \sigma_{xx}z dA = 0, \tag{3}$$

where M_b is the bending moment. For a linear elastic material, the constitutive equation can be written

$$\sigma_{xx} = \varepsilon_{xx}E. \tag{4}$$



Assuming that cross-sections remain flat and perpendicular to the neutral axis, the compatibility equation is given by

$$\frac{L}{R} = \frac{(1 + \varepsilon_{xx})L}{R - y}, \tag{5}$$

where ε_0 is the strain at the center line and R is the radius of curvature of the centerline. Solving for ε_{xx} in (5) gives

$$\varepsilon_{xx} = \frac{(-y)}{R} = (-y) \kappa,$$

The axial strain in pure bending is: $\epsilon_{xx} = (-y) \kappa$.

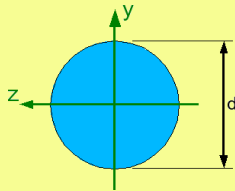
Insert the axial strain in the constitutive equation

$$\sigma_{xx} = E(-y) \kappa. \quad (6)$$

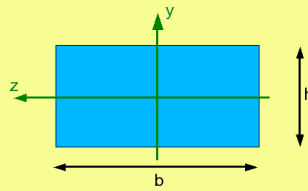
Insert the stress expression into the moment equilibrium (2), and assume that the coordinate system is located at the center of mass of the cross-section

$$\kappa = \frac{M_b}{EI_{zz}}. \quad (7)$$

Moment of Inertia: $I_{zz} = \int y^2 dA$



$$I_{zz} = \frac{\pi d^4}{64} \approx \frac{d^4}{20.4}$$



$$I_{zz} = \frac{bh^3}{12}$$

Note: Uniaxial: $F = \epsilon \cdot (EA)$
 Bending: $M_b = \kappa \cdot (EI)$
 Torsion: $M_t = \phi' \cdot (\mu I_z)$

Equation (6) to (7) now yields

$$\sigma_{xx} = \frac{M_b(-y)}{I_{zz}} \quad (8)$$

To find the displacements as a function of the applied loads utilize the following well-known relation

$$\kappa = \frac{1}{R} = \frac{|v''|}{(1 + v'^2)^{3/2}}, \quad (9)$$

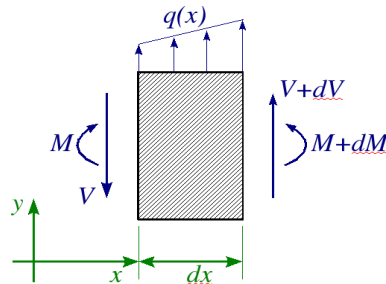
where v is the displacement in the y -direction. Assume small displacements and rotations

$$\kappa = \frac{d^2v}{dx^2}. \quad (10)$$

Equation (7) and (10) yield

$$EI_{zz} \frac{d^2v}{dx^2} = M. \quad (11)$$

To simplify this equation further, consider the force and moment equilibrium of an infinitesimal volume element



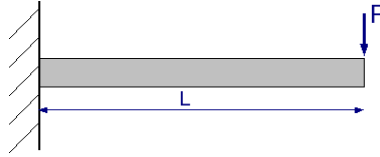
$$\begin{aligned} \uparrow: \quad & (V + dV) - V + qdx = 0 \\ \Rightarrow \quad & \frac{dV}{dx} + q = 0 \end{aligned} \quad (12)$$

$$\begin{aligned} (x + dx) \odot: \quad & (M + dM) - M + Vdx - q\frac{dx}{2}dx = 0 \\ \Rightarrow \quad & \frac{dM}{dx} + V = 0 \end{aligned} \quad (13)$$

Equation (11) can now finally be written as

$$\boxed{\frac{d^2}{dx^2} \left(EI_{zz} \frac{d^2 v}{dx^2} \right) = q} \quad (14)$$

8.2 Deflection of a Cantilever Beam



The deflection of the cantilever beam is given by

$$\frac{d^2 v(x)}{dx^2} = \kappa(x) = \frac{M(x)}{EI} = \frac{-P(L-x)}{EI}$$

Introducing the boundary conditions the deflection can be written

$$v(x) = -\frac{Px^2}{6EI}(3L-x)$$

Define δ to be the deflection at the tip of the cantilever beam:

$$\delta = -v(x=L) = \frac{PL^3}{3EI}$$

giving

$$P = \left(\frac{3EI}{L^3} \right) \delta.$$

8.3 Elastic Buckling

Consider a simply-supported beam of length L that is subjected to an axial compressive force F . Let the deflection of the beam be $w(x)$, then the moment is given by $M = Fw$. Recall that for an Euler-Bernoulli beam,

$$M = -EI \frac{d^2 w}{dx^2}, \quad (1)$$

which together with the moment becomes

$$\frac{d^2 w}{dx^2} + \frac{F}{EI} w = 0. \quad (2)$$

The solution to this ODE is given by

$$w(x) = A \sin \left(\sqrt{\frac{F}{EI}} x \right) + B \cos \left(\sqrt{\frac{F}{EI}} x \right). \quad (3)$$

For a simply supported beam the boundary conditions are $w(0) = w(L) = 0$, giving

$$B = 0$$

$$A \sin \left(\sqrt{\frac{F}{EI}} L \right) = 0.$$

Non-trivial solutions only exists if

$$\sqrt{\frac{F}{EI}} L = n\pi, \quad \text{where } n = 1, 2, 3. \quad (4)$$

The critical load occurs for $n = 1$ giving

$$F_{crit} = \frac{\pi^2 EI}{L^2}. \quad (5)$$

For other boundary conditions the buckling equation can be written

$$F_{crit} = C \frac{\pi^2 EI}{L^2} = \frac{\pi^2 EI}{L'^2}$$

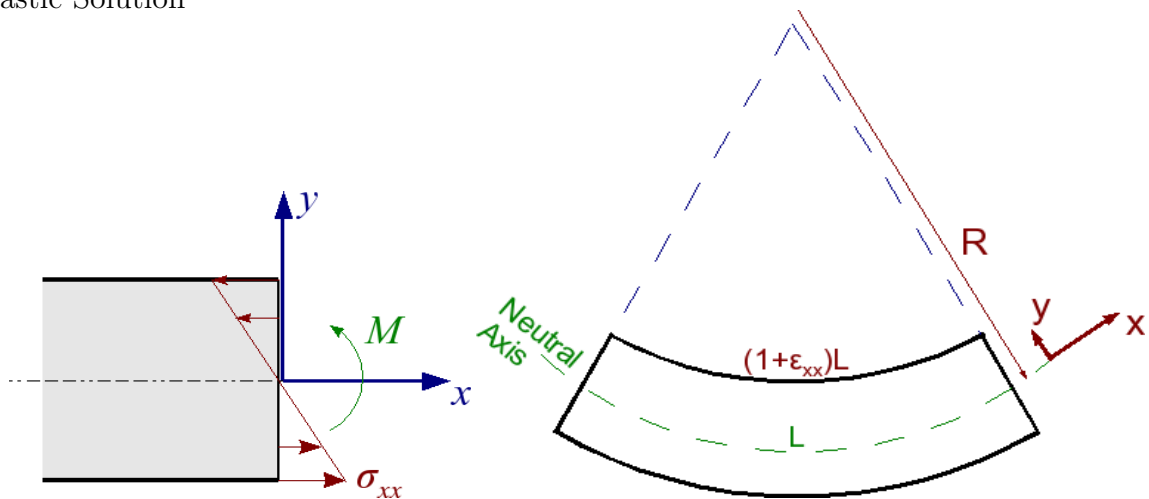
where $L' = KL$.

8.4 Elastic-Plastic Beam Bending

Consider a beam bending problem based on the following assumptions:

- Pure bending (no transverse forces)
- Rectangular cross-section (with a width of b and a height of h)

Elastic Solution



Moment equilibrium:

$$\int_A \sigma_x(-y)dA = M \quad (1)$$

Constitutive Equation:

$$\sigma_x = \varepsilon_x E \quad (2)$$

Compatibility:

$$\frac{L}{R} = \frac{(1 + \varepsilon_x)L}{R - y} \quad (3)$$

Equations (2) and (3) give

9.1 Energy release rate, crack driving force

$$G = \frac{\pi\sigma^2 a}{E}$$

9.2 Relation between G and K_I

$$G = \frac{K_I^2}{E^*}$$

9.3 Conditions for plane strain LEFM

$$B, a \geq 2.5 \left(\frac{K_I}{\sigma_Y} \right)^2$$

9.4 Mode I stress field, rectangular coordinates

$$\begin{aligned} \sigma_{xx} &= \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right] \\ \sigma_{yy} &= \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left[1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right] \\ \sigma_{xy} &= \frac{K_I}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \end{aligned}$$

9.5 Derive the J -integral

The potential energy of a cracked two-dimensional body (assuming no body forces and constant tractions) is

$$\Pi(a) = \int_A W dA - \int_{\Gamma_T} T_i u_i ds, \quad (1)$$

where W is the strain energy density. Differentiate with respect to the crack length a :

$$\frac{d\Pi}{da} = \int_A \frac{dW}{da} - \int_{\Gamma} T_i \frac{du_i}{da} ds. \quad (2)$$

Note that we can replace Γ_T with Γ since $du_i/da = 0$ on Γ_u . So far, we have used the coordinate system x_1x_2 , which is located at the center of the edge crack. Now introduce a new coordinate system X_1X_2 located at the tip of the crack. The relation between the two coordinate systems is

$$X_i = x_i - a\delta_{i1}.$$

The chain rule gives {memory guideline: $\phi = \phi(a, X_1(a))$ }

$$\frac{d}{da} = \frac{\partial}{\partial a} + \frac{\partial X_1}{\partial a} \frac{\partial}{\partial X_1} = \frac{\partial}{\partial a} - \frac{\partial}{\partial X_1} = \frac{\partial}{\partial a} - \frac{\partial}{\partial x_1}.$$

Equation (2) can now be written

$$\frac{d\Pi}{da} = \int_A \left(\frac{\partial W}{\partial a} - \frac{\partial W}{\partial x_1} \right) dA - \int_{\Gamma} T_i \left(\frac{\partial u_i}{\partial a} - \frac{\partial u_i}{\partial x_1} \right) ds. \quad (3)$$

Utilize the following ‘trick’

$$\frac{\partial W}{\partial a} = \frac{\partial W}{\partial \varepsilon_{ij}} \frac{\partial \varepsilon_{ij}}{\partial a} = \sigma_{ij} \frac{\partial \varepsilon_{ij}}{\partial a}.$$

Therefore

$$\int_A \frac{\partial W}{\partial a} dA = \int_A \sigma_{ij} \frac{\partial \varepsilon_{ij}}{\partial a} dA = \left\{ \begin{array}{l} \text{principle of} \\ \text{virtual work} \end{array} \right\} = \int_\Gamma T_i \frac{\partial u_i}{\partial a} ds.$$

Hence (3) becomes

$$\frac{d\Pi}{da} = - \int_A \frac{\partial W}{\partial x_1} dA + \int_\Gamma T_i \frac{\partial u_i}{\partial x_1} ds.$$

Use the divergence theorem ($\int_A B_{i,i} dA = \int_\Gamma B_i n_i ds$, where n_i is the outward normal to Γ , i.e. $n_1 ds = dx_2$):

$$- \frac{d\Pi}{da} = \int_\Gamma \left(W n_1 - T_i \frac{\partial u_i}{\partial x_1} \right) ds \equiv J.$$

9.6 Prove that the J -integral is path independent

Let Γ_1 and Γ_2 denote two curves going counter clockwise around a crack tip, both starting and ending on the two traction free crack surfaces. Furthermore, let S_1 and S_2 be the two paths on the crack faces that are required to close the path $\Gamma_1 + \Gamma_2 + S_1 + S_2$. Finally, let J_1 denote the value obtained by the J -integral for the contour Γ_1 . Form

$$J_1 - J = \oint_{\Gamma + \Gamma_1 + S_1 + S_2} \left(W dx_2 - T_i \frac{\partial u_i}{\partial x_1} ds \right)$$

Use the divergence theorem:

$$\begin{aligned} J_1 - J &= \int_A \left[\frac{\partial W}{\partial x_1} - \frac{\partial}{\partial x_j} \left(\sigma_{ji} \frac{\partial u_i}{\partial x_1} \right) \right] dA \\ &= \int_A \left[\frac{\partial W}{\partial \varepsilon_{ij}} \frac{\partial \varepsilon_{ij}}{\partial x_1} - \sigma_{ji,j} \frac{\partial u_i}{\partial x_1} - \sigma_{ji} \frac{\partial}{\partial x_1} \frac{\partial u_i}{\partial x_j} \right] dA \\ &= \int_A \left[\sigma_{ij} \frac{\partial \varepsilon_{ij}}{\partial x_1} - \sigma_{ij} \frac{\partial}{\partial x_1} (u_{i,j}) \right] dA \\ &= 0 \end{aligned}$$

Hence $J_1 = J$ and J is independent of path.

9.7 Crack extension criteria for an elastic material under uniaxial tension

The stress distribution in mode I is

$$\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} \tilde{\sigma}_{ij}(\theta) F(a/w)$$

where $F(a/w)$ is a compensation for finite size. The strains ε_{ij} are related to the stresses by Hooke’s law, both are concentrated as $1/\sqrt{r}$. The fracture criterion can be stated as:

- The crack advances when the energy release rate equals a material specific energy release rate, $G_{IC} = 2\chi_s$, where χ_s is the surface free energy.

- The crack advances when at the crack at a typical distance of order b the tensile stress $\sigma_{\theta\theta}$ reaches the ideal cohesive strength σ_{ic} ,

$$\sigma_{\theta\theta} = \sigma_{ic} = \frac{1}{e} \sqrt{\frac{2\chi_s E}{(1-\nu^2)b}},$$

where e is the base of the natural logarithm.

- The crack advances when

$$K_I = K_{IC} = \sqrt{\frac{G_{IC} E}{1-\nu^2}}.$$

9.8 Crack advance criteria for a plastic non-hardening material in mode I

The results presented here are obtained by analogy from mode III. The size of the plastic zone in small scale yielding (SSY) is

$$s = \frac{1}{\pi} \left(\frac{K_I}{Y} \right)^2.$$

The equivalent stress is constant inside the plastic zone, but the equivalent strain is concentrated as

$$\varepsilon_e = \varepsilon_0 \frac{s}{r},$$

where $\varepsilon_0 = Y/E$ is the equivalent strain at yield. The crack advance criterion is that the equivalent strain averaged over a representative volume element (RVE) ρ reaches a critical value ε^f ,

$$\varepsilon^f \approx \frac{\left(1 - \frac{1}{n}\right) \ln\left(\frac{1}{p_0}\right)}{\sinh\left[\left(1 - \frac{1}{n}\right) \sqrt{3} \frac{\sigma_m}{\sigma_e}\right]},$$

where p_0 is the initial porosity, $\sigma_e = Y$, $\sigma_m = \sigma_{ii}/3$, and n is the strain hardening exponent. This is satisfied at the crack tip when K_I reaches a critical value to expand the plastic zone to a critical size s_c , where

$$s_c = \frac{1}{\pi} \left(\frac{K_{IC}}{Y} \right)^2 \quad \text{and} \quad K_{IC} = \sqrt{\varepsilon^f \rho \pi E Y}.$$

This means that the fracture criterion can be written $K_I = K_{IC}$. Other equivalent criteria can be stated: The crack opening displacement $COD = s\varepsilon_0$ reaches a critical value $CCOD = s_c\varepsilon_0 = \varepsilon^f \rho$; or in small scale yielding the energy release rate reaches a critical value

$$G_I = G_{IC} = \frac{K_{IC}^2 (1-\nu^2)}{E} = \pi Y \varepsilon^f \rho (1-\nu^2).$$

9.9 Crack advance criteria in a power law hardening material

Consider a material with the constitutive equation

$$\varepsilon_e = \alpha \varepsilon_0 \left(\frac{\sigma_e}{\sigma_0} \right)^n,$$

where σ_e and ε_e are the yield stress and yield strain, respectively. It can be shown that the crack tip fields are given by the HRR-fields

$$\begin{aligned}\sigma_{ij} &= \sigma_0 \left(\frac{J}{\alpha \sigma_0 \varepsilon_0 I_n r} \right)^{1/(1+n)} \tilde{\sigma}_{ij}(\theta, n) \\ \varepsilon_{ij} &= \varepsilon_0 \left(\frac{J}{\alpha \sigma_0 \varepsilon_0 I_n r} \right)^{n/(1+n)} \tilde{\varepsilon}_{ij}(\theta, n) \\ \sigma_e &= \sigma_0 \left(\frac{J}{\alpha \sigma_0 \varepsilon_0 I_n r} \right)^{1/(1+n)} \tilde{\sigma}_e(\theta, n) \\ \varepsilon_e &= \varepsilon_0 \left(\frac{J}{\alpha \sigma_0 \varepsilon_0 I_n r} \right)^{n/(1+n)} \tilde{\varepsilon}_e(\theta, n)\end{aligned}$$

J is a field parameter that characterizes the strength of the local field in a sense very similar to the energy release rate G_I that characterizes the elastic field of a brittle solid. In a material with limited ductility where the crack advances with a finite plastic zone size, the contour integral can be evaluated outside s_c where it will be in the linear elastic material, where it gives

$$J = G_I = \frac{K_I^2(1 - \nu^2)}{E}.$$

Under these conditions J can still be interpreted as a energy release rate.

10.1 *Facts about BCC, FCC, and HCP (number of atoms per structure cell, e.g. of materials, slip systems, stacking sequence)*

Body-centered cubic crystal structure:

- 2 atoms per structure cell;
- e.g.: Alpha Iron and Tungsten;
- Not close packed, $\{110\}$ planes have highest atomic density, but $\langle 111 \rangle$ are close packed.

Face-centered cubic crystal structure:

- 4 atoms per structure cell;
- e.g.: Al, Copper, Gold, Silver and Nickel;
- stacking sequence: ABCABC...;
- 12 slip systems: 4 sets of octahedral planes $\{111\}$, each having three slip directions $\langle 110 \rangle$.

Hexagonal close-packed structure:

- planes and directions are specified by the Miller-Bravais system $(hkil)$, where h , k and i refer to three symmetrical directions in the basal plane, and l is along the c -axis ($i = -(h + k)$);
- stacking sequence: ABAB...;
- 3 slip systems: one slip plane (0001) and three slip directions, $\langle 11\bar{2}0 \rangle$;
- e.g.: Zn.

10.2 *Give some examples of structure-sensitive and structure-insensitive properties of metals*

Structure-sensitive: electrical conductivity, yield stress, fracture strength and creep strength.

Structure-insensitive: elastic constants, melting point, density, specific heat, coefficient of thermal expansion.

10.3 *Mention three types of lattice defects and give examples of each of them*

Point defects: vacancies, interstitial atoms and impurity atoms;

Line defects: dislocations;

Surface defects: grain boundaries, stacking faults and twinned regions.

10.4 *Edge dislocations: Burgers vector and movement*

Burgers vector is always perpendicular to the dislocation line. An edge dislocation can leave the slip plane by diffusion controlled climb.

10.5 *Screw dislocations: Burgers vector, movement and stress field*

The dislocation line is parallel to the Burgers vector. A screw dislocation can leave the slip plane by cross-slip. Creates the stress field

$$\tau_{\phi z} = \frac{Gb}{2\pi r}$$

10.6 Dislocation dissociation

$$b_1^2 > b_2^2 + b_3^2$$

10.7 Shockley partials in FCC lattice

$$\frac{a_0}{2} [10\bar{1}] \longrightarrow \frac{a_0}{6} [2\bar{1}\bar{1}] + \frac{a_0}{6} [11\bar{2}]$$

10.8 Definition of Burgers vector

$$\mathbf{b} = \oint_c \frac{\partial \mathbf{u}}{\partial s} ds$$

where c is a right-handed circuit around the dislocation.

10.9 Properties of \mathbf{b}

- \mathbf{b} is preserved along a dislocation,
- a dislocation line cannot terminate inside a crystal,
- a dislocation can only terminate on a free surface, close on itself creating a loop, or join other dislocations at a node.

10.10 Plastic strain produced when a dislocation moves a distance x on a slip plane in a crystal

The strain produced when a dislocation moves a distance x in a crystal of width l and height h is

$$\gamma = \frac{xb}{lh} \quad \text{which can be written} \quad d\gamma = \frac{bd(\text{area})}{V}.$$

If there are N dislocations that each move an average distance dx then

$$\gamma = \frac{Nbdx}{lh}.$$

Let $\rho = N/(lh)$ be the dislocation density, then the plastic strain can be written

$$\gamma = \rho b dx.$$

10.11 Stress fields around a positive edge dislocation and a positive screw dislocation

Edge dislocation

$$\begin{aligned} \sigma_{rr} = \sigma_{\theta\theta} &= -\frac{\mu b}{2\pi(1-\nu)r} \sin \theta? \\ \sigma_{r\theta} &= \frac{\mu b}{2\pi(1-\nu)r} \sin \theta? \\ \sigma_{zz} &= \nu(\sigma_{rr} + \sigma_{\theta\theta}) \end{aligned}$$

Screw dislocation

$$\sigma_{\theta z} = \frac{\mu b}{2\pi r}$$

Note, the stress fields are only valid when $r > \mathcal{O}(b)$.

10.12 Line energy of dislocations

The strain energy per unit volume for a screw dislocation is given by

$$W = \int_0^{\varepsilon_{ij}} \sigma_{ij} d\varepsilon_{ij} = 2 \int_0^{\varepsilon_{\theta z}} \sigma_{\theta z} d\varepsilon_{\theta z} = \sigma_{\theta z} \varepsilon_{\theta z} = \frac{\sigma_{\theta z}^2}{2\mu}.$$

The elastic energy per unit length of dislocation for a screw dislocation therefore becomes

$$\begin{aligned} \mathcal{E}_s &= \int_{r_c}^R \frac{\sigma_{\theta z}^2}{2\mu} 2\pi r dr + \mathcal{E}_{core} \\ &= \frac{\mu b^2}{4\pi} \ln\left(\frac{R}{r_c}\right) + \mathcal{E}_{core} \\ &= \frac{\mu b^2}{4\pi} \ln\left(\frac{\alpha R}{r_c}\right) \end{aligned}$$

where r_c is the core radius and $\alpha = \mathcal{O}(1)$. If R is approximated from

$$\rho \simeq \frac{1}{\pi R^2}$$

then we get

$$\mathcal{E} \simeq \frac{Gb^2}{2}$$

which typically is about 3 eV. A similar calculation yields the same result for an edge dislocation.

10.13 Volume change due to a dislocation

First, it is obvious that a screw dislocation does not result in any dilatation. Furthermore, for an edge dislocation, integrating ε_{ii} around the dislocation also results in zero dilatation. A more detailed analysis reveals that there is a very small volume change due to the dislocation core. But this volume change is so small that for most practical purposes plastic flow can be considered to conserve volume.

10.14 'Force' on a dislocation

If a dislocation in a crystal moves under the action of an externally applied stress, the resulting displacements on the boundary will cause the external forces to do work on the crystal. Since the strain energy of the crystal will not be altered by a small displacement of the dislocation in the center of a very large crystal, the work must be dissipated as a temperature rise within the crystal. We consider this dissipation as having resulted from the displacement of a fictitious force applied normal to the dislocation line by the external stresses. The plastic work increment is related to the shear stress σ_s as

$$dW = \sigma_s d\gamma^p V = \sigma_s b t dx$$

where t is the thickness. The thermodynamic driving force (per unit length) becomes

$$f_x = \frac{1}{t} \frac{\partial W}{\partial x} = \sigma_s b$$

where σ_s is the resolved shear stress in the direction of \mathbf{b} .

10.15 Line tension of a dislocation

Since a dislocation possess a large elastic energy per unit length, it will always tend to shorten its length between two points inside the crystal by gliding or climbing. Thus, it will behave as if it were subjected to a line tension T all along its length

$$T = \frac{\partial U}{\partial L} = \frac{\mathcal{E} \Delta L}{\Delta L} = \mathcal{E}.$$

The work done by the applied shear stress σ_s is stored in terms of an increase in dislocation length.

$$\Delta W = \frac{f \Delta A}{2} = \frac{\sigma_s b \Delta A}{2} = \mathcal{E} \Delta L.$$

But from the geometry of a curved dislocation that is pinned at two points (at a distance L apart)

$$\Delta A \simeq 2R \Delta L \quad \Rightarrow \quad \mathcal{E} = T = \sigma_s b R.$$

This gives the curvature force relation

$$\frac{1}{R} = \frac{\sigma_s b}{\mathcal{E}} \quad \text{and also} \quad \sigma_s = \frac{\mathcal{E}}{bR}.$$

The maximum value of R is $L/2$ giving

$$\sigma_{s,peak} = \frac{2\mathcal{E}}{bL}.$$

10.16 Difference between a jog and a kink

The steps in dislocations which form in the process of intersection are called *jogs*. Jogs lying in the slip plane and can be eliminated by glide motion of the dislocation are called *kinks*.

10.17 Plastic resistance mechanisms in metals

■ Intrinsic resistance

- Lattice resistance
- Dislocation resistance
- Grain boundary resistance

■ Extrinsic mechanisms

- Solute resistance
- Precipitate particle resistance
- Dispersed particle resistance

10.18 Lattice resistance

The intrinsic lattice resistance is induced by the variation in core energy due to dislocation glide. The relation between the variation of core energy between neighboring lattice rows and the lattice resistance is given by

$$\tau_l = \frac{\pi \Delta \mathcal{E}_{core}}{b^2} \quad \text{or} \quad \hat{\tau}_l = \frac{1}{b} \frac{\partial \mathcal{E}}{\partial y}.$$

Simple models have shown that this energy decreases exponentially with the width of the core, while the core width is inversely related to the ideal shear strength of the lattices. At $T = 0\text{K}$: (1) for FCC metals, $\hat{\tau}_l$ is neglectable; (2) for BCC metals, $\hat{\tau}_l \approx [5 \cdot 10^{-3}\mu, 1.0\mu]$; (3) for covalent materials, $\hat{\tau}_l \approx [1 \cdot 10^{-3}\mu, 2.0 \cdot 10^{-2}\mu]$

10.19 Particle controlled resistance

When a dislocation touches or otherwise interacts with a particle to test its strength, it does so by wrapping itself around the particle to exert increasingly larger components of the line tension force on the particle in the direction of advance. Thus, the evoked particle resistance \hat{K} at any instance is balanced by the components of line tension force of the cusped dislocation. The maximum force a dislocation can exert on a particle in this way is equal to twice the line tension $2\mathcal{E}$. Hence, any particle with strength $\hat{K}/(2\mathcal{E}) > 1$ is impenetrable by dislocations. A dislocation can overcome such particles only by going around them. When $\hat{K}/(2\mathcal{E}) < 1$, the dislocation overcomes the particle by cutting it.

10.20 Dispersed particle resistance

When *impenetrable* particles with $\hat{K}/(2\mathcal{E}) > 1$ are distributed randomly in a plane with mean center-center spacing l and having an overall volume fraction c , the flow stress is governed by bowing of dislocations through the gaps of average spacing l in semicircular segment configurations. This gives rise to a plastic resistance of

$$\hat{\tau} = \beta \frac{2\mathcal{E}}{bl} = \beta \frac{2\mathcal{E}}{br_0} \sqrt{\frac{3c}{2\pi}}$$

where r_0 is the actual particle radius and $\beta (\approx 0.85)$ is a statistical factor accounting for the variation in particle spacings. Clearly, for a given particle size the maximum plastic resistance is proportional to $c^{0.5}$, while for a given particle volume fraction $\hat{\tau}$ depends on $1/\sqrt{r_0}$ over the range in which $\hat{K}/(2\mathcal{E}) > 1$.

10.21 Precipitate particle resistance

When *penetrable* particles with $\hat{K}/(2\mathcal{E}) < 1$ are dispersed randomly in a plane, dislocations sample them and penetrate them without the need to bow to semicircular configurations.

Assume spherical particles of radius r and volume fraction c , and with a mean spacing l between particles in a given plane

$$c = \frac{2}{3} \frac{\pi r^2}{l^2}, \quad \text{sometimes written} \quad c = \frac{\pi r_0^2}{l^2}.$$

The relation between the peak resistive force \hat{K} and lattice resistance of the particle $\hat{\tau}_p$ is

$$\hat{K} = 2rb\hat{\tau}_p.$$

Define λ to be the sampling length (i.e. distance between particles along the dislocation), and σ_s the applied shear stress acting on the glide plane, then we have

$$K = \sigma_s b \lambda. \quad (1)$$

According to Friedel: for each contact lost a new one is generated, when this happens the dislocation sweeps the area l^2 . Also recall $1/R = \sigma_s b / \mathcal{E}$. The geometrical relationship between λ and l can be taken as

$$l^2 = \frac{\lambda^3}{2R}. \quad (2)$$

Equations (1) and (2) now gives

$$\sigma_s = \tau_p = \left[\frac{K^3}{2\mathcal{E}l^2b^2} \right]^{0.5}$$

which can be written as

$$\hat{\tau}_p = \frac{2\mathcal{E}}{bl} \left(\frac{\hat{K}}{2\mathcal{E}} \right)^{1.5}.$$

The plastic resistance of the alloy then becomes

$$\hat{\tau}_p \simeq \frac{2\mathcal{E}}{bl} \left(\frac{\hat{K}}{2\mathcal{E}} \right)^{1.5} = \frac{2\mathcal{E}}{br_0} \left[\frac{3c}{2\pi} \right]^{0.5} \left(\frac{\hat{K}}{2\mathcal{E}} \right)^{1.5}. \quad (3)$$

For many mechanisms the particle strength $\hat{K}/(2\mathcal{E})$ depends on particle size. This dependence is often linear and introduces a technologically important possibility of maximizing the plastic resistance at constant volume fraction of particles by particle size control. Thus, in the range of precipitation strengthening where $\hat{K}/(2\mathcal{E}) = K'r/(2\mathcal{E})$, Eqn. (3) transforms to

$$\hat{\tau}_p = \left(\frac{K'}{b} \right)^{1.5} \left(\frac{3c}{2\pi} \right)^{0.5} \left(\frac{rb}{2\mathcal{E}} \right)^{0.5}$$

where $K' = d\hat{K}/dr$ is the coefficient of the particle size-strength connection, we see that when c is constant, the plastic resistance is proportional to $r^{0.5}$, and that the peak strength

$$\hat{\tau}_{p,peak} = \frac{K'}{b} \left(\frac{3c}{2\pi} \right)^{0.5} \simeq 2\hat{\tau}_{lp} \left(\frac{c}{\pi} \right)^{0.5}$$

is achieved at a particle size $r_{peak} = 2\mathcal{E}/K' = \mathcal{E}/(\hat{\tau}_{lp}b)$.

10.22 Dislocation resistance

Glide dislocations in a slip plane encounter many dislocations of other slip systems that spread through the plane. Such forest dislocations are cut in a number of ways. If both the glide dislocation and the forest dislocations are of edge character, a simple jog with energy $\sim \mu b^3/10$ is formed. To find the corresponding \hat{K} we have to assume that the forest dislocation has an effective cross section w , then we can write

$$\frac{\hat{K}w}{2} = \frac{\mu b^3}{10} = 0.2b \frac{\mu b}{2} = 0.2b\mathcal{E}$$

which gives

$$\frac{\hat{K}}{2\mathcal{E}} = 0.2 \frac{b}{w} \approx 0.2.$$

It is therefore clear that we can treat the dislocation resistance in an analogous fashion to particle resistance, thus

$$\hat{\tau}_{disl} = \frac{2\mathcal{E}}{bl} \left(\frac{\hat{K}}{2\mathcal{E}} \right)^{1.5}.$$

But $\hat{K}/(2\mathcal{E})$ can be taken as a constant, $1/l = \sqrt{\rho}$, and $\mathcal{E} = \mu b^2/2$ giving

$$\hat{\tau}_{disl} = \alpha \mu b \sqrt{\rho}$$

where α is a constant in the range 0.3 – 0.4.

10.23 Solute resistance

Individual solute atoms are usually weak and act on the dislocation line collectively in a complex manner. The resulting plastic resistance have been shown to be of the form

$$\hat{\tau}_{ss} = \beta \mu \left(\frac{\hat{K}}{2\mathcal{E}} \right)^{4/3} \cdot c^{2/3}$$

where β is of the order of 1.

10.24 Total plastic resistance of a metal

The total athermal resistance can be found by superposition

$$\hat{\tau}_{total} = \hat{\tau}_l + \hat{\tau}_{ss} + \hat{\tau}_p + \hat{\tau}_{disl}.$$

10.25 Temperature and strain rate dependence of the plastic shear resistance of a metal

The overall temperature dependence of the plastic shear resistance at a given strain rate has the following behavior: first the resistance goes down and then reaches a plateau at around half the melting point and then continues to decrease further towards zero plastic resistance at the melting point.

Above $T_m/2$ diffusion becomes an important consideration in undoing dislocation structures resulting from strain hardening making it possible to obtain steady state creep. Below $T_m/2$ diffusion is unimportant and obstacles controlling the plastic resistance tend to be relatively stable. In the range between 0 K and $T_m/2$, however, it is possible in many instances to shear obstacles at stress levels σ_s less than the athermal levels of resistance $\hat{\tau}$, through thermally activated processes. The key elements of thermally activated glide are the force distance curves $K = K(y)$ of obstacles, where y is the distance of penetration of a dislocation into the obstacle at a force $K < \hat{K}$ where \hat{K} is the peak resistive force of the obstacle. If the dislocation can be aided to go from y_1 to y_2 under constant applied stress σ_s by thermal fluctuations the obstacle would be overcome and effectively long range dislocation glide can be achieved. The energy barrier for this process is

$$\Delta G^* = \Delta F - \Delta W = \int_{y_1}^{y_2} K(y) dy - K_a(y_2 - y_1) = \int_{K_a}^{\hat{K}} \Delta y(K) dK.$$

To simplify the analysis, we will now consider an obstacle for which $K(y) = \hat{K}$ for $y \in [0, 2r]$ (this is the case for obstacles where the shear resistance is comprised of an increase of internal interface energy). In this simple case

$$\Delta G^* = 2r(\hat{K} - K_a) = 2r\hat{K} \left(1 - \frac{K_a}{\hat{K}} \right).$$

Also, from above, $K_a/\hat{K} = (\sigma_s/\hat{\tau})^{2/3}$ giving

$$\Delta G^* = \Delta G_0 \left[1 - \left(\frac{\sigma}{\hat{\tau}} \right)^{2/3} \right]$$

where $\Delta G_0 = 2r\hat{K}$. The probability of obtaining the required assistance from thermal fluctuations is given by Boltzmann's expression

$$\exp \left[-\frac{\Delta G^*}{kT} \right].$$

Once a successful thermal fluctuation is accomplished the dislocation line sweeps out a small area increment of order l^2 and in general results in an increment of plastic strain bl^2/V . If there are n similarly positioned dislocation segments in the volume element V and the frequency of oscillation of the dislocation segment in front of the obstacle is ν_G then the overall plastic strain rate under the applied stress σ for an obstacle field with athermal resistance $\hat{\tau}$ becomes

$$\dot{\gamma} = \dot{\gamma}_0 \exp \left[-\frac{\Delta G^*}{kT} \right] \quad \text{with} \quad \dot{\gamma}_0 = n\nu_G \frac{bl^2}{V}$$

or since n/V is likely to be of order $1/l^3$ giving $\dot{\gamma}_0 = b\nu_G/l$. The above developed expression can alternatively be written as

$$\frac{\sigma_s}{\hat{\tau}} = \left[1 - \frac{T}{T_0} \right]^{1.5}; \quad T_0 = \frac{\Delta G_0}{k \ln(\dot{\gamma}_0/\dot{\gamma})}.$$

T_0 is a strain rate dependent 'cut-out' temperature of the glide obstacle under consideration; for many mechanisms $T_0 < T_m/2$. Since there will always be a temperature independent additive of the flow stress $\hat{\tau}_\mu$, the overall dependence will first decrease and then reach a non-zero plateau at temperatures higher than T_0 .

In general, for other obstacle interactions

$$\Delta G^* = \Delta G_0 \left[1 - \left(\frac{T}{T_0} \right)^{p/q} \right]^q$$

where p and q are of order unity or less, or alternatively

$$\dot{\gamma} = \dot{\gamma}_0 \exp \left\{ -\frac{\Delta G_0}{kT} \left[1 - \left(\frac{\sigma_s}{\hat{\tau}} \right)^{p/q} \right] \right\}.$$

10.26 Strain rate sensitivity of flow stress

Let's consider the case of a boxed-shaped obstacle force-distance curve, from above

$$\dot{\gamma} = \dot{\gamma}_0 \exp \left\{ -\frac{\Delta G_0}{kT} \left[1 - \left(\frac{\sigma_s}{\hat{\tau}} \right)^{2/3} \right] \right\}$$

This leads to

$$\ln \dot{\gamma} = \ln \dot{\gamma}_0 - \frac{\Delta G_0}{kT} + \frac{\Delta G_0}{kT} \left(\frac{\sigma}{\hat{\tau}} \right)^{2/3}.$$

Define the stress exponent of the strain rate by

$$m \equiv \frac{d(\ln \dot{\gamma})}{d(\ln \sigma)} = \frac{2}{3} \frac{\Delta G_0}{kT} \left(\frac{\sigma}{\hat{\tau}} \right)^{2/3}$$

where a typical value of m is in the range 80 – 160.

10.27 Strain hardening at low temperatures

When a solid is plastically strained, glide dislocations that produce the plastic strain cut each other, become pinned and entangled, and accumulate. This results in increased dislocation interactions, and an increase in the dislocation resistance which is referred to as *strain hardening*. The process is very complex and in detail has defied accurate description. We will examine it by a simple form of dimensional analysis. We start out with the relation for the dislocation resistance

$$\tau = \tau_{disl} = \alpha\mu b\sqrt{\rho}, \quad \alpha \approx 0.2 - 0.4$$

where α could be temperature dependent. When due to strain hardening, due to an increment of strain $d\gamma$ the dislocation density increases by $d\rho$ the plastic resistance increases by

$$d\tau = \frac{\alpha\mu b}{2} \frac{d\rho}{\sqrt{\rho}}.$$

The plastic strain increment, however, is

$$d\gamma = \frac{d(b\sum\Delta a_i)}{V} = bd\left(\frac{l\Lambda_t}{V}\right) = bLd\left(\frac{\Lambda_t}{V}\right)$$

where $d\sum\Delta a_i$ is the increment over the entire area swept by dislocations. If we assume that dislocations traverse a mean free length L during these sweeps

$$\sum_i \Delta a_i = L\Lambda_t$$

where Λ_t is the total mobile length of dislocations and Λ_t/V is the total mobile line length/volume. For the specific increment of strain under consideration we assume (or imply) that this acting length is stored in the body upon the end of the increment when the dislocations have moved the length L . This gives

$$d\left(\frac{\Lambda_t}{V}\right) \simeq d\rho$$

for the increase of dislocation density stored. Then, $d\gamma = bld\rho$. By self similarity, we expect that the storage distance L is likely to be a multiple C of the mean dislocation spacing l , i.e. $L = Cl$ where $l = 1/\sqrt{\rho}$. Then, $d\gamma = bCd\rho/\sqrt{\rho}$ and the strain hardening rate

$$\frac{d\tau}{d\gamma} \simeq \frac{\alpha}{2C}\mu.$$

Computer experiments and other estimates puts $C \approx 25$ or so. This gives for the hardening rate h normalized with μ as

$$\frac{h}{\mu} \simeq \frac{\alpha}{2C} \in \left[\frac{1}{250}, \frac{1}{125} \right]$$

10.28 Deformation at elevated temperatures in the presence of diffusion

If deformation is administered above $T_m/2$, static thermal recovery can occur concurrently with deformation and at a steady state undo the effect of strain hardening. The undoing occurs inside tight clusters that pin the strain hardening induced dislocation network. This permits glide controlled

spontaneous elimination of large dislocation groups. The process is complex but we can again formulate a quick dimensional model. In tight clusters edge dislocations can become eliminated by climbing. This gives

$$\frac{d\rho}{dt} = -\frac{\rho}{t_a}$$

where t_a is the characteristic annihilation time. Solution of a load-diffusion equation gives

$$\frac{1}{t_a} \simeq Db^2\rho^2$$

where D is the self diffusion constant. Then

$$\frac{d\rho}{dt} = -\beta Db^2\rho^3$$

where β is a numerical constant. However, the overall dislocation density relates to the plastic (dislocation) resistance as

$$\tau = \alpha\mu b\sqrt{\rho}$$

where we understand τ to be governed only by the dislocation resistance. Thus

$$\frac{d\rho}{dt} = \frac{d}{dt} \left(\frac{\tau}{\alpha\mu b} \right)^2 = \frac{2}{\alpha\mu b} \frac{\tau}{\alpha\mu b} \frac{d\tau}{dt},$$

and upon substitution of the relation for reduction of dislocation density in its form related to the plastic resistance as

$$\frac{d\rho}{dt} = -\beta b^2 D \left(\frac{\tau}{\alpha\mu b} \right)^6$$

we have

$$\frac{1}{\alpha\mu} \left(\frac{d\tau}{dt} \right) = -\frac{\beta b^3 D}{2} \left(\frac{\tau}{\alpha\mu b} \right)^5.$$

Now considering that in a deformation situation τ increases due to strain due to our relation that we developed earlier

$$\frac{d\tau}{d\gamma} = \frac{\alpha\mu}{2C}$$

which we now consider as

$$\left(\frac{d\tau}{d\gamma} \right)_t = \frac{\alpha\mu}{2C}.$$

And, furthermore, τ decreases due to thermal recovery according to the above expression which we interpret as

$$\left(\frac{\partial\tau}{\partial t} \right)_\gamma = -\frac{\alpha\mu\beta b^2 D}{2} \left(\frac{\tau}{\alpha\mu b} \right)^5.$$

We note that under the two effects of straining and thermal recovery we have

$$d\tau = \left(\frac{\partial\tau}{\partial\gamma} \right)_t d\gamma + \left(\frac{\partial\tau}{\partial t} \right)_\gamma dt.$$

We note that a steady state with $d\tau = 0$ is possible when

$$\left(\frac{\partial\tau}{\partial\gamma} \right)_t \dot{\gamma}_{ss} + \left(\frac{\partial\tau}{\partial t} \right)_\gamma = 0$$

for here we get

$$\dot{\gamma}_{ss} = \frac{bC}{\alpha^6} \frac{D}{b^2} \left(\frac{\tau}{\mu} \right)^5$$

and since during deformation the applied stress and the reference resistance will retain a critical ratio we have the generalization

$$\dot{\gamma}_{ss} = \dot{\gamma}_0 \frac{D}{b^2} \left(\frac{\sigma_s}{\mu} \right)^m$$

where m is generally of order 5 for pure metals as modelled and $\dot{\gamma}_0$ now collects together a number of model sensitive parameters to which we don't want to commit ourselves. The self diffusion constant

$$D = D_0 \exp\left(-\frac{Q_D}{kT}\right)$$

where Q_D is the activation energy of self diffusion and $D_0 = zb^2\nu_D$ is the pre-exponential factor, where z is a local coordination number of sites between atom exchanges which can occur with vacancies which control the diffusion process.

$$z \simeq \mathcal{O}(3-6) \quad \text{and the atom frequency} \quad \nu_D \simeq 10^{13} \text{ s}^{-1}$$

10.29 Diffusional flow

Diffusional flow occurs by point (vacancy) transport. It can be shown that

$$\dot{\gamma}_{df} = \frac{16D_V\sigma\Omega}{b^2kT} \left[1 + \frac{\pi}{2} \frac{\delta}{d} \frac{D_B}{D_V} \right]$$

where Ω is the atomic volume, C_0 the thermal equilibrium concentration of vacancies, δ the grain boundary thickness, and d the grain size. Furthermore,

$$D_V = D_0 \exp\left(-\frac{Q_V}{kT}\right)$$

$$D_B = D_0 \exp\left(-\frac{Q_B}{kT}\right)$$

$$Q_B \simeq 0.6Q_V$$

At high temperatures, volume diffusion dominates $\dot{\gamma}_{df} \propto 1/d^2$, and at lower temperatures $\dot{\gamma}_{df} \propto 1/d^3$.

10.30 Connection between local ($\hat{\tau}$) and global (\hat{Y})

The deformation has to be compatible: deforming grains must continue to fit together. An upper bound solution can be found by assuming uniform strain everywhere. Five arbitrary slip systems are required.

$$dW = \hat{Y} d\varepsilon^p = \left\langle \sum_{i=1}^5 \hat{\tau} d\gamma_i \right\rangle = \hat{\tau} \left\langle \sum d\gamma_i \right\rangle$$

where $\langle \dots \rangle$ denotes an average value. This gives the Taylor factor m_T

$$\frac{\hat{Y}}{\hat{\tau}} = \frac{\langle \sum^5 d\gamma_i \rangle}{d\varepsilon^p} = m_T$$

For both FCC and BCC materials $m_T = 3.1$. Mechanism inspired phenomenology.

11.1 Plastic yielding under combined stresses

For a rate independent isotropic material the equivalent stress according to Von Mises is given by the empirical relation

$$\bar{\sigma} = \sqrt{\frac{1}{2} [(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]}.$$

If k is the yield strength in shear and Y is the yield strength in tension then we get $k = Y/\sqrt{3}$, and yielding will simply occur when $\bar{\sigma} = Y$. The equivalent stress for the case when all stress components are present becomes

$$\bar{\sigma} = \left(\frac{1}{2} [(\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2] + 3\sigma_{12}^2 + 3\sigma_{23}^2 + 3\sigma_{31}^2 \right)^{1/2}$$

which equivalently can be written as

$$\bar{\sigma} = \sqrt{\frac{3}{2} s_{ij} s_{ij}} = \sqrt{3J_2}.$$

In a similar fashion, Tresca's yield condition is defined by

$$\bar{\tau} = \frac{1}{2} (\sigma_{max} - \sigma_{min}),$$

yielding will occur when $\bar{\tau} = k$. As crystals are plastically deformed, the stress for plastic flow, called the flow stress, usually increases. We can now introduce a work equivalent plastic strain increment $d\bar{\varepsilon}^p$

$$dW^p = \bar{\sigma} d\bar{\varepsilon}^p = \left\{ \begin{array}{l} \text{for a} \\ \text{tension test} \end{array} \right\} = Y(\varepsilon^p) d\varepsilon^p.$$

The normal plastic strains should preserve volume $\varepsilon_{ii}^p = 0$. It can be shown that the equivalent plastic strain can be calculated from

$$d\bar{\varepsilon}^p = \sqrt{\frac{2}{3} d\varepsilon_{ij}^p d\varepsilon_{ij}^p}$$

which in expanded form becomes

$$d\bar{\varepsilon}^p = \left\{ \frac{2}{9} [(d\varepsilon_{11}^p - d\varepsilon_{22}^p)^2 + (d\varepsilon_{22}^p - d\varepsilon_{33}^p)^2 + (d\varepsilon_{33}^p - d\varepsilon_{11}^p)^2] + \frac{1}{3} [(d\gamma_{12}^p)^2 + (d\gamma_{23}^p)^2 + (d\gamma_{31}^p)^2] \right\}^{1/2}.$$

For the case of pure tension $d\bar{\varepsilon}^p = d\varepsilon_{33}^p$, and for the case of pure shear $d\bar{\varepsilon}^p = d\gamma_{23}^p/\sqrt{3}$, this is the background for the definition of the shear strain increment

$$d\bar{\gamma}^p = \sqrt{3} d\bar{\varepsilon}^p.$$

The individual strain increments are proportional to the components of the unit normal vector on the yield surface in the appropriate directions of stress, giving the associated flow rule

$$\frac{d\varepsilon_{11}^p}{d\varepsilon^p} = \frac{1}{\bar{\sigma}} \left[\sigma_{11} - \frac{1}{2}(\sigma_{22} + \sigma_{33}) \right]; \quad \text{cycl.}$$

$$\frac{d\gamma_{12}^p}{d\bar{\gamma}^p} = \frac{3\sigma_{12}}{\bar{\sigma}}; \quad \text{cycl.}$$

Note, since only the current direction of dislocation motion is determined by the current stress, the current stress determines only the current strain increments and not their total values as in elasticity. The concept of critical shear stress for slip and a stress strain relation can be considered valid only when applied to a region which is large compared both to mean spacing between dislocation sources and the mean distance of dislocation travel. The fact that the strain increment components plotted as vectors in six dimensional stress space are always normal to the yield locus is equivalent to the principal of maximum plastic resistance which states:

For any plastic strain increment, the state of stress actually occurring gives an increment of work which equals or exceeds the work which would be done by that strain increment $d\varepsilon_{ij}^p$, with any other state of stress within or on the yield locus. In equation form, if σ_{ij}^ represents any state of stress within or on the yield locus,*

$$(\sigma_{ij} - \sigma_{ij}^*) d\varepsilon_{ij}^p \geq 0.$$

11.2 Necking in tension (athermal idealization)

Necking will occur when the decrease in cross-sectional area is more rapid than the increase of flow stress due to strain-hardening.

$$dP = YdA + AdY.$$

Necking will occur when $dP = 0$. Also,

$$dV = Adl + ldA = 0 \Rightarrow \frac{dA}{A} = -\frac{dl}{l} = -d\varepsilon,$$

which leads to the necking condition

$$\frac{dY}{d\varepsilon^p} = Y, \quad \frac{d\bar{\sigma}}{d\varepsilon^p} = \bar{\sigma}.$$

For the case when the strain hardening behavior is given by

$$Y = Y_0 \varepsilon^n \quad (n < 1.0)$$

the necking condition becomes $\varepsilon_n = n$.

11.3 General strategies for approximate solutions in elasticity and plasticity

The solution of specific problems in elastic and plastic or rigid plastic behavior in general involve considerable complexities. Specific solutions of problems are often only accessible through numerical techniques which will not be considered here. Instead, we will consider a selection of specific problems in elastic behavior and plastic non-hardening behavior by approximate methods which are designed to bound the exact solution, and with some care can give very useful insight into the exact solution.

First we consider elastic behavior. In elasticity we know the solution of problems requires satisfaction of: equilibrium, compatibility, constitutive equations and boundary conditions of imposed stress and displacement. When such a solution is obtained it is unique and the elastic strain energy associated with it is less than any other solution that does not satisfy all these conditions, or only satisfies some of them. Thus, in elasticity most approximate solutions are based on the minimum potential energy principle. We will here use this approach to develop some useful bounding solutions for the elastic properties of quasi-randomly arrayed heterogeneous solids. We will start out by noting that in elasticity the shear and the bulk behavior of a solid are physically uncoupled and that the elastic strain energy due to dilatation is uncoupled from the elastic strain energy of the shear process. Based on this observation and the minimum elastic strain energy principle we want to determine the elastic properties of heterogeneous media made up of say n different component materials of isotropic properties each occupying a given volume fraction c_i . Each component possesses a shear modulus and a bulk modulus

$$\mu_i = \frac{d\tau_i}{d\gamma_i} \quad \text{and} \quad K_i = \frac{d\sigma_i}{d\varepsilon_i}$$

where τ_i is the shear stress, γ_i is the shear strain, σ_i the mean normal stress, and ε_i the dilatation. We consider a solid in which the components are roughly equiaxed and are statistically random distributed with no particular order. If under some condition or applied stress the exact answer was known we could obtain the overall elastic strain energy in any particular component part as

$$\begin{aligned} dU_i &= \frac{1}{2}(\sigma\varepsilon)_i dV_i + \frac{1}{2}(\tau\gamma)_i \\ &= \frac{1}{2} \frac{\sigma_i^2}{K_i} dV_i + \frac{1}{2} \frac{\tau_i^2}{\mu_i} dV_i \\ &= \frac{1}{2} K_i \varepsilon_i^2 dV_i + \frac{1}{2} \mu_i \gamma_i^2 dV_i \end{aligned}$$

where for the shear energy we are considering as a generic example only one component. Then the overall elastic strain energy of the composite would be

$$U_c = \sum_{i=1}^n \left[\frac{1}{2} \int_{V_i} (\sigma\varepsilon)_i dV_i + \frac{1}{2} \int_{V_i} (\tau\gamma)_i dV_i \right].$$

For the exact solution this strain energy U_c is a minimum in relation to any variation of the solution. We could obtain the elastic constants of this uniaxial form from two separate experiments. From a dilatation experiment

$$\frac{1}{2} \sigma_c \varepsilon V = \frac{1}{2} K_c \varepsilon^2 V = U_c = \sum_{i=1}^n \int_{V_i} \frac{1}{2} \sigma_i \varepsilon_i dV_i.$$

Then

$$K_c = \frac{d^2(U_c/V)}{d\varepsilon^2} = \frac{1}{V} \frac{d^2}{d\varepsilon^2} \left[\sum_{i=1}^n \frac{1}{2} \int_{V_i} K_i \varepsilon_i^2 dV_i \right].$$

In a related shear experiment we find

$$\mu_c = \frac{d^2(U_c/V)}{d\gamma^2} = \frac{1}{V} \frac{d^2}{d\gamma^2} \left[\sum_{i=1}^n \int_{V_i} \mu_i \gamma_i^2 dV_i \right].$$

In general the exact answer for the stress and strain distribution in the interior, in the components is not available. Therefore, we are interested in obtaining approximate solutions. We will do so by satisfying either equilibrium or compatibility separately. This provides bounds to the answer.

11.4 The upper bound theorem for a rigid-plastic solid

In a rigid-plastic continuum, deformation must occur under any system of loads P_k for which a distribution of displacements can be found such that

- the displacement boundary conditions, if any, are satisfied,
- the displacements can be differentiated to give a strain, with no change in volume anywhere, and
- the resulting plastic work done throughout the material, found from the resulting equivalent strain, is less than the work done by the external loads acting through the assumed displacements:

$$\sum_k P_k dp_k > \int_V \bar{\sigma}_Y d\bar{\varepsilon}^p dV$$

where $\bar{\sigma}_Y$ is the equivalent flow stress.

11.5 The lower bound theorem for a rigid-plastic solid

In a rigid-plastic continuum there can be no plastic deformation under loads for which a stress distribution can be found which

- everywhere satisfies the equilibrium equations,
- is in equilibrium with external loads, and,
- is everywhere within the yield locus.

11.6 The self consistent method

The self consistent method is based on the fundamental solution of Eshelby (1957) which states that for an ellipsoidal inclusion in an infinite medium the elastic stress and strain field in the interior is uniform when the body as a whole is subjected to a distant uniform stress field. Then we get $d\sigma_{ij}^m = C_{ijkl}^m d\varepsilon_{kl}^m$ for inclusion m , and $d\sigma_{ij} = C_{ijkl} d\varepsilon_{kl}$ for the composite. The Eshelby solution states

$$d\sigma^i = B^i(C^i, C)d\sigma.$$

Consider now a heterogeneous medium with n different component phases with known elastic properties and known volume fractions c_i . The self consistent method considers n reference Eshelby problems for each one, one particular component is considered as a spherical inclusion in the composite of unknown and to be determined elastic properties. Since, all n components fill the entire volume, the overall field of the component, whether that is stress, strain, or elastic strain energy is made up of the volume fraction average of the individual fields. This is the so-called self consistent statement, i.e.

$$\sum_{i=1}^n c_i d\sigma^i = d\sigma,$$

but with the stress concentration tensor B^i introduced

$$\sum_{i=1}^n c_i B^i(C^i, C)d\sigma = d\sigma.$$

This is the self consistent statement and furnishes as many equations as there are unknown components of elastic constants. The closed form solution for the bulk and shear modulus of an initially isotropic composite with isotropic components becomes

$$\sum_{i=1}^n \frac{c_i}{1 + \left(\frac{\mu_i}{\mu} - 1\right) \beta^*} = 1$$

$$\sum_{i=1}^n \frac{c_i}{1 + \left(\frac{K_i}{K} - 1\right) \alpha^*} = 1$$

where

$$\alpha^* = \frac{1 + \nu}{3(1 - \nu)}, \quad \beta^* = \frac{2(4 - 5\nu)}{15(1 - \nu)}$$

where ν is the composite Poisson's ration given by

$$\nu = \frac{3K - 2\mu}{6K + 2\mu} = \frac{1 - \frac{2\mu}{3K}}{2 + \frac{2\mu}{3K}}$$

The self consistent results are generally very good when the components are of light concentration.

11.7 Plasticity analysis by slip line fields

Consider a rigid non-hardening material for application in plane strain. For this situation $d\varepsilon_{33}^p = 0$ giving $\sigma_{33} = (\sigma_{11} + \sigma_{22})/2$. By plugging this in the yield criterion we get

$$\bar{\sigma} = Y = \frac{\sqrt{3}}{2}(\sigma_1 - \sigma_3)$$

but since we also have $k = Y/\sqrt{3}$, we get

$$\sigma_1 - \sigma_2 = \pm 2k$$

when considering principal stresses. Similarly, we define the mean normal stress as $\sigma = (\sigma_1 + \sigma_2)/2$. Consider a coordinate system α, β that is parallel to the principal shear directions and rotated an angle φ with respect to the 1, 2 plane. Then by Mohr's circle we get

$$\begin{aligned} \sigma_{11} &= \sigma - 2 \sin 2\varphi, \\ \sigma_{22} &= \sigma + 2 \sin 2\varphi, \\ \sigma_{12} &= k \cos 2\varphi. \end{aligned}$$

By inserting these equations into the equilibrium equations, and then consider the 1, 2 axes to parallel to α , and β ($\sin 2\varphi = 0$, $\cos 2\varphi = 1$) we get

$$\begin{aligned} \frac{\partial \sigma}{\partial x_1} - 2k \frac{\partial \varphi}{\partial x_1} &= 0, \\ \frac{\partial \sigma}{\partial x_2} + 2k \frac{\partial \varphi}{\partial x_2} &= 0. \end{aligned}$$

Integrating these two equations

$$\begin{aligned} \sigma - 2k\varphi &= \text{const.} && \text{along } \alpha\text{-line} \\ \sigma + 2k\varphi &= \text{const.} && \text{along } \beta\text{-line} \end{aligned}$$

12.1 Finite deformation considerations

The method described here may be called an isomorphic mapping of space. That is, we consider a correspondence between points \mathbf{x} in a reference or initial space and points \mathbf{X} in a space mapped from this initial space. This is represented by the transformation

$$\mathbf{x} \rightarrow \mathbf{X}. \quad (1)$$

The space or region mapped out by \mathbf{X} will be of different shape, size and position to that mapped out by \mathbf{x} . Equation (1) may also be written

$$\mathbf{X} = \mathbf{u} + \mathbf{x}.$$

Here \mathbf{X} , \mathbf{x} , \mathbf{u} are vectors in three-dimensional space and the representation used for them is by the same *fixed* Cartesian co-ordinate axis system. By considering the change in the length of a infinitesimal line element during the deformation it is easy to derive the Lagrangian (or Eulerian) strain tensor. It is also possible to show that

$$dV = Jdv,$$

where $J = \det(\partial\mathbf{X}/\partial\mathbf{x})$. A homogeneous transformation is one in which $\partial X_\alpha/\partial x_\beta$ are independent of position. In this case we directly obtain

$$\mathbf{X} = \mathbf{D}\mathbf{x}.$$

For transformations which describe real deformations, it is clear that \mathbf{D} will be a real non-singular matrix. The polar factorization theorem can be stated as follows:

Every real non-singular matrix is uniquely expressible as a product of a real orthogonal matrix and a positive-definite real symmetric matrix.

Also: an orthonormal real set of eigenvectors can be chosen for a real symmetric matrix. The reciprocal of an orthogonal matrix equals its transpose. The finite strain tensor can be written as

$$2\boldsymbol{\eta} = \mathbf{D}^T\mathbf{D} - \mathbf{E}.$$

12.2 Derivation of the Lagrangian strain tensor

Suppose that two material particles, before the motion, have coordinates (a_i) , $(a_i + da_i)$; after the motion, let their respective coordinates be (x_i) , $(x_i + dx_i)$. Then the initial and final distances between these neighboring particles are given by

$$ds_0^2 = da_i da_i,$$

$$ds^2 = dx_i dx_i.$$

Let the displacement vector be defined by $u_i \equiv x_i - a_i$, then $ds^2 - ds_0^2$ is

$$\begin{aligned}
 ds^2 - ds_0^2 &= dx_i dx_i - da_i da_i \\
 &= \frac{\partial x_t}{\partial a_i} da_i \frac{\partial x_t}{\partial a_j} da_j - \delta_{ij} da_i da_j \\
 &= \left[\frac{\partial x_t}{\partial a_i} \frac{\partial x_t}{\partial a_j} - \delta_{ij} \right] da_i da_j \\
 &= \left[\left(\delta_{it} + \frac{\partial u_t}{\partial a_i} \right) \left(\delta_{jt} + \frac{\partial u_t}{\partial a_j} \right) - \delta_{ij} \right] da_i da_j \\
 &= \left[\frac{\partial u_i}{\partial a_j} + \frac{\partial u_j}{\partial a_i} + \frac{\partial u_t}{\partial a_i} \frac{\partial u_t}{\partial a_j} \right] da_i da_j
 \end{aligned}$$

Define the Lagrangian strain tensor as

$$E_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial a_j} + \frac{\partial u_j}{\partial a_i} \right) + \frac{1}{2} \frac{\partial u_t}{\partial a_i} \frac{\partial u_t}{\partial a_j},$$

and hence,

$$ds^2 - ds_0^2 = 2E_{ij} da_i da_j.$$

12.3 Derivation of the Eulerian strain tensor

$$\begin{aligned}
 ds_0^2 &= da_i da_i, \\
 ds^2 &= dx_i dx_i.
 \end{aligned}$$

Let the displacement vector be defined by $u_i \equiv x_i - a_i$, then

$$\begin{aligned}
 ds^2 - ds_0^2 &= dx_i dx_i - da_i da_i \\
 &= \left[\delta_{ij} - \frac{\partial a_t}{\partial x_i} \frac{\partial a_t}{\partial x_j} \right] dx_i dx_j \\
 &= \left[\delta_{ij} - \left(\delta_{ti} - \frac{\partial u_t}{\partial x_i} \right) \left(\delta_{tj} - \frac{\partial u_t}{\partial x_j} \right) \right] dx_i dx_j \\
 &= \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{\partial u_t}{\partial x_i} \frac{\partial u_t}{\partial x_j} \right] dx_i dx_j \\
 &= 2e_{ij} dx_i dx_j
 \end{aligned}$$

where

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

13.1 Constitutive similarities between an ideal gas and an ideal rubber

Compressing an ideal gas is similar to deforming rubber in that they both deform without storing internal energy and both go back to original shape upon unloading. To show this consider a quasistatic reversible process

$$dE = TdS - PdV. \quad (1)$$

The total differential of Helmholtz free energy

$$dA = -PdV - SdT$$

gives the Maxwell relation

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial S}{\partial V}\right)_T. \quad (2)$$

Equations (1) and (2) can now be combined to yield

$$\frac{\partial E}{\partial V} = T \left(\frac{\partial P}{\partial T}\right)_V - P,$$

which for an ideal gas, $PV = nRT$, results in

$$\frac{\partial E}{\partial V} = 0.$$

13.2 Definition of tensile creep compliance and tensile stress relaxation modulus

The tensile creep compliance, $D_c(t)$, is defined by

$$D_c(t) = \frac{\varepsilon(t)}{\sigma_0}.$$

And the tensile stress relaxation modulus, $E_r(t)$, is defined by

$$E_r(t) = \frac{\sigma(t)}{\varepsilon_0}.$$

The characteristic relaxation time is defined as the time at which the stress has been reduced down to $1/e \approx 37\%$ of the initial stress (in a stress relaxation test). Also, note that the time dependence of D_c and E_r is weaker for a crosslinked or semi-crystalline material than for a corresponding uncrosslinked amorphous material.

13.3 Time temperature superposition

For rheologically simple materials, the time-temperature superposition makes it possible to extrapolate mechanical data obtained within a narrow time interval to much shorter and longer time scales where no actual measurements have been made. This procedure has been generally found to hold with amorphous polymers (at temperatures up to $T_g + 100^\circ\text{C}$) for measurements made at small strains in regions 2, 3 and 4.

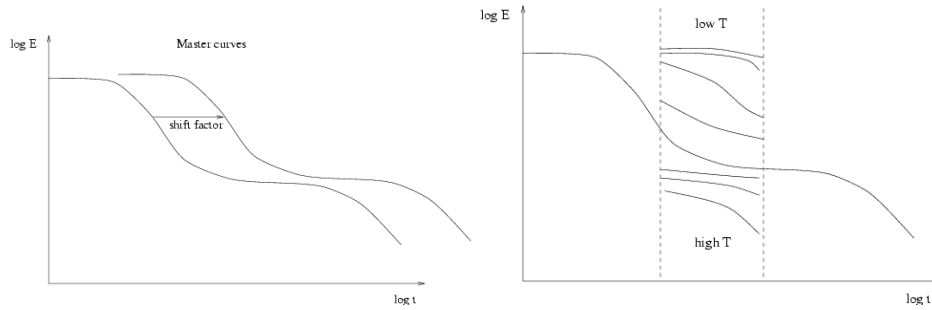
The amount of horizontal shift or “shift factor” necessary to effect superposition can be calculated by use of the WLF (Williams, Landel, Ferry) equation:

$$\log a_T(T) = \frac{-C_1(T - T_0)}{C_2 + (T - T_0)},$$

where T_0 is a reference temperature and C_1 and C_2 are constants that are the same for almost all amorphous polymers. The constants depend, however, on the choice of reference temperature. At the glass transition temperature, for example, the constants are $C_1 = 17.44$ and $C_2 = 51.6$. These constants amounts to a shift factor of about 3°C per decade time.

13.4 How to obtain a master curve

A master curve for a material can be obtained by performing experiments under a restricted time interval but using different temperatures.



The master curve for the specific temperature is then obtained by holding the curve segment corresponding to the specific temperature fixed and shifting the other curves horizontally until one continuous curve is obtained. Note, however, that this does not work for semi crystalline materials since the curves will not fit upon horizontal shifting. The reason for this is that not everything 'speeds up' the same when the temperature is raised. Also note that $\log E - T$ curves can be determined directly from the set of curves shown in the figure above.

13.5 Boltzmann's equation for linear viscoelastic materials

Consider a body that is subjected to the load $d\sigma$ at time τ . If the material is linear viscoelastic then the strain response is given by

$$d\varepsilon(t) = D_c(t - \tau)d\sigma.$$

By virtue of the linear and time invariant properties of the material we can generalize this equation and obtain

$$\varepsilon(t) = \int_{-\infty}^t D_c(t - \tau) \frac{d\sigma(\tau)}{d\tau} d\tau$$

for an amorphous polymer under uniaxial loading. $D_c(t - \tau)$ is called the kernel and has to be determined by experiments. It can similarly be shown that

$$\sigma(t) = \int_{-\infty}^t E(t - \tau) \frac{d\varepsilon(\tau)}{d\tau} d\tau.$$

The variables used in the first form of Boltzmann's equation can be interpreted as follows: τ stands for stress-input time, t stands for strain-output time, and $(t - \tau)$ stands for polymer memory time.

13.6 Connection between the creep compliance and the stress relaxation modulus

The connection between creep compliance and stress relaxation modulus can be determined by the Laplace transform,

$$\mathcal{L}[f(t)] \equiv F(P) \equiv \int_0^{\infty} e^{-pt} f(t) dt.$$

By applying the Laplace transformation to the two integral forms of Boltzmann's equation we obtain

$$\mathcal{L}[\sigma(t)] = \frac{1}{p^2 \mathcal{L}[D(t)]}$$

which can be rearranged as

$$\int_0^t E(t-\tau)D(\tau)d\tau = \int_0^t D(t-\tau)E(\tau)d\tau = t.$$

The product $E_r(t)D_c(t)$ is close to unity in region 1 and 3, but closer to zero in region 2 and 4. This can be used as a means of determining in which region of mechanical equivalence a polymer is in.

Furthermore, McLoad developed the approximation

$$D_c(t)E_r(t) \simeq \frac{\sin mt}{m\pi}$$

where m is the negative slope of the master curve.

13.7 The correspondence principle

Assume that the stress is spatially separable, i.e. $\sigma(\mathbf{x}, t) = f_1(\mathbf{x})f_2(t)$, then Boltzmann's equation becomes

$$\varepsilon(\mathbf{x}, t) = f_1(\mathbf{x}) \int_0^t D_c(t-\tau) \frac{df_2(\tau)}{d\tau} d\tau,$$

which for the case of creep

$$f_2(\tau) = \sigma_0 H(\tau),$$

where $H(\tau)$ is the Heaviside step function, leads to

$$\varepsilon(\mathbf{x}, t) = f_1(\mathbf{x})\sigma_0 D_c(t).$$

Hence, for creep loading, linear elasticity solutions can be used if E is replaced by $1/D_c(t)$.

Similarly, for the case when the strain is spatially separable and the loading consists of a constant strain; we can determine the linear viscoelastic response by replacing E by $E_r(t)$.

13.8 ODE representation of Boltzmann's equation

Boltzmann's equation can equivalently be represented as a linear ODE with constant coefficients

$$a_n \frac{d^n \varepsilon}{dt^n} + \dots + a_0 \varepsilon = b_m \frac{d^m \sigma}{dt^m} + \dots + b_0 \sigma.$$

In a relaxation test, the right hand side of the equation above becomes zero, and the solution to the differential equation can be written as

$$\varepsilon(t) = \sum_i^n c_i e^{p_i t}.$$

Mechanical memory of a material is the ability of the material to eventually return to the original state of strain. Note that an elastic material has complete and instantaneous recovery. Thus, a material exhibits complete recovery if, and only if, all roots of the characteristic equation are negative. Furthermore, sometimes a material has optical memory (something that can be measured by birefringence).

Applicability of linear viscoelasticity: in region 1, the strain has to be $\lesssim 1\%$; increases sharply above T_g , becomes $\simeq 100\%$ strain close to $T_g + 50^\circ \text{ C}$.

13.9 Constitutive relation for an ideal rubber

The constitutive relation for an ideal rubber can, somewhat simplistically, be written

$$\sigma_x = \frac{3\rho RT}{M_C} \left(\lambda - \frac{1}{\lambda^2} \right)$$

13.10 Constitutive relations for a Maxwell body

For a Maxwell body the strain rate is given by

$$\dot{\epsilon} = \frac{\sigma}{\eta} + \frac{\dot{\sigma}}{E}$$



For a stress relaxation experiment ($\dot{\epsilon} = 0$) the constitutive relation becomes

$$\sigma = \sigma_0 \exp\left(\frac{-t}{\tau}\right),$$

where $\tau = \eta/E$. Furthermore, the characteristic relaxation time is defined by $\tau = t$, which leads to $\sigma = \sigma_0/e \approx 0.37\sigma_0$.

13.11 Viscoelastic damping

Consider a viscoelastic system that is subjected to a sinusoidal strain. Due to the material behavior the stress response will be out of phase. Introduce the following definitions:

E' = The fraction of the stress which follows the imposed strain without any delay, divided by the strain itself. Is called the *storage modulus*.

E'' = The fraction of the stress which follows the imposed strain with a delay of 90° divided by the strain. Is called the *loss modulus*.

Can also define a complex modulus by

$$E^*(\omega) = E'(\omega) + iE''(\omega),$$

and a loss tangent

$$\tan \delta = \frac{E''(\omega)}{E'(\omega)}$$

13.12 Linear Viscoelasticity Theory

When subjected to an external loading agent many materials do not exhibit a purely elastic or purely viscous response, but a combination of the two. The simplest way to model this behavior is through linear viscoelasticity. This material representation has been used and studied extensively for many years, but despite this there are some aspects of the theory that can be difficult to grasp at first, and also since other more complicated models often are generalizations of this theory, a relatively detailed derivation is given below.

The foundation of linear viscoelasticity theory is the Boltzmann's ? superposition principle which is discussed next.

Boltzmann's Superposition Principle.

One way to state the Boltzmann's superposition principle is through the statement:

Each loading step makes an independent contribution to the final state.

This idea can be used to formulate an integral representation of linear viscoelasticity. The strategy is to perform an experiment in which a step function in strain is applied, $\varepsilon(t) = \varepsilon_0 H(t)$, and the stress response $\sigma(t)$ is measured. Then a stress relaxation modulus can be defined by $G(t) = \sigma(t)/\varepsilon_0$. Note that ε_0 does not have to be infinitesimal due to the assumed superposition principle.

To develop a model capable of predicting the stress response due to an arbitrary strain history, start by decomposing the strain history into a sum of infinitesimal strain steps:

$$\varepsilon(t) = \sum_i \Delta\varepsilon_i H(t - \tau_i) \quad (1)$$

the stress response can therefore directly be written

$$\sigma(t) = \sum_i \Delta\varepsilon_i G(t - \tau_i). \quad (2)$$

In the limit as the number of strain increments goes to infinity, the stress response (2) becomes

$$\sigma(t) = \int_{-\infty}^t G(t - \tau) d\varepsilon(\tau) = \int_{-\infty}^t G(t - \tau) \frac{d\varepsilon(\tau)}{d\tau} d\tau. \quad (3)$$

Note that if $G(t) = G_0$, then $\sigma(t) = G_0\varepsilon(t)$. If only the response in one loading mode (i.e. uniaxial loading) is of interest, then it is sufficient to determine the stress relaxation modulus for that loading mode and then by using Equation (3) the response due to any imposed deformation can be obtained.

If Equation (3) is generalized to a three-dimensional deformation state for an isotropic material, the following relationship is obtained:

$$\mathbf{T}(t) = \int_0^t 2G(t - \tau) \dot{\varepsilon} d\tau + \mathbf{I} \int_0^t K(t - \tau) \dot{\phi} d\tau \quad (4)$$

where $G(t)$ is the stress relaxation shear modulus, $\dot{\varepsilon}$ the rate of change of deviatoric strains, $K(t)$ the stress relaxational bulk modulus, and $\dot{\phi}$ the rate of change of volumetric strains. That is, only two relaxation moduli need to be determined to predict any arbitrary deformation. The corresponding relationship for a general anisotropic material is

$$\sigma_{ij}(t) = G_{ijkl}(0)\varepsilon_{kl}(t) + \int_0^t \varepsilon_{kl}(t - s) \frac{dG_{ijkl}(s)}{ds} ds. \quad (5)$$

Note, to be able to predict the stress response at any arbitrary strain history it is sufficient to know the stress relaxation modulus, and to be able to follow a stress history the creep compliance needs to be known.

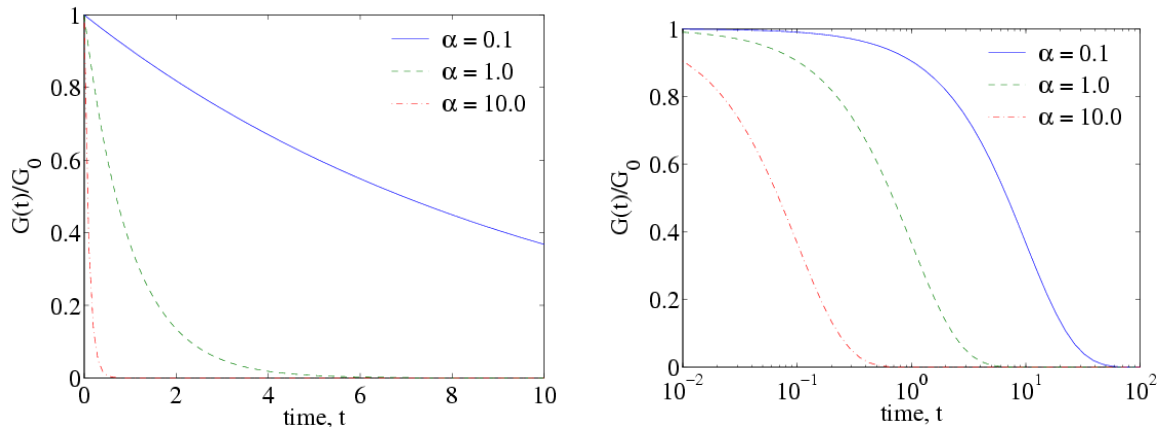
Example 1. Consider once again a general one-dimensional loading case. To exemplify the model consider first a case in which

$$G(t) = \begin{cases} G_0 \exp(-\alpha_0 t) & \text{if } t \geq 0, \\ 0 & \text{if } t < 0 \end{cases} \quad (6)$$

and

$$\varepsilon(t) = \begin{cases} 0 & \text{if } t < 0, \\ \dot{\varepsilon} t & \text{if } t \geq 0, \end{cases} \quad (7)$$

see Figure below.

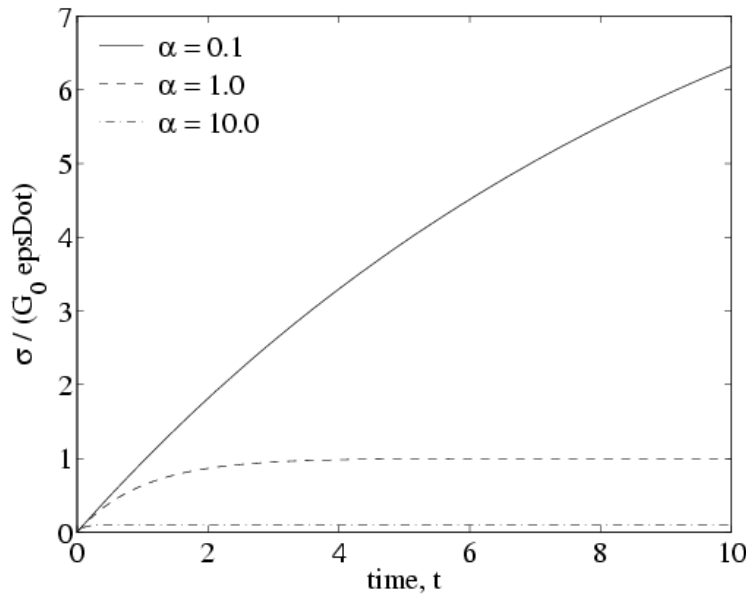


Equation (3) then gives

$$\sigma(t) = \int_0^t G_0 \dot{\epsilon} \exp[-\alpha_0(t - \tau)] d\tau,$$

yielding

$$\sigma(t) = \frac{G_0 \dot{\epsilon}}{\alpha_0} [1 - \exp(-\alpha_0 t)]. \quad (8)$$

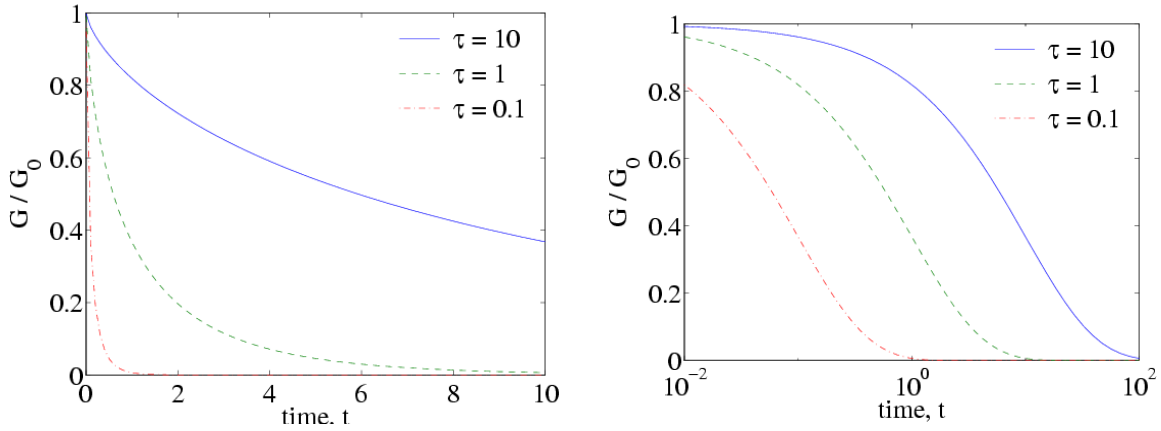


The result is plotted in the figure above, illustrating that large α_0 corresponds to fast relaxation. From (8) it is also clear that the stress response is always predicted to be proportional to the applied strain rate. And even if a relaxation spectrum is chosen, the Boltzmann's superposition principle does not allow for a sigmoidal shaped stress-strain response. ■

Another commonly used functional form of the relaxation modulus is the stretched exponential:

$$G(t) = G_0 \exp \left[- \left(\frac{t}{\tau_0} \right)^\beta \right] \quad (9)$$

which is plotted in the figure below.



If we again consider a constant strain rate loading situation, the stress response becomes

$$\sigma(t) = \int_0^t G_0 \dot{\epsilon} \exp \left[- \left(\frac{t}{\tau_0} \right)^\beta \right] dt$$

which is not easy to express in elementary functions, but it is clear that $\sigma(t)$ is still proportional to $\dot{\epsilon}$.

Example 2. As a last example consider

$$G(t) = \begin{cases} G_0 \exp(-\alpha_0 t) & \text{if } t \geq 0, \\ 0 & \text{if } t < 0 \end{cases} \quad (10)$$

and

$$\varepsilon(t) = \begin{cases} 0 & \text{if } t < 0, \\ \varepsilon_0 \sin(\omega_0 t) & \text{if } t \geq 0, \end{cases} \quad (11)$$

giving

$$\begin{aligned} \sigma(t) &= \int_0^t G_0 \exp(-\alpha t) \varepsilon_0 \omega_0 \cos(\omega_0 \tau) d\tau \\ &= \frac{G_0 \varepsilon_0 \omega_0}{\alpha_0^2 + \omega_0^2} [\alpha_0 \cos(\omega_0 t) + \omega_0 \sin(\omega_0 t) - \alpha_0 \exp(-\alpha_0 t)]. \end{aligned} \quad (12)$$

■

It is also possible to formulate the whole theory for the case when the stress is the driving quantity. If in this case the creep compliance is defined as $J(t) = \varepsilon(t)/\sigma$, the resulting strain can be calculated from

$$\varepsilon(t) = \int_{-\infty}^t J(t - \tau) \frac{d\sigma(\tau)}{d\tau} d\tau. \quad (13)$$

Storage and Loss Moduli.

As a final illustration will also be shown how the theory can be applied to a sinusoidally driving strain state specified by

$$\varepsilon(t) = \varepsilon_0 \sin(\omega t). \quad (14)$$

The resulting stress response can be written:

$$\sigma(t) = \int_0^\infty G(s)\omega\varepsilon_0 \cos[\omega(t-s)] ds \quad (15)$$

where $s \equiv t - \tau$. This equation can be expanded into

$$\begin{aligned} \sigma(t) = \varepsilon_0 \sin(\omega t) \left[\omega \int_0^\infty G(s) \sin(\omega s) ds \right] \\ + \varepsilon_0 \cos(\omega t) \left[\omega \int_0^\infty G(s) \cos(\omega s) ds \right]. \end{aligned} \quad (16)$$

Note that the integrals only converge if

$$\lim_{s \rightarrow \infty} G(s) = 0. \quad (17)$$

By defining two frequency-dependent functionals: the storage modulus $G'(\omega)$ and the loss modulus $G''(\omega)$, the stress response can be written

$$\sigma(t) = \varepsilon_0 [G'(\omega) \sin(\omega t) + G''(\omega) \cos(\omega t)]. \quad (18)$$

or alternatively

$$\sigma(t) = \sigma_0 \sin(\omega t + \delta) \quad (19)$$

$$= \sigma_0 \sin(\omega t) \cos \delta + \sigma_0 \cos(\omega t) \sin \delta \quad (20)$$

hence

$$\varepsilon_0 G'(\omega) = \sigma_0 \cos \delta \quad (21)$$

$$\varepsilon_0 G''(\omega) = \sigma_0 \sin \delta \quad (22)$$

giving

$$\frac{G''}{G'} = \tan \delta \quad (23)$$

It is often convenient to introduce a complex variable based notation

$$G^* = \frac{\sigma^*}{\varepsilon^*} = G' + iG'' \quad (24)$$

It is also possible to consider a stress driven oscillation giving a complex compliance:

$$J^* = \frac{\varepsilon^*}{\sigma^*} = \frac{1}{G^*} = J' - iJ'' \quad (25)$$

The relationships between J' , J'' , G' and G'' are:

$$J' = \frac{G'}{G'^2 + G''^2} \quad (26)$$

$$J'' = \frac{G''}{G'^2 + G''^2} \quad (27)$$

$$G' = \frac{J'}{J'^2 + J''^2} \quad (28)$$

$$G'' = \frac{J''}{J'^2 + J''^2} \quad (29)$$

Spectra.

Several different means of specifying viscoelastic mechanical properties have been given. Specifically, relaxation functions, creep functions and complex moduli have been discussed. Another way of characterizing the material response is through spectra. To introduce the concept of a relaxation spectrum consider the relaxation modulus

$$G(t) = \sum_n G_n \exp \left[\frac{-t}{\tau_n} \right]. \quad (30)$$

In the limit as $n \rightarrow \infty$ the summation is replaced by an integral:

$$G(t) = \int_0^\infty f(\tau) \exp \left[\frac{-t}{\tau} \right] d\tau. \quad (31)$$

The function $f(\tau)$ is called the relaxation time spectrum. In practice it is often more convenient to use a logarithmic time scale

$$G(t) = \int_{-\infty}^{+\infty} H(\tau) \exp \left[\frac{-t}{\tau} \right] d(\ln \tau) + G(\infty). \quad (32)$$

Similarly, a retardation time spectrum can be defined by

$$J(t) = \int_{-\infty}^{+\infty} L(\tau) \left[1 - \exp \left(\frac{-t}{\tau} \right) \right] d(\ln \tau) + J(\infty). \quad (33)$$

It is possible to solve for $H(t)$ and $L(t)$ by using Laplace transforms, see ? for details.

Relationships Between Different Viscoelastic Functions.

The formal relationship between the relaxation modulus $G(t)$ and the creep compliance $J(t)$ can be derived by taking the Laplace transformation of Equations (3) and (13)

$$\tilde{\sigma}(s) = s\tilde{G}(s)\tilde{\varepsilon}(s) \quad (34)$$

$$\tilde{\varepsilon}(s) = s\tilde{J}(s)\tilde{\sigma}(s) \quad (35)$$

which can be rewritten as

$$\tilde{G}(s) = \frac{1}{s^2\tilde{J}(s)}. \quad (36)$$

Based on the Laplace limit theorems it can be shown ? that:

$$\lim_{t \rightarrow 0} J(t) = \lim_{t \rightarrow 0} \frac{1}{G(t)} \quad (37)$$

$$\lim_{t \rightarrow \infty} J(t) = \lim_{t \rightarrow \infty} \frac{1}{G(t)} \quad (38)$$

Also since $\mathcal{L}^{-1}(1/s^2) = t$ we directly get:

$$\int_0^t G(t-\tau)J(\tau)d\tau = \int_0^t J(t-\tau)G(\tau)d\tau = t. \quad (39)$$

Differential Form of the Integral Representation.

In this section will be shown that the integral form

$$\sigma(t) = \int_{-\infty}^t G(t-\tau) \frac{d\varepsilon(\tau)}{d\tau} d\tau. \quad (3\text{-rep})$$

can also be written in differential form as

$$P(D)\sigma(t) = Q(D)\varepsilon(t) \quad (40)$$

where $P(D)$ and $Q(D)$ are polynomials of $D \equiv d/dt$.

To show this start by taking the Laplace transform of Equation (40):

$$P(s)\tilde{\sigma}(s) - \frac{1}{s} \sum_{k=1}^N p_k \sum_{r=1}^k s^r \sigma^{(k-r)}(0) = Q(s)\tilde{\varepsilon}(s) - \sum_{k=1}^N q_k \sum_{r=1}^k s^r \varepsilon^{(k-r)}(0). \quad (41)$$

The Laplace transform of (3) is

$$\tilde{\sigma}(s) = s\tilde{G}(s)\tilde{\varepsilon}(s), \quad (34\text{-rep})$$

demonstrating that the two forms are equal if

$$s\tilde{G}(s) = \frac{\tilde{Q}(s)}{\tilde{P}(s)} \quad (42)$$

and

$$\sum_{r=k}^N p_r \sigma_{ij}^{r-k}(0) = \sum_{r=k}^N q_r \varepsilon^{r-k}(0), \quad k = 1, 2, \dots, N \quad (43)$$

which is a restriction on the initial conditions.

Rheological Models—Maxwell Model.

The Maxwell rheological model constitutes a linear spring ($\sigma = E\varepsilon_1$) and a linear dashpot ($\dot{\varepsilon}_2 = \sigma/\eta$) in series. The rate of change in strain of the system is given by

$$\dot{\varepsilon} = \frac{\dot{\sigma}}{E} + \frac{\sigma}{\eta} \quad (44)$$

which is the differential representation. Now consider a stress relaxation experiment $\varepsilon(t) = \varepsilon_0 H(t)$ giving

$$\frac{d\sigma}{dt} + \frac{E}{\eta}\sigma = 0, \quad (\text{for } t > 0)$$

having the solution

$$\sigma(t) = \sigma_0 \exp\left[\frac{-t}{\eta/E}\right]. \quad (45)$$

Hence the stress relaxation function for the Maxwell model is

$$G(t) = G_0 \exp\left[\frac{-t}{\eta/E}\right].$$

In this section the key aspects of linear viscoelasticity theory has been presented. It has been shown that to characterize the material only one² functional form needs to be determined. The material functional can be determined through one creep, stress relaxation or oscillatory experiment. Once the material dependent functional has been determined the response due to any arbitrary imposed deformation or loading can be directly calculated.

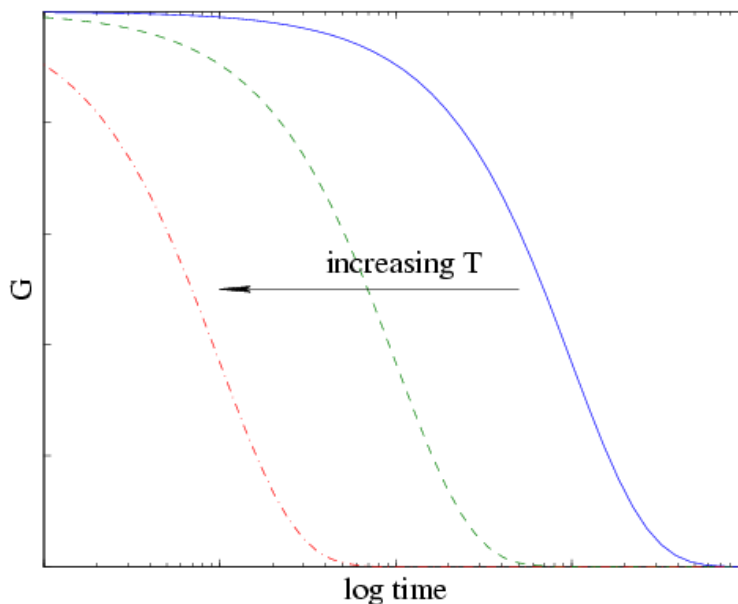
²Only one material function is required for an incompressible isotropic material subjected to a one-dimensional loading situation. For an isotropic material subjected to a general loading situation two material functionals need to be determined, and for an anisotropic material the number of functional are dependent on the the material symmetry.

13.13 The Use of Shift Functions to Generalize Linear Viscoelasticity Theory

For many materials the domain in which linear viscoelasticity theory give good predictions is unfortunately relatively small. Based on experimental observations it turns out that the influence of variations in external parameters (such as temperature and aging time), which contribute to the limited applicability of the theory, can be accounted for by using a shift function approach. The reason for the success of this simple idea is that when the material functional is plotted using appropriate log-scales, changes in these external parameters do not change the shape of the plotted curve to any significant degree, only shift it.

Time-Temperature Equivalence.

So far the discussion has been for a general viscoelastic material and can therefore be applied also to a polymer. But when considering polymers a number of complications become apparent. One of the more important issues that need to be recognized is the strong temperature dependence of the material. It has been shown experimentally that in many cases the temperature dependence can be modeled by a scaling of time using what has been termed the *time-temperature equivalence*. The basis for this principle is shown in the figure below illustrating that if the experimentally observed stress relaxation modulus is plotted as a function of logarithmic time, the shape of the resulting curves is the same for a wide interval of temperatures.



In fact, the only significant difference between the curves is a horizontal shift. This observation suggests that if the relaxation modulus is known at one temperature (i.e. the ‘master curve’ is known) then the relaxation modulus at any other temperature is obtained if the horizontal shift factor $a_T = a_T(T)$ is known. Any material that has this property is called a *rheologically simple material*.

The time shifts can be written

$$\log t_{T_0} - \log t_T = \log a_T \quad (1)$$

where t_T is the time at temperature T and t_{T_0} the time at temperature T_0 . Equation (1) gives $a_T = t_{T_0}/t_T$ or $t_T = t_{T_0}/a_T$, hence the behavior at a temperature of T becomes exactly the same as

the behavior at the reference temperature T_0 if the time is *accelerated* by the factor a_T . In general the temperature is a function of time $T = T(t_{T_0})$, so instead of $t_T = t_{T_0}/a_T$ it is necessary to write

$$dt_T = \frac{dt_{T_0}}{a_T(T(t_{T_0}))} \quad (2)$$

giving

$$t_T = \int_0^{t_{T_0}} \frac{dt'_{T_0}}{a_T(T(t'_{T_0}))}. \quad (3)$$

The effective time experienced by the material—the material time—is a function of temperature and wall clock time. For a rheologically simple material, the scaling of time with temperature occurs in all viscoelastic quantities such as G , J , J' , J'' , $\tan \delta$, etc. And the scaling constant must be the same for all quantities for the material to be rheologically simple.

Example 3. To exemplify this idea consider a simple Maxwell element: $G(t) = G_0 \exp(-t)$. If the material is rheologically simple the relaxation modulus becomes

$$G(t, T) = G_0 \exp[-a_T(T)t].$$

The influence of $a_T(T)$ on the stress-strain behavior was examined in Example 1. ■

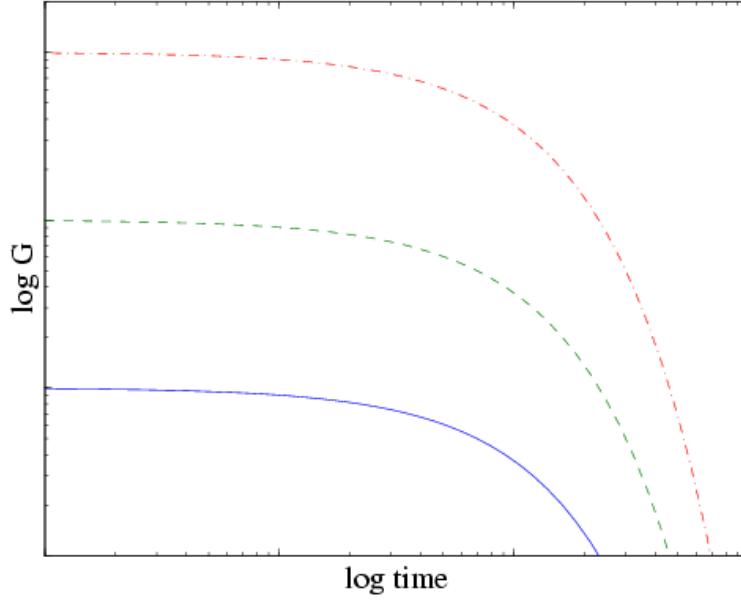
One commonly quoted representation of a_T is the WLF-equation ?:

$$\log a_T(T) = \frac{C_1(T - T_0)}{C_2 + T - T_0} \quad (4)$$

where $C_1 = 17.4$ and $C_2 = 51.6$ K. This relationship is often used for amorphous polymers in the temperature range $T \in [T_g - 50 \text{ K}, T_g + 50 \text{ K}]$.

Vertical Shifts.

As will be discussed in more detail below, the stress relaxation modulus (and also the creep compliance) curves when plotted as a function of logarithmic time often turn out to have the same shape not only for different temperatures but also for variations in other parameters (such as aging time). But to create a master curve in these cases it is often necessary to also use vertical shifts (on a log-scale), see the figure below.



$$\log G^\alpha - \log G^{\alpha_0} = \log b \quad (5)$$

giving

$$b = \frac{G^\alpha}{G^{\alpha_0}}. \quad (6)$$

In summary, the integral formulation

$$\sigma(t) = \int_{-\infty}^t G(t-\tau) \frac{d\varepsilon(\tau)}{d\tau} d\tau. \quad (3\text{-rep})$$

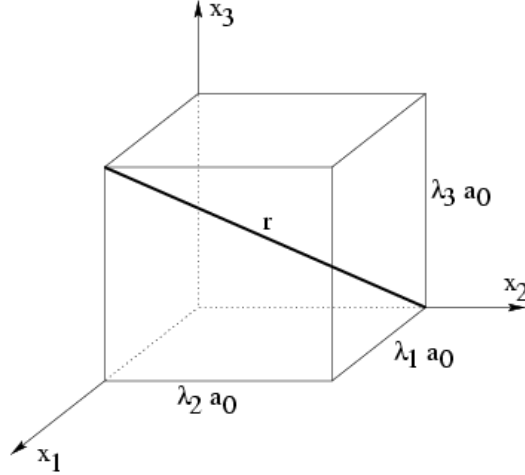
becomes

$$\sigma(t) = \int_0^t b(t)G(\hat{t}(t) - \hat{t}(\tau)) \frac{d\varepsilon(\tau)}{d\tau} d\tau \quad (7)$$

when both vertical shift $b(\theta_1(t))$ and horizontal shift $\hat{t}(t) = \hat{t}(\theta_2(t))$, where θ_1 and θ_2 are external parameters such as temperature, are considered.

13.14 Constitutive Modeling of the Equilibrium Response of Elastomers

Consider an elastomeric body \mathcal{B} in its reference configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ with the corresponding material points labeled by $\mathbf{p} \in \mathcal{B}_0$. It is assumed that the boundary $\partial\mathcal{B}_0$ of the region \mathcal{B}_0 is regular enough to ensure the validity of the divergence theorem, and that the exterior normal \mathbf{n}_0 to \mathcal{B}_0 is defined for almost every point \mathbf{p} of $\partial\mathcal{B}_0$, where ‘almost everywhere’ means that the set of points where \mathbf{n}_0 is not defined has the area measure zero. Denote by $\chi_t(\mathbf{p}) : \mathcal{B}_0 \times \mathbb{R} \rightarrow \mathbb{R}^3$ a macroscopic motion of \mathcal{B}_0 in a time interval $t \in [0, t_1] \subset \mathbb{R}_+$ which maps any material point \mathbf{p} to the point $\mathbf{x} = \chi_t(\mathbf{p}) \in \mathbb{R}^3$ in the deformed configuration $\mathcal{B}_t = \chi_t(\mathcal{B}_0) \subset \mathbb{R}^3$. In the following the reference configuration is taken to be stress-free with homogeneous reference temperature $\theta_0 \in \mathbb{R}_+$. The total deformation gradient defined by $\mathbf{F} = \partial_{\mathbf{p}} \chi(\mathbf{p}, t)$ can be decomposed into distortional and dilatational parts: $\mathbf{F} = (J)^{1/3} \mathbf{F}^*$ where $J = \det(\mathbf{F})$. To get a physical picture of the deformation process of an elastomer assume that on average the chain molecules can be considered to be located along the diagonals of a unit cell located in principal stretch space as illustrated in the figure below (this is the eight chain assumption of ?.)



Denote the side lengths of the unit cell in the reference state by a_0 and the undeformed chain length by r_0 (it then directly follows that $r_0 = a_0\sqrt{3}$.) Further take the macromolecules to be freely jointed with n rigid links each of length l . For this chain model the average end-to-end distance in the absence of an external force field is $l\sqrt{n}$. By defining $\{\lambda_i^* | i = 1, 2, 3\}$ to be the applied principal distortional stretches the effective distortional chain length becomes $r = a_0[(\lambda_1^*)^2 + (\lambda_2^*)^2 + (\lambda_3^*)^2]^{1/2}$, giving the effective distortional chain stretch

$$\bar{\lambda}^* = \left[\frac{(\lambda_1^*)^2 + (\lambda_2^*)^2 + (\lambda_3^*)^2}{3} \right]^{1/2} = \sqrt{\frac{\text{tr } \mathbf{C}^*}{3}} = \sqrt{\frac{\text{tr } \mathbf{B}^*}{3}},$$

where $\mathbf{B}^* = (J)^{-2/3}\mathbf{B}$. Based on this physical model, an *eight-chain material* is defined as an isotropic thermoelastic material whose strain energy density W only depends on the two invariants $\bar{\lambda}^*(\mathbf{B}^*)$, $J(\mathbf{F})$, and the temperature θ . By noting that the effective chain stretch is related to the first invariant of \mathbf{B}^* through $\bar{\lambda}^* = [I_1(\mathbf{B}^*)/3]^{1/2}$ it follows that the strain energy density can be written $\bar{W}(\bar{\lambda}^*, J, \theta)$, or alternatively $\bar{W}(I_{1^*}, J, \theta)$ where $I_{1^*} := I_1(\mathbf{B}^*) = \text{tr}(\mathbf{B}^*)$. To determine the strain energy density, W , first use the experimental observation that the internal energy is not a function of the applied distortional stretch, i.e. $e(J, \theta)$. The specific heat at constant volume, defined by $c_v = \partial e(J, \theta)/\partial \theta$, can then be written

$$c_v(J, \theta) = \frac{\partial \psi(\bar{\lambda}^*, J, \theta)}{\partial \theta} + \eta(\bar{\lambda}^*, J, \theta) + \theta \frac{\partial \eta(\bar{\lambda}^*, J, \theta)}{\partial \theta}. \quad (1)$$

where the definition of the Helmholtz free energy $\psi(\bar{\lambda}^*, J, \theta) = e(J, \theta) - \theta \eta(\bar{\lambda}^*, J, \theta)$ has been used. Since the first two terms of the right hand side of (1) have to cancel to satisfy the Clausius-Duhem inequality the specific heat becomes

$$c_v(J, \theta) = \theta \frac{\partial \eta(\bar{\lambda}^*, J, \theta)}{\partial \theta}. \quad (2)$$

Further assume that the material is almost incompressible and that the temperature does not vary too much such that c_v , to a first order approximation, can be taken to be a constant. Equation (2) then yields

$$\psi(\bar{\lambda}^*, J, \theta) = c_v \theta (1 - \ln \theta) + e_1(J) - \theta \eta(\bar{\lambda}^*, J). \quad (3)$$

Assuming small volumetric deformations, the linearized relationship between the Cauchy stress \mathbf{T} and the volumetric deformation J is taken as

$$\frac{\partial \bar{W}}{\partial J} = \mathbf{T} \propto \kappa (J - 1) \mathbf{1} \quad (4)$$

giving the convex relationship $e_1(J) = \kappa[J^2/2 - J + 1/2]/\rho_0$ which when inserted into (3) gives

$$\bar{W}(\bar{\lambda}^*, J, \theta) = \rho_0 c_v \theta [1 - \ln \theta] + \kappa \left[\frac{J^2}{2} - J + \frac{1}{2} \right] - \theta \rho_0 \eta(\bar{\lambda}^*). \quad (5)$$

Note that the dependence on J in $\eta(\bar{\lambda}^*, J)$ has been neglected due to the the assumption of small volume change. It now only remains to determine how the entropy depends on the effective chain stretch. By assuming the molecules to be freely jointed with a fixed bond length the entropy can be determined from the statistical mechanics relation $[\rho_0 \eta] \propto N k_B \ln \Omega(r)$ where $\Omega(r)$ is the probability distribution of the end-to-end distance of the molecular chain and N is the number of chains per unit reference volume. Flory [?] showed that the probability distribution under these conditions can be written

$$\Omega(r) = \frac{1}{2\pi^2 r} \int_0^\infty q \sin(qr) \left[\frac{\sin ql}{ql} \right]^n dq. \quad (6)$$

One approximation of (6) good for $n \gg 1$ and $r \approx n$ is the Langevin expression attributed to Kuhn and Gr \ddot{u} hn [?]:

$$\Omega(r) = \frac{A'}{l^3} \left[\frac{\sinh \beta}{\beta} \right]^n \exp \left[\frac{-\beta r}{l} \right] \quad (7)$$

where $\beta = \mathcal{L}^{-1}(r/(nl))$ and $\mathcal{L}(x) = \coth(x) - 1/x$ is the Langevin function. By inserting (7) into (5) the strain energy density can be written

$$\begin{aligned} \bar{W}(\bar{\lambda}^*, J, \theta) = \rho_0 c_v \theta [1 - \ln \theta] + \kappa \left[\frac{J^2}{2} - J + \frac{1}{2} \right] \\ - N k_B \theta n \ln \left(\frac{\sinh \beta}{\beta} \right) + N k_B \theta \beta \lambda^{lock} \bar{\lambda}^* + W_0 \end{aligned} \quad (8)$$

where

$$\beta = \mathcal{L}^{-1} \left(\frac{\bar{\lambda}^*}{\lambda^{lock}} \right), \quad \lambda^{lock} = \sqrt{n}. \quad (9)$$

The Cauchy stress for an eight-chain material can then be obtained from the continuum mechanics expression

$$\begin{aligned} \mathbf{T} = \frac{2}{J} \left[\hat{W}_{1^*} + \hat{W}_{2^*} I_{1^*} \right] \mathbf{B}^* - \frac{2}{J} \hat{W}_{2^*} (\mathbf{B}^*)^2 + \\ \left[\frac{\partial \hat{W}}{\partial J} - \frac{2I_{1^*}}{3J} \hat{W}_{1^*} - \frac{4I_{2^*}}{3J} \hat{W}_{2^*} \right] \mathbf{1}, \end{aligned} \quad (10)$$

which in this case with no dependence on I_{2^*} can be simplified to

$$\mathbf{T} = \frac{2}{J} \hat{W}_{1^*} \text{dev}[\mathbf{B}^*] + \frac{\partial \hat{W}}{\partial J} \mathbf{1} \quad (11)$$

or when expressed in terms of the effective chain stretch $\bar{\lambda}^*$

$$\mathbf{T} = \frac{1}{J} \frac{1}{3\bar{\lambda}^*} \frac{\partial \bar{W}}{\partial \bar{\lambda}^*} \text{dev}[\mathbf{B}^*] + \frac{\partial \bar{W}}{\partial J} \mathbf{1}. \quad (12)$$

The Cauchy stress can then be calculated from (12) giving

$$\mathbf{T} = \frac{-\theta}{3J\bar{\lambda}^*} \frac{d[\rho_0 \eta(\bar{\lambda}^*)]}{d\bar{\lambda}^*} \text{dev}[\mathbf{B}^*] + \kappa [J - 1] \mathbf{1}. \quad (13)$$

From the chain rule

$$\frac{\partial[\rho_0\eta(r(\bar{\lambda}^*))]}{\partial\bar{\lambda}^*} = \frac{\partial[\rho_0\eta]}{\partial r} \frac{\partial r}{\partial\bar{\lambda}^*} = \frac{\partial[\rho_0\eta]}{\partial r} \frac{1}{\frac{\partial}{\partial r} \left[\frac{r}{l\sqrt{n}} \right]} = l\sqrt{n} \frac{\partial[\rho_0\eta]}{\partial r}$$

it is clear that it is sufficient to determine how the entropy of a single macromolecule depends on its end-to-end distance. In the limit $n \rightarrow \infty$, Equation (7) becomes a Gaussian distribution

$$\Omega(r) = \left[\frac{3}{2\pi nl^3} \right]^{3/2} \exp \left[\frac{-3r^2}{2nl^2} \right]. \quad (14)$$

It is easy to show that the change in entropy with chain length for the Langevin expression therefore can be written

$$\frac{\partial[\rho_0\eta]}{\partial r} = \frac{\partial[Nk \ln \Omega(r)]}{\partial r} = \frac{-Nk_B}{l} \mathcal{L}^{-1} \left(\frac{r}{nl} \right),$$

and that the corresponding expression for Gaussian chains becomes

$$\frac{\partial[\rho_0\eta]}{\partial r} = \frac{\partial[Nk \ln \Omega(r)]}{\partial r} = -\frac{3Nk_B r}{nl^2}.$$

Equation (13) can now be written

$$\mathbf{T} = \frac{Nk_B\theta}{3J} \frac{\lambda^{\text{lock}}}{\bar{\lambda}^*} \mathcal{L}^{-1} \left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}} \right) \text{dev}[\mathbf{B}^*] + \kappa[J-1]\mathbf{1}, \quad (15)$$

where $\lambda^{\text{lock}} = \sqrt{n}$. For the special case of incompressible uniaxial deformation Equation (15) simplifies to

$$\sigma = \frac{Nk_B\theta}{3} \frac{\lambda^{\text{lock}}}{\bar{\lambda}^*} \mathcal{L}^{-1} \left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}} \right) \left[\lambda^2 - \frac{1}{\lambda} \right] \quad (16)$$

and for simple shear defined by $\mathbf{F} = \mathbf{1} + \gamma \mathbf{e}_1 \otimes \mathbf{e}_2$ the shear stress is given by

$$T_{12} = \frac{Nk_B\theta}{3J} \frac{\lambda^{\text{lock}}}{\bar{\lambda}^*} \mathcal{L}^{-1} \left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}} \right) \gamma \quad (17)$$

where $\bar{\lambda}^* = \sqrt{1 + \gamma^2/3}$. The initial shear modulus of the material is given by $\mu_0 = \frac{\partial T_{12}}{\partial \gamma} |_{\gamma=0}$ giving

$$\mu_0 = \frac{Nk_B\theta_0}{3} \lambda^{\text{lock}} \mathcal{L}^{-1} \left(\frac{1}{\lambda^{\text{lock}}} \right) \quad (18)$$

which when inserted in (15) gives the Cauchy stress as

$$\mathbf{T} = \frac{\theta}{\theta_0} \frac{\mu_0}{J\bar{\lambda}^*} \frac{\mathcal{L}^{-1} \left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}} \right)}{\mathcal{L}^{-1} \left(\frac{1}{\lambda^{\text{lock}}} \right)} \text{dev}[\mathbf{B}^*] + \kappa[J-1]\mathbf{1}. \quad (19)$$

For the special case of incompressible uniaxial deformation the corresponding equation becomes

$$\sigma = \frac{\mu_0}{\bar{\lambda}^*} \frac{\mathcal{L}^{-1} \left(\frac{\bar{\lambda}^*}{\lambda^{\text{lock}}} \right)}{\mathcal{L}^{-1} \left(\frac{1}{\lambda^{\text{lock}}} \right)} \left[\lambda^2 - \frac{1}{\lambda} \right]. \quad (20)$$

The constitutive relationship for the case of Gaussian chains is directly obtained by replacing the inverse Langevin function by the first term in its series expansion $\mathcal{L}^{-1}(x) \approx 3x$, giving

$$\mathbf{T} = \frac{\theta}{\theta_0} \frac{\mu_0}{J} \text{dev}[\mathbf{B}^*] + \kappa[J - 1]\mathbf{1}. \quad (21)$$

14.1 List of Symbols

Direct notation is used throughout, with the same conventions as in \mathcal{B} , \mathcal{B}_0 and \mathcal{B}_t .

$\mathcal{B}_t \subset \mathbb{R}^3$	position of the material body \mathcal{B} at time t
$\mathbf{p} \in \mathcal{B}_0$	position of a material point in the reference configuration
$\mathbf{x} \in \mathcal{B}_t$	position of a material point in the current configuration
$\mathbf{F} \in \text{Lin}^+$	deformation gradient
a_0, a	area element in the reference and current configuration
v_0, v	volume element in the reference and current configuration
\mathbf{n}_0, \mathbf{n}	normal to the surface in the reference and current configuration
ρ_0, ρ	mass density in the reference and current configuration
\mathbf{T}	Cauchy stress
\mathbf{S}	first Piola-Kirchhoff stress
\mathbf{S}^{pk2}	second Piola-Kirchhoff stress
\mathbf{b}	specific body force (i.e. per unit mass)
$\boldsymbol{\tau}$	Kirchhoff stress
e	specific internal energy
η	specific entropy
θ	absolute temperature
\mathbf{g}_0, \mathbf{g}	temperature gradient in the reference and current configuration
ψ	specific Helmholtz free energy
W	strain energy density per unit reference volume
r	specific heat supply
\mathbf{t}	Cauchy traction
h_0, h	heat flux in the reference and current configuration
\mathbf{q}_0, \mathbf{q}	heat flux vector in the reference and current configuration

14.2 Elements of Tensor Algebra and Analysis

- ▶ $\mathbf{A} \cdot \mathbf{B} := \text{tr}(\mathbf{A}\mathbf{B}^T) = A_{ij}B_{ij}, \forall \mathbf{A}, \mathbf{B} \in \text{Lin}.$
- ▶ For all vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$:

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

$$(\mathbf{a} \otimes \mathbf{b})(\mathbf{c} \otimes \mathbf{d}) = (\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \otimes \mathbf{d}).$$

- ▶ The rank $r(\mathbf{A})$ of a tensor \mathbf{A} is the dimension of the range of the linear transformation \mathbf{A} .
- ▶ Derivatives are identified with linear transformations. Let $f : D \rightarrow Y$ where $D \subset X$, then $Df(\mathbf{x}) = \partial_{\mathbf{x}}f(\mathbf{x})$ is a linear transformation from X to Y . The value of the transformation at $\mathbf{u} \in X$ is denoted $Df(\mathbf{x})[\mathbf{u}] = \partial_{\mathbf{x}}f(\mathbf{x})[\mathbf{u}]$, which for inner product spaces also can be written $Df(\mathbf{x}) \cdot \mathbf{u} = \partial_{\mathbf{x}}f(\mathbf{x}) \cdot \mathbf{u}$.
- ▶ The cofactor of $\mathbf{A} \in \text{Lin}$ is $\text{cof } \mathbf{A} := \partial_{\mathbf{A}} \det \mathbf{A}$ which if $\mathbf{A} \in \text{invLin}$ can be written $(\det \mathbf{A})\mathbf{A}^{-T}$
- ▶ A number $v \in \mathbb{R}_+$ and a vector $\mathbf{e} \in \mathcal{V}$ are said to be a *singular value* and a *singular vector* of $\mathbf{F} \in \text{Lin}$ if they are an eigenvalue and an eigenvector of $\sqrt{\mathbf{F}\mathbf{F}^T}$. When $\mathbf{F} \in \text{invLin}$ is a deformation gradient, the singular values of \mathbf{F} are called the principal stretches and the singular vectors the principal directions.

- ▶ Let $W = \rho_0 \psi$ be the strain energy per unit reference volume, and $W_i := \partial W / \partial I_i$.
- ▶ The invariants of \mathbf{B} can be written:

$$\begin{aligned} I_1 &= \text{tr } \mathbf{B} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \\ I_2 &= \frac{1}{2} [\text{tr}(\mathbf{B}^2) - (\text{tr } \mathbf{B})^2] = \lambda_1^2 \lambda_2^2 + \lambda_2^2 \lambda_3^2 + \lambda_3^2 \lambda_1^2 \\ I_3 &= \det \mathbf{B} = \lambda_1^2 \lambda_2^2 \lambda_3^2 \end{aligned}$$

14.3 Kinematics of Continuous Bodies

- ▶ Consider a continuum body \mathcal{B} with reference configuration $\mathcal{B}_0 \subset \mathbb{R}^3$ and material points labeled by $\mathbf{p} \in \mathcal{B}_0$. Assume that the boundary $\partial \mathcal{B}_0$ of the region \mathcal{B}_0 is regular enough to ensure the validity of the divergence theorem, and that the exterior normal \mathbf{n}_0 to \mathcal{B}_0 is defined for almost every point \mathbf{p} of $\partial \mathcal{B}_0$, where ‘almost everywhere’ means that the set of points where \mathbf{n}_0 is not defined has the area measure zero.
- ▶ Each open region $\mathcal{B}_t \subset \mathbb{R}^3$ whose boundary has the chosen degree of regularity is called an *admissible region*.
- ▶ The value $\mathbf{x} = \boldsymbol{\chi}(\mathbf{p}, t)$ is the position of the material point $\mathbf{p} \in \mathcal{B}_0$ at time $t \in [t_1, t_2] \subset \mathbb{R}$. The partial mapping $\boldsymbol{\chi}(\cdot, t)$ is the configuration at t . The spatial set $\{\boldsymbol{\chi}(\mathbf{p}, t) \in \mathbb{R}^3 : \mathbf{p} \in \mathcal{B}\}$ is the current region occupied by the body at time t . The deformation gradient is defined by $\mathbf{F} = \partial_{\mathbf{p}} \boldsymbol{\chi}(\mathbf{p}, t)$.
- ▶ We shall associate with each body \mathcal{B} a set Σ , the *state space*, and another set Π , the *class of processes*. The elements σ of Σ are the *states* of the body and the elements π of Π are the *processes*. Each process is a function $\pi : [0, t_\pi] \rightarrow \Sigma$. The value $\sigma(t)$ is the state of the body at time $t \in [0, t_\pi]$. The pair (Σ, Π) is called a *system*.
- ▶ Let $[t_1, t_2] \subset \mathbb{R}$ be a time interval, \mathcal{B} an admissible region and ϕ a continuously differentiable function defined on an open set containing the closure of $\mathcal{B} \times [t_1, t_2]$ such that $\nabla \phi \neq \mathbf{0}$ at every point where $\phi = 0$. A moving surface in \mathcal{B} on $[t_1, t_2]$ is a family $\{S_t, t \in [t_1, t_2]\}$ of closed oriented surfaces in \mathcal{B} given by

$$S_t = \{\mathbf{p} \in \text{cl } \mathcal{B} : \phi(\mathbf{p}, t) = 0\}, \quad t \in [t_1, t_2].$$

The spacetime set U composed of the spacetime points on the singular surface, given by

$$U = \{(\mathbf{p}, t) \in \text{cl } \mathcal{B} \times [t_1, t_2] : \phi(\mathbf{p}, t) = 0\}$$

is a three-dimensional hypersurface.

- ▶ The jump $[f]$ and the mean value $\langle f \rangle$ of f on the singular surface are defined by $[f] = f^+ - f^-$ and $\langle f \rangle = \frac{1}{2}(f^+ + f^-)$, respectively.
- ▶ Let the operator ∇ denote the referential gradient, and the superimposed dot the material time derivative:

$$\nabla f(\mathbf{p}, t) = \text{Grad } f(\mathbf{p}, t) = \partial_{\mathbf{p}} f(\mathbf{p}, t), \quad \dot{f}(\mathbf{p}, t) = \partial_t f(\mathbf{p}, t)$$

- ▶ Lines, areas and volumes are deformed according to: $d\mathbf{l} = \mathbf{F}d\mathbf{l}_0$, $d\mathbf{a} = \text{cof } \mathbf{F}d\mathbf{a}_0$, $dv = \det \mathbf{F}dv_0$.

- Let $f(\mathbf{p}, t) = \tilde{f}(\mathbf{x}, t)$. The spatial gradient and the partial time derivative of f are denoted by $\text{grad } f = \partial_{\mathbf{x}} \tilde{f}(\mathbf{x}, t)$ and $\partial \tilde{f} / \partial t = \partial_t \tilde{f}(\mathbf{x}, t)$, respectively.

- • Deformation gradient

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R} = \sum \lambda_i \mathbf{l}_i \otimes \mathbf{r}_i$$

- Right stretch tensor

$$\mathbf{U} = \sum \lambda_i \mathbf{r}_i \otimes \mathbf{r}_i = \mathbf{R}^T \mathbf{V} \mathbf{R}$$

- Left stretch tensor

$$\mathbf{V} = \sum \lambda_i \mathbf{l}_i \otimes \mathbf{l}_i = \mathbf{R} \mathbf{U} \mathbf{R}^T$$

- Rotation tensor

$$\mathbf{R} = \sum \mathbf{l}_i \otimes \mathbf{r}_i$$

- Eigenvectors

$$\mathbf{l}_i = \mathbf{R} \mathbf{r}_i$$

- Left Cauchy Green tensor (Finger tensor)

$$\mathbf{B} = \mathbf{F} \mathbf{F}^T = \mathbf{V}^2 = \mathbf{R} \mathbf{C} \mathbf{R}^T = \sum \lambda_i^2 \mathbf{l}_i \otimes \mathbf{l}_i$$

- Right Cauchy Green tensor

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} = \mathbf{U}^2 = \mathbf{R}^T \mathbf{B} \mathbf{R} = \sum \lambda_i^2 \mathbf{r}_i \otimes \mathbf{r}_i$$

- Cauchy stress (true stress)

$$\mathbf{T} = \sum \sigma_i \mathbf{l}_i \otimes \mathbf{l}_i$$

- Piola-Kirchhoff stress

$$\mathbf{S} = \sum s_i \mathbf{l}_i \otimes \mathbf{r}_i$$

- Second Piola-Kirchhoff stress

$$\mathbf{S}^{\text{pk2}} = \sum s_i^{\text{pk2}} \mathbf{r}_i \otimes \mathbf{r}_i$$

14.4 Balance Equations

- 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.
- Piola's transformation: Let \mathbf{q}_0 be a continuously differentiable vector field in the reference description. The interpretation of \mathbf{q}_0 as a flux vector is that if \mathcal{B}_0 is any oriented surface in the reference configuration with normal \mathbf{n}_0 , then the integral

$$\int_{\mathcal{B}_0} \mathbf{q}_0 \cdot \mathbf{n}_0 \, da_0 = \int_{\mathcal{B}_t} \mathbf{q} \cdot \mathbf{n} \, da$$

is the rate at which the quantity under consideration flows through $\partial \mathcal{B}_t$.

This directly leads to $\mathbf{q}_0 = (\text{cof } \mathbf{F})^T \mathbf{q}$, and $\text{Div } \mathbf{q}_0 = \det \mathbf{F} \, \text{div } \mathbf{q}$ outside the singular surface.

- Balance of mass

$$M = \int_{\mathcal{B}_t} \rho dv, \quad \boxed{\rho = \rho_0/J}, \quad \partial_t \rho + \operatorname{div}(\rho \mathbf{v}) = 0.$$

- Let \mathbf{f} be the resultant Cauchy traction acting on a body:

$$\mathbf{f} = \int_{\partial \mathcal{B}_0} \mathbf{S} \mathbf{n}_0 da_0 = \int_{\partial \mathcal{B}_t} \mathbf{T} \mathbf{n} da.$$

- Balance of linear momentum: material form

$$\int_{\partial \mathcal{B}_0} \mathbf{S} \mathbf{n}_0 da_0 + \int_{\mathcal{B}_0} \rho_0 \mathbf{b} dv_0 = \frac{d}{dt} \int_{\mathcal{B}_0} \rho_0 \mathbf{v} dv_0,$$

and in the current configuration

$$\int_{\partial \mathcal{B}_t} \mathbf{T} \mathbf{n} da + \int_{\mathcal{B}_t} \rho \mathbf{b} dv = \frac{d}{dt} \int_{\mathcal{B}_t} \rho \mathbf{v} dv$$

and the corresponding local forms are

$$\boxed{\operatorname{Div} \mathbf{S} + \rho_0 \mathbf{b} = \rho_0 \dot{\mathbf{v}}}, \quad \text{and} \quad \operatorname{div} \mathbf{T} + \rho \mathbf{b} = \rho \dot{\mathbf{v}}.$$

- Balance of angular momentum: material form in the reference configuration

$$\int_{\partial \mathcal{B}_0} (\mathbf{x} - \mathbf{x}_0) \times \mathbf{S} \mathbf{n}_0 da_0 + \int_{\mathcal{B}_0} \rho_0 (\mathbf{x} - \mathbf{x}_0) \times \mathbf{b} dv_0 = \frac{d}{dt} \int_{\mathcal{B}_0} \rho_0 (\mathbf{x} - \mathbf{x}_0) \times \mathbf{v} dv_0.$$

Note, the balance of angular momentum implies the balance of linear momentum, or the equation of balance of angular momentum is satisfied iff the equation of linear momentum is satisfied and the Cauchy stress is symmetric. The local form is $\boxed{\mathbf{S} \mathbf{F}^T = \mathbf{F} \mathbf{S}^T}$.

- Theorem of virtual work: let (\mathbf{f}, \mathbf{b}) be a system of forces on \mathcal{B} during a motion χ . Then a necessary and sufficient condition that the momentum laws be satisfied is that given a region $\mathcal{R} \subset \mathcal{B}_t$ and time $t \in \mathbb{R}$,

$$\int_{\partial \mathcal{R}} \mathbf{f}(\mathbf{n}) \cdot \mathbf{w} da + \int_{\mathcal{R}} \mathbf{b} \cdot \mathbf{w} dv = \int_{\mathcal{R}} \rho \dot{\mathbf{v}} \cdot \mathbf{w} dv$$

for every infinitesimal rigid displacement \mathbf{w} .

- Let $h_0(\mathbf{n}_0)$ be the heat influx per unit referential area. Then

$$h_0(\mathbf{n}_0) = - \sum_{i=1}^3 (\mathbf{n}_0 \cdot \mathbf{e}_i) h_0(\mathbf{e}_i) = - \left[\sum_{i=1}^3 h_0(\mathbf{e}_i) \mathbf{e}_i \right] \cdot \mathbf{n}_0 \equiv -\mathbf{q}_0 \cdot \mathbf{n}_0$$

proves the existence of a referential heat flux vector \mathbf{q}_0 that does not depend on \mathbf{n}_0 .

- Relations between the different stress measures

$$\begin{aligned} \mathbf{S} &= J \mathbf{T} \mathbf{F}^{-T}, & \mathbf{T} &= \frac{1}{J} \mathbf{S} \mathbf{F}^T \\ \mathbf{S}^{\text{pk2}} &= J \mathbf{F}^{-1} \mathbf{T} \mathbf{F}^{-T} = \mathbf{F}^{-1} \mathbf{S}, & \mathbf{T} &= \frac{1}{J} \mathbf{F} \mathbf{S}^{\text{pk2}} \mathbf{F}^T \\ \boldsymbol{\tau} &= J \mathbf{T} = \mathbf{S} \mathbf{F}^T \end{aligned}$$

- By introducing the specific internal energy e , we can state the material rate form of the balance of energy as

$$\int_{\partial \mathcal{B}_0} (\mathbf{v} \cdot \mathbf{S} \mathbf{n}_0 - \mathbf{q}_0 \cdot \mathbf{n}_0) da_0 + \int_{\mathcal{B}_0} \rho_0 (\mathbf{v} \cdot \mathbf{b} + r) dv_0 = \frac{d}{dt} \int_{\mathcal{B}_0} \rho_0 \left(e + \frac{\mathbf{v}^2}{2} \right) dv_0,$$

or in local form expressed per unit reference volume

$$\boxed{\mathbf{S} \cdot \dot{\mathbf{F}} - \text{Div } \mathbf{q}_0 + \rho_0 r = \rho_0 \dot{e}},$$

or per unit current volume

$$\mathbf{T} \cdot \mathbf{L} - \text{div } \mathbf{q} + \rho r = \rho \dot{e}.$$

- The existence of the absolute temperature and entropy is postulated for general nonequilibrium processes. It is assumed that these quantities satisfy the Clausius-Duhem inequality. By introducing the specific entropy η and the absolute temperature $\theta \in \mathbb{R}_+$ the material form of the Clausius-Duhem inequality becomes:

$$\int_{\partial \mathcal{B}_0} \frac{-\mathbf{q}_0 \cdot \mathbf{n}_0}{\theta} da_0 + \int_{\mathcal{B}_0} \frac{\rho_0 r}{\theta} dv_0 \leq \frac{d}{dt} \int_{\mathcal{B}_0} \eta \rho_0 dv_0.$$

The local material form expressed per unit reference volume

$$-\text{Div } \frac{\mathbf{q}_0}{\theta} + \frac{\rho_0 r}{\theta} \leq \rho_0 \dot{\eta}$$

which also can be written

$$\rho_0 \dot{e} - \mathbf{S} \cdot \dot{\mathbf{F}} + \frac{\mathbf{q}_0 \cdot \mathbf{g}_0}{\theta} \leq \rho_0 \theta \dot{\eta}$$

where $\mathbf{g}_0 := \partial_{\mathbf{p}} \theta$ is the referential gradient of the temperature. Or in terms of the current configuration

$$\rho \dot{e} - \mathbf{T} \cdot \mathbf{L} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \leq \rho \theta \dot{\eta}.$$

- By introducing the specific Helmholtz free energy per unit mass $\psi := e - \theta \eta$, the Clausius-Duhem inequality can be restated as the dissipation inequality

$$\rho_0 \dot{\psi} - \mathbf{S} \cdot \dot{\mathbf{F}} + \rho_0 \eta \dot{\theta} + \frac{\mathbf{q}_0 \cdot \mathbf{g}_0}{\theta} \leq 0$$

or

$$\boxed{\rho \dot{\psi} - \mathbf{T} \cdot \mathbf{L} + \rho \eta \dot{\theta} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \leq 0.}$$

14.5 The First Law of Thermodynamics

- For a process $\pi \in \Pi$ and a region $\mathcal{R} \subset \mathcal{B}$ the work $w(\pi, \mathcal{R})$ done by \mathcal{R} in π is

$$w(\pi, \mathcal{R}) = - \int_0^{t_\pi} \left[\int_{\partial \mathcal{R}} \mathbf{v} \cdot \mathbf{S} \mathbf{n}_0 da_0 + \int_{\mathcal{R}} \mathbf{v} \cdot \mathbf{b} dv_0 \right] dt$$

and the net heat gained by \mathcal{R} in π is

$$q(\pi, \mathcal{R}) = \int_0^{t_\pi} \left[- \int_{\partial \mathcal{R}} \mathbf{q}_0 \cdot \mathbf{n}_0 da_0 + \int_{\mathcal{R}} r dv_0 \right] dt.$$

- ▶ First law of thermodynamics: $w(\pi, \mathcal{R}) = q(\pi, \mathcal{R})$ for every cyclic process π and every region \mathcal{R} .

14.6 The Principle of Material Frame Indifference

- ▶ A mapping $i : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is said to be an isometry if $|i(\mathbf{x}) - i(\mathbf{y})| = |\mathbf{x} - \mathbf{y}|$ for every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$. A change of frame is a family $i = \{i_t, t \in \mathbb{R}\}$ of isometries. It is of the form

$$i_t(\mathbf{x}) = \mathbf{R}(t)(\mathbf{x} - \mathbf{x}_0) + \mathbf{x}'_0, \quad \mathbf{x} \in \mathbb{R}^3, \quad t \in \mathbb{R}$$

where $\mathbf{R}(\cdot) : \mathbb{R} \rightarrow \text{Orth}$, and $\mathbf{x}'_0 : \mathbb{R} \rightarrow \mathbb{R}^3$ are functions and $\mathbf{x}_0 \in \mathbb{R}^3$ a point.

- ▶ The internal energy \bar{e} is a local state function on $(\Sigma, \Pi, \mathcal{B})$ defined by $e(\sigma, \mathbf{p}) = u(\sigma, \mathbf{p}) - \frac{1}{2}\rho_0(\mathbf{p}) \mathbf{v}(\sigma, \mathbf{p})^2$, where u is the specific total energy.
- ▶ The internal energy is objective, i.e. for every process π and every change of frame i we have $e((i \circ \pi)(t), \cdot) = e(\pi(t), \cdot)$ for every region \mathcal{R} and every $t \in [0, t_\pi]$.

14.7 Isotropic Functions

- ▶ A subset \mathcal{V} of Sym is said to be *isotropic* if for every $\mathbf{A} \in \mathcal{V}$ and every $\mathbf{Q} \in \text{Orth}$ also $\mathbf{Q}\mathbf{A}\mathbf{Q}^T \in \mathcal{V}$.
- ▶ A scalar-valued function $h : \mathcal{V} \rightarrow \mathbb{R}$ is said to be isotropic if its domain is isotropic and $h(\mathbf{Q}\mathbf{A}\mathbf{Q}^T) = h(\mathbf{A})$ for every $\mathbf{A} \in \mathcal{V}$ and every $\mathbf{Q} \in \text{Orth}$.
- ▶ A tensor-valued function $\mathbf{G} : \mathcal{V} \rightarrow \text{Lin}$ is said to be isotropic if its domain is isotropic and $\mathbf{G}(\mathbf{Q}\mathbf{A}\mathbf{Q}^T) = \mathbf{Q}\mathbf{G}(\mathbf{A})\mathbf{Q}^T$ for every $\mathbf{A} \in \mathcal{V}$ and every $\mathbf{Q} \in \text{Orth}$.
- ▶ A subset \mathcal{V} of Lin is said to be *objective* if for every $\mathbf{A} \in \mathcal{V}$ and every $\mathbf{Q} \in \text{Orth}$ also $\mathbf{Q}\mathbf{A} \in \mathcal{V}$. A scalar valued function and a tensor valued function are said to be objective if $h(\mathbf{Q}\mathbf{A}) = h(\mathbf{A})$ and $\mathbf{G}(\mathbf{Q}\mathbf{A}) = \mathbf{Q}\mathbf{G}(\mathbf{A})$, respectively.

14.8 Constitutive Equations

- ▶ There are 19 unknown field variables in the governing equations developed above ($\mathbf{x}, \mathbf{S}, \mathbf{q}_0, e, \eta, \theta, \rho$) but only 8 equations. The remaining 11 equations are the constitutive equations: $e(\cdot), \eta(\cdot), \mathbf{S}(\cdot), \mathbf{q}_0(\cdot)$. Candidate arguments for the constitutive equations are: $\mathbf{p}, \mathbf{F}, \dot{\mathbf{F}}, \partial_{\mathbf{p}}\mathbf{F}, \theta, \dot{\theta}, \partial_{\mathbf{p}}\theta, \rho, \dot{\rho}, \{\xi\}$, etc.
- ▶ An adiabatic thermoelastic material is defined by $e(\cdot), \eta(\cdot), \mathbf{S}(\cdot)$ being functions of \mathbf{F} and θ .
- ▶ A thermoelastic material is defined by $e(\cdot), \eta(\cdot), \mathbf{S}(\cdot), \mathbf{q}_0(\cdot)$ being functions of $\mathbf{F}, \theta, \mathbf{g}_0$.
- ▶ A viscous body with heat conduction is defined by $e(\cdot), \eta(\cdot), \mathbf{S}(\cdot), \mathbf{q}_0(\cdot)$ being functions of $\mathbf{F}, \dot{\mathbf{F}}, \theta, \mathbf{g}_0$.
- ▶ A process in which θ and \mathbf{F} are constants in space and time is called an equilibrium process. The total stress can be decomposed into equilibrium and dynamic components:

$$\mathbf{S}(\mathbf{F}, \theta, \mathbf{g}_0, \dot{\mathbf{F}}) = \mathbf{S}_d(\mathbf{F}, \theta, \mathbf{g}_0, \dot{\mathbf{F}}) + \mathbf{S}_e(\mathbf{F}, \theta).$$

- ▶ A viscous body with heat conduction satisfies the dissipation inequality (i.e. the Clausius-Duhem inequality) if and only if the following three conditions hold:

1. the constitutive functions $\psi(\cdot)$, $\eta(\cdot)$, $e(\cdot)$ are independent of the non-equilibrium variables \mathbf{g}_0 , $\dot{\mathbf{F}}$
2. the following equilibrium thermostatic relations hold

$$\begin{aligned}\mathbf{S}_e(\mathbf{F}, \theta) &= \rho_0 \frac{\partial \psi(\mathbf{F}, \theta)}{\partial \mathbf{F}} \\ \eta(\mathbf{F}, \theta) &= -\frac{\partial \psi(\mathbf{F}, \theta)}{\partial \theta} \\ e(\mathbf{F}, \theta) &= -\theta^2 \frac{\partial}{\partial \theta} \left[\frac{\psi(\mathbf{F}, \theta)}{\theta} \right]\end{aligned}$$

3. the following dissipation inequality holds

$$\mathbf{S}_d(\mathbf{F}, \theta, \mathbf{g}_0, \dot{\mathbf{F}}) \cdot \dot{\mathbf{F}} - \mathbf{q}_0(\mathbf{F}, \theta, \mathbf{g}_0, \dot{\mathbf{F}}) \cdot \mathbf{g}_0 / \theta \geq 0$$

- The principle of frame indifference causes further restrictions on the constitutive equations: $\mathbf{S}_e(\mathbf{U}, \theta)$, $e(\mathbf{U}, \theta)$, $\psi(\mathbf{U}, \theta)$, $\eta(\mathbf{U}, \theta)$. For the non-equilibrium response ($\mathbf{L} \equiv \text{grad } \mathbf{v} = \partial_{\mathbf{x}} \mathbf{v}$, $\mathbf{g} \equiv \text{grad } \theta = \partial_{\mathbf{x}} \theta$): $\mathbf{S}_d(\mathbf{F}, \theta, \mathbf{g}, \mathbf{D})$, $\mathbf{q}_0(\mathbf{F}, \theta, \mathbf{g}, \mathbf{D})$ and

$$\begin{aligned}\mathbf{S}_d(\mathbf{R}\mathbf{F}, \theta, \mathbf{R}\mathbf{g}, \mathbf{R}\mathbf{D}\mathbf{R}^T) &= \mathbf{R}\mathbf{S}_d(\mathbf{F}, \theta, \mathbf{g}, \mathbf{D}) \\ \mathbf{q}_0(\mathbf{R}\mathbf{F}, \theta, \mathbf{R}\mathbf{g}, \mathbf{R}\mathbf{D}\mathbf{R}^T) &= \mathbf{q}_0(\mathbf{F}, \theta, \mathbf{g}, \mathbf{D})\end{aligned}$$

Or in terms of \mathbf{C} :

$$\mathbf{S}_e = 2\rho_0 \mathbf{F} \frac{\partial \psi}{\partial \mathbf{C}}$$

- Heat conduction law: Fourier's law:

$$\mathbf{q}_0 = \mathbf{K}(\mathbf{C}, \theta) \mathbf{g}_0$$

where \mathbf{K} is a positive semidefinite heat conductivity tensor.

- Elastic Fluid: $\psi(J, \theta)$
- Specific heat $c = \partial_{\theta} e$
- Green strain: $\mathbf{E}_G = \frac{1}{2} [\mathbf{U}^2 - \mathbf{1}] = \frac{1}{2} [\mathbf{C} - \mathbf{1}]$, Logarithmic strain $\mathbf{E} = \ln \mathbf{U}$.

14.9 Modeling of Hyperelastic Materials

DEFINITION 0.1 The field variables $\phi(\cdot)$, $\mathbf{T}(\cdot)$, $\eta(\cdot)$, $\mathbf{q}(\cdot)$ of a *thermoelastic material* only depend on the state variables \mathbf{F} , θ , \mathbf{g} .

THEOREM 0.1 To satisfy the Clausius-Duhem inequality the Cauchy stress for a thermoelastic material has to satisfy

$$\boxed{\mathbf{T}(\mathbf{F}, \theta) = \frac{1}{J} \frac{\partial W(\mathbf{F}, \theta)}{\partial \mathbf{F}} \mathbf{F}^T.} \quad (1)$$

Proof: The Clausius-Duhem inequality for a thermoelastic material can be written

$$\rho \dot{\psi} - \mathbf{T} \cdot \mathbf{L} + \rho \eta \dot{\theta} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \leq 0. \quad (2)$$

Differentiating ψ and inserting into (2) yields

$$\rho(\partial_{\mathbf{F}}\psi) \cdot \dot{\mathbf{F}} + \rho(\partial_{\theta}\psi)\dot{\theta} + \rho(\partial_{\mathbf{g}}\psi) \cdot \dot{\mathbf{g}} - \mathbf{T} \cdot \mathbf{L} + \rho\eta\dot{\theta} + \frac{\mathbf{q} \cdot \mathbf{g}}{\theta} \leq 0, \quad (3)$$

which must hold for any process leading to

$$\partial_{\mathbf{g}}\psi = 0, \quad \eta = -\partial_{\theta}\psi, \quad \mathbf{q} \cdot \mathbf{g}/\theta \leq 0. \quad (4)$$

Recalling that $\mathbf{T} \cdot \mathbf{L} = \mathbf{T}\mathbf{F}^{-T} \cdot \dot{\mathbf{F}}$ and $\rho = \rho_0/J$ directly leads to (1). \square

THEOREM 0.2 By imposing objectivity on a thermoelastic material the Cauchy stress has to satisfy

$$\mathbf{T}(\mathbf{C}, \theta) = \frac{2}{J} \mathbf{F} \frac{\partial W(\mathbf{C}, \theta)}{\partial \mathbf{C}} \mathbf{F}^T. \quad (5)$$

Proof: To satisfy objectivity, a change of observer must imply $\mathbf{T}(\mathbf{F}) = \mathbf{R}\mathbf{T}(\mathbf{U})\mathbf{R}^T$ and $W(\mathbf{F}, \theta) = W(\mathbf{U}, \theta) = W(\mathbf{C}, \theta)$, which when inserted into (1) gives

$$\mathbf{T}(\mathbf{U}, \theta) = \mathbf{R} \left[\frac{1}{J} \frac{\partial W(\mathbf{U}, \theta)}{\partial \mathbf{U}} \mathbf{U}^T \right] \mathbf{R}^T, \quad (6)$$

or when expressed in terms of \mathbf{C} gives (5). \square

THEOREM 0.3 For an isotropic material Equation (5) becomes

$$\mathbf{T} = \frac{2}{J} (W_1 + W_2 I_1) \mathbf{B} - \frac{2}{J} W_2 \mathbf{B}^2 + W_3 \mathbf{1} \quad (7)$$

where $W(I_1(\mathbf{C}), I_2(\mathbf{C}), I_3(\mathbf{F}), \theta)$ and $W_1 := \partial W / \partial I_1(\mathbf{C})$, etc.

Proof: Equation (1) can be written

$$\mathbf{T}(I_1, I_2, J, \theta) = \frac{2}{J} \mathbf{F} \frac{\partial W}{\partial I_i} \frac{\partial I_i}{\partial \mathbf{C}} \mathbf{F}^T,$$

and by using $\partial_{\mathbf{C}} I_1 = \mathbf{1}$, $\partial_{\mathbf{C}} I_2 = I_1 \mathbf{1} - \mathbf{C}$, and $\partial_{\mathbf{C}} I_3 = \frac{J}{2} \mathbf{F}^{-1} \mathbf{F}^{-T}$ the proposed equation (7) directly follows. \square

THEOREM 0.4 If the deformation gradient is decomposed into dilatational and distortional components $\mathbf{F} = J^{1/3} \mathbf{F}^*$, then the Clausius-Duhem inequality implies

$$\mathbf{T} = \frac{1}{J} \frac{\partial W}{\partial \mathbf{F}^*} \mathbf{F}^{*T} + \frac{\partial W}{\partial J} \mathbf{1} - \frac{1}{3J} \left(\frac{\partial W}{\partial \mathbf{F}^*} \cdot \mathbf{F}^* \right) \mathbf{1}. \quad (8)$$

Proof: By using the chain rule in index notation Equation (1) can be written

$$T_{ij} = \frac{1}{J} \frac{\partial W}{\partial F_{mn}^*} \frac{\partial F_{mn}^*}{\partial F_{ij}} + \frac{1}{J} \frac{\partial W}{\partial J} \frac{\partial J}{\partial F_{ik}} F_{jk}$$

giving

$$T_{ij} = \frac{1}{J} \frac{\partial W}{\partial F_{mn}^*} \frac{\partial [J(\mathbf{F})^{-1/3} F_{mn}]}{\partial F_{ik}} + \frac{\partial W}{\partial J} \delta_{ij}$$

which when expanded equates to (8). \square

THEOREM 0.5 If the deformation gradient is decomposed into dilatational and distortional components $\mathbf{F} = J^{1/3}\mathbf{F}^*$, then the Clausius-Duhem inequality and objectivity gives

$$\mathbf{T} = \frac{2}{J}\mathbf{F}^* \frac{\partial W}{\partial \mathbf{C}^*} \mathbf{F}^{*T} + \frac{\partial W}{\partial J} \mathbf{1} - \frac{2}{3J} \left(\frac{\partial W}{\partial \mathbf{C}^*} \cdot \mathbf{C}^* \right) \mathbf{1}. \quad (9)$$

Proof: Directly analogous to the previous proof. \square

THEOREM 0.6 If the deformation gradient is decomposed into dilatational and distortional components $\mathbf{F} = J^{1/3}\mathbf{F}^*$, then the Cauchy stress for an isotropic material has to be

$$\mathbf{T} = \frac{2}{J} [W_{1^*} + W_{2^*} I_{1^*}] \mathbf{B}^* - \frac{2}{J} W_{2^*} (\mathbf{B}^*)^2 + \frac{\partial W}{\partial J} \mathbf{1} - \frac{2I_{1^*}}{3J} W_{1^*} \mathbf{1} - \frac{4I_{2^*}}{3J} W_{2^*} \mathbf{1}, \quad (10)$$

where $W_{1^*} \equiv \partial W / \partial I_1(\mathbf{C}^*)$. Proof: Directly analogous to the previous proof. \square

15.1 The phase rule

The number of degrees of freedom is given by

$$f = n + 2 - p$$

where n is the number of components and p is the number of phases.

15.2 The microcanonical ensemble

The partition function Ω is a measure of the number of configurations in the ensemble

$$s = -k \sum_i p_i \ln p_i = k \ln \Omega.$$

15.3 The canonical ensemble

Considering a system having a very large number of degrees of freedom. The system is characterized by (macroscopic) thermodynamic variables (N, V, T are fixed in the system). Now, consider an ensemble containing a very large number of such systems. Let

$$\begin{aligned} \mathcal{A} &= \text{number of systems in the ensemble} \\ a_i &= \text{number of systems in state } i \text{ (i.e. having energy } E_i) \\ \mathcal{E} &= \text{total energy of the ensemble} \end{aligned}$$

giving

$$\mathcal{A} = \sum a_i, \quad \mathcal{E} = \sum a_i E_i.$$

The state of the ensemble can be characterized by the occupation numbers $\mathbf{a} = \{a_1, a_2, \dots\}$. The probability of finding a system in state i is

$$P_i = \frac{\langle a_i \rangle}{\mathcal{A}} = \frac{a_i^*}{\mathcal{A}}.$$

Further consider a set of all possible ensembles. Since each ensemble has the same energy they have the same probability of occurring. Let $W(\mathbf{a})$ be the number of occurrences of the ensemble specified by \mathbf{a} giving

$$W(\mathbf{a}) = \frac{\mathcal{A}!}{a_1! a_2! \dots}$$

Also define \mathbf{a}^* to be the most common ensemble in the set, then \mathbf{a}^* can be found from

$$\frac{\partial}{\partial a_j} \left\{ \ln W(\mathbf{a}) - \alpha \sum a_k - \beta \sum a_k E_k \right\} = 0$$

giving

$$p_i = \frac{e^{-\beta E_j}}{\sum e^{-\beta E_k}}.$$

The partition function becomes

$$Q(N, V, E) = \sum_j e^{-\beta E_j} = \sum_E \Omega(N, V, E) e^{-E/(kT)}.$$