Continuum Mechanics

Continuum Mechanics and Constitutive Equations

Continuum mechanics pertains to the description of mechanical behavior of materials under the assumption that the material is a uniform continuum. It is a "black box" approach with the goal of predicting mechanical behavior in the absence of understanding for engineering and scientific calculation. There is a strong parallel between the black box approach of continuum mechanics and the description of a thermodynamic system with which you may be familiar.

For Materials Scientists and Engineers, continuum mechanics provides a language and a framework for understanding the physical and morphological basis for mechanical behavior. For example, by using the tensoral nature of modulus a materials engineer can describe and understand the modulus and fracture strength of a single crystal silicon wafer with reference to the crystallographic orientation of the material. A materials engineer uses the terminology of continuum mechanics to describe die swell in extrusion of a polymer filament. Similarly, the piezoelectric behavior of ceramic crystals is described using tensoral continuum mechanical descriptions.

The tensoral description of stress, strain and rate of strain in continuum mechanics leads to the basic definition of tensoral moduli, compliances and viscosities. These parameters are examples of **constitutive parameters**, that is constants that describe the constitution of the "black box". There are an unlimited number of **constitutive constants** each related to a particular response to a particular perturbation of a continuum system and it is important to understand what a constitutive constant can and can not do. First, in and of itself a constitutive constant, such as the thermal expansion coefficient, the modulus, conductivity, does not lead to any type of understanding of a material. A constitutive parameter and constitutive equation predicts a response usually under a set of strict limits. Knowing the tensile modulus will not in and of itself enable an understanding of the shear compliance or the bulk modulus. In order to draw broader consequences from a given constitutive parameter a model for the mechanical behavior must be considered based on our understanding of structure and morphology for a given material.

The combination of morphology and continuum mechanics has proven to be a powerful tool in understanding the mechanical behavior of materials. For example, the lamellar crystallites in a polyethylene blown film are known to orient in the film plane for low density polyethylene and normal to the machine direction for high density polyethylene from small-angle x-ray scattering measurements. The tensile modulus for low-density polyethylene has roughly the same value in the machine and transverse directions for this reason making the material useful for packaging applications. Additionally, this same continuum/morphological model for the microstructure predicts low water vapor transmission for low density polyethylene films which is also advantageous in packaging applications. High density films display low moduli in the machine direction and higher transverse moduli with high moisture transmission rates.

Stress

We will consider systems where the principle stresses are applied in one of the three Cartesian directions. You have learned in your introductory mechanics class that the coordinate system for any system can be rotated to this condition using devices such as Mohr's circle and associated mathematical expressions. A review of such coordinate system rotations is given in Mechanical Metallurgy by Dieter in Chapter 2. We will also only consider surface forces, that is a force that acts on a surface. Then, we do not consider body forces such as the force due to gravity, centrifugal force, thermal expansion, or magnetic forces.

Under these conditions a force is described by a magnitude, in Newtons, and a direction along one of the three principle axes. A parameter described by a direction and a magnitude is called a vector. Consider a surface force in the z-direction acting on a cubic element of material. The surface on which the force acts can be one of the three types of surfaces available on the cubic element. A surface is described by the normal direction in the most compact form. That is the plane formed by the x-y axes is called the z-surface because the normal to this plane points in the z-direction. Then, a z-surface force acting on the z-surface results in a tensile stress on the cubic volume element,

$$_{zz} = F_z/A_z \qquad (1)$$

The z-force can act on two other surfaces, x and y, x being the y-z plane and y being the x-z plane. The corresponding stresses, $_{zx}$ and $_{zy}$ are best considered with regard to a deck of cards. Consider a deck of cards where the friction between each pair of cards is constant and where the bottom card is fixed while the force F_z is applied in the plane of the top card, in the z-direction of the y-z plane. The top card will move causing a deformation of the stack as shown in Figure 1.

Figure 1. Shear Deformation
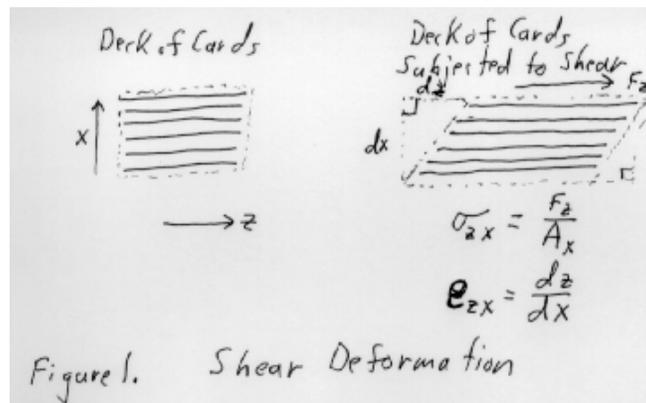
For the z-force there are two types of shear stresses that can be applied to a cubical volume element,

$$_{zx} = F_z/A_x \qquad \text{and} \qquad _{zy} = F_z/A_y \qquad (2)$$

For each of the three surface force vectors there are three types of surfaces on which they can act. Then surface stress is a 9 component second order tensor. A second order tensor is a

collection of values that have a magnitude and two directions. In Cartesian coordinates we can write the stress tensor, σ_{ij}, as,

$$\underline{\underline{\sigma_{ij}}} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \qquad (3)$$

There are many different nomenclatures used in the literature even where Cartesian coordinates are used. For instance, the normal stresses, σ_{xx}, σ_{yy}, σ_{zz}, are sometimes written, σ_x, σ_y, σ_z. The shear stresses, σ_{zx} and the like, are sometimes written, τ_{zx}. The indicies are often written 1, 2, 3 rather than x, y, z. Moreover, a nine-component stress tensor can be equally defined in cylindrical coordinates, for uniaxial tension or pipe flow, or in cylindrical coordinates through simple coordinate transformations that you are familiar with from Calculus classes.

Although 9 components are needed to describe an arbitrary state of stress, generally we can assume that there are no rotational forces acting on the cubical element for purposes of a continuum analysis. This assumption leads to the simplification that the stress matrix of equation (3) is a symmetric matrix, that is $\sigma_{ij} = \sigma_{ji}$. This can be demonstrated for one pair of symmetric shear stresses, for instance σ_{xy} and σ_{yx}, Figure 2. The dashed line in figure 2 is a torsional bar which must have not rotational torque is the system is not subjected to rotational motion. Two stresses, σ_{xy} and σ_{yx}, are applied to the system. The torsional element is subjected to two rotational forces shown. These two forces must balance under these conditions leaving $F_y = F_x$ and $\sigma_{xy} = \sigma_{yx}$. (For each off diagonal torsional element the solid body has two symmetric torsional elements which when summed lead to the same result.)

Figure 2. Demonstration That $\sigma_{xy} = \sigma_{yx}$. Dashed Line is a torsional Element
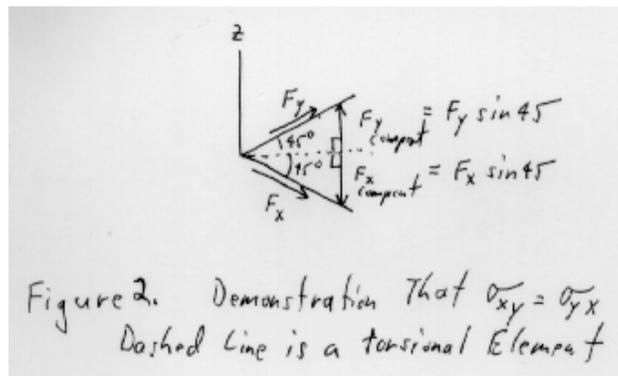
Then, for systems not subject to rotation we can rewrite the stress matrix as a 6 component matrix,

$$\underline{\underline{\sigma_{ij}}} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} \qquad (4)$$

Usually, we are not interested in the hydrostatic component to stress since this can only lead to volumetric expansion or contraction. For a material in the atmosphere the hydrostatic component of stress is a tensile stress whose magnitude is the atmospheric pressure, P and which is applied equally to the faces of the Cartesian system. The hydrostatic pressure is the first of three scalar **invariants** for the stress tensor. An invariant is a scalar value derived from a tensor that does not change with rotation or conversion of the coordinate system. The hydrostatic pressure, P, can be obtained from the stress tensor by summation of the tensile or **normal stress** components,

$$P = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3} = \frac{I_{1,}}{3} = \frac{\sigma_{ii}}{3} \qquad (5)$$

Where "$I_{1,}$" is the first invariant of the stress tensor. The latter expression is an example of the use of **"Einstein" tensor notation** where repeated indices indicate summation over that index.

Usually it is desirable to remove hydrostatic pressure from consideration of the stress. The stress tensor described above is, in this context, called **the total stress tensor** and is sometimes denoted , while the deviatory or extra stress tensor excluding hydrostatic stress is denoted, ,

$$\underline{\underline{\sigma}} = \underline{\underline{\tau}} = \underline{\underline{\tau}} - P\underline{\underline{\delta}} = \underline{\underline{\tau}} = \underline{\underline{\sigma}} - P\underline{\underline{\delta}} = \begin{vmatrix} \sigma_{xx} - P & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} - P & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} - P \end{vmatrix} \qquad (6)$$

where   is the identity tensor with unit values on the diagonal components and zeros elsewhere.

The other two invariants for the stress tensor are given by,

$$I_{2,} = \frac{1}{2}\left(\sigma_{ik}\sigma_{ki} - \sigma_{ii}\sigma_{kk} \right) = \begin{vmatrix} \sigma_{22} & \sigma_{23} \\ \sigma_{23} & \sigma_{33} \end{vmatrix} + \begin{vmatrix} \sigma_{11} & \sigma_{13} \\ \sigma_{13} & \sigma_{33} \end{vmatrix} + \begin{vmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{vmatrix} \qquad (7)$$

$$I_{3,} = \frac{1}{6}\left(2\sigma_{ij}\sigma_{jk}\sigma_{ki} - 3\sigma_{ij}\sigma_{ji}\sigma_{kk} + \sigma_{ii}\sigma_{jj}\sigma_{kk} \right) = \begin{vmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{vmatrix} \qquad (8)$$

where Einstein notation has been used in the first expressions.

Rotation of coordinate system can be achieved using matrix math. This will be considered only where it is necessary later in the course.

It is often useful to consider deviatory normal stresses, σ_{11}, σ_{22}, σ_{33}, in terms of the first and second normal stress differences,

$$\sigma_1 = \tau_{11} - \tau_{22} = \sigma_{11} - \sigma_{22} \qquad (9)$$

$$\tau_2 = \tau_{22} - \tau_{33} = \sigma_{22} - \sigma_{33} \tag{10}$$

since it is not possible to independently measure the normal stress components of the deviatory stress tensor.

Strain:

Figure 1 defines a shear component of the strain in terms of the derivative of the z and x dimensions of a cubic material element,

$$e_{zx} = dz/dx = e_{31} = dx_3/dx_1$$

Strain (e is sometimes called the **displacement tensor**) is a second order tensor with nine components defined by tensile, e_{ii}, and shear, e_{ij}, components,

$$\underline{\underline{e_{ij}}} = \begin{matrix} e_{xx} & e_{xy} & e_{xz} \\ e_{xy} & e_{yy} & e_{yz} \\ e_{xz} & e_{yz} & e_{zz} \end{matrix} \tag{11}$$

With the stress tensor we removed the hydrostatic pressure since it did not give rise to some types of mechanical deformation, for example flow of an incompressible fluid. Similarly the total strain tensor is usually decomposed into two tensors, **the strain tensor**, ε_{ij}, and the **vorticity or rotation tensor**, ω_{ij},

$$\varepsilon_{ij} = \frac{\left(e_{ij} + e_{ji}\right)}{2} \tag{12}$$

$$\omega_{ij} = \frac{\left(e_{ij} - e_{ji}\right)}{2} \tag{13}$$

The strain tensor is a symmetric 6 component tensor while the vorticity tensor is an antisymmetric 3 component tensor. The vorticity tensor reflects the extent of rotational motion which has occurred on application of stress.

The dilatometric (volume) strain is approximated by $\Delta = \varepsilon_{ii}$ (using Einstein notation). This can be removed from the strain to describe the deviatory strain tensor, ε',

$$\underline{\underline{\varepsilon}}' = \underline{\underline{\varepsilon}} - \frac{\Delta}{3}\underline{\underline{\delta}} \tag{14}$$

5

Rate of Strain:

Figure 3. Creep Measurement for Solid —; Liquid(- - -); and Viscoelastic (......)
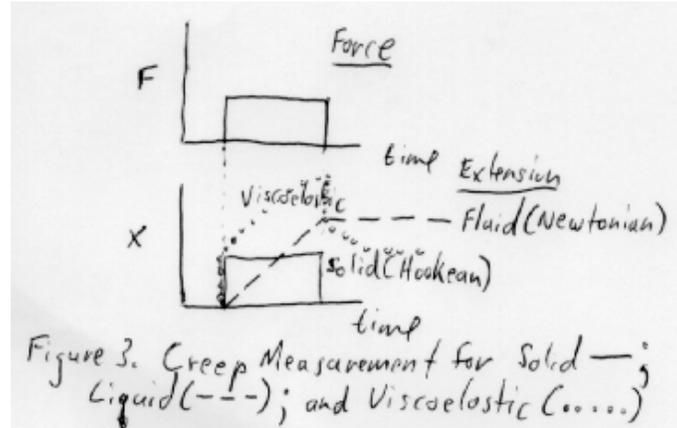
Figure 3 shows the behavior in time of three samples displaying the three major categories of mechanical response in materials. At a certain time a fixed shear stress is applied to the sample and the deformation, x, of the sample as a function of time is observed. For a Hookean solid the response in terms of deformation is instantaneous. When the stress is removed the material completely recovers to the initial length, x. For a Newtonian fluid the rate of change of length, strain rate, is constant. The sample deforms at a constant rate until the stress is removed at which time the extent of deformation remains constant, dashed line in lower plot. A viscoelastic displays a combination of these two behaviors, there is an initial and immediate deformation reminiscent of Hookean behavior, followed by a region of flow, dotted curve in lower graph. Following removal of the stress there is some immediate recovery of the deformation similar to Hookean behavior as well as some permanent set to the material indicated by the failure of the material to return to the horizontal axis. For viscoelastic and viscous materials the rate of strain is the dominant response to an applied stress.

The rate of strain tensor, $\dot{\underline{\underline{\epsilon}}}$, is the derivative of the strain tensor with respect to time,

$$\dot{\underline{\underline{\epsilon}}} = \frac{d\underline{\underline{\epsilon}}}{dt} = \frac{d\underline{v}}{d\underline{x}} \qquad (15)$$

or equivalently the velocity gradient tensor. Consider ϵ_{12},

$$\epsilon_{12} = \frac{dx_1}{dx_2}, \quad \dot{\epsilon}_{12} = \frac{d\epsilon_{12}}{dt} = \frac{d\frac{dx_1}{dx_2}}{dt} = \frac{d\frac{dx_1}{dt}}{dx_2} = \frac{dv_1}{dx_2} \qquad (16)$$

Constitutive Equations:

As mentioned above a constitutive equation relates a response to the perturbation associated with the response. For mechanical properties the response can be considered the strain or rate of strain and we define the **compliance**, J, (sign conventions may vary)

$$J = \frac{}{_0} \qquad (17)$$

where the subscript "0" indicates that the stress is constant therefore defining a creep measurement such as shown in figure 3.

The modulus, E, is defined in the context of a stress relaxation experiment (constant strain),

$$E = \frac{}{_0} \qquad (18)$$

For a Hookean elastic the modulus and compliance are inverse parameters. For time dependent response such as in viscoelastic materials there are complex relationships between the time dependent modulus and time dependent compliance.

The **viscosity**, , is defined in parallel to the modulus, (sign conventions may vary)

$$= \frac{}{\dot{}_0} \qquad (19)$$

Equations 17, 18 and 19 define the ideal behavior expected for a Hookean elastic (17 and 18) and for a Newtonian fluid (19).

Since the stress, strain and strain rate are tensoral quantities, equations 17 to 19 must correctly be written in tensor form, this will be discussed below.

Normal stresses which develop in polymer flow and lead to die swell and related phenomena are described by low strain rate idealized constitutive equations,

$$_1 = \frac{_1}{\dot{}^2_0} \quad \textbf{and} \quad _2 = \frac{_2}{\dot{}^2_0} \qquad (20)$$

Elastic Constants (Tensoral Analysis):

In the most generic sense we can consider each component of the total stress tensor as having a relationship with each component of the total strain tensor. The elastic constant (modulus) tensor would then have 9 x 9 = 81 possible components. For $_{ij}$ and $_{kl}$ we would have,

$$_{ij} = C_{ijkl}\,_{kl} \ \textbf{where} C_{ijkl} \ \textbf{has 81 componen} \qquad (21)$$

Since both ε_{ij} and ε_{kl} are symmetric tensors, that is $\varepsilon_{ij} = \varepsilon_{ji}$, the modulus tensor displays 36 independent components,

$$
\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{bmatrix} =
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\
c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\
c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\
c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66}
\end{bmatrix}
\begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{31} \\ 2\varepsilon_{12} \end{bmatrix}
\tag{22}
$$

If the elastic constant matrix is independent of orientation of the material, the material is called **mechanically isotropic** (meaning same form). Materials such as a multigrain metal or an amorphous polymer are usually isotropic. If the elastic constants matrix changes with the material orientation the material is called **mechanically anisotropic**. Materials such as a silicon wafer, an aluminum pop can or a fiber are highly anisotropic in mechanical response.

Generally the elastic constant matrix is symmetric based on a generalized association between strain an energy in mechanical deformation (see Malvern, "Introduction to the Mechanics of a Continuous Media p. 285 for instance). Then the 36 term elastic tensor reduces to 21 independent parameters.

Generallyl, materials display some degree of mechanical symmetry. For a plane of symmetry in the 12 plane (3 normal), the elastic constant matrix can be shown to reduce to 13 independent constants since many of the elastic constants can be shown to be 0,

$$
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\
c_{12} & c_{22} & c_{23} & 0 & 0 & c_{26} \\
c_{13} & c_{23} & c_{33} & 0 & 0 & c_{36} \\
0 & 0 & 0 & c_{44} & c_{45} & c_{46} \\
0 & 0 & 0 & c_{45} & c_{55} & c_{56} \\
c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66}
\end{bmatrix}
\qquad \text{Plane of Symmetry} \tag{23}
$$

If 3 otrhogonal planes of symmetry exist, such as in a biaxially oriented sheet, the elastic constant matrix reduces to 9 independent parameters,

$$
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\
c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{66}
\end{bmatrix}
\qquad \text{3 Orthogonal Symmetry Planes} \tag{23}
$$

For an isotropic material the elastic constants are independent of the orientation of the coordinate axes and the elastic constant matrix can be reduced to 2 independent moduli.

$$
\begin{bmatrix}
+2\mu & & & 0 & 0 & 0 \\
& +2\mu & & 0 & 0 & 0 \\
& & +2\mu & 0 & 0 & 0 \\
0 & 0 & 0 & \mu & 0 & 0 \\
0 & 0 & 0 & 0 & \mu & 0 \\
0 & 0 & 0 & 0 & 0 & \mu
\end{bmatrix}
\qquad \text{Isotropic Material} \qquad (23)
$$

Then a tensile stress strain measurement and a shear measurement will fully characterize the mechanical response of an isotropic material.

Generally, we consider much simpler scenarios of mechanical deformation and the traditional nomenclature for tensile and shear tests should be compared with the matrix description given above. Equation 18 can be written,

$$
_{11} = E \,_{11} \quad \textbf{and} \quad _{12} = G \,_{12} \qquad (24)
$$

where E is the tensile modulus and G is the shear modulus. A tensile stress in the x-direction produces contraction in the y and z directions described by the **Poisson ratio**, ,

$$
_{22} = \,_{33} = - \,_{11} = - \frac{_{11}}{E} \quad \textbf{Isotropic Materia} \qquad (25)
$$

For an incompressible material such as a rubber = 0.50. For metals the value is generally 0.33. For an isotropic material we know that there are only two independent moduli, equation 23, so E, G and can be related,

$$
G = \frac{E}{2(1+ \ )} \qquad (26)
$$

We can also consider a modulus associated with dilatometric deformation (deformation that results in a volume change). The bulk modulus, K, related hydrostatic pressure, P, to the dilatation, $= \,_{11} + \,_{22} + \,_{33}$,

$$
K = \frac{P}{} = \frac{1}{} \qquad (27)
$$

where is the compressibility. Again, the new modulus can be related to the two original moduli,

$$K = \frac{E}{3(1-2\nu)} = \frac{EG}{(9G-3E)} \qquad (28)$$

Lame's constant, λ, is used to describe the effects of dilatation on tensile stress,

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \qquad (29)$$

We have,

$$\sigma_{11} = 2G\,\varepsilon_{11} + \lambda\Delta \qquad (30)$$

This should be compared with the matrix elements of equation 23.

For an isotropic material with all components of stress subject to small strain we consider that a tensile stress, σ_{11}, leads only to tensile strains, ε_{11}, $\varepsilon_{22}=-\nu\varepsilon_{11}$, $\varepsilon_{33}=-\nu\varepsilon_{11}$. Then,

$$\varepsilon_{ii} = \frac{1}{E}\left(\sigma_{ii} - \nu\left(\sigma_{jj} + \sigma_{kk}\right)\right) \qquad (31)$$

Shear stress produces only one shear strain,

$$\sigma_{ij} = G\,\varepsilon_{ij} \qquad (32)$$

where G is the shear modulus.

Elastic Strain Energy:

The area under a stress-strain curve is equal to the energy expended in deformation, Figure 4.

Figure 4. Energy, U, associated with Strain.
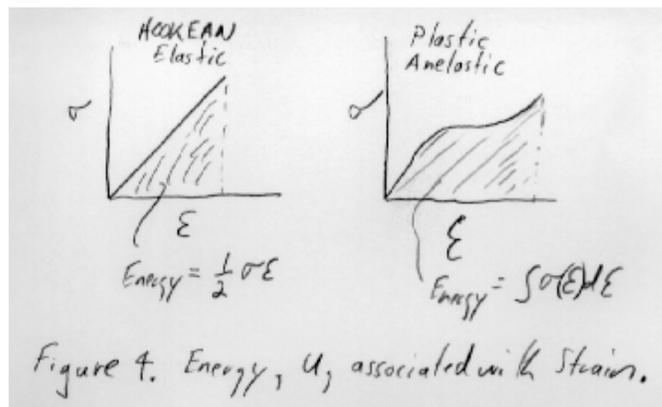
The relationship between strain energy and stress and strain can be obtained by considering that energy is equal to the applied force, F, times the change in distance over which the force acts,

$$dU = F(x)dx = xF(\varepsilon)d\varepsilon \qquad (33)$$

where x is a unit length. The force in the first graph of Figure 4 follows the function,

$$F(\varepsilon) = AE\varepsilon = x^2 E\varepsilon \qquad (34)$$

where A is the unit area associated with stress. Then we have,

$$dU = F(x)dx = V_{unit} E\varepsilon\, d\varepsilon \qquad (35)$$

where V is a unit volume. Dividing the energy by the unit volume provides the strain energy density, U_0. Integration of equation (35) yields,

$$U_0 = \int_{\varepsilon=0} E\varepsilon\, d\varepsilon = \frac{1}{2}E\varepsilon^2 = \frac{1}{2}\sigma\varepsilon \qquad (36)$$

This expression is valid for tensile stress and shear stress. For a general 3-d stress tensor we can obtain using similar logic,

$$U_0 = \frac{1}{2}\sigma_{ij}\varepsilon_{ij} \qquad (37)$$

using Einstein notation. Using equations (31) and (32),

$$U_0 = \frac{1}{2E}\sigma_{ii}^2 - \frac{\nu}{2E}\left(\sigma_{ii}\sigma_{jj} - \sigma_{ii}^2\right) + \frac{1}{4G}\left(\sigma_{ij}\sigma_{ij} - \sigma_{ii}\sigma_{jj}\right) \qquad (38)$$

using Einstein notation. Using equation (30),

$$U_0 = \frac{1}{2}\lambda\varepsilon^2 + G\varepsilon_{ii}^2 + \frac{1}{4}G\left(\varepsilon_{ii}\varepsilon_{jj} - \varepsilon_{ii}^2\right) \qquad (39)$$

From equation (39), the derivative of the strain energy density with respect to any strain component yields the corresponding stress component and similarly, from equation (38) the derivative with respect to any stress component yields the corresponding strain component,

$$\frac{\partial U_0}{\partial \varepsilon_{ij}} = \sigma_{ij} \quad \textbf{and} \quad \frac{\partial U_0}{\partial \sigma_{ij}} = \varepsilon_{ij} \qquad (40).$$

Extension of Continuum Concepts to Materials Science:

As was mentioned above, continuum mechanics considers a material to be composed of a continuum with no structural features. In this way engineering properties can be predicted and used in design. As a materials scientist we know some of the details of various engineering materials and the basic assumption of continuum mechanics is clearly incorrect. However, we can use the continuum framework to develop more complicated descriptions of materials.

We can first consider the most rudimentary details of materials. All materials are composed of atoms that may be bonded together with covalent or ionic bonds. Deformation of a material can lead to slight deformation of these bonds and to some extent this is the simplest view of a Young's modulus. Consider the atom, A, in figure 5, subject to a displacement, u. Displacement from the equilibrium position in a crystal, for instance, is usually considered in terms of the atomic potential energy diagram, ϕ(u).

Figure 5. Atom "A", is displaced a distance "u" Resulting in force F_A(u) associated with the symmetric (+u is same as -u) potential energy ϕ(u).

$$F_A(u) = \frac{d\phi}{du}$$
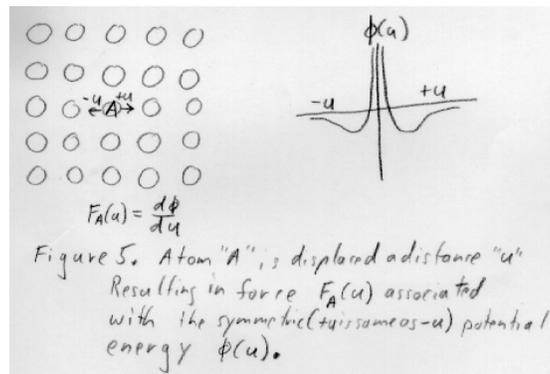
The potential energy, ϕ(u), can be a complex function but any normal function can be described in terms of a Taylor series expansion about a known point such as the equilibrium point, u = 0,

$$\phi(u) = \phi_0 + \frac{d\phi}{du}\bigg|_0 u + \frac{1}{2}\frac{d^2\phi}{du^2}\bigg|_0 u^2 + ... \qquad (41)$$

The force, F = dϕ/du, is 0 at u = 0 so the first derivative is zero. (Additionally, the potential is symmetric so that all odd power derivatives must be equal to 0.) Then we can write the force, F, in terms of the remaining derivatives ignoring higher order terms, u^4, u^6, for small displacements,

$$F = \frac{d\phi}{du} = \frac{d^2\phi}{du^2}\bigg|_0 u \qquad (42)$$

This equation is of the form of Hook's Law, $F = k_{spr} u$ where k_{spr} is the spring constant, related to the Young's Modulus. Then the Young's Modulus, E, is proportional to the second derivative of the potential energy for atomic displacement at the equilibrium atomic position. This is our first consideration of the relationship between structure and mechanical properties.