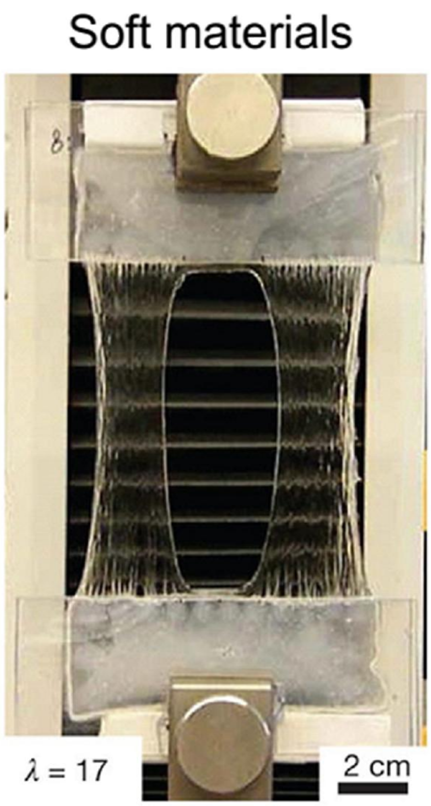
Lecture 3: Fracture mechanics of Hyper-elastic solids + Energy Momentum Tensor (J integral for large deformation)

Motivation: Most traditional materials used in engineering structures are sufficiently stiff so that the deformation can be described adequately by small strain theory. Recent advances in soft materials have created new soft materials such as double network hydrogels that can support very large deformation before failure. The figure below shows the deformed configuration of an initial straight crack in a sheet. Clearly, one cannot expect linear theory to be able to describe such large deformation.



Sun et al., Nature, 2012,489,133-136

Linear theory breaks down for two reasons:

1. The kinematics used in linear theory assumes small displacements, small displacement gradients and small rotation.
2. The material model used in linear theory assumes that strain is directly proportional to stress.

To dealt with the first, we need to use large deformation theory, which allows us to distinguish between reference (in this lecture chosen to be the stress free body) configuration and the deformed configuration. To deal with the second, we have to consider more realistic material model describing the material response to stress. In this and the following lecture we limit ourselves to elastic solids in which the stress state is uniquely determined by the deformation gradient.

Notations and Brief Review of Large Deformation continuum mechanics

A 2nd order Carteisan tensor (linear transformation from E^3 *(Euclidean space)* to E^3 is denoted by $\tilde{A}$. I will use the dyadic notation, so $\tilde{A} = A_{ij}\vec{e}_i\vec{e}_j$ with respect to an orthornormal basis $\{\vec{e}_i\}$ ($\vec{e}_i \bullet \vec{e}_j = \delta_{ij}$). Vectors will be denoted by $\vec{b} = b_i\vec{e}_i$. The value of $\tilde{A}$ on a vector $\vec{b}$ is denoted by

$$\tilde{A}\vec{b} \equiv A_{ij}\vec{e}_i\vec{e}_j \bullet b_k\vec{e}_k = A_{ij}b_k\vec{e}_i \underbrace{\vec{e}_j \bullet \vec{e}_k}_{\delta_{jk}} = A_{ik}b_k\vec{e}_i .$$

The transpose of trace of $\tilde{A}$ is the tensor $\tilde{A}^T = A_{ji}\vec{e}_i\vec{e}_j$. The trace of $\tilde{A}$ is the scalar defined by $tr\tilde{A} = A_{ii}$. The product of two 2nd order tensors $\tilde{A}$ and $\tilde{B}$ is another 2nd order tensor $\tilde{A}\tilde{B} \equiv A_{ik}B_{kj}\vec{e}_i\vec{e}_j$. The gradient of a vector function $\vec{v} = \vec{v}(x_i)$ with respect to $\vec{x} = x_i\vec{e}_i$ is the 2nd order tensor denoted by $\nabla_x\vec{v} = \dfrac{\partial v_i}{\partial x_j}\vec{e}_i\vec{e}_j$. For the sake of simplicity, I will use the same orthonormal basis for vectors and tensors in the deformed and reference configuration.

Review of continuum mechanics relevant for the these two lectures

Due to time limitations, the review below will be very brief and narrowly focused.

Kinematics

We use a Cartesian coordinate system with origin O with a fixed orthornormal basis $\{\vec{e}_i\}$. We assume the elastic body B is initially (*t = 0*) stress free and use this configuration as the reference configuration. We identify a material point in B with their position vector $\vec{x} = x_i\vec{e}_i$. At time t, the material point $\vec{x}$ moves to the position $\vec{y} = \vec{f}(\vec{x},t)$ with respect to the same coordinate system. We define the displacement vector of the material point $\vec{u} = \vec{u}(\vec{x},t)$ by

$$\vec{u} = \vec{y} - \vec{x} \qquad (3.1)$$

We assume that the function $\vec{f}$ which carries a material point $\vec{x}$ to its deformed position $\vec{y}$ is one to one and smooth. The deformation gradient tensor $\tilde{F} = F_{ij}\vec{e}_i\vec{e}_j$ is the linear transformation that completely characterizes the deformation in a small neighborhood containing the material point $\vec{x}$, that is

$$d\vec{y} = \tilde{F}d\vec{x}, \quad \tilde{F} = \nabla_x\vec{f} \Rightarrow F_{ij} = \delta_{ij} + \frac{\partial u_i}{\partial x_j} \qquad (3.2)$$

Since $\vec{f}$ is one to one, $\left|det\tilde{F}\right| > 0$ is non-zero. Physical consideration that the volume of a material element cannot vanish demands that $det\tilde{F} > 0$. The stretch ratio λ of any small line element $d\vec{x} = |d\vec{x}|\vec{t}$ with its origin at $\vec{x}$, after deformation becomes $d\vec{y}$,

$$\lambda^2 = \frac{|d\vec{y}|^2}{|d\vec{x}|^2} = \tilde{F}t \bullet \tilde{F}\vec{t} = \vec{t} \bullet \underbrace{\left(\tilde{F}^T\tilde{F}\right)}_{\tilde{C}}\vec{t} \qquad (3.3)$$

where $\tilde{C} = \tilde{F}^T\tilde{F}$ is the right Cauchy-Green tensor. It is easy to show that $\tilde{C}$ is symmetric and positive definite ($det\tilde{F} > 0$, $\tilde{F}$ is invertible and cannot have a zero eigenvalue) and therefore all eigenvalues of $\tilde{C}$ is positive (denoted by λ_i^2) and $\tilde{C}$ has an orthornormal eigenbasis $\vec{E}_i$. Therefore, the representation of $\tilde{C}$ in principal coordinates is:

$$\tilde{C} = \sum_{i=1}^{3} \lambda_i^2 \vec{E}_i \vec{E}_i \quad \text{(no sum on } i\text{)} \qquad (3.4)$$

The eigenvectors $\vec{E}_i$ of $\tilde{C}$ are called principal directions of strain, they are arranged such that $\lambda_1^2 \geq \lambda_2^2 \geq \lambda_3^2 > 0$. For obvious reasons, $\lambda_i > 0$ are called principal stretch ratios. From (3.4), it is not difficult to show the Polar Decomposition Theorem where $\tilde{F}$ can be decomposed into

$$\tilde{F} = \tilde{R}\tilde{U} = \tilde{V}\tilde{R} \qquad (3.5)$$

where $\tilde{R}$ is an orthogonal tensor, $\tilde{U}$ and $\tilde{V}$ are positive definite symmetric tensors,

$$\tilde{U} = \sum_{i=1}^{3} \lambda_i \vec{E}_i \vec{E}_i \qquad \tilde{V} = \sum_{i=1}^{3} \lambda_i \left(\tilde{R}\vec{E}_i\right)\left(\tilde{R}\vec{E}_i\right) \qquad \text{(no sum on i)} \qquad (3.6)$$

The tensors $\tilde{R}$, $\tilde{U}$ and $\tilde{V}$ in (3.5) are unique. Physically, the equation $\tilde{F} = \tilde{R}\tilde{U}$ states that the local deformation in the neighborhood of a material $\vec{X}$ can be considered as a pure stretch, followed by a rigid body rotation.

Balance Laws

In these lectures I will neglected body forces and consider only quasi-static theory. The derivation of force and angular momentum balance are identical to those in small strain theory provided that we derived them in the deformed configuration. In short, the Cauchy stress or true stress tensor $\tilde{\tau} = \tau_{ij}\vec{e}_i\vec{e}_j = \tau_{ji}\vec{e}_i\vec{e}_j$ is symmetric due to angular momentum balance and satisfies

$$\nabla_y \bullet \tilde{\tau} = \vec{0} \Leftrightarrow \frac{\partial \tau_{ij}}{\partial y_j}\vec{e}_i = \vec{0} \qquad \vec{y} \in \vec{f}(B) \qquad (3.7a)$$

$$\tilde{\tau} = \tilde{\tau}^T \Leftrightarrow \tau_{ij} = \tau_{ji} \qquad \vec{y} \in \vec{f}(B) \qquad (3.7b)$$

Note that differentiation in (3.7a) *is with respect to the deformed coordinates* and the three scalar PDEs in (3.7) are defined in the deformed body, which is the image of the body *B* under $\vec{f}$, denoted by $\vec{f}(B)$. However, in order to determine the deformation, we must know the reference configuration *B*; therefore it is necessary to express the balance laws in the reference configuration. To see how this is done, we note that by the divergence theorem, (3.7a) is equivalent to

$$\oiint_s \tau_{ij} n_j ds_y = 0 \Leftrightarrow \oiint_s \tilde{\tau}\vec{n} ds_y = \vec{0} \qquad (3.8)$$

for *any* close surface *s* inside $\vec{f}(B)$, where $\vec{n}$ is the unit outward normal vector to *s.* Physically, it states that the total traction force acting on any material surface must be zero (since there are no body and inertia forces). We now use a change of variable integration formula to convert (3.8) to a surface integral in the reference configuration. Specifically, one can show

$$\vec{n} ds_y = J\tilde{F}^{-T}\vec{m} ds_x \qquad J \equiv det\tilde{F} \qquad (3.9)$$

where $\vec{n}$ is the image of $\vec{m}$ under $\vec{f}$, and ds_x is surface area in the reference configuration corresponding to ds_y, thus,

$$\oiint_{\partial\Omega_t} \tilde{\tau}(\vec{y},t)\vec{n}(\vec{y},t) ds_y = \oiint_{\partial\Omega_0} \underbrace{\tilde{\tau}\left(\vec{f}(\vec{x},t),t\right) J(\vec{x},t)\tilde{F}^{-T}(\vec{x},t)}_{\tilde{\sigma}(\vec{x},t)} \vec{m}(\vec{x}) ds_x = 0 \qquad (3.10a)$$

Define the 1st Piola-Kirchhoff stress tensor (also called the Nominal stress tensor)

$$\tilde{\sigma}(\vec{x},t) \equiv \tilde{\tau}\left(\vec{f}(\vec{x},t),t\right) J(\vec{x},t)\tilde{F}^{-T}(\vec{x},t) \quad \text{or} \quad \tilde{\sigma} = J\tilde{\tau}\tilde{F}^{-T} \qquad (3.10b)$$

Equation (3.10a) tells us that

$$\oiint_{\partial\Omega_0} \tilde{\sigma}(\vec{x},t)\vec{m}(\vec{x}) ds_x = 0 \qquad (3.10c)$$

Now, apply divergence theorem in the reference configuration *B*, and noting that (3.10c) holds for any close surface in *B*, we obtain the force balance equation in the reference coordinates (note derivative is respect to x_i)

$$\nabla_x \bullet \tilde{\sigma} = 0 \Leftrightarrow \frac{\partial \sigma_{ij}}{\partial x_j}\vec{e}_i = 0, \qquad \vec{x} \in B \qquad (3.11)$$

The vector $\tilde{\sigma}(\vec{x},t)\vec{m}(\vec{x})$ is the Piola traction, it has units of true force/reference area and points in the same direction as the Cauchy traction. Using (3.10b), the angular momentum balance $\tau_{ij} = \tau_{ji}$ becomes:

$$\tilde{F}\tilde{\sigma}^T = \tilde{S}\tilde{\sigma} \tag{3.12}$$

Equation (3.12) shows that the 1st Piola stress generally *non-symmetric*. Furthermore, it appears that angular momentum balance in the reference configuration leads to an additional set of PDE's to be satisfied. However, it can be shown that angular momentum balance is automatically satisfied for *hyper-elastic* materials (see definition below).

Constitutive law for Hyper-elastic solids

A *homogeneous* hyper-elastic solid is a solid that has a strain energy density function *W* which depends only on the deformation gradient, and such that

$$\sigma_{ij} = \frac{\partial W}{\partial F_{ij}} \tag{3.13}$$

Here the material is assumed to satisfy Material Objectivity. In simple language, this means the constitutive behavior of the material is the same if it is observed in a rotated frame of reference.

In this notes I considered only isotropic, homogeneous and *incompressible* hyperelastic solids. For incompressible isotropic hyperelastic solids, *W* can only depends on the two principal invariants of the right Cauchy Green tensor, that is,

$$W(\tilde{F}) = \Phi(I_1, I_2) \tag{3.14a}$$

where

$$I_1 = tr\tilde{C}, \quad I_2 = \frac{1}{2}\left[\left(tr\tilde{C}\right)^2 - tr\tilde{C}^2\right] \tag{3.14b}$$

In principal coordinates,

$$I_1 = \sum_{i=1}^{3} \lambda_i^2, \quad I_2 = \frac{1}{2}\left[\lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2\right] \tag{3.14c}$$

Note that since the material is incompressible, the invariant

$$J = det\,\tilde{F} = 1 \Rightarrow \lambda_1\lambda_2\lambda_3 = 1 \tag{3.14d}$$

imposes a constraint on the deformation. It can be shown that, for an incompressible solid, the 1st Piola stress is related to the work function by

$$\sigma_{ij} = \frac{\partial W}{\partial F_{ij}} - p\left(\tilde{F}^{-1}\right)_{ji} \Leftrightarrow \tilde{\sigma} = \frac{\partial W}{\partial \tilde{F}} - p\tilde{F}^{-T} \tag{3.15}$$

Using (3.10b) and J = 1, the Cauchy stress tensor is given by

$$\tilde{\tau} = \frac{\partial W}{\partial \tilde{F}} \tilde{F}^T - p\tilde{I} \Leftrightarrow \tau_{ij} = \frac{\partial W}{\partial F_{ij}} F_{ji} - p\delta_{ij} \tag{3.16}$$

Hence *p* can be interpreted as a constitutively indeterminate workless pressure which is used to enforce incompressibility. For isotropic material, $\frac{\partial W}{\partial F_{ij}}$ can be evaluated using (3.14a,b) and the chain rule, after some calculations, this results in

$$\tilde{\sigma} = 2\left[\frac{\partial \Phi}{\partial I_1} + I_2 \frac{\partial \Phi}{\partial I_2}\right]\tilde{F} - 2\frac{\partial \Phi}{\partial I_2}\tilde{F}\tilde{C} - p\tilde{F}^{-T} \tag{3.17}$$

Example: For a neo-Hookean solid (ideal rubber), $\Phi(I_1, I_2) = \frac{\mu_0}{2}(I_1 - 3)$, where μ_0 is the small strain shear modulus. Thus,

$$\tilde{\sigma} = \mu_0 \tilde{F} - p\tilde{F}^{-T} \tag{3.18}$$

For example, in simple uniaxial tension of a long straight bar oriented in the 1 direction, the only non-vanishing components of the deformation gradient tensor are the diagonal elements, these are

$$F_{11} = \lambda, F_{22} = F_{33} = 1/\sqrt{\lambda} \tag{3.19}$$

The pressure *p* is determined by the traction free boundary condition $S_{22} = S_{33} = 0 \Rightarrow \frac{\mu_0}{\lambda} = p$, so the only non-vanishing component of the 1st Piola stress tensor is

$$\sigma_{11} = \mu_0\left(\lambda - \frac{1}{\lambda^2}\right) \tag{3.20}$$

J integral in large deformation hyperelastic solid: Energy Momentum tensor of Eshelby

J.D Eshelby,"The elastic energy-momentum tensor", J. of elasticity, vol. 5, 321-335, 1975

In the absence of body forces and neglecting inertia, define the *energy momentum tensor*

$$P_{ij} = W\delta_{ij} - \sigma_{kj} u_{k,i} \tag{3.21}$$

where *W* is the strain energy density function. The notation $_{,j}$ denotes partial derivatives with respect to x_j. Recall the first Piola stress σ_{ij} is the gradient of the work function, that is,

$$\sigma_{ij} = \frac{\partial W}{\partial F_{ij}} = \frac{\partial W}{\partial u_{i,j}} \tag{3.22}$$

It is straightforward to verify that

$$P_{ij},_j = 0 \qquad (3.23)$$

in a region of B where the displacements and deformations are continuously differentiable. Equation (3.23) implies that, in any simply connected region $\Omega \subset B$ where the fields are continuously differentiable,

$$\oiiint\limits_{\Omega} P_{ij},_j \, dV = \oiint\limits_{\partial\Omega} P_{ij} m_j dS \qquad (3.24)$$

where $\partial\Omega$ is the boundary of Ω and $\vec{m}$ is the unit normal vector to the closed surface $\partial\Omega$. Here we seek an interpretation of the energy momentum tensor.

Consider the simple case of a point defect inside a Hyperelastic body subjected to some external loads. If we move this defect by $\delta\vec{\xi} = \delta\xi_m \vec{e}_m$ with the external load fixed, the potential energy of the body will change by δE. In the following, we will show that

$$\delta E = -F_k \delta\xi_k \,, \qquad (3.25a)$$

where

$$F_k = \oiint\limits_{S} P_{kj} m_j dS = \oint\limits_{S} \left[W m_k - \sigma_{ij} m_j u_i,_k \right] dS \,. \qquad (3.25b)$$

This is the generalization of the J integral (with i =1) in small strain theory. Note that $\vec{F} = F_i \vec{e}_i$ is the configuration force associated with the change in position of the defects (the net traction force acting on the defects is exactly zero). In (3.25b), *S* is any closed surface inside B that encloses the defect (assuming that there is only one defect in B). The surface integral is independent of the surface as long as it does not enclose any other defects due to (3.23).

Eshelby's proof of (3.25a,b) is summarized below:

For the time being, assume that dead traction are prescribed on the body, we will later see that (3.25a,b) is independent of the loading system (just as the J integral is independent of the loading system).

The movement of the defect will cause the elastostatic fields to change. This causes changes in the total strain energy of the system as well as the potential energy of the loading device. To compute these changes, Eshelby splits the problem into two steps.

Step 1: Denote the elastostatic state *before moving the defect* (beginning of step 1) by

$$u_i(x_j), W\left(u_{i,j}(x_k)\right) \equiv W\left(x_k\right), \sigma_{ij}(x_k) \tag{3.26}$$

At the beginning of step 1, the total strain energy of the system is

$$\int_B W(x_j)dV \tag{3.27}$$

and the potential energy of the loading device is

$$-\oint_{\partial B} \sigma_{ij} m_j u_i dS \tag{3.28}$$

Now, translate this elastostatic solution by $\delta\xi_m$, i.e.,

$$\begin{aligned} &u_i(x_j) \to u_i(x_j - \delta\xi_j), \\ &W\left(u_{i,j}(x_k)\right) \to W\left(u_{i,j}(x_k - \delta\xi_k)\right), \\ &\sigma_{ij}(x_j) \to \sigma_{ij}(x_j - \delta\xi_j) \end{aligned} \tag{3.29}$$

It should be noted that these translated fields satisfy all the field equations. *However, these translated fields do not satisfy the boundary conditions. Indeed, the boundary condition (e.g. the surface traction and displacements on the boundary) will be changed due to this shift. Indeed, if the original traction on the boundary is*

$$\sigma_{ij} m_j \tag{3.30a}$$

then the traction at <u>the end of step one</u> is

$$\approx \left(\sigma_{ij} - \sigma_{ij,k}\, \delta\xi_k\right) m_j \tag{3.30b}$$

whereas the displacement on the surface of the body at the end of step one will be

$$\approx u_i - u_{i,k}\, \delta\xi_k \tag{3.30c}$$

Note in this argument Eshelby assumed that these fields can be extrapolated slightly passed their domain of definition. Finally, at the end of step one, the strain energy of the body is

$$\int_B W(x_j - \delta\xi_j)dV \approx \int_B W(x_j)dV - \int_B W_{,i}\, \delta\xi_i dV \tag{3.31}$$

where we used the notation $W\left(u_{i,j}(x_k)\right) = W\left(x_k\right)$.

Step 2 *In step 2, we will adjust the tractions (in doing so we will change the potential energy of the body) so that the original boundary conditions are satisfied. The idea is to compute the change of the potential energy of the body as a result of this adjustment.*

At the end of step one, the traction is on the boundary is $\approx\left(\sigma_{ij}-\sigma_{ij},_k\,\delta\xi_k\right)m_j$ and at the end of step 2 it is $\sigma_{ij}m_j$ so with error on the order of $\delta\xi_k$ it is $\sigma_{ij}m_j$ throughout the adjustment. The surface displacement changes from $\approx u_i-u_i,_k\,\delta\xi_k$ at the end of step one to u_i^F, which denote the displacement at the end of step 2. The external work done on the body during from the beginning of step two to the end is

$$\oint_{\partial B}\left[\sigma_{ij}+O\left(\delta\xi_j\right)\right]\left[u_i^F-\left(u_i-u_i,_k\,\delta\xi_k\right)\right]m_j dS \qquad (3.32)$$

Since $\left[u_i^F-\left(u_i-u_i,_k\,\delta\xi_k\right)\right]$ is of order $\delta\xi_k$, the slight change of traction during the adjustment make contribution on the order of $\left|\delta\xi_k\right|^2$ [1], so the external work done on the body from the beginning of step 2 to the end is:

$$\oint_{\partial B}\sigma_{ij}m_j\left[u_i^F-\left(u_i-u_i,_k\,\delta\xi_k\right)\right]m_j dS \qquad (3.33)$$

Energy conservation implies that the change in elastic strain energy of the body from the beginning of step 2 to the end is equal to the external work done and given by (3.33).

Thus, the total change in strain energy from the beginning of step 1 to the end of step 2 is

$$\begin{aligned}&\left[\int_B W(x_j)dV-\int_B W,_i\,\delta\xi_i dV\right]+\oint_{\partial B}\sigma_{ij}m_j\left[u_i^F-\left(u_i-u_i,_k\,\delta\xi_k\right)\right]dS-\int_B W(x_j)dV\\ &=-\int_B W,_i\,\delta\xi_i dV+\oint_{\partial B}\sigma_{ij}m_j\left[u_i^F-\left(u_i-u_i,_k\,\delta\xi_k\right)\right]dS\end{aligned} \qquad (3.34)$$

The potential energy of the loading device at the end of step 2 is

$$-\oint_{\partial B}\sigma_{ij}m_j u_i^F dS \qquad (3.35)$$

The change in potential energy due to the loading mechanism from the beginning of step one to the end of step 2 is

[1] As pointed out by Eshelby, this means the imposition of dead traction boundary condition is not necessary.

$$-\oint_{\partial B} \sigma_{ij} \left[u_i^F - u_i \right] m_j dS \qquad (3.36)$$

Adding these changes in energy, we have

$$\delta E = -\delta\xi_k \left[\int_{\partial B} W \delta_{kj} m_j dS - \oint_{\partial B} \sigma_{ij} u_{i,k} m_j dS \right] = -\delta\xi_k \underbrace{\int_{\partial B} \left(W \delta_{kj} - \sigma_{ij} u_{i,k} \right) m_j dS}_{F_k} \quad (3.36)$$

which is (3.25a,b). Note that F_k is independent of path, so ∂B can be replaced by any closed surface that encloses the defect. Finally, we note that Eshelby's argument assumes that the energy of the defect is bounded, which need not to be the case.

For the special case of a two dimensional *traction free* crack, for example, a plane strain crack with crack faces on the $x_1 x_2$ plane and a straight crack front in the x_3 direction, the only relevant component of energetic force is F_1 . Here ∂B is any simple path that starts from the lower crack face, goes around the crack tip, and ends on the top crack face.