Institute of Thermomechanics ASCR

THERMODYNAMIC FOUNDATION OF MATERIAL MODELS

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Contents

Uniaxial problem

Nominal stress and small strain

$$\boxed{\sigma = \frac{F}{A} \quad \text{and} \quad \epsilon = \frac{\Delta l}{l}}$$

A = the initial cross section
l = the initial length

First law

Internal energy $$u = U/V$$

Heat power $$\dot{q} = \dot{Q}/V$$

Mechanical power $$\dot{w} = \dot{W}/V = \frac{F}{Al}\frac{\mathrm{d}}{\mathrm{d}t}(\Delta l) = \sigma\dot{\epsilon}$$

$$\boxed{\dot{q} + \dot{w} = \dot{u}}$$

Second law

Entropy $$\eta = S/V$$

Heat content inequality

$$\boxed{\dot{\eta} \geq \frac{\dot{q}}{T}}$$

Dissipation inequality

$$\dot{\eta} \geq \frac{\dot{q}}{T}$$

Dissipation inequality

$$T\dot{\eta} \geq \dot{q}$$

Dissipation inequality

$$T\dot{\eta} \geq \dot{q} = \dot{u} - \dot{w}$$

Dissipation inequality

$$T\dot{\eta} \geq \dot{q} = \dot{u} - \dot{w}$$

$$\dot{w} + T\dot{\eta} \geq \dot{u}$$

Dissipation inequality

$$T\dot{\eta} \geq \dot{q} = \dot{u} - \dot{w}$$

Legendre transform

Dissipation inequality

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Legendre transform

$T\dot{\eta} = (T\eta)^{\cdot} - \dot{T}\eta$

Dissipation inequality

$$T\dot{\eta} \geq \dot{q} = \dot{u} - \dot{w}$$

Legendre transform

$T\dot{\eta} = (T\eta)^{\cdot} - \dot{T}\eta$

$-\eta\dot{T} + \dot{w} \geq \dot{u} - (T\eta)^{\cdot}$

Dissipation inequality

$$T\dot{\eta} \geq \dot{q} = \dot{u} - \dot{w}$$

Legendre transform

$T\dot{\eta} = (T\eta)^{\cdot} - \dot{T}\eta$

$-\eta\dot{T} + \dot{w} \geq \dot{u} - (T\eta)^{\cdot} = (u - T\eta)^{\cdot}$

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$\psi := u - T\eta$ Helmholtz free energy

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$\psi := u - T\eta$ Helmholtz free energy

$$\boxed{-\eta\dot{T} + \dot{w} \geq \dot{\psi}}$$

The Helmholtz free energy (1/2)

Isothermal process

$$\Delta w \geq \psi_2 - \psi_1$$

Cyclic loading

$$1 \xrightarrow{L} 2 \xrightarrow{U} 1$$

$$\left.\begin{array}{l} \Delta w_L \geq \psi_2 - \psi_1 \\ \Delta w_U \geq \psi_1 - \psi_2 \end{array}\right\} \quad \Rightarrow \quad \Delta w_L \geq \psi_2 - \psi_1 \geq -\Delta w_U$$

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…assuming $\Delta w_L > 0$ and $\Delta w_U < 0$

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$$\boxed{\psi = \text{strain energy}}$$

The Helmholtz free energy (2/2)

First law

$$\Delta q + \Delta w = u_2 - u_1$$

Isothermal process

$$\Delta w \simeq \psi_2 - \psi_1$$

Tensile test

$$\Delta q = \quad ? \quad \Delta w$$

The Helmholtz free energy (2/2)

First law

$$\Delta q + \Delta w = u_2 - u_1$$

Isothermal process

$$\Delta w \simeq \psi_2 - \psi_1$$

Tensile test

$$\Delta q = 10 \times \Delta w$$

Thermoelasticity

Assumption

$$\exists \psi(\epsilon, T) : \quad \dot{\psi} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \frac{\partial \psi}{\partial T}\dot{T}$$

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$$-\eta \dot{T} + \dot{w} \geq \dot{\psi}$$

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$$-\eta \dot{T} + \sigma \dot{\epsilon} \geq \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \frac{\partial \psi}{\partial T}\dot{T}$$

Thermoelasticity

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Dissipation inequality

$$-\left(\eta + \frac{\partial \psi}{\partial T}\right)\dot{T} + \left(\sigma - \frac{\partial \psi}{\partial \epsilon}\right)\dot{\epsilon} \geq 0$$

Thermoelasticity

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$$\exists \psi(\epsilon, T): \qquad \dot{\psi} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \frac{\partial \psi}{\partial T}\dot{T}$$

Dissipation inequality

$$-\left(\eta + \frac{\partial \psi}{\partial T}\right)\dot{T} + \left(\sigma - \frac{\partial \psi}{\partial \epsilon}\right)\dot{\epsilon} \geq 0$$

$$\boxed{\eta = -\frac{\partial \psi}{\partial T} \quad \text{and} \quad \sigma = \frac{\partial \psi}{\partial \epsilon}}$$

Thermoelasticity – zeroing brackets

Denote

$$\eta + \frac{\partial \psi}{\partial T} = f(\epsilon, T)$$

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$$\exists\, \epsilon, T : \quad f(\epsilon, T) \neq 0$$

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$$\exists\, \epsilon, T : \;\; f(\epsilon, T) \neq 0$$

For $\dot{\epsilon} = 0$ it follows

$$-\left(\eta + \frac{\partial \psi}{\partial T}\right) \dot{T} \geq 0$$

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$$\eta + \frac{\partial \psi}{\partial T} = f(\epsilon, T)$$

Assume

$$\exists\, \epsilon, T : \;\; f(\epsilon, T) \neq 0$$

For $\dot{\epsilon} = 0$ it follows

$$-f(\epsilon, T)\dot{T} \geq 0$$

But $\dot{T}$ is arbitrary, thus

$$\boxed{f(\epsilon, T) \equiv 0} \qquad \text{necessary condition}$$

Thermoelasticity – heat transfer

Defining relation

$$u = \psi + T\eta$$

Thermoelasticity – heat transfer

Defining relation

$$\dot{u} = (\psi + T\eta)^{\cdot} = \dot{\psi} + \dot{T}\eta + T\dot{\eta}$$

Thermoelasticity – heat transfer

Defining relation

$$\dot{u} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \frac{\partial \psi}{\partial T}\dot{T} + \dot{T}\eta + T\dot{\eta}$$

Thermoelasticity – heat transfer

Defining relation

$$\dot{u} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \underline{\frac{\partial \psi}{\partial T}\dot{T}} + \underline{\dot{T}\eta} + T\dot{\eta}$$

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Defining relation

$$\dot{u} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \underline{\frac{\partial \psi}{\partial T}\dot{T}} + \underline{\dot{T}\eta} + T\dot{\eta}$$

$\dot{u} = \sigma\dot{\epsilon} + T\dot{\eta}$ (model)

Thermoelasticity – heat transfer

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$$\dot{u} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \underline{\frac{\partial \psi}{\partial T}\dot{T}} + \underline{\dot{T}\eta} + T\dot{\eta}$$

$\dot{u} = \sigma\dot{\epsilon} + T\dot{\eta}$ (model)
$\dot{u} = \dot{w} + \dot{q}$ (1st law)

Thermoelasticity – heat transfer

Defining relation

$$\dot{u} = \frac{\partial \psi}{\partial \epsilon}\dot{\epsilon} + \underline{\frac{\partial \psi}{\partial T}\dot{T}} + \underline{\dot{T}\eta} + T\dot{\eta}$$

Corollary

$$\left.\begin{aligned} \dot{u} &= \sigma\dot{\epsilon} + T\dot{\eta} \quad \text{(model)} \\ \dot{u} &= \dot{w} + \dot{q} \qquad \text{(1st law)} \end{aligned}\right\} \Rightarrow \boxed{\dot{\eta} = \frac{\dot{q}}{T} \quad \text{(ideal process)}}$$

Thermoelasticity – summary

Free energy setup

$$\exists\, \psi(\epsilon, T) \quad \Rightarrow \quad \sigma = \frac{\partial \psi}{\partial \epsilon}\,, \quad \eta = -\frac{\partial \psi}{\partial T}$$

Heat transfer

$$\dot{\eta} = \frac{\dot{q}}{T} \quad \Rightarrow \quad \dot{q} = T\dot{\eta}$$

Duhamel-Neumann model

Thermal expansion

$$\epsilon = \frac{\sigma}{E} + \alpha \Delta T$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha\Delta T)$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

Free energy

$$\psi(\epsilon, T) = \int \sigma \, \mathrm{d}\epsilon$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

Free energy

$$\psi = \frac{1}{2} E \epsilon^2 - E \alpha \Delta T \epsilon + f(T)$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

Free energy

$$\psi = \frac{1}{2} E \epsilon^2 - E \alpha \Delta T \epsilon + f(T)$$

Entropy

$$\eta = -\frac{\partial \psi}{\partial T}$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

Free energy

$$\psi = \frac{1}{2} E \epsilon^2 - E \alpha \Delta T \epsilon + f(T)$$

Entropy

$$\eta = E \alpha \epsilon - f'(T)$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

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$$\psi = \frac{1}{2} E \epsilon^2 - E \alpha \Delta T \epsilon + f(T)$$

Entropy

$$\eta = E \alpha \epsilon - f'(T)$$

Heat exchange

$$\dot{q} = T \dot{\eta} = T(E \alpha \dot{\epsilon} - f''(T) \dot{T})$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

Free energy

$$\psi = \frac{1}{2} E \epsilon^2 - E \alpha \Delta T \epsilon + f(T)$$

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$$\eta = E \alpha \epsilon - f'(T)$$

Heat exchange

$$\dot{q} = \alpha T E \dot{\epsilon} - T f''(T) \dot{T}$$

Duhamel-Neumann model

Thermal expansion

$$\sigma = E(\epsilon - \alpha \Delta T)$$

Free energy

$$\psi = \frac{1}{2} E \epsilon^2 - E \alpha \Delta T \epsilon + f(T)$$

Entropy

$$\eta = E \alpha \epsilon - f'(T)$$

Heat exchange

$$\dot{q} = \alpha T E \dot{\epsilon} - T f''(T) \dot{T}$$

$$\boxed{\dot{q} = \alpha T E \dot{\epsilon} + c \dot{T}}$$

…note that $c = \mathrm{function(T)}$

Numerical example

$$\dot{q} = \alpha T E \dot{\epsilon} + c\dot{T} = \alpha T \dot{\sigma}$$

Tensile test 100 MPa

$$\Delta q = \alpha T \sigma = 10^{-5} \times 300 \times 10^{8} = 3 \times 10^{5} \quad \mathrm{J/m^3}$$

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Mechanical work

$$\Delta w = \frac{\sigma^2}{2E} = \frac{(10^8)^2}{2 \times 2 \times 10^{11}} = 0.25 \times 10^{5} \quad \mathrm{J/m^3}$$

Recap

- The Helmholtz free energy (HFE) is the strain (stored) energy.
- HFE substantially differs from the internal energy.
- The dissipation inequality restricts the HFE structure.
- Thermoelasticity is the ideal proces $(\dot{\eta} = \dot{q}/T)$.
- Specific heat capacity of solids is independent of stress.