Chapter Title	Thermoelastic Bar Theory		
Copyright Year	2013		
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Comp. by: JNagalakshmi Stage: Proof Chapter No.: 889 Title Name: ETS Date:1/3/13 Time:09:15:55 Page Number: 1

2 Thermoelastic Bar Theory

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7 Overview

The simplest quasi-static and dynamic laboratory 8 experiments concerning material behavior of 9 solids are performed using uniaxial tension and 10 compression tests. This requires 11 a thermomechanical theory in one space dimen-12 sion which corresponds to the motion of thin bars 13 described by a single material coordinate. One 14 considers here a general Lagrangian description 15 of the thermodynamic bar theory which allows to 16 17 take into account the heat exchanges across the lateral surface of a bar with its environment. 18 Balance laws and entropy inequality in differen-19 20 tial form and the corresponding jump conditions are described. For thermoelastic heat-conducting 21 materials, thermodynamic restrictions, energy 22 23 and entropy identities, and dissipative aspects are derived. One discusses additional restrictions 24 in the form of thermostatic stability conditions 25 versus dynamic stability conditions. The results 26 are appropriate in solving one-dimensional prob-27 lems in nonlinear thermo-elastodynamics and are 28 29 related with central ideas in the analysis of quasilinear hyperbolic systems of conservation 30 laws, for example, the need to consider 31

discontinuous solutions, since even for smooth 32 initial data, the thermoelastic system may 33 develop discontinuous solutions within a finite 34 time. The need to impose entropy conditions in 35 order to select physical meaningful solutions and 36 to ensure the uniqueness of weak solutions (as in 37 ▶ Heat Conduction and Viscosity as Structuring 38 Mechanisms for Shock Waves in Thermoelastic 39 Materials). It is shown that the thermoelastic 40 model has a constitutive deficiency to describe 41 solid-solid phase transitions. One way to over- 42 come this inconvenience is to augment the 43 thermoelastic model to include physical effects 44 as viscosity or time of relaxation considered in 45 ► Maxwellian rate-type thermo-viscoelastic bar 46 theory – an approach to non-monotone 47 thermoelasticity. 48

Thermodynamic Theory in One Space 49 Dimension 50

One considers a thin bar \mathcal{B} of length L in its 51 unstressed reference configuration having 52 a constant cross-sectional area A along its axis 53 OX. Suppose that the motion of the bar is only 54 longitudinal and is described by a function 55 $x = \chi(X, t), X \in [0, L], t \ge 0$ with the property 56 that $\chi(X, t)$ is injective and bicontinuous with 57 respect to X for any fixed t. X is the initial coordinate (or Lagrangian coordinate), x is the actual 59 axial coordinate (or Eulerian coordinate), and t 60 denotes time. $\chi(\cdot, t)$ is called the *deformation* 61 (or *configuration*) of the bar \mathcal{B} at time t. 62

R. Hetnarski (ed.), *Encyclopedia of Thermal Stresses*, DOI 10.1007/978-94-007-2739-7, © Springer Science+Business Media Dordrecht 2013

2

Whenever χ is continuously differentiable, the 63 functions $v(X,t) = \frac{\partial \chi}{\partial t}(X,t)$ and 64 $\varepsilon(X,t) = \frac{\partial \chi}{\partial X}(X,t) - 1 > -1$ denote the particle 65 velocity and the strain at point X and time t, 66 respectively. Moreover, we assume that all the 67 thermomechanical field quantities are uniform 68 over a cross section, that is, they only depend on 69 X and t. 70

If $\varrho = \varrho(X)$ denotes the mass density in the reference configuration, then in the Lagrangian description, the role of the conservation of mass is only to determine the current mass density $\varrho_a = \varrho_a(x,t)$, once the motion χ is known, through relation $\varrho(X) = \varrho_a(x,t) \frac{\partial \chi}{\partial X}(X,t)$.

The balance of linear momentum for a portion of the bar occupying the interval (X_1, X_2) requires

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{X_1}^{X_2} \varrho v(X, t) A \mathrm{d}X = A \sigma(X, t) \Big|_{X=X_1}^{X=X_2} + \int_{X_1}^{X_2} \varrho b(X, t) A \mathrm{d}X,$$
(1)

where $\sigma = \sigma(X, t)$ denotes the axial stress (force per unit area in the reference configuration) and b = b(X, t) denotes a distributed longitudinal load per unit mass.

The balance of energy (the first law of thermodynamics) for the same piece of bar requires

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{X_1}^{X_2} \varrho\left(\frac{v^2}{2} + e\right) A \mathrm{d}X = A(\sigma v - q) \Big|_{X=X_1}^{X=X_2} + \int_{X_1}^{X_2} \varrho(bv + r) A \mathrm{d}X + \int_{A_{lat}} \tilde{q} \mathrm{d}s,$$
(2)

where e = e(X, t) is the internal energy per unit mass, q = q(X, t) is the axial heat flux per unit cross-sectional area of the bar, $\tilde{q} = \tilde{q}(X, t)$ is the heat flux per unit area across the lateral surface of the bar \mathcal{A}_{lat} between X_1 and X_2 , and r = r(X, t) is the heat supply per unit mass, in the reference configuration.

The balance laws have to be supplemented with the Clausius-Duhem inequality (second law of thermodynamics) which for the interval (X_1, X_2) takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{X_{1}}^{X_{2}} \varrho \eta A \mathrm{d}X \ge -A \frac{q}{\theta} (X, t) \Big|_{X=X_{1}}^{X=X_{2}} + \int_{X_{1}}^{X_{2}} \frac{\varrho r}{\theta} A \mathrm{d}X + \int_{A_{lat}} \frac{\tilde{q}}{\theta} \mathrm{d}s,$$
(3)

where $\eta = \eta(X, t)$ is the entropy per unit mass 97 and $\theta = \theta(X, t)$ is the absolute temperature. 98

Traditionally one distinguishes two situations. 99 The first one corresponds to the case when the 100 thermomechanical variables are smooth (smooth 101 processes). The second one corresponds to the 102 case when the motion χ is continuous, but some 103 of the quantities $v, \varepsilon, \theta, \sigma, e, \eta$, and q have jump 104 discontinuities across a smooth curve X = S(t) in 105 the t - X plane, being smooth function of (X, t) 106 everywhere else (discontinuous processes). This 107 curve is called a strong wave discontinuity (for 108 instance, shock wave, phase boundary) propagat- 109 ing with the speed S. We name X > S(t) as the + 110 side of the discontinuity and X < S(t) as the -111 side of the discontinuity. 112

Consider f = f(X, t) one of the above quantities, and suppose there exists a single discontinuity X = S(t) in the interval (X_1, X_2) . Then, one 115 shows that 116

$$f(X_2,t) - f(X_1,t) = \int_{X_1}^{X_2} \frac{\partial f}{\partial X} dX + \llbracket f \rrbracket(t),$$

$$\frac{d}{dt} \int_{X_1}^{X_2} f dX = \int_{X_1}^{X_2} \frac{\partial f}{\partial t} dX - \dot{S}\llbracket f \rrbracket(t),$$
(4)

where $[\![f]\!](t) = f^+(t) - f^-(t) = f(S(t) + 0, t)$ 117 -f(S(t) - 0, t) denotes the jump across the discontinuity curve. Moreover, according to 119 Hadamard's lemma ([1, 2, Section 173]), we have 120

$$\frac{\mathbf{d}\llbracket f \rrbracket(t)}{\mathbf{d}t} = \begin{bmatrix} \frac{\partial f}{\partial t} \end{bmatrix} + \dot{S}(t) \begin{bmatrix} \frac{\partial f}{\partial X} \end{bmatrix}.$$
 (5)

The definition of the particle velocity v and 121 strain ε , on one side, and the continuity condition 122 of the motion χ , on the other side, lead in the 123 smooth case to the differential compatibility relation between v and ε and, in the discontinuous 125 case, to the kinematic jump condition, 126 respectively: 127

Thermoelastic Bar Theory

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial X}, \qquad \llbracket v \rrbracket + \dot{S} \llbracket \varepsilon \rrbracket = 0. \tag{6}$$

By using relations (4) in the integral forms 128 (1)–(3), one gets, for the smooth case, the balance 129 laws and Clausius-Duhem inequality in their 130 differential form and, for the discontinuous 131 case, the balance laws and entropy inequality 132 across a wave discontinuity: 133

$$\varrho \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial X} + \varrho b, \qquad \varrho \dot{S} \llbracket v \rrbracket + \llbracket \sigma \rrbracket = 0 \quad (7)$$

$$\varrho \frac{\partial}{\partial t} \left(\frac{v^2}{2} + e \right) = \frac{\partial}{\partial X} (\sigma v - q) + \varrho (bv + r) + \frac{2}{R} \tilde{q},$$
$$\varrho \dot{S} \left[\left[\frac{v^2}{2} + e \right] \right] + \left[\sigma v - q \right] = 0$$
(8)

$$\varrho \frac{\partial \eta}{\partial t} \ge -\frac{\partial}{\partial X} \left(\frac{q}{\theta} \right) + \frac{2}{R} \frac{\tilde{q}}{\theta} + \frac{\varrho r}{\theta},
- \varrho \dot{S} \llbracket \eta \rrbracket + \llbracket \frac{q}{\theta} \rrbracket \ge 0.$$
(9)

Here we have assumed that the bar \mathcal{B} is circu-134 lar with radius R. 135

By using relations (6) and (7) in (8), one can 136 rewrite the PDEs system and the corresponding 137 jump relations under the form 138

$$\frac{\partial \varepsilon}{\partial t} = \frac{\partial v}{\partial X}, \qquad \varrho \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial X} + \varrho b,$$

$$\varrho \frac{\partial e}{\partial t} = \sigma \frac{\partial \varepsilon}{\partial t} - \frac{\partial q}{\partial X} + \varrho r + \frac{2}{R} \tilde{q}$$
(10)

$$\begin{split} \llbracket v \rrbracket + \dot{S} \llbracket \varepsilon \rrbracket &= 0, \qquad \varrho \dot{S} \llbracket v \rrbracket + \llbracket \sigma \rrbracket &= 0, \\ \varrho \dot{S} \llbracket e \rrbracket + < \sigma > \llbracket v \rrbracket - \llbracket q \rrbracket &= 0, \end{split}$$
(11)

where $\langle f \rangle = \frac{1}{2}(f^+ + f^-)$, and we have used the 139 identity $[\![ab]\!] = \langle a \rangle [\![b]\!] + \langle b \rangle [\![a]\!].$ 140

In thermodynamics it is useful to use the 141 Helmholtz free energy $\psi = e - \theta \eta$ as 142 a thermodynamic potential. Then the Clausius-143 144 Duhem inequality $(9)_1$ takes the form

$$-\varrho \frac{\partial \psi}{\partial t} + \sigma \frac{\partial \varepsilon}{\partial t} - \varrho \eta \frac{\partial \theta}{\partial t} - \frac{q}{\theta} \frac{\partial \theta}{\partial X} \ge 0, \quad (12)$$

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and the jump entropy inequality $(9)_2$ becomes 145

$$\frac{\dot{S}}{\langle\theta\rangle}(\varrho[\psi] - \langle\sigma\rangle[\varepsilon] + \varrho[\theta]\langle\eta\rangle) - \frac{[\theta]}{\langle\theta\rangle}\left\langle\frac{q}{\theta}\right\rangle \ge 0.$$
(13)

It is useful to note here the role of the 146 Clausius-Duhem inequality. For smooth 147 thermomechanical fields, this expression of the 148 second law of thermodynamics is used to restrict 149 the form of the constitutive relations. On the other 150 side, for the discontinuous thermomechanical 151 fields, it becomes an additional constraint that 152 weak solutions have to satisfy (see also > Heat 153 Conduction and Viscosity as Structuring Mecha- 154 nisms for Shock Waves in Thermoelastic 155 Materials). 156

Heat-Conducting Thermoelastic Bars 157

Convective Heat Transfer with the Environment

In the one-dimensional bar theory, the heat 160 absorption or emission through the lateral surface 161 of the bar is by no means unimportant. For 162 instance, in quasi-static loading or unloading 163 tests on shape memory alloy bars, the latent heat 164 of the phase transformation results in heating (or 165 cooling) of the specimen in the neighborhood of 166

the transformation front (see [3]). A test 167 conducted in an air environment or water envi- 168 ronment leads to different thermomechanical 169 results (see also ► Pseudoelasticity and Shape 170 Memory Effect – A Maxwellian Approach). 171

A good way to model such circumstances is to 172 suppose that the heat flux \tilde{q} across the lateral 173 surface of the bar satisfies Newton's convective 174 law of heat transfer 175

$$\tilde{q}(X,t) = -\omega(\theta(X,t) - \theta_{ext}(X,t)), \qquad (14)$$

where θ_{ext} is the ambient temperature and 176 $\omega = \text{ const.} > 0$ is a heat transfer coefficient, 177 which depends upon both the constitution of the 178 bar and the conditions of the environment. This 179 law expresses the fact that the rate of heat loss/ 180

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4

gain of a body is proportional to the difference in 181 temperatures between the body and its surround-182 ings. Let us note that \tilde{q} is zero in two situations: 183 first, when the temperature of the environment 184 coincides with the temperature of the bar at 185 each X and t, which is not easy to be accom-186 plished in practice when θ is not constant, and 187 second, when placing the bar in an adiabatic 188 environment, for example, a vacuum and $\omega = 0$. 189

190 The Thermoelastic Model

The reference density ρ , the body force b, and the 191 heat supply r are viewed as externally prescribed 192 fields. The other thermomechanical variables are 193 connected through constitutive relations that 194 the characterize material response. 195 A constitutive theory is determined by selecting 196 a class of independent (prime) variables and 197 a class of dependent variables, derived from the 198 prime variables via constitutive relations. 199

One considers here thermomechanical theo-200 ries in which χ and θ are prime variables. One 201 advantage of this choice is that these quantities 202 can be directly measured experimentally. The 203 others such as the internal energy e, entropy η , 204 axial force σ , axial heat flux q, and lateral flux \tilde{q} 205 are considered as dependent variables since they 206 are derived from the prime variables by constitu-207 tive relations. 208

In determining the general form of phenome-209 nological constitutive theories, one imposes on 210 the constitutive relations some principles, like the 211 principle of equipresence, the principle of mate-212 rial frame indifference, and the principle of com-213 patibility with the Clausius-Duhem inequality 214 (see [4] and [5] for the general form of constitu-215 tive theories in several space dimensions). 216

217 Thermodynamic Considerations

A *state* of the bar is any pair $S = (\chi(X), \theta(X))$, 218 $X \in [0, L]$ where $\chi(X)$ and $\theta(X)$ are a deformation 219 and temperature field over \mathcal{B} . One takes ε , θ , and 220 the temperature gradient θ_X as independent vari-221 ables of the constitutive theory. By including the 222 temperature gradient, one incorporates the effect 223 224 of heat conduction. The remaining

thermomechanical variables are determined by 225 constitutive relations satisfying the principle of 226 equipresence: 227

$$\sigma = \sigma_{eq}(\varepsilon, \theta, \theta_X), \quad \psi = \psi_{eq}(\varepsilon, \theta, \theta_X),$$

$$\eta = \eta_{eq}(\varepsilon, \theta, \theta_X), \quad q = Q(\varepsilon, \theta, \theta_X).$$
(15)

By anticipating that the constitutive functions 228 of thermoelastic materials characterize the equilibrium states of some thermo-viscous materials, 230 we have used consistently the index *eq* (see 231 Maxwellian Rate-Type Thermo-Viscoelastic 232 Bar Theory). 233

A smooth *process* of the bar will be any pair 234 $S(t) = (\chi(X,t), \theta(X,t)), t \in [0, t_0]$ of smooth 235 time-dependent fields over \mathcal{B} which satisfies 236 the balance equations (10) and the constitutive 237 relations (14) and (15). 238

The Clausius-Duhem inequality must be sat- 239 isfied for all smooth thermomechanical pro- 240 cesses. Let us note that a process can be realized 241 by a proper choice of the externally prescribed 242 fields *b* and *r*. When the constitutive functions are 243 brought into (12), one gets 244

$$\begin{pmatrix} \sigma_{eq} - \varrho \frac{\partial \psi_{eq}}{\partial \varepsilon} \rangle \dot{\varepsilon} - \varrho \left(\eta_{eq} + \frac{\psi_{eq}}{\partial \theta} \right) \dot{\theta} \\ - \varrho \frac{\partial \psi_{eq}}{\partial \theta_X} \dot{\theta}_X - \frac{Q}{\theta} \theta_X \ge 0,$$
 (16)

where dot denotes time derivative. The values ε , 245 θ , θ_X , $\dot{\varepsilon}$, $\dot{\theta}$, and $\dot{\theta}_X$ can be assigned independently. 246 Since the inequality is to be satisfied for all inde- 247 pendent variations of $\dot{\varepsilon}$, $\dot{\theta}$, and $\dot{\theta}_X$, which occur 248 linearly, the coefficients of these terms have to 249 vanish separately, that is, 250

$$\frac{\psi_{eq}}{\partial \theta_X} = 0, \quad \sigma = \sigma_{eq}(\varepsilon, \theta) = \varrho \frac{\partial \psi_{eq}}{\partial \varepsilon},
\eta = \eta_{eq}(\varepsilon, \theta) = -\frac{\partial \psi_{eq}}{\partial \theta},$$
(17)

and, in addition, a residual thermal dissipation 251 inequality has to be satisfied 252

$$D_{th} = -\frac{1}{\theta}Q(\varepsilon, \theta, \theta_X)\theta_X \ge 0.$$
(18)

Thus, the Clausius-Duhem inequality places severe restrictions on the form of the constitutive functions. The free energy of the thermoelastic material has to be independent of θ_X , and it is a potential for the stress and entropy functions.

Let us note that in a thermoelastic material for any smooth fields ε and θ , the only dissipative mechanism is the thermal dissipation (18). If one considers the Fourier law for axial heat conduction, that is, $Q = -\kappa(\varepsilon, \theta)\theta_X$, then (18) requires that the heat conduction coefficient κ has to be positive.

On the other side, when the motion of a bar 265 involves a propagating discontinuity, then 266 according to the jump entropy inequality $(9)_2$, 267 strain and temperature discontinuous fields con-268 stitute a source of dissipation in thermoelastic 269 materials (see also > Heat Conduction and 270 Viscosity as Structuring Mechanisms for Shock 271 Waves in Thermoelastic Materials). 272

Even in the isothermal case, a strain discontinuity constitutes a source of dissipation in an elastic nonlinear material defined by relation $\sigma = \sigma_{eq}(\varepsilon)$. Indeed, according to (13), the dissipation inequality takes the form

$$\dot{S}\left(\varrho\psi_{eq}(\varepsilon^{+}) - \varrho\psi_{eq}(\varepsilon^{-}) - \frac{1}{2}(\sigma_{eq}(\varepsilon^{+}) + \sigma_{eq}(\varepsilon^{-}))(\varepsilon^{+} - \varepsilon^{-})\right) \ge 0.$$
(19)

By using, in this isothermal case, the expres-278 sion $(20)_1$ of the free energy determined below, 279 one gets a useful geometrical meaning of the 280 dissipation induced by a shock wave. That is, 281 the coefficient of \hat{S} in (19) is just the signed area 282 between the graph of $\sigma = \sigma_{eq}(\varepsilon)$ and the chord 283 which joins $(\varepsilon^{-}, \sigma_{eq}(\varepsilon^{-}))$ and $(\varepsilon^{+}, \sigma_{eq}(\varepsilon^{+}))$. 284 Let us note that if the stress response function 285

Let us note that if the stress response function $\sigma = \sigma_{eq}(\varepsilon, \theta)$ can be determined experimentally, then the free energy function $\psi = \psi_{eq}(\varepsilon, \theta)$, the entropy $\eta = \eta_{eq}(\varepsilon, \theta)$, the internal energy $e = e_{eq}(\varepsilon, \theta) = \psi_{eq} + \theta \eta_{eq}$, as well as the specific 289 heat at constant strain $C = C_{eq}(\varepsilon, \theta)$ are uniquely 290 determined, modulo an additive function of tem-291 perature $\phi = \phi(\theta)$ by relations 292

$$\begin{split} \psi_{eq}(\varepsilon,\theta) &= \int_{\varepsilon_0}^{\varepsilon} \frac{1}{\varrho} \sigma_{eq}(s,\theta) \mathrm{d}s + \phi(\theta), \\ \eta_{eq}(\varepsilon,\theta) &= -\int_{\varepsilon_0}^{\varepsilon} \frac{1}{\varrho} \frac{\partial \sigma_{eq}(s,\theta)}{\partial \theta} \mathrm{d}s - \frac{\mathrm{d}\phi(\theta)}{\mathrm{d}\theta} \end{split}$$
(20)

$$C_{eq}(\varepsilon,\theta) \equiv \frac{\partial e_{eq}}{\partial \theta} \equiv \theta \frac{\partial \eta_{eq}}{\partial \theta} \equiv -\theta \frac{\partial^2 \psi_{eq}(\varepsilon,\theta)}{\partial \theta^2}$$
$$= -\theta \int_{\varepsilon_0}^{\varepsilon} \frac{1}{\varrho} \frac{\partial^2 \sigma_{eq}(s,\theta)}{\partial \theta^2} ds - \theta \frac{d^2 \phi(\theta)}{d\theta^2},$$
(21)

where ε_0 is an arbitrary reference strain.

It is known that from calorimetric measurements, it is possible to determine the specific heat 295 $C_{eq}(\varepsilon_0, \theta)$ at a constant strain ε_0 over an interval 296 of temperature. Consequently, this information is 297 sufficient to determine the additive function 298 $\phi = \phi(\theta)$ as solution of the differential equation 299

$$\frac{\mathrm{d}^2\phi(\theta)}{\mathrm{d}\theta^2} = -\frac{C_{eq}(\varepsilon_0,\theta)}{\theta} \tag{22}$$

up to an arbitrary linear function of θ , which can 300 be established once the free energy and the 301 entropy at a given state, respectively $\psi(\varepsilon_0, \theta_0)$ 302 and $\eta(\varepsilon_0, \theta_0)$, are given. 303

Energy Identities By using relations $(9)_1$, (14), and (17), one derives the following entropy identity for smooth fields of a thermoelastic bar:

$$\varrho \frac{\partial \eta_{eq}(\varepsilon,\theta)}{\partial t} + \frac{\partial}{\partial X} \left(\frac{q}{\theta}\right) + \frac{2\omega}{R} \frac{(\theta - \theta_{ext})}{\theta} - \frac{\varrho r}{\theta} = \frac{D_{th}}{\theta},$$
(23)

where the right term in (23) represents the total 308 entropy production corresponding to a smooth 309 process of the thermoelastic bar. 310

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From (17) one derives also the following energy identity for smooth fields:

$$\varrho \frac{e_{eq}(\varepsilon,\theta)}{\partial t} = -\dot{W} + \dot{Q},$$
(24)

where $\dot{W} = -\sigma_{eq}(\varepsilon, \theta)\dot{\varepsilon}$ is the *rate of work* and 313 $\dot{Q} = v_{eq}(\varepsilon, \theta)\dot{\varepsilon} + \varrho C_{eq}(\varepsilon, \theta)\dot{\theta}$ is the rate of heat. 314 The term $v_{eq}(\varepsilon, \theta) = -\theta \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} = -\varrho \theta \frac{\partial^2 \psi_{eq}(\varepsilon, \theta)}{\partial \theta \partial \varepsilon}$ 315 denotes the latent heat with respect to strain and 316 characterizes the heat released or absorbed by 317 a body upon change of strain at constant temper-318 ature. On the other side, one sees from relation 319 (24) that the specific heat C_{eq} characterizes the 320 amount of heat required to change a body's tem-321 perature by a given amount by keeping the defor-322 mation fixed. While the sign of the latent heat 323 depends on the sign of $\frac{\partial \sigma_{eq}}{\partial \theta}$, the sign of the spe-324 cific heat at constant strain is supposed always 325 positive. The Clausius-Duhem inequality says 326 nothing about the sign of C_{eq} . Its positiveness, as 327 we shall see below, is related to the stability of the 328 body. Moreover, experience shows that there is no 329 substance for which this condition is violated. 330

The *heat propagation equation* for a thermoelastic bar endowed with the Fourier's heat conduction law is then obtained from the balance of energy $(10)_3$ and the constitutive relations (14) and (20)-(21) as

$$\varrho C_{eq}(\varepsilon,\theta) \frac{\partial \theta}{\partial t} = \varrho \theta \frac{\partial^2 \psi_{eq}(\varepsilon,\theta)}{\partial \varepsilon \partial \theta} \frac{\partial \varepsilon}{\partial t} + \frac{\partial}{\partial X} \left(k \frac{\partial \theta}{\partial X} \right) - \frac{2\omega}{R} (\theta - \theta_{ext}) + \varrho r.$$
(25)

336 Isentrope and Thermal Expansion

For a thermoelastic body, there is another natural 337 choice of independent variables. Instead of using 338 ε and θ as independent variables in the constitu-339 tive equations, one employs the strain ε and the 340 entropy η . This is possible because C_{eq} is always 341 supposed strictly positive and, according to (21), 342 η_{eq} must be a strictly increasing function of θ for 343 each fixed ε . Therefore, the 344 equation $\eta = \eta_{eq}(\varepsilon, \theta)$ can be solved for θ in a unique 345

manner as $\theta = \tilde{\theta}(\varepsilon, \eta)$. The internal energy is 346 then defined by $e = \tilde{e}(\varepsilon, \eta) = e_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))$ and 347 the stress by $\sigma = \tilde{\sigma}(\varepsilon, \eta) = \sigma_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))$. By 348 using the identities $\eta = \eta_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))$, for any 349 pair (ε, η) and $\theta = \tilde{\theta}(\varepsilon, \eta_{eq}(\varepsilon, \theta))$, for any pair 350 (ε, θ) , and relations (17), one shows that, in this 351 case, the internal energy is a thermodynamic 352 potential for the stress and temperature, that is, 353 $\sigma = \tilde{\sigma}(\varepsilon, \eta) = \varrho \frac{\tilde{e}(\varepsilon, \eta)}{\partial \varepsilon}$ and $\theta = \tilde{\theta}(\varepsilon, \eta) = \frac{\tilde{e}(\varepsilon, \eta)}{\partial \eta}$. 354 The specific heat at constant strain is then given 355 by $\tilde{C}(\varepsilon, \eta) = C_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta)) = \tilde{\theta}(\varepsilon, \eta) \left(\frac{\partial \tilde{\theta}(\varepsilon, \eta)}{\partial \eta}\right)^{-1}$. 356

Isentrope. Since we are using as independent ³⁵⁷ variables the strain ε and the temperature θ , it is ³⁵⁸ useful to remind here the equation of an ³⁵⁹ isentrope. By differentiating the relation ³⁶⁰ $\eta_{eq}(\varepsilon, \theta) = \eta^* = \text{const.}$ and by using the thermo-³⁶¹ dynamic relations (17), one gets that an isentrope ³⁶² in the (θ, ε) plane is a solution $\theta = \theta_I(\varepsilon)$ of the ³⁶³ differential equation ³⁶⁴

$$\frac{\mathrm{d}\theta}{\mathrm{d}\varepsilon} = \frac{\theta}{\varrho C_{eq}(\varepsilon,\theta)} \frac{\partial \sigma_{eq}(\varepsilon,\theta)}{\partial \theta}.$$
 (26)

If the initial condition is $\theta_I(\varepsilon^*) = \theta^*$, then this 365 isentrope will be labelled with the value 366 $\eta^* = \eta_{eq}(\varepsilon^*, \theta^*)$. 367 Let us note that if $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} < 0$, the temperature 368 *decreases* along the isentrope, while if 369 $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} > 0$, the temperature *increases* along the 370 isentrope. Moreover, according to (24), an isen-371 tropic process occurs when the rate of heat \dot{Q} is 372 zero. 373

Some dimensionless combinations are often 374 used. For instance, sometimes it is convenient to 375 introduce the *Grüneisen coefficient* which is 376 defined as 377

$$\Gamma(\varepsilon,\theta) = -\frac{1+\varepsilon}{\varrho C_{eq}(\varepsilon,\theta)} \frac{\partial \sigma_{eq}(\varepsilon,\theta)}{\partial \theta}, \qquad (27)$$

characterizing the temperature changes along an 378 isentrope. Indeed, according to (26), we have 379 $\frac{d\theta}{\theta} = -\Gamma(\varepsilon, \theta) \frac{d\varepsilon}{1+\varepsilon}$, that is, it is the negative 380 slope of the isentrope in the $\log \theta - \log(1+\varepsilon)$ 381 plane. The Grüneisen coefficient can have 382

a profound effect on the existence and qualitative
behavior of steady, structured shock waves
(see ▶ Heat Conduction and Viscosity as
Structuring Mechanisms for Shock Waves in
Thermoelastic Materials). Depending on its
sign, a compressive shock discontinuity can be
of heating type or of cooling type.

390 *The coefficient of thermal expansion* at 391 constant stress is introduced as

$$\alpha(\varepsilon,\theta) = -\frac{\partial \sigma_{eq}(\varepsilon,\theta)}{\partial \theta} \left(\frac{\partial \sigma_{eq}(\varepsilon,\theta)}{\partial \varepsilon}\right)^{-1} \quad (28)$$

and characterizes the temperature changes along an isobar ($\sigma = \sigma_{eq}(\varepsilon, \theta) = \text{const.}$) in the $\theta - \varepsilon$ plane. Thus, α is positive when the material expands upon heating at constant pressure, which is true in most situations.

The Grüneisen coefficient and the coefficient 397 of thermal expansion have the same sign if the 398 thermostatic stability conditions, given below, 399 are satisfied. Typically one expects to be positive. 400 However, materials in which Γ or α changes sign 401 are not uncommon, perhaps the most familiar 402 being water, which contracts upon heating near 403 its freezing point. Other materials which have 404 a negative coefficient of thermal expansion are 405 certain iron-nickel alloys or the near-equiatomic, 406 cold-worked Nitinol exhibiting shape memory 407 effect [6]. 408

409 Thermostatic Stability Conditions

Let us note that the second law of thermodynam-410 ics places no restrictions on the sign of $\frac{\partial \sigma_{eq}(z,\theta)}{\partial \theta}$ 411 and $\frac{\partial \sigma_{eq}(\varepsilon,\theta)}{\partial \varepsilon}$. This high degree of generality may 412 introduce into the constitutive equations 413 improper effects for real materials. Therefore, in 414 general, based on physical or experimental facts, 415 additional restrictions, called a priori inequal-416 ities, are imposed on the constitutive function 417 $\sigma = \sigma_{eq}(\varepsilon, \theta).$ 418

For instance, according to Gibbsian thermostatics (see [7]), a necessary condition for a point ϵ_{21} (ϵ, η) to be *thermostatically stable* is that

$$-\tilde{e}(\varepsilon,\eta) - \frac{\partial \tilde{e}(\varepsilon,\eta)}{\partial \varepsilon}(\varepsilon^* - \varepsilon) - \frac{\partial \tilde{e}(\varepsilon,\eta)}{\partial \eta}(\eta^* - \eta) \ge 0,$$
(29)

for any (ε^*, η^*) in the domain of $\tilde{e}(\cdot, \cdot)$. That 422 means (ε, η) is a point of convexity for 423 $e = \tilde{e}(\varepsilon, \eta)$, that is, the Hessian matrix 424

$$\begin{pmatrix} \frac{\partial^2 \tilde{e}}{\partial \eta^2} \frac{\partial^2 \tilde{e}}{\partial \eta \partial \varepsilon} \\ \frac{\partial^2 \tilde{e}}{\partial \varepsilon \partial \eta} \frac{\partial^2 \tilde{e}}{\partial \varepsilon^2} \end{pmatrix}$$
(30)

is positive semi-definite at (ε, η) . Therefore, the 425 following restrictions have to be satisfied: 426

$$\frac{\partial^{2}\tilde{e}}{\partial\eta^{2}} \geq 0, \quad \frac{\partial^{2}\tilde{e}}{\partial\varepsilon^{2}} \geq 0, \quad \frac{\partial^{2}\tilde{e}}{\partial\eta^{2}}\frac{\partial^{2}\tilde{e}}{\partial\varepsilon^{2}} - \left(\frac{\partial^{2}\tilde{e}}{\partial\eta\partial\varepsilon}\right)^{2} \geq 0$$
(31)

or equivalently

 $\tilde{e}(\varepsilon^*,\eta^*)$

$$\frac{\partial \tilde{\theta}(\varepsilon,\eta)}{\partial \eta} \ge 0, \quad \frac{\partial \tilde{\sigma}(\varepsilon,\eta)}{\partial \varepsilon} \ge 0, \\
\frac{\partial \tilde{\theta}(\varepsilon,\eta)}{\partial \eta} \frac{\partial \tilde{\sigma}(\varepsilon,\eta)}{\partial \varepsilon} - \left(\frac{\partial \tilde{\sigma}(\varepsilon,\eta)}{\partial \eta}\right)^2 \ge 0.$$
(32)

One can show that the necessary and sufficient 428 conditions which ensure the *Gibbsian thermo-* 429 *static stability* (29) are the positiveness of the 430 specific heat and the positiveness of the deriva- 431 tive of the stress with respect to ε along an 432 isotherm: 433

$$C_{eq}(\varepsilon, \theta) \ge 0$$
 and $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon} \ge 0.$ (33)

Indeed, this assertion follows from relations 434

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$$\begin{aligned} \frac{\partial \tilde{\theta}(\varepsilon,\eta)}{\partial \eta} &= \frac{\tilde{\theta}(\varepsilon,\eta)}{\tilde{C}(\varepsilon,\eta)} \ge 0\\ \frac{\partial \tilde{\sigma}(\varepsilon,\eta)}{\partial \varepsilon} &= \frac{\partial \sigma_{eq}(\varepsilon,\tilde{\theta}(\varepsilon,\eta))}{\partial \varepsilon} + \frac{\theta}{\varrho C_{eq}(\varepsilon,\tilde{\theta}(\varepsilon,\eta))}\\ \left(\frac{\partial \sigma_{eq}(\varepsilon,\tilde{\theta}(\varepsilon,\eta))}{\partial \theta}\right)^2 \ge 0,\\ \frac{\partial^2 \tilde{e}}{\partial \eta^2} \frac{\partial^2 \tilde{e}}{\partial \varepsilon^2} - \left(\frac{\partial^2 \tilde{e}}{\partial \eta \partial \varepsilon}\right)^2 &= \frac{\tilde{\theta}(\varepsilon,\eta)}{\varrho \tilde{C}(\varepsilon,\theta)} \frac{\partial \sigma_{eq}(\varepsilon,\tilde{\theta}(\varepsilon,\eta))}{\partial \varepsilon} \ge 0, \end{aligned}$$
(34)

obtained by using the chain rule and differentiating the identity $\eta = \eta_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))$ with respect to ε and η .

Another way to prove these assertions is the following. By using the free energy function $\psi = \psi_{eq}(\varepsilon, \theta)$, one derives from (29) that a necessary condition for a point (ε, θ) to be thermostatically stable is that the following inequality

$$\psi_{eq}(\varepsilon^*, \theta^*) - \psi_{eq}(\varepsilon, \theta) - \frac{\partial \psi_{eq}(\varepsilon, \theta)}{\partial \varepsilon} (\varepsilon^* - \varepsilon) - \frac{\partial \psi_{eq}(\varepsilon^*, \theta^*)}{\partial \theta} (\theta^* - \theta) \ge 0$$
(35)

444 be satisfied for all $(\varepsilon^*, \theta^*)$ in the domain of 445 definition of ψ_{eq} .

The consequences of this inequality are the following. Let (ε, θ) be fixed and $(\varepsilon^*, \theta^*) = (\varepsilon + \lambda \overline{\varepsilon}, \theta + \lambda \overline{\theta})$ a point in the domain of definition of ψ_{eq} for sufficiently small λ . Let us introduce the function

$$\delta(\lambda) = \psi_{eq}\left(\varepsilon + \lambda \overline{\varepsilon}, \theta + \lambda \overline{\theta}\right) - \psi_{eq}(\varepsilon, \theta) \\ - \frac{\partial \psi_{eq}(\varepsilon, \theta)}{\partial \varepsilon} \lambda \overline{\varepsilon} - \frac{\partial \psi_{eq}(\varepsilon + \lambda \overline{\varepsilon}, \theta + \lambda \overline{\theta})}{\partial \theta} \lambda \overline{\theta}$$
(36)

which has the following properties: $\delta(0) = 0$ and 452 $\delta'(0) = 0$. According to (35), one gets

$$\delta''(0) = \frac{\partial^2 \psi_{eq}(\varepsilon, \theta)}{\partial \varepsilon^2} \,\overline{\varepsilon}^2 - \frac{\partial^2 \psi_{eq}(\varepsilon, \theta)}{\partial \theta^2} \,\overline{\theta}^2 \ge 0,$$

for any pair($\overline{\varepsilon}, \overline{\theta}$). (37)

Thermoelastic Bar Theory

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Immediate consequences of this inequality are 453

$$\frac{\partial^2 \psi_{eq}(\varepsilon,\theta)}{\partial \varepsilon^2} = \frac{1}{\varrho} \frac{\partial \sigma(\varepsilon,\theta)}{\partial \varepsilon} \ge 0, -\frac{\partial^2 \psi_{eq}(\varepsilon,\theta)}{\partial \theta^2} = \frac{C_{eq}(\varepsilon,\theta)}{\theta} \ge 0.$$
(38)

Therefore, the Gibbsian stability condition 454 reads in the following terms: the free energy 455 function $\psi_{eq}(\varepsilon, \theta)$ has to be convex in ε for each 456 θ and concave in θ for each ε . 457

Dynamic Stability Conditions

A natural physical condition to be imposed on the 459 constitutive functions is to require the existence 460 of real sound speeds (or, equivalently, accelera- 461 tion waves) with finite propagation velocity in the 462 adiabatic case. This is called *dynamic stability* 463 *condition* since it ensures in this case the stability 464 of the solutions of the equations of motion. 465

The system composed by $(10)_{1,2}$ and (25) 466 describing the motion of an isolated (r = 0, 467 $\omega = 0$) thermoelastic bar in the absence of axial 468 heat conduction ($\kappa = 0$) is called the *adiabatic* 469 *thermoelastic system* and can be written as 470

$$\frac{\partial}{\partial t} \begin{pmatrix} v \\ \varepsilon \\ \theta \end{pmatrix} - \begin{pmatrix} 0 & \frac{1}{\varrho} \frac{\partial \sigma_{eq}}{\partial \varepsilon} & \frac{1}{\varrho} \frac{\partial \sigma_{eq}}{\partial \theta} \\ 1 & 0 & 0 \\ \frac{\theta}{\varrho C_{eq}} \frac{\partial \sigma_{eq}}{\partial \theta} & 0 & 0 \end{pmatrix} \frac{\partial}{\partial X} \begin{pmatrix} v \\ \varepsilon \\ \theta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$
(39)

This system is suitable for the description of 471 wave propagation since the heat conductivity, or 472 other physical mechanisms like viscosity, can be 473 ignored outside the narrow transition zones 474 corresponding to wave discontinuity. The type 475 of this system is given by the eigenvalues and 476 the right eigenvectors of the above matrix. 477

The eigenvalues are solution of the equation 478

$$\lambda \left[\lambda^2 - \left(\frac{1}{\varrho} \frac{\partial \sigma_{eq}}{\partial \varepsilon} + \frac{\theta}{\varrho^2 C_{eq}} \left(\frac{\partial \sigma_{eq}}{\partial \theta} \right)^2 \right) \right] = 0. \text{ This sys-}_{479}$$
tem is *strictly hyperbolic* if the three eigenvalues 480 are real and distinct and the corresponding right 481 eigenvectors are linearly independent. One shows 482 that this happens if and only if 483

$$U^{2}(\varepsilon,\theta) \equiv \frac{1}{\varrho} \frac{\partial \sigma_{eq}}{\partial \varepsilon} + \frac{\theta}{\varrho^{2} C_{eq}} \left(\frac{\partial \sigma_{eq}}{\partial \theta}\right)^{2} > 0.$$
(40)

In this case, the eigenvalues, which corre-484 spond to the characteristic directions of the 485 hyperbolic system, are $\lambda_1(\varepsilon, \theta) = -U(\varepsilon, \theta)$, 486 $\lambda_2(\varepsilon,\theta) = 0$, and $\lambda_3(\varepsilon,\theta) = U(\varepsilon,\theta)$, and $U(\varepsilon,\theta)$ 487 is called the adiabatic sound speed at the state 488 (ε, θ) . It is obvious that the hyperbolicity condi-489 tion, that is, the dynamic stability condition (40), 490 is satisfied when the thermostatic stability condi-491 tions (33) are fulfilled. The reverse statement is 492 not true. The dynamic stability condition ensures 493 that initial and boundary value problems for the 494 adiabatic thermoelastic system (39) are well 495 posed, or correctly set, in the sense of Hadamard 496 (see [8]). 497

Phase Transitions in Thermoelastic Solids On 498 the other side, circumstances when $\frac{\partial \sigma_{eq}}{\partial \varepsilon} < 0$ on 499 certain intervals of strain and temperature cannot 500 be excluded since they contain the essence of the 501 physics of phase transformations. Indeed, 502 a classical constitutive viewpoint in phenomeno-503 logical modelling of phase-transforming mate-504 rials is based on non-monotone thermoelasticity 505 506 theories and started at the end of nineteenth century with the equation of van der Waals for 507 thermoelastic fluids. The van der Waals fluid is 508 characterized by non-monotone pressure-specific 509 volume relations and is a prototype of continuum-510 mechanical models of two-phase materials. In 511 solid mechanics such an approach based on non-512 monotone stress-strain relation for certain ranges 513 of temperature has been initiated by Ericksen [9] 514 515 in 1975 in an isothermal and one-dimensional context and has been followed by numerous and 516 important studies (see, for instance, [10] and the 517 references therein). 518

When $\frac{\partial \sigma_{eq}}{\partial \varepsilon}$ is *negative*, and sufficiently large, 519 the adiabatic thermoelastic system (39) has com-520 plex eigenvalues over some regions in the $\theta - \varepsilon$ 521 plane called elliptic regions of state space, and 522 the system is of mixed type. The system does not 523 have more the nature of wave propagation prob-524 lem, and the initial and boundary value problems 525 are ill posed. In general, the solution fails to be 526

unique or is continuously dependent on initial 527 data. The multiplicity of solutions at the contin- 528 uum level can be viewed as arising from 529 a constitutive deficiency, reflecting the need to 530 specify additional pieces of constitutive informa- 531 tion. Indeed, phase transitions are strongly dissi- 532 phenomena, but for thermoelastic pative 533 materials, the only source of dissipation as we 534 have seen is the thermal dissipation (18). There- 535 fore, there is a need to find simple and appropriate 536 dissipative mechanisms to be included in the 537 constitutive description of thermoelastic mate- 538 rials such that the model will be able to describe 539 the process of phase transformation, that is, the 540 nucleation and propagation of phases. 541

One way to introduce a dissipative mechanism 542 is the thermodynamical framework developed by 543 Abeyaratne and Knowles presented extensively 544 in [10]. A different approach to the problem of 545 phase transformations is to augment the 546 thermoelastic constitutive equation $\sigma = \sigma(\varepsilon, \theta)$ 547 by introducing rate-type effects as in [11]. This 548 formulation is considered in \triangleright Maxwellian ratetype thermo-viscoelastic bar theory – an 550 approach to non-monotone thermoelasticity. 551

Cross-References

▶ Heat Conduction and Viscosity as Structuring 553 Mechanisms for Shock Waves in 554 Thermoelastic Materials 555 Maxwellian Rate-Type Thermo-Viscoelastic 556 Bar Theory – An Approach to Non-Monotone 557 Thermoelasticity 558 Pseudoelasticity and Shape Memory Effect – 559 A Maxwellian Rate-Type Approach 560

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