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DYNAMIC THERMOELASTIC PHASE TRANSITIONS

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Abstract—This paper summarizes some recent work carried out jointly with R. Abeyaratne on the continuum modeling of phase transitions in thermoelastic tensile bars. The specific model considered involves a particular Helmholtz free energy potential governing the bulk response of the material as well as a kinetic relation controlling the phase transition. Inertia is taken into account. The discussion here is based on an adiabatic model.

1. INTRODUCTION

This paper briefly summarizes some recent work by R. Abeyaratne and the author on the continuum dynamics of solid–solid phase transitions in one-dimensional tensile bars composed of a particular thermoelastic material. The subject of continuum modeling of phase transitions has been studied at some length in recent years; an extensive sample of some of the resulting literature may be found in the references listed in the papers by Abeyaratne and Knowles (1993a,b, 1994a,b) and Abeyaratne *et al.* (1994), as well as in the review article by Huo and Müller (1993). Some of the literature cited in these references pertains only to purely mechanical models, suppressing thermal effects, and still other papers among those listed consider only quasi-static processes, corresponding to some problems studied rather widely in the experimental literature.

The discussion to be given here involves an adiabatic theory that omits effects due to heat condition, but incorporates other thermal effects as well as inertia; the emphasis is placed on the nature of propagating strain discontinuities. A distinction is made between *shock waves* and propagating *phase boundaries*, though both are moving strain jumps. At phase boundaries, the kinetics of the underlying phase transition must be invoked, while at shock waves such information is not needed and in fact cannot be accommodated. Both types of discontinuities are necessarily subject to the classical entropy inequality.

Detailed arguments supporting the present results are omitted here; they may be found in Abeyaratne and Knowles (1994a).

2. FIELD EQUATIONS AND JUMP CONDITIONS

Consider a tensile bar that occupies the interval $(-\infty, \infty)$ of the x-axis in the reference state. During a motion of the bar, a particle located at x in the reference state is carried at time t to $x+u(x, t)$, where u is the displacement. The associated strain and particle velocity are given by $\gamma = u_x$, $v = u_t$, respectively; subscripts indicate partial derivatives. The nominal stress, absolute temperature, entropy per unity mass and internal energy per unit mass at this particle at time t are denoted by $\sigma(x, t)$, $\theta(x, t) > 0$, $\eta(x, t)$ and $\varepsilon(x, t)$, respectively. While the displacement is required to be continuous, all of the other quantities listed above are allowed to suffer jumps at moving points of discontinuity. (If heat conduction were accounted for, θ would also be required to be continuous.) Away from such discontinuities, such derivatives as arise are assumed to exist.

Where the fields are smooth, the following field equations must hold:

$$v_x = \gamma_t \tag{1}$$

$$\sigma_x = \rho v_t \tag{2}$$

$$\sigma\gamma_t = \rho\varepsilon_t \tag{3}$$

and the following inequality must also be satisfied:

$$\eta_t \geqslant 0. \tag{4}$$

In eqns (2) and (3), ρ is the (constant) referential mass density.

If $x = s(t)$ is the location at time t of a moving jump in the field quantities, one must fulfill the following jump conditions:

$$\overset{+}{v} - \bar{v} + (\overset{+}{\gamma} - \bar{\gamma})\dot{s} = 0 \tag{5}$$

$$\overset{+}{\sigma} - \bar{\sigma} - \rho(\overset{+}{v} - \bar{v})\dot{s} = 0 \tag{6}$$

$$\{\rho(\overset{+}{\varepsilon} - \bar{\varepsilon}) - (1/2)(\overset{+}{\sigma} + \bar{\sigma})(\overset{+}{\gamma} - \bar{\gamma})\}\dot{s} = 0 \tag{7}$$

$$(\overset{+}{\eta} - \bar{\eta})\dot{s} \leqslant 0. \tag{8}$$

Here $\overset{+}{v} - \bar{v}$, for example, stands for $v(s(t)+, t) - v(s(t)-, t)$.

The assumed smoothness of u is responsible for both eqns (1) and (5), the global balance of momentum yields eqns (2) and (6), global balance of energy—the "first law"—implies eqns (3) and (7), and the requirement that the rate of entropy production be positive leads to eqns (4) and (8).

3. A THERMOELASTIC MATERIAL

We now assume the bar is thermoelastic, which means that there is an internal energy potental $\hat{\varepsilon}$, determined by the material, such that $\varepsilon(x, t) = \hat{\varepsilon}(\gamma(x, t), \eta(x, t))$, and for which the following constitutive relations hold:

$$\sigma = \rho\hat{\varepsilon}_\gamma(\gamma, \eta) \tag{9a}$$

$$\theta = \hat{\varepsilon}_\eta(\gamma, \eta). \tag{9b}$$

Let $\psi(x, t) = \varepsilon(x, t) - \theta(x, t)\ \eta(x, t)$ be the Helmholtz free energy. If the specific heat $c = \hat{\varepsilon}_\eta / \hat{\varepsilon}_{\eta\eta}$ is positive as assumed here, the relation (9b) is invertible to give $\eta = \hat{\eta}(\gamma, \theta)$, and one may introduce the Helmholtz potential $\hat{\psi}(\gamma, \theta) = \hat{\varepsilon}(\gamma, \hat{\eta}(\gamma, \theta)) - \theta\hat{\eta}(\gamma, \theta)$. The relations (9a,b) may then be replaced by the following equivalent ones:

$$\sigma = \rho\hat{\psi}_\gamma(\gamma, \theta), \quad \eta = -\hat{\psi}_\theta(\gamma, \theta). \tag{10}$$

Abeyaratne and Knowles (1993b) give an explicit $\hat{\psi}(\gamma, \theta)$ upon which their quasi-static study in that paper, as well as the present dynamic investigation, is based. To describe with minimum detail those features of this particular $\hat{\psi}$ that are needed for present purposes, it

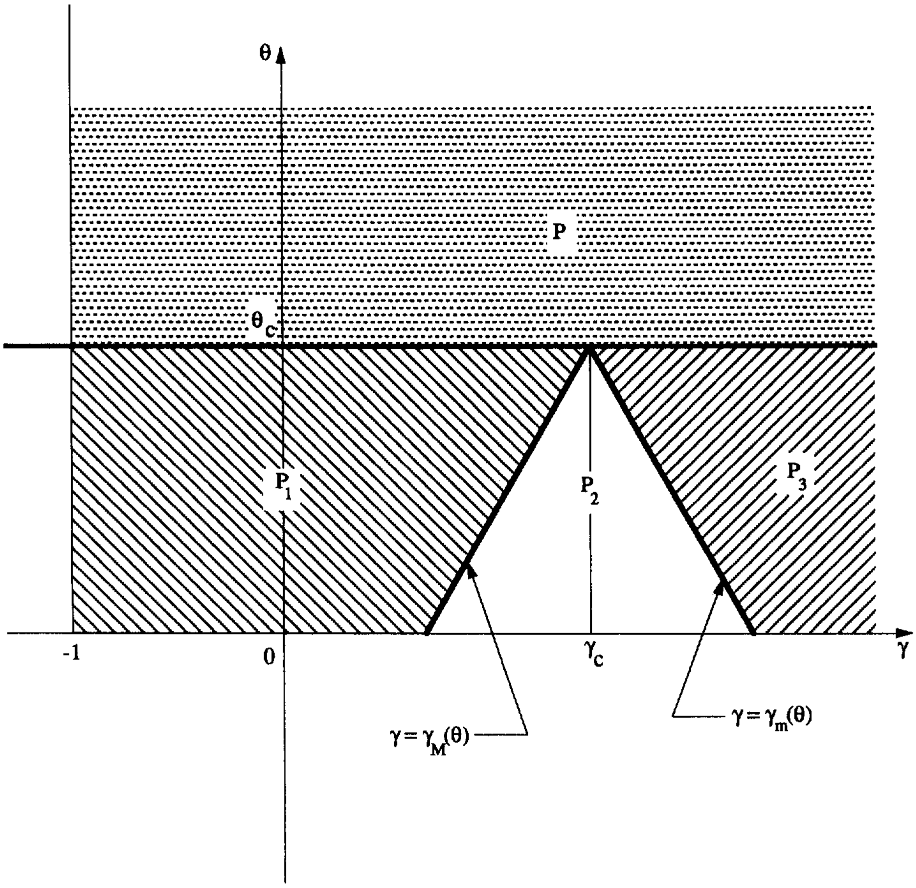

Fig. 1. The strain–temperature plane.

is necessary to refer to the γ, θ plane, which is sketched in Fig. 1. The expression for the model $\hat{\psi}$ is given sectionally on this plane. Each of the subregions P, P_1, P_2, P_3 shown in the figure is identified with a phase of the material. The boundaries between P_1 and P_2 and between P_2 and P_3 are described, respectively, by

$$\gamma = \gamma_M(\theta) = \gamma_c + M(\theta - \theta_c), \quad \gamma = \gamma_m(\theta) = \gamma_c + m(\theta - \theta_c), \tag{11}$$

where $\gamma_c > 0$, $\theta_c > 0$, M and m are material constants. Above the critical temperature θ_c, the material can exist in only one phase, corresponding to the region P. Below this temperature, it can exist in the low-strain corresponding to P_1, in the high-strain phase corresponding to P_3 and in an intermediate phase associated with P_2. We shall not be concerned with temperatures above θ_c, where only a single phase is possible, so we do not give an explicit formula for $\hat{\psi}$ on the region P. On P_1 and P_3, we take

$$\hat{\psi}(\gamma, \theta) = \begin{cases} \dfrac{\mu}{2\rho}\gamma^2 - \dfrac{\alpha\mu}{\rho}\gamma(\theta - \theta_T) - c\theta \log(\theta/\theta_T) & \text{on } P_1, \\ \dfrac{\mu}{2\rho}(\gamma - \gamma_T)^2 - \dfrac{\alpha\mu}{\rho}(\gamma - \gamma_T)(\theta - \theta_T) - c\theta \log(\theta/\theta_T) + \dfrac{\lambda_T}{\theta_T}(\theta - \theta_T) & \text{on } P_3. \end{cases} \tag{12}$$

Here the material constants μ, α and c are, respectively, the elastic modulus, the coefficient of thermal expansion and the specific heat at constant strain, which for simplicity are all taken to be constant and the same in both the high- and low-strain phases. The constants

γ_T, θ_T and λ_T are the transformation strain, the transformation temperature and the latent heat at the transformation temperature, respectively; their physical meaning is discussed in detail by Abeyaratne and Knowles (1993b, 1994a,b). There are restrictions on the material constants just listed—some equalities, some inequalities—that we shall not repeat here; they may be found in the papers cited. One restriction ensures that states in the intermediate phase are always dynamically unstable in the sense described by Abeyaratne and Knowles (1993c). We shall not consider here any processes in the bar that include states in the intermediate phase, so we omit the formula for $\hat{\psi}$ on P_2 corresponding to those in eqn (12).

The Helmholtz potential described above and given in more detail by Abeyaratne and Knowles (1993b) is a "two-well potential" in a sense specified there. Multiple-well potentials are commonly used in describing phase transitions.

We consider only two-phase processes in the bar in which the state (γ, θ) at any particle is always in either the low-strain phase region P_1 $[\gamma < \gamma_M(\theta)]$ or the high-strain phase region $[\gamma > \gamma_m(\theta)]$. We refer to the latter inequalities as the phase segregation restrictions; they ultimately play a major role. For processes of this kind, the fundamental relations (1)–(8) can be readily specialized to the material at hand. The thermomechanical coupling parameter α turns out to introduce some troublesome non-linearities in the resulting jump conditions; we therefore assume from here on that $\alpha = 0$. The field equations (1)–(3) for the two-phase processes to be studied then specialize to

$$\gamma_t - v_x = 0 \tag{13a}$$

$$a^2\gamma_x - v_t = 0 \tag{13b}$$

$$\theta_t = 0, \tag{13c}$$

where the fields are smooth; because of eqn (13c), the inequality (4) is automatically satisfied. In eqn (13b), $a = (\mu/\rho)^{1/2}$ is the acoustic speed common to both phases.

To specialize the jump conditions (5)–(8), one must distinguish between two possible situations: at a *shock wave*, the states $(\bar{\gamma}, \bar{\theta})$ and $(\overset{+}{\gamma}, \overset{+}{\theta})$ on either side of the discontinuity belong to the same phase, i.e. to the same region P_1 or P_3. At a *phase boundary*, these states belong to different phases. At a shock wave in either phase of the material, eqns (5)–(8) become

$$(\overset{+}{\gamma} - \bar{\gamma})\dot{s} + \overset{+}{v} - \bar{v} = 0 \tag{14}$$

$$a^2(\overset{+}{\gamma} - \bar{\gamma}) + \dot{s}(\overset{+}{v} - \bar{v}) = 0 \tag{15}$$

$$(\overset{+}{\theta} - \bar{\theta})\dot{s} = 0 \tag{16}$$

$$\dot{s}\log(\overset{+}{\theta}/\bar{\theta}) \leqslant 0. \tag{17}$$

It is readily seen that eqns (14)–(17) are equivalent to the following:

$$\text{either} \begin{cases} \dot{s} = \pm a, \\ (\overset{+}{\gamma} - \bar{\gamma})\dot{s} + \overset{+}{v} - \bar{v} = 0, \quad \overset{+}{\gamma} \neq \bar{\gamma}, \quad \overset{+}{v} \neq \bar{v}, \\ \overset{+}{\theta} = \bar{\theta}, \end{cases} \quad \text{or} \quad \begin{cases} \dot{s} = 0, \\ \overset{+}{\gamma} = \bar{\gamma}, \ \overset{+}{v} = \bar{v}. \\ \overset{+}{\theta} \neq \bar{\theta}. \end{cases} \tag{18}$$

In the first alternative in eqn (18), the discontinuity propagates with the acoustic speed $\dot{s} = \pm a$ and involves jumps in strain and particle velocity, but not in temperature. In the second alternative, the discontinuity is stationary in the Lagrangian sense, which corresponds to a jump—this time in temperature but not in strain or particle velocity—that moves *with* the particles of the body. It is thus like a contact discontinuity in gas dynamics. Note that in either of the cases in eqn (18), the entropy inequality is trivially satisfied; this is an artifact of the present material and would not occur for a material characterized by a more general, non-piecewise-quadratic, two-well potential. In addition, for our material, the velocity of a shock wave is known *a priori*; for more general material models, this would not be the case. For this reason, it might be better to call these discontinuities acoustic waves, rather than shock waves; their amplitudes, nevertheless, need not be small.

Turning to the case of a propagating phase boundary, we suppose next that the high-strain phase is on the left side of the jump, the low-strain phase on the right. For the present material (with $\alpha = 0$), the basic jump conditions (5)–(8) specialize under the present circumstances to

$$(\overset{+}{\gamma}-\bar{\gamma})\dot{s}+\overset{+}{v}-\bar{v} = 0 \tag{19}$$

$$a^2(\overset{+}{\gamma}-\bar{\gamma}+\gamma_T)+(\overset{+}{v}-\bar{v})\dot{s} = 0 \tag{20}$$

$$\{c(\overset{+}{\theta}-\bar{\theta})+(a^2\gamma_T/2)(\overset{+}{\gamma}+\bar{\gamma}-\gamma_T)+\lambda_T\}\dot{s} = 0 \tag{21}$$

$$\{\log(\overset{+}{\theta}/\bar{\theta})+\lambda_T/(c\theta_T)\}\dot{s} \leqslant 0. \tag{22}$$

In contrast to the case for shock waves in this material, the jump conditions (19)–(22) do not determine the phase boundary velocity $\dot{s}$ in terms of material constants. Moreover, by eliminating the vs between eqns (19) and (20), one can express $\dot{s}^2$ in terms of the strains $\overset{\pm}{\gamma}$; this expression can be used to show that $|\dot{s}|$ must be smaller than the acoustic speed a. The entropy inequality (22) determines the direction in which a phase boundary can propagate if the temperatures $\overset{\pm}{\theta}$ on either side are known. In particular, in the special case $\lambda_T = 0$ of vanishing latent heat, eqn (22) implies that the phase boundary cannot move into the hotter material.

It may be observed that, for the present special choice of thermoelastic material, thermal and mechanical effects are completely uncoupled in the differential equations (13) as well as in the jump conditions (18) at shock waves, but this is not the case for the jump conditions (19)–(22) at a phase boundary. In this sense, the present model appears to be the simplest one that retains non-trivial effects due to the occurrence of a phase transition.

4. EVOLUTION OF DISCONTINUITIES

Let us suppose that, at time $t = 0$, our doubly-infinite bar is in a given piecewise homogeneous state with a discontinuity at the origin: thus

$$\gamma(x,0), v(x,0), \theta(x,0) = \begin{cases} \gamma_L, v_L, \theta_L & \text{for } x < 0, \\ \gamma_R, v_R, \theta_R & \text{for } x > 0, \end{cases} \tag{23}$$

where the six given γs, vs and θs are constants. We shall only consider data for which the state (γ_L, θ_L) on the left is in the high-strain phase, while (γ_R, θ_R) is in the low-strain phase; some of the issues surrounding this by-no-means innocuous limitation on the initial data are interesting, especially in the adiabatic theory presently under discussion. We avoid these issues here; they are discussed—through not fully resolved—by Abeyaratne and Knowles (1993a,c,d). We now consider the initial value problem in which γ, ψ and θ are sought satisfying the initial conditions (23), the differential equations (13) and the jump conditions (18) or (19)–(22) at shock waves or phase boundaries, respectively. This is called the Riemann problem; it is the natural problem to study if one wishes to investigate the way in which a given discontinuity evolves in a dynamical system of partial differential equations.

Although some light can be shed on the structure of the most general scale-invariant solutions of the scale-invariant Riemann problem posed above [see Abeyaratne and Knowles (1994a)], we leave this aside here and describe only the nature of one class of solutions constructed in that reference. In this class, the solutions are piecewise constant:

$$\gamma(x,t), v(x,t), \theta(x,t) = \begin{cases} \gamma_L, v_L, \theta_L & \text{for } x < -at, \\ \gamma', v', \theta' & \text{for } -at < x < 0, \\ \bar{\gamma}, \bar{v}, \bar{\theta} & \text{for } 0 < x < \dot{s}t, \\ \overset{+}{\gamma}, \overset{+}{v}, \overset{+}{\theta} & \text{for } \dot{s}t < x < at, \\ \gamma_R, v_R, \theta_R & \text{for } x > at, \end{cases} \tag{24}$$

where the strains, particle velocities and temperatures bearing primes, pluses and minuses are all unknown constants, and the phase boundary velocity $\dot{s}$—assumed to be subsonic with respect to the acoustic speed—is *also* an unknown (positive) constant. Moreover, the unknown strains and temperatures, once they are determined, must be forced to satisfy the phase segregation restrictions described earlier: the states (γ', θ') and $(\bar{\gamma}, \bar{\theta})$ must be in the high-strain phase, possibly separated by a contact discontinuity, while $(\overset{+}{\gamma}, \overset{+}{\theta})$ must be in the low-strain phase.

For a candidate of the form (24), the fields are constant where they are smooth, so the differential equations (13) are trivially satisfied. Thus the issue of whether there is a solution—and if so, how many—reduces to an analysis of the appropriate jump conditions. In Abeyaratne and Knowles (1994a), such an analysis is carried out. It is shown there that, for a suitable class of given data, there is a one-parameter family of solutions of the form (24) for the Riemann problem, in which each of the nine unknowns in eqn (24) is expressed as an explicitly determined function of the parameter $\dot{s}$, with all phase segregation restrictions satisfied. The parameter $\dot{s}$ itself remains undetermined after all of the jump conditions and initial conditions have been enforced. Thus for this class of initial data, the Riemann problem fails to have a unique solution, having instead the one-parameter family of solutions described above. An analogous lack of uniqueness arises in the purely mechanical theory of the dynamics of phase transitions, in the thermomechanical theory that accounts for heat conduction, and in the quasi-static model; see Abeyaratne and Knowles (1993a,b, 1994b). We have taken the view that, in any one of these settings, this lack of uniqueness is a constitutive deficiency to be remedied by importing from materials science some information about the physics of the phase transition.

5. THE NOTION OF DRIVING TRACTION

Consider a piece of the bar that occupies the interval $[x_1, x_2]$ in the reference configuration. During an adiabatic thermomechanical process in the bar, the entropy production rate $\Gamma(t)$ for this piece of the bar is given by

$$\Gamma(t) = \frac{d}{dt}\int_{x_1}^{x_2} \rho\eta(x,t)\,dx. \tag{25}$$

Let us temporarily relinquish the assumption that the bar is thermoelastic, operating instead in the absence of any constitutive law. Suppose that in the piece of the bar under consideration above, the fields are smooth except at the moving strain discontinuity $x = s(t)$. Then $\Gamma(t)$ in eqn (25) may be decomposed into two parts:

$$\Gamma(t) = \Gamma_{\text{bulk}}(t) + \Gamma_s(t), \tag{26}$$

where

$$\Gamma_{\text{bulk}}(t) = \int_{x_1}^{x_2} \rho\eta_t(x,t)\,dx \tag{27a}$$

$$\Gamma_s(t) = -\rho(\overset{+}{\eta} - \bar{\eta})\dot{s}; \tag{27b}$$

Γ_{bulk} arises from the local dissipation in the material at each particle, and Γ_s represents the rate of entropy production by the moving discontinuity. Since the second law of thermodynamics requires that $\Gamma(t) \geqslant 0$ for every piece of the bar, Γ_{bulk} and Γ_s must be separately non-negative; this leads to eqns (4) and (8).

A useful alternative description of Γ_s involves the notion of driving traction f acting on the discontinuity at $x = s(t)$; f is defined as

$$f = -[[\rho\eta]]\langle\theta\rangle, \tag{28}$$

where, for any field $g(x, t)$, we have written $[[g]] = \overset{+}{g} - \overset{-}{g}$, $\langle g\rangle = (\overset{+}{g} + \overset{-}{g})/2$. Then

$$\Gamma_s = \frac{f\dot{s}}{\langle\theta\rangle}, \tag{29}$$

and $\Gamma_s \geqslant 0$ requires that

$$f\dot{s} \geqslant 0. \tag{30}$$

By using the definition (28), the energy jump condition (7) and the fact that $\varepsilon = \psi + \theta\eta$, one can derive an alternative representation for f that reveals the relation between driving traction as defined in the present adiabatic framework and its counterpart in other settings:

$$f = [[\rho\psi]] - \langle\sigma\rangle[[\gamma]] + \langle\rho\eta\rangle[[\theta]]. \tag{31}$$

The main significance of eqn (31) is that it remains valid for non-adiabatic thermomechanical processes as well as adiabatic ones; it has been derived without appeal to any constitutive law. In a theory that accounts for heat conduction, temperature is continuous, and eqn (31) reduces to $f = [[\rho\psi]] - \langle\sigma\rangle[[\gamma]]$, which is the form of the driving traction used in Abeyaratne and Knowles (1994b). For quasi-static, isothermal processes, one has $[[\sigma]] = [[\theta]] = 0$, and f as given in eqn (31) specializes to $f = [[\psi]] - \sigma[[\chi]]$, where σ is the common value of the stress on either side of the slowly moving discontinuity; this is precisely the jump in the Gibbs free energy, often called the "driving force" in a phase transition.

A detailed discussion of the notion of driving traction in a three-dimensional thermomechanical setting that accounts for inertia and heat conduction is given by Abeyaratne and Knowles (1990).

If we now reinstate the assumption that the bar is thermoelastic, we find first from eqns (3), (9) and (27a) that $\Gamma_{\text{bulk}} = 0$ for any such material, and then that the formula (31) for f becomes

$$f = \rho\{[[\psi]] - \langle\psi_{,\gamma}\rangle[[\gamma]] - \langle\psi_{\theta}\rangle[[\theta]]\}. \tag{32}$$

Suppose the moving discontinuity is a phase boundary in the special thermoelastic material introduced in Section 3, and assume that the high-strain phase is on the left. Then eqn (32) can be shown to specialize to

$$f = -\rho\langle\theta\rangle\{c\log(\overset{+}{\theta}/\overset{-}{\theta}) + \lambda_T/\theta_T\}. \tag{33}$$

On the other hand, at a shock wave that is not a contact discontinuity, one finds that $f = 0$, so that a shock wave is dissipation-free in this special material. This would not be true for a more general two-well potential. Contact discontinuities are dissipation-free because $\dot{s} = 0$.

6. THE KINETIC RELATION

Extra constitutive information is needed to single out a physically acceptable solution to the Riemann problem and thus provide a determinate theory of the evolution of the discontinuity studied in Section 4. To ascertain an appropriate additional constitutive assumption, we start first from the fact that, for a thermoelastic material, $\Gamma = (f/\langle\theta\rangle)\dot{s}$. Next, we appeal to the theory of irreversible processes, as described for example by Kestin (1979), and identify $f/\langle\theta\rangle$ as an affinity and $\dot{s}$ as its conjugate flux on the basis of the form of Γ. We then postulate a relation of the kind used in irreversible thermodynamics: the affinity is a materially-determined function of the conjugate flux, so that in the present case

$$f/\langle\theta\rangle = \varphi(\dot{s}). \tag{34}$$

In view of the entropy inequality (30), φ must conform to the requirement that

$$\varphi(\dot{s})\dot{s} \geqslant 0. \tag{35}$$

If φ is continuous as assumed here, eqn (35) requires that $\varphi(0) = 0$.

Let us now return to the one-parameter family of solutions to the Riemann problem of Section 4, recalling that $\dot{s}$ is the free parameter. In this family of solutions, all physical quantities, in particular $\overset{+}{\theta}$ and $\overset{-}{\theta}$, are determined as functions of $\dot{s}$. Upon substituting the expressions for $\overset{+}{\theta}$ and $\overset{-}{\theta}$ in terms of $\dot{s}$ into eqn (33), one has a formula for the driving traction f in terms of $\dot{s}$. Substitution of this expression for f into the kinetic relation (34) furnishes a single equation for the determination of the phase boundary velocity $\dot{s}$.

Under certain assumptions on the material parameters and on the nature of the kinetic response function $\varphi(\dot{s})$, it is shown by Abeyaratne and Knowles (1994a) that there is a range of initial data for which this equation has a unique solution $\dot{s}$. This value of $\dot{s}$ then singles out from the family of solutions to the Riemann problem the one that is preferred by the specified kinetics.

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