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# The structure of shock and interphase layers for a heat conducting Maxwellian rate-type approach to solid-solid phase transitions

## Part I: Thermodynamics and admissibility

**Abstract** We consider a thermoelastic model for phase transforming materials which can adequately describe the evolution with respect to the temperature of the hysteresis loop both in compression and tension tests. The specificity of this model is that the Grüneisen coefficient changes its sign. The model is augmented by considering a dissipative mechanism governed by a Maxwellian rate-type constitutive equation that can describe stress relaxation phenomena toward equilibrium between phases. Existence and uniqueness of traveling wave solutions are investigated. One derives that the admissibility condition induced by the Maxwellian rate-type approach, coupled or not with Fourier heat conduction law is related to the chord criterion with respect to the Hugoniot locus. We investigate the structure of profile layers and we focus on their thermodynamic properties. The influence of the exothermic or endothermic character of phase transitions on the inner structure of interphase layers is captured. A phenomenon of temperature overshoot/undershoot with respect the front state temperature and Hugoniot back state temperature inside an interphase layer is revealed.

**Keywords** Phase transitions · Thermoelasticity · Shocks · Entropy · Traveling waves · Admissibility

## 1 Introduction

The subject of non-linear wave propagation which causes changes not only in stress or motion, but also in heat and temperature has attracted the interest of both theoreticians and experimentalist. We mention here for example, as background references, the comprehensive analysis of Drumheller [1] and the extensive review article by Menikoff and Plohr [2].

The study of steady, structured shock waves or *traveling waves* is an important subject in the theory of waves both from theoretical and experimental point of view. From a mathematical perspective the study of traveling waves provides *admissibility criteria* for discontinuous solutions of adiabatic thermoelastic theories which derive from associated dissipative systems (Liu [3], Slemrod [4], [5], Pego [6], Ngan and Truskinovsky [7]). Steady shock waves were first analyzed in Newtonian fluids. It has been shown that discontinuous solutions, called shock waves, arising in inviscid flow equations have a physical sense as limits of traveling wave profiles, named shock layers, of viscous, heat-conducting fluids (Weyl [8], Gilbarg [9], Hamad [10] and the literature therein). In metallic materials, impact-induced traveling waves have been experimentally observed in the 1960's (see for instance Barker [11]). The structure of these steady shock waves, which is due to the viscous effects governing the viscoplastic flow of metals, has been recently investigated and revisited by

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Molinari and Ravichandran [12]. For thermoelastic materials a complete study of traveling waves structured only by heat conduction has been made by Dunn and Fosdick [13].

The subject of this paper is devoted to the study of some new thermo-mechanical aspects concerning the propagation of steady, structured waves in materials which can exist in different solid phases and can undergo reversible stress- and temperature-induced phase transitions, like shape memory alloys (SMAs). These materials exhibit significant local temperature changes both in quasistatic and dynamic experiments. That is due to the large amount of latent heat released (absorbed) during the phase transformation process. Temperature measurements have been done in the quasistatic case (Leo *et al* [14], Shaw and Kyriakides [15]), but they are exceedingly difficult to be realized during shock wave experiments, and too little is known about the temperature variation across impact-induced propagating phase boundaries and about their internal structure.

From crystallographic point of view these materials are defined by a crystalline structure and the transition from one phase to another is characterized by a rapid transition in the crystalline lattice. In continuum mechanics, the thermoelasticity theory with non-convex stored energy has become a common constitutive framework to model such materials (e.g. Abeyaratne and Knowles [16] and the references). The theory of thermoelastic materials undergoing solid-solid phase transformations requires additional constitutive information that governs the evolution of a phase boundary.

One way is to introduce from the onset a nucleation criterion for the initiation of phase transition and a kinetic relation which relates the interface velocity and the driving force of phase transformation (e.g. Truskinovsky [17], Abeyaratne and Knowles [18]). These additional constitutive relations are sufficient to ensure unique solutions for initial-boundary value problems. In this approach the transition from one stable phase of the material to another one is an *instantaneous* process and the propagating interface separating two distinct phases is a surface of zero thickness across which the thermo-mechanical variables suffer a jump.

A second way is to regularize the problem by augmenting the constitutive thermoelastic law in such a way that the stress depends additionally on other physical mechanisms which usually are rate-type effects and/or strain-gradient effects. Using this approach a nucleation criterion is no more necessary and the thermomechanical instabilities associated with the formation and propagation of phases occur in a natural way (e.g. Vainchtein [19] using only strain-rate effects, Făciu and Mihailescu-Suliciu [20] using strain-rate and stress-rate effects, and Ngan and Truskinovsky [21] using strain-rate effects and strain-gradient effects). In this approach, the study of traveling wave solutions reveals that the propagating interface separating two distinct phases becomes a transition layer of finite thickness where the thermomechanical variables vary rapidly, but continuously. Due to the strain-rate effects the transition from one stable phase of the material to another one is *no more an instantaneous* process, but it requires a small phase transition time.

This framework has been mainly used to derive kinetic relations for the sharp interface theory. These are obtained by using the traveling wave solutions for the augmented theory, which may include various combinations of strain-rate, strain gradient, heat conduction and convective heat transfer effects and by removing these effects in a suitable limit process. One considers that the kinetic laws obtained in this way incorporate microscale processes associated with the transformation of one microstructure to another (e.g. lattice in the case of a crystalline solid). For instance, such kinetics laws have been investigated by Slemrod [5], Turteltaub [22], Ngan and Truskinovsky [7], [21] in the case where non-isothermal "viscosity-capillarity" models are coupled with heat conduction inside the phase transition front. The case of non-isothermal Kelvin-Voigt model coupled with heat conduction and convection has been investigated by Vainchtein [23]. Depending on the properties of these kinetic relations different thermo-mechanical aspects related with the propagation of a phase boundary can be captured. For example, one gets a thermal trapping effect when the phase transition progresses only for sufficiently large values of the driving force (e.g. [7], [21], [23]), or a "stick-slip" behavior of the phase boundary motion in the case of a non-monotone kinetic law (e.g. [22], [7], [21], [23]). Similar non-monotonic kinetic laws have been already observed for a related non-isothermal Ginzburg-Landau model (e.g. Umantsev [24] and the literature therein).

There exists a considerable literature on dynamics of martensitic phase boundaries for the non-isothermal case. We recall here the pure thermal approach which neglect inertia, but take into account convective heat exchange with ambient medium and radiation (Leo *et al* [14], Bruno *et al* [25]). When both inertia and heat release are taken into account we mention Abeyaratne and Knowles [26], [27], Knowles [28] and the references.

The novelty of this work consists in the fact that we consider a different augmented model of a phase transforming thermoelastic material, with the special property that the Grüneisen coefficient changes its sign on the constitutive domain, which corresponds to an important feature of a SMA. The study of its traveling wave solutions reveals important thermomechanical consequences on the internal structure of propagating phase

boundaries. Moreover, we show that it is possible that in the limiting case of vanishing of the augmented-effects the resulting sharp interface theory can lose important information concerning the thermal behavior inside the transition front.

We briefly introduce in Sect. 2 the dynamic thermomechanic bar theory in Lagrangian description. Based on experimental observations on pseudoelastic NiTi (Shaw [29]), in Sect. 3 we describe the constitutive assumptions for a thermoelastic three phase material, i.e. a material which can exist in the austenitic phase  $A$  and in two variants of martensite  $M^\pm$ , one obtained in tension ( $\sigma > 0$ ) and the other in compression ( $\sigma < 0$ ) tests. As usual, for phase transforming materials (see for example Abeyaratne et al [30]) the stress-strain relation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  at fixed temperature  $\theta$  is non-monotone on certain strain intervals. The particular feature of our assumptions, in agreement with the experimental behavior in [29], is that  $\frac{\partial \sigma_{eq}}{\partial \theta}$  is positive on that part of the constitutive domain in the  $\varepsilon - \theta$  plane associated with  $A \leftrightarrow M^+$  phase transformations and it is negative on the complementary part associated with  $A \leftrightarrow M^-$  phase transformations. This behavior reflects experimental observations related with the shape memory effect and the fact that in traction tests the hysteresis loop moves upwards, while in compression tests it moves downwards in the  $\varepsilon - \sigma$  plane, as the temperature grows. Therefore, it follows that the Grüneisen coefficient, which typically is positive, changes its sign in the  $\varepsilon - \theta$  plane and this behavior has an important effect on the structure of interphase layers. Further, we recall the thermodynamic relations arising from the Clausius-Duhem inequality, the Gibbsian thermostatic stability conditions, and on the other side the dynamic stability condition which ensures the existence of a real sound speed for the thermoelastic material. Consequently, we associate the stable/unstable phases of the material with the domain of hyperbolicity/ellipticity of the dynamic thermoelastic PDE system. We end this section by describing the jump relations across a first order discontinuity for the adiabatic system of thermoelasticity and by characterizing the Hugoniot locus in the  $\varepsilon - \theta$  plane and in the  $\varepsilon - \sigma$  plane.

In order to identify meaningful weak solutions for the quasilinear adiabatic thermoelastic system we augment in Sect. 4 the constitutive law  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  by assuming that the stress depends additionally not only on strain rate  $\dot{\varepsilon}$  (as in Vainchtein [23]), but also on the stress rate  $\dot{\sigma}$ . Thus, we introduce a dissipative regularizing term which includes stress relaxation phenomena toward equilibrium between phases. Hence, we consider the following approach which combines aspects of both the Maxwell and KelvinVoigt models, i.e.  $\sigma = \sigma_{eq}(\varepsilon, \theta) + \mu \dot{\varepsilon} - \tau \dot{\sigma}$ , where  $\mu > 0$  is a "viscosity" coefficient and  $\tau > 0$  is a time of relaxation. Next, we describe the necessary and sufficient restrictions imposed by the Clausius-Duhem inequality on this Maxwellian rate-type model. It is obvious that for phase transforming materials the use of the term "viscosity" for the Kelvin-Voigt model, or for this Maxwellian rate-type model is improper since there is no "viscosity" in such materials. In fact there are the rate-type effects which introduce physical mechanisms allowing for describing non-instantaneous phase transitions, and thus, to get an internal structure in a propagating phase boundary. Due to certain tradition concerning the terminology and due to analogies with similar constitutive equations used in fluid mechanics or in viscoelasticity, and for simplicity reasons in the following we shall often use the term "viscosity effect" instead of "rate-type effects".

In order to exhibit the inner structure of shock and interphase layers corresponding to this augmented thermomechanic theory, Sect. 5 is devoted to a detailed analysis of traveling wave solutions. Since for  $\tau = 0$  our rate-type constitutive equation reduces to the Kelvin-Voigt model in solid mechanics, which is equivalent with the Navier-Stokes equation for one-dimensional flows, from our analysis one can retrieve classical results obtained in studying steady wave solutions for viscous, heat conducting fluids. Let us recall that Gilbarg [9] has given a sufficient set of conditions on the equation of state, which includes Weyl's fluids [8], to prove the existence of one-dimensional shock layers and has investigated their limit behavior for small viscosity and heat conductivity. His constitutive restrictions correspond to a convex relation between pressure and specific volume and to a positive Grüneisen coefficient. A direct consequence of these constitutive assumptions is that the admissible shocks are of compressive heating type. The non-convex case in non-isothermal gas dynamics has been considered later by Liu [31] and it leads to the occurrence of shocks of expansive cooling type. He proposed an admissibility condition of Oleinik type [32], called extended entropy condition, which is just a chord criterion with respect to the Hugoniot locus. His proof assumes there is no heat conduction. When both viscosity and heat conduction are considered in the structure of the profile layer Gilbarg's result for the non-convex case has been extended by Pego [6].

Starting from our special constitutive assumptions we pursue two main objectives in Sect. 5. First, we discuss the existence and uniqueness of traveling wave solutions for the augmented PDEs system. In this way we answer the question, which is the admissibility condition induced by the Maxwellian rate-type approach, coupled or not with Fourier heat conduction law. Second, we investigate the inner structure of profile layers, the capacity of heat conduction and/or relaxation ("viscous") dissipative mechanisms to structure shock waves

and phase transition fronts and the effect of Grüneisen coefficient. The questions to be answered are: 1) what happens when the "viscous" added effect and the heat conductivity effect vanish ?; 2) does the adiabatic thermoelastic wave structure with sharp interfaces inherits the wave structure of the augmented theory ?

We find that *the chord criterion with respect to the Hugoniot locus in the  $\varepsilon - \sigma$  plane* is, in general, a necessary and sufficient condition for the existence and uniqueness of "viscous", heat conducting profile layers. It should be noted that this is an extremely practical *admissibility condition* for discontinuous solutions of the adiabatic thermoelastic system because it does not depend on the considered dissipative mechanism.

We also show that there may exist a non-physical situation, and we characterize it from thermodynamical point of view, when a strong discontinuity satisfies the chord criterion, but a "viscous", heat-conducting profile layer does not exist if the "viscosity effect" is dominated by the heat conductivity effect, like in the example given by Pego [6].

It is useful to note here that this chord criterion involves that the admissible propagating phase boundaries are supersonic or sonic with respect to the front state, and subsonic or sonic with respect to the back state of the front wave, as in gas dynamics. That means the chord criterion is consistent with Lax conditions [33]. Unlike this admissibility condition, generated by the rate-type effects in the augmented models, the presence of both "viscosity" and strain-gradient terms, which introduces dissipation and dispersion mechanisms, allows propagating phase boundaries which are subsonic or sonic with respect to both front and back states of the wave (e.g. Slemrod [5], Ngan and Truskinovsky [7], [21] and the literature therein). These phase boundaries are referred in [7] and [21] as kinks.

We consider separately the cases when the Grüneisen coefficient is positive, negative or changes its sign inside the profile layer. We find that when the Grüneisen coefficient changes sign inside the layer, the temperature variation is non-monotone, and even more, it reaches lower/larger values than the initial and final temperature for compressive/expansive wave discontinuity. This finding could be also important for interpreting experimental results. Thus, the profile layer of the temperature displays an asymmetric spike-layer form which is in agreement with the exothermic or endothermic character of phase transformation. On the other side, this behavior implies that, in this case, the adiabatic thermoelastic temperature structure with sharp interface does not inherit the structure of the augmented theory.

We investigate the basic difference between the effect of "viscosity" and heat conduction on the structure of the profile layers. We illustrate that when the only structuring mechanism is the heat conduction the temperature is continuous, but the strain may be discontinuous having isothermal jumps inside the profile layer. Finally, we show that the entropy production in a "viscous", thermally conducting profile layer generated by the Maxwellian rate-type approach does not depend on "viscosity" or heat conduction. Moreover, we show that when the "viscosity effect" dominates the heat conductivity effect then the variation of entropy inside the profile layer is monotone, while in the opposite case the entropy variation is non-monotone and even more its values can become inside the profile layer lower than the entropy front state and/or larger than the entropy of the Hugoniot back state.

For a quantitative analysis of these features an explicit piecewise linear model based on experimental results of the type obtained by Shaw [29] will be considered in Part II [35] and investigated numerically.

## 2 Thermomechanic bar theory. Lagrangian description

We consider a thin cylindrical bar with length  $L$ , constant cross-sectional area, constant mass density  $\rho$  (mass per unit length) in an unstressed reference configuration, which corresponds to a defined phase of the material. Let the function  $x = \chi(X, t)$  express the *longitudinal motion* of the bar and  $\theta = \theta(X, t) > 0$  express the *absolute temperature*. The first gives the actual position  $x$  occupied at the time  $t$  by a particle labelled  $X \in [0, L]$  in the reference configuration. The function  $\chi(X, t)$  is assumed to be injective and bi-continuous with respect to  $X$ . Whenever  $\chi(X, t)$  is differentiable we denote by  $\varepsilon(X, t) = \frac{\partial \chi}{\partial X} - 1 > -1$  the *strain* at point  $X$  and by  $v = v(X, t) = \frac{\partial \chi}{\partial t}$  the *particle velocity*. We denote by  $\sigma = \sigma(X, t)$  the *nominal stress* (longitudinal force per unit area in the reference configuration), by  $e = e(X, t)$  the *specific internal energy* per unit mass, by  $\eta = \eta(X, t)$  the *specific entropy* per unit mass, by  $q = q(X, t)$  the *axial heat flux*, by  $r = r(X, t)$  the *lateral heat exchange* of the bar with its surrounding. At points  $(X, t)$  where  $v, \varepsilon, \theta, \sigma, e, q$  and  $r$  are smooth functions the compatibility equation between strain and particle velocity, the balance of momentum and the balance of energy become

$$\frac{\partial \varepsilon}{\partial t} - \frac{\partial v}{\partial X} = 0, \quad \rho \frac{\partial v}{\partial t} - \frac{\partial \sigma}{\partial X} = 0, \quad \rho \frac{\partial e}{\partial t} - \sigma \frac{\partial \varepsilon}{\partial t} + \frac{\partial q}{\partial X} = r. \quad (1)$$

If we suppose that across a curve  $X = S(t)$  in the  $X - t$  plane at least one of the quantities  $v, \varepsilon, \theta, \sigma, e, q$  experience jumps then the continuity of the motion  $\chi$ , the balances of momentum and of energy require

$$\dot{S}[\varepsilon] + [v] = 0, \quad \rho \dot{S}[v] + [\sigma] = 0, \quad \rho \dot{S}[e] + \langle \sigma \rangle [v] - [q] = 0. \quad (2)$$

Such a curve is usually called a *strong discontinuity*, or a *first order discontinuity*. Here  $\dot{S}(t)$  denotes the speed of propagation of the discontinuity and for any quantity  $f = f(X, t)$  we have used the notations  $[[f]](t) = f^+(t) - f^-(t) = f(S(t)^+, t) - f(S(t)^-, t)$  and  $\langle f \rangle(t) = \frac{1}{2}(f^+(t) + f^-(t))$ . We name  $X > S(t)$  as the + side and  $X < S(t)$  as the - side of the discontinuity.

The second law of thermodynamics in the form of the Clausius-Duhem inequality and the corresponding jump relation read

$$\rho \frac{\partial \eta}{\partial t} \geq -\frac{\partial}{\partial X} \left( \frac{q}{\theta} \right) + \frac{r}{\theta}, \quad -\rho \dot{S}[[\eta]] + \left[ \left[ \frac{q}{\theta} \right] \right] \geq 0. \quad (3)$$

We note that for smooth processes the Clausius-Duhem inequality is used to restrict the form of the constitutive relations, while for non-smooth processes, i.e. solutions with jump discontinuities, it becomes an additional constraint that weak solutions must satisfy.

### 3 Three phase materials - the thermoelastic case

#### 3.1 Constitutive assumptions

Solid-solid phase transformations are responsible for the remarkable properties of SMAs. They are well understood and explained at crystallographic level. Basically, there are two relevant phases associated with SMAs, the austenite (stable at high temperatures) and the martensite (stable at low temperatures). While the austenite has a well-ordered body-centered cubic structure that presents only one variant, the martensite can form even twenty four variants. For an uniaxial test at a given temperature, it is enough to consider a material which exists in the austenite phase  $A$ , for sufficiently small values of strain, and in two variants of martensite  $M^+$  and  $M^-$ . One variant is obtained for sufficiently large tensile strain and the other variant for sufficiently large compressive strain, respectively. In general, this deformation behavior for single crystal and polycrystalline NiTi was observed to be asymmetric in tension and in compression (Gall *et al* [34]).

From phenomenological point of view the reversible phase transformations in crystalline solids have been successfully studied using the theory of thermoelasticity with non-convex free-energy or, equivalently, with non-monotone stress-strain relation for certain interval of temperature (e.g. Abeyaratne and Knowles [16] and the references therein). In this paper we consider such a stress-strain-temperature relation

$$\sigma = \sigma_{eq}(\varepsilon, \theta), \quad (4)$$

in order to characterize the response of a three phase shape memory alloy in traction and compression tests. This phenomenological constitutive equation can be determined starting from isothermal stress-strain curves obtained experimentally at very low strain-rates over an interval of temperature and from the macroscopic observations which accompany the evolution of inhomogeneous deformation. A typical example is given by the pseudoelastic responses of a nearly equiatomic polycrystalline NiTi alloy under uniaxial traction tests reported by Shaw and Kyriakides [15] and Shaw [29, Fig.3] for temperatures between 15 °C and 55 °C.

The above mentioned set of uniaxial displacement controlled tests conducted in nearly isothermal conditions are characterized by hysteresis loops having the following characteristics. The bar, initially in the phase of low stretch (austenite), starts to deform elastically in a homogeneous manner. This homogeneity is lost shortly after a maximum stress  $\sigma = \sigma_M^+(\theta)$ , which corresponds to the strain level  $\varepsilon = \varepsilon_M^+(\theta)$  (see Fig. 1). Thus, the beginning of a stress decay is followed immediately by a significant stress-drop which accompanies the first nucleation of martensite. The forward  $A \rightarrow M^+$  phase transformation produces a well defined upper stress plateau with small oscillations. Along it the transformation occurs in a localized way, i.e through nucleation events and subsequent growth of the high stretch phase (martensite) into the austenite phase. Once the transformation is complete the specimen starts again to deform elastically and homogeneously while the slope of the stress-strain relation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is again positive.

During unloading the stress decreases nonlinearly while the specimen deforms homogeneously in the new martensite phase. This homogeneity is lost shortly after a minimum stress  $\sigma = \sigma_m^+(\theta)$  has been reached (see Fig. 1), which corresponds to the strain  $\varepsilon = \varepsilon_m^+(\theta)$ . After a sudden stress rise, unstable transformation from



martensite to austenite proceeds along a lower stress plateau by the propagation of distinct phase fronts along the length of the unloaded specimen.

Since along the loading and unloading stress plateaus the coexistence of two solid phases is allowed and, in general, multiple co-existent phase distributions are possible for a single axial stress state it is natural and common to consider the slope of the stress-strain relation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  negative for  $\varepsilon \in (\varepsilon_M^+(\theta), \varepsilon_m^+(\theta))$ . We will see later in what way the monotone increasing/decreasing stress-strain relations  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  are associated with the so called stable/unstable states of the material.

While the monotone increasing parts of the stress-strain relations  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  can be chosen in such a way to fit known quasi-static isothermal experiments like in Shaw [29, Fig.3], the monotone decreasing part of these curves cannot be determined in a direct way from such experiments. Consequently, in general, they are chosen in a conventional way which is illustrated in the example considered in Part II of this paper [35].

Let us note that for theories like those developed by Abeyaratne *et al* [30] based on additional constitutive information in the form of driving force and nucleation criteria an explicit form for  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  on the unstable interval  $\varepsilon \in (\varepsilon_M^+(\theta), \varepsilon_m^+(\theta))$  is necessary only in so far as the Maxwell stress need to be determined. On the other side, theories which include rate-type effects, like in our case, possess their own kinetics due to the intrinsic dissipation mechanism incorporated ([19], [20], [21]). Thus, the form of the descending part of the constitutive equation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  will only affect the kinetics of phase transformation, i.e. the rate at which the transformation takes place in the unstable interval. Indeed, it was shown, for the isothermal case, in Făciu and Molinari [36, Part II, Sect. 2, relations (11)-(12)] how the slope of the equilibrium curve influences the growth/decay of a perturbation of an equilibrium state.

The same type of deformation behavior, but in general asymmetric, can be observed in compression tests. Therefore, we suppose in the following that the pairs of strain and stress ( $\varepsilon = \varepsilon_M^\pm(\theta), \sigma = \sigma_M^\pm(\theta)$ ) and ( $\varepsilon = \varepsilon_m^\pm(\theta), \sigma = \sigma_m^\pm(\theta)$ ) associated with the changes of slope of the equilibrium stress-strain relation at constant temperature (see Fig. 1) can be determined experimentally. Using this information we can plot a phase diagram in the  $\varepsilon - \theta$  plane, like in Fig. 2, which contains essential constitutive information on phase transformation.

In the following we assume (see also Abeyaratne *et al* [30]) there are two critical temperatures  $\theta_m$  and  $\theta_M$  such as, for  $\theta > \theta_M$  the material only exists in its austenite form no matter what the stress level is, whereas for  $\theta < \theta_m$  the material only exists in its martensitic forms. For  $\theta \in [\theta_m, \theta_M]$  all three phases are available to the material. The thermomechanical assumptions we consider here are.

**H1)** The boundary curves  $\varepsilon = \varepsilon_m^\pm(\theta)$ ,  $\varepsilon = \varepsilon_M^\pm(\theta)$  of the phase diagram in the  $\varepsilon - \theta$  plane (see Fig. 2) are *continuously differentiable* and have the following properties:

$$\begin{aligned} \frac{d\varepsilon_M^+(\theta)}{d\theta} > 0, \quad \frac{d\varepsilon_M^-(\theta)}{d\theta} < 0 \quad \text{for } \theta \in (\theta_m, \theta_M); \quad \frac{d\varepsilon_m^+(\theta)}{d\theta} > 0, \quad \frac{d\varepsilon_m^-(\theta)}{d\theta} < 0 \quad \text{for } \theta < \theta_m \\ \varepsilon_M^+(\theta_m) = \varepsilon_M^-(\theta_m), \quad \varepsilon_m^-(\theta_M) = \varepsilon_M^-(\theta_M), \quad \varepsilon_m^+(\theta_M) = \varepsilon_M^+(\theta_M). \end{aligned} \quad (5)$$

**H2)** The stress response function  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is *continuous, piecewise-smooth* and satisfies the following properties. **a)** At each temperature  $\theta > \theta_M$ ,  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is a monotonically *increasing* function of strain. **b)** At each temperature  $\theta \in [\theta_m, \theta_M]$  (see Fig. 1) the function  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is: a monotonically *increasing* function of strain for  $\varepsilon < \varepsilon_m^-(\theta)$ , for  $\varepsilon \in (\varepsilon_M^-(\theta), \varepsilon_M^+(\theta))$  and for  $\varepsilon > \varepsilon_m^+(\theta)$ ; a monotonically *decreasing* function of strain over the intervals  $(\varepsilon_m^-(\theta), \varepsilon_M^-(\theta))$  and  $(\varepsilon_M^+(\theta), \varepsilon_m^+(\theta))$ . **c)** At each temperature  $\theta < \theta_m$ ,  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is a monotonically *increasing* function of strain for  $\varepsilon < \varepsilon_m^-(\theta)$  and  $\varepsilon > \varepsilon_m^+(\theta)$  while on the remaining interval  $(\varepsilon_m^-(\theta), \varepsilon_m^+(\theta))$  it is monotonically *decreasing*.

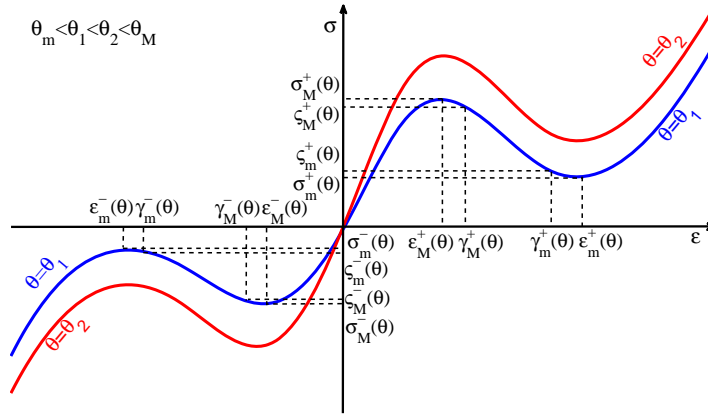
It is well known that the pseudoelastic hysteresis is strongly influenced by the temperature. Indeed, according to the traction tests reported by Shaw [29] the hysteresis loop moves *upward* as the temperature grows. On the other side, for compression tests, the hysteresis loop moves *downward* as the temperature grows. Consequently, we consider the following natural assumption.

**H3)** There exists a monotone curve  $\varepsilon = \varepsilon_t(\theta)$  across which  $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta}$  changes the sign (Fig. 2), i.e.

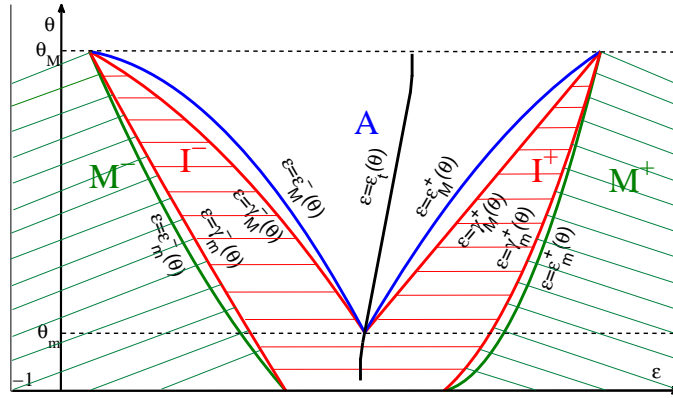
$$\begin{aligned} \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} > 0, \quad \text{for } \varepsilon > \varepsilon_t(\theta); \quad \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} < 0, \quad \text{for } \varepsilon < \varepsilon_t(\theta), \\ \varepsilon_M^-(\theta) < \varepsilon_t(\theta) < \varepsilon_m^+(\theta), \quad \text{for } \theta \in (\theta_m, \theta_M) \quad \text{and} \quad \varepsilon_m^-(\theta) < \varepsilon_t(\theta) < \varepsilon_m^+(\theta), \quad \text{for } \theta < \theta_m. \end{aligned} \quad (6)$$

Concerning the *smoothness assumptions* of relation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  we distinguish two cases.

**S1)** First, we consider  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  a *smooth function* (at least of class  $C^2$ ) on its domain of definition.



**Fig. 1** Evolution of the stress-strain curves with respect to temperature:  $\theta \in (\theta_m, \theta_M)$  - pseudoelastic range.



**Fig. 2** Phase diagram in the  $\varepsilon - \theta$  plane: A phase - blank area;  $M^\pm$  phase - oblique lines area;  $I^\pm$  region - horizontal lines area.

**S2)** Second, we suppose  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  a *continuous and piecewise smooth function* on its domain of definition. More precisely, it is smooth on each domain delimitate by the curves  $\varepsilon = \varepsilon_M^\pm(\theta)$ ,  $\varepsilon = \varepsilon_m^\pm(\theta)$ , and  $\varepsilon = \varepsilon_l(\theta)$  across which  $\frac{\partial \sigma_{eq}}{\partial \varepsilon}$ ,  $\frac{\partial \sigma_{eq}}{\partial \theta}$ ,  $\frac{\partial^2 \sigma_{eq}}{\partial \theta^2}$  may have jump discontinuities. A typical example is given in Part II [35] where a continuous piecewise linear relation is considered.

### 3.2 Thermodynamic considerations for the thermoelastic model

If one uses the Helmholtz free energy  $\psi = e - \theta \eta$ , the entropy inequality (3)<sub>1</sub> takes the form

$$-\rho \frac{\partial \psi}{\partial t} + \sigma \frac{\partial \varepsilon}{\partial t} - \rho \eta \frac{\partial \theta}{\partial t} - \frac{q}{\theta} \frac{\partial \theta}{\partial X} \geq 0. \quad (7)$$

It is well known that the following restrictions on the free energy  $\psi = \psi_{eq}(\varepsilon, \theta)$ , entropy  $\eta = \eta_{eq}(\varepsilon, \theta)$  and dissipation of the thermoelastic model (4) are imposed by the second law of thermodynamics (7)

$$\sigma_{eq}(\varepsilon, \theta) = \rho \frac{\partial \psi_{eq}(\varepsilon, \theta)}{\partial \varepsilon}, \quad \eta_{eq}(\varepsilon, \theta) = -\frac{\partial \psi_{eq}(\varepsilon, \theta)}{\partial \theta}, \quad D_{th} = -\frac{q}{\theta} \frac{\partial \theta}{\partial X} \geq 0. \quad (8)$$

Indeed, in this case, for any smooth fields  $\varepsilon$  and  $\theta$  there exists only thermal dissipation. Since we consider the Fourier law for axial heat conduction, i.e.  $q = -\kappa \frac{\partial \theta}{\partial X}$ , we recall that (8)<sub>3</sub> requires  $\kappa > 0$ .

Let us first consider the smooth case **S1)**. The stress response function  $\sigma = \sigma_{eq}(\varepsilon, \theta)$ , determined mainly from quasistatic experiments, defines a unique free energy function  $\psi_{eq}(\varepsilon, \theta)$ , modulo an additive function of

temperature  $\phi = \phi(\theta)$ , as well as, the entropy  $\eta = \eta_{eq}(\varepsilon, \theta)$ , the internal energy  $e = e_{eq}(\varepsilon, \theta) = \psi_{eq} + \theta \eta_{eq}$  and the specific heat at constant strain  $C = C_{eq}(\varepsilon, \theta)$  by relations

$$\psi_{eq}(\varepsilon, \theta) = \int_{\varepsilon_0}^{\varepsilon} \frac{1}{\rho} \sigma_{eq}(s, \theta) ds + \phi(\theta), \quad \eta_{eq}(\varepsilon, \theta) = - \int_{\varepsilon_0}^{\varepsilon} \frac{1}{\rho} \frac{\partial \sigma_{eq}(s, \theta)}{\partial \theta} ds - \frac{d\phi(\theta)}{d\theta}, \quad (9)$$

$$C_{eq}(\varepsilon, \theta) \equiv \frac{\partial e_{eq}}{\partial \theta} \equiv \theta \frac{\partial \eta_{eq}}{\partial \theta} \equiv -\theta \frac{\partial^2 \psi_{eq}(\varepsilon, \theta)}{\partial \theta^2} = -\theta \int_{\varepsilon_0}^{\varepsilon} \frac{1}{\rho} \frac{\partial^2 \sigma_{eq}(s, \theta)}{\partial \theta^2} ds - \theta \frac{d^2 \phi(\theta)}{d\theta^2}, \quad (10)$$

where  $\varepsilon_0$  is an arbitrary reference strain.

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

$$\frac{d^2 \phi(\theta)}{d\theta^2} = - \frac{C_{eq}(\varepsilon_0, \theta)}{\theta}, \quad (11)$$

up to an arbitrary linear function of  $\theta$ , which can be established once the free energy and the entropy at a given state, respectively  $\psi_{eq}(\varepsilon_0, \theta_0)$  and  $\eta_{eq}(\varepsilon_0, \theta_0)$  are given.

Moreover, according to assumption **S1**) the free energy  $\psi_{eq}(\varepsilon, \theta)$  and the entropy  $\eta_{eq}(\varepsilon, \theta)$  are at least of  $C^1$  class and the specific heat  $C_{eq}(\varepsilon, \theta)$  is at least of  $C^0$  class on the domain of definition. If the weaker assumption **S2**) is fulfilled one shows that the free energy is of class  $C^1$ , the entropy as well as the internal energy are of class  $C^0$ , while the specific heat is a discontinuous function on its domain of definition.

We recall the following energy identity for smooth fields (**first law of thermodynamics**)

$$\rho \frac{\partial e_{eq}(\varepsilon, \theta)}{\partial t} = \sigma_{eq}(\varepsilon, \theta) \frac{\partial \varepsilon}{\partial t} - \theta \frac{\partial \sigma_{eq}}{\partial \theta} \frac{\partial \varepsilon}{\partial t} + \rho C_{eq} \frac{\partial \theta}{\partial t}, \quad (12)$$

where the first right-term with minus sign is the *rate of work*, while the second and the third right-term describe the contribution of the *latent heat* and *specific heat*, respectively, to the *rate of heat* of the thermoelastic material.

Often are employed the strain  $\varepsilon$  and the entropy  $\eta$ , rather than  $\varepsilon$  and the temperature  $\theta$ , as independent variables. This is possible because the specific heat at constant strain  $C_{eq}(\varepsilon, \theta)$  is always strictly positive and, according to (10),  $\eta_{eq}(\varepsilon, \theta)$  must be a strictly increasing function of  $\theta$  for each fixed  $\varepsilon$ . It follows that the equation (9)<sub>2</sub> can be solved for  $\theta$  in a unique manner as  $\theta = \tilde{\theta}(\varepsilon, \eta)$ . The internal energy is then defined by  $e = \tilde{e}(\varepsilon, \eta) = e_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))$  and the stress by  $\sigma = \tilde{\sigma}(\varepsilon, \eta) = \sigma_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))$ . Moreover, in this case the internal energy is a thermodynamic potential for the stress and temperature, i.e.  $\sigma = \tilde{\sigma}(\varepsilon, \eta) = \rho \frac{\tilde{e}(\varepsilon, \eta)}{\partial \varepsilon}$  and  $\theta = \tilde{\theta}(\varepsilon, \eta) = \frac{\tilde{e}(\varepsilon, \eta)}{\partial \eta}$ . The specific heat at constant strain is then given by  $\tilde{C}(\varepsilon, \eta) = \tilde{\theta}(\varepsilon, \eta) \left( \frac{\partial \tilde{\theta}(\varepsilon, \eta)}{\partial \eta} \right)^{-1}$ . Let us note that by using the chain rule we get

$$\frac{\partial \tilde{\sigma}(\varepsilon, \eta)}{\partial \varepsilon} = \frac{\partial \sigma_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))}{\partial \varepsilon} + \frac{\tilde{\theta}(\varepsilon, \eta)}{\rho C_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))} \left( \frac{\partial \sigma_{eq}(\varepsilon, \tilde{\theta}(\varepsilon, \eta))}{\partial \theta} \right)^2. \quad (13)$$

Since we will use as independent variables the strain  $\varepsilon$  and the temperature  $\theta$  it is useful to recall here the equation of an *isentrope*. By differentiating relation  $\eta_{eq}(\varepsilon, \theta) = \eta^* = \text{const.}$  and by using relations (8) we get that an isentrope in the  $\varepsilon - \theta$  plane is a solution  $\theta = \theta_I(\varepsilon)$  of the differential equation

$$\frac{d\theta}{d\varepsilon} = \frac{\theta}{\rho C_{eq}(\varepsilon, \theta)} \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta}. \quad (14)$$

Let us note that if  $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} < 0$  the temperature *decreases* along the isentrope, while if  $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} > 0$  the temperature *increases* along the isentrope.

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

$$\Gamma = \Gamma(\varepsilon, \theta) = - \frac{1 + \varepsilon}{\rho C_{eq}(\varepsilon, \theta)} \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta}, \quad (15)$$



and characterizes the temperature changes along an isentrope. Indeed, according to (14) we have  $\frac{d\theta}{\theta} = -\Gamma(\varepsilon, \theta) \frac{d\varepsilon}{1+\varepsilon}$ , i.e it is the negative slope of the isentrope in the  $\log \theta - \log(1 + \varepsilon)$  plane.

The coefficient of thermal expansion at constant stress is defined as

$$\alpha(\varepsilon, \theta) = -\left(\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta}\right) \left(\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon}\right)^{-1}. \quad (16)$$

and characterizes the temperature changes along an isobar ( $\sigma = \text{const.}$ ) in the  $\varepsilon - \theta$  plane.

Usually  $\Gamma$  and  $\alpha$  are positive for most metals although there are known exceptions. Let us note that according to our assumption **H3**,  $\Gamma$  changes its sign across the curve  $\varepsilon = \varepsilon_t(\theta)$  (Fig. 2). Moreover,  $\alpha$  changes also its sign in the  $\varepsilon - \theta$  plane. Such behavior, when the thermal expansion coefficient is negative during martensitic - austenitic transformation has been reported by Uchil et al [37] in near-equiatomic, cold-worked Nitinol exhibiting shape memory effect.

### 3.3 Stability conditions. Constitutive domains of stable/unstable phases.

According to the Gibbsian thermostatics (Coleman and Noll [38]), a necessary condition for a point  $(\varepsilon, \eta)$  to be *thermodynamically stable* is that  $\tilde{e}(\varepsilon^*, \eta^*) - \tilde{e}(\varepsilon, \eta) - \frac{\partial \tilde{e}(\varepsilon, \eta)}{\partial \varepsilon}(\varepsilon^* - \varepsilon) - \frac{\partial \tilde{e}(\varepsilon, \eta)}{\partial \eta}(\eta^* - \eta) \geq 0$ , for any  $(\varepsilon^*, \eta^*)$  in the domain of  $\tilde{e}(\cdot, \cdot)$ . One shows that conditions  $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon} \geq 0$  and  $C_{eq}(\varepsilon, \theta) = -\theta \frac{\partial^2 \psi_{eq}(\varepsilon, \theta)}{\partial \theta^2} > 0$  are necessary and sufficient to ensure the Gibbsian thermostatic stability.

A natural physical condition to be imposed on the constitutive functions is to require the existence of real and finite sound speeds (acceleration waves) in the adiabatic case. We call it *dynamic stability condition* since it ensures the stability of the solutions of the equations of motion. One shows that it is a weaker condition on  $\sigma_{eq}(\varepsilon, \theta)$  than the *thermodynamic stability condition*.

The system of equations (1) describing the motion of an isolated ( $r = 0$ ) thermoelastic bar (4) in the absence of conductivity ( $\kappa = 0$ ) is called the *adiabatic thermoelastic system*, and can be written as

$$\frac{\partial}{\partial t} \begin{pmatrix} v \\ \varepsilon \\ \theta \end{pmatrix} - \begin{pmatrix} 0 & \frac{1}{\rho} \frac{\partial \sigma_{eq}}{\partial \varepsilon} & \frac{1}{\rho} \frac{\partial \sigma_{eq}}{\partial \theta} \\ 1 & 0 & 0 \\ \frac{\theta}{\rho C_{eq}} \frac{\partial \sigma_{eq}}{\partial \theta} & 0 & 0 \end{pmatrix} \frac{\partial}{\partial X} \begin{pmatrix} v \\ \varepsilon \\ \theta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \quad (17)$$

This system is appropriate for the description of wave propagation since the heat conductivity can be ignored outside the narrow transition zones. The type of system is given by the eigenvalues and the right eigenvectors of the above matrix. The eigenvalues are solution of the equation  $\lambda [\lambda^2 - (\frac{1}{\rho} \frac{\partial \sigma_{eq}}{\partial \varepsilon} + \frac{\theta}{\rho^2 C_{eq}} (\frac{\partial \sigma_{eq}}{\partial \theta})^2)] = 0$ . This system is strictly hyperbolic if the three eigenvalues are real and distinct, and the corresponding right eigenvectors are linearly independent. One shows that this happens if and only if

$$\lambda^2(\varepsilon, \theta) \equiv \frac{1}{\rho} \frac{\partial \sigma_{eq}}{\partial \varepsilon} + \frac{\theta}{\rho^2 C_{eq}} \left(\frac{\partial \sigma_{eq}}{\partial \theta}\right)^2 > 0. \quad (18)$$

In this case the non-zero characteristic direction  $\lambda(\varepsilon, \theta)$  is called the *sound speed* at the state  $(\varepsilon, \theta)$ .

It is obvious that the hyperbolicity condition (18) is fulfilled for any pair  $(\varepsilon, \theta)$  such that  $\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon} \geq 0$ , i.e. for  $\varepsilon \in (\infty, \varepsilon_m^-(\theta)) \cup (\varepsilon_M^-(\theta), \varepsilon_M^+(\theta)) \cup (\varepsilon_m^+(\theta), \infty)$ . When the slope of the isotherm  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  becomes negative the system may change type becoming an elliptic one. Therefore, we consider an additional assumption which allows to define the constitutive domain of phases.

**H4** Let us suppose that at each temperature  $\theta \in [\theta_m, \theta_M]$  there exists at least a value  $\varepsilon^* \in (\varepsilon_m^-(\theta), \varepsilon_M^-(\theta))$  and at least a value  $\varepsilon^* \in (\varepsilon_M^+(\theta), \varepsilon_m^+(\theta))$  such that  $\lambda^2(\varepsilon^*, \theta) < 0$ , i.e. the hyperbolicity condition is violated. Then one proves there exists  $\varepsilon = \gamma_M^\pm(\theta)$  and  $\varepsilon = \gamma_m^\pm(\theta)$  (Fig. 2) such that

$$\varepsilon_m^-(\theta) < \gamma_m^-(\theta) < \gamma_M^-(\theta) < \varepsilon_M^-(\theta) < \varepsilon_M^+(\theta) < \gamma_M^+(\theta) < \gamma_m^+(\theta) < \varepsilon_m^+(\theta) \quad (19)$$

with the property that

$$\begin{aligned}\lambda^2(\varepsilon, \theta) &> 0 \text{ for } \varepsilon \in (\infty, \gamma_m^-(\theta)) \cup (\gamma_M^-(\theta), \gamma_M^+(\theta)) \cup (\gamma_m^+(\theta), \infty), \\ \lambda^2(\varepsilon, \theta) &< 0 \text{ for } \varepsilon \in (\gamma_m^-(\theta), \gamma_M^-(\theta)) \cup (\gamma_M^+(\theta), \gamma_m^+(\theta)).\end{aligned}$$

We also suppose that *at each temperature*  $\theta < \theta_m$  there exists at least an  $\varepsilon^* \in (\varepsilon_m^-(\theta), \varepsilon_m^+(\theta))$  such that the hyperbolicity condition is violated. Then one proves there exists  $\varepsilon = \gamma_m^-(\theta)$  and  $\varepsilon = \gamma_m^+(\theta)$  such that

$$\lambda^2(\varepsilon, \theta) > 0 \text{ for } \varepsilon \in (\infty, \gamma_m^-(\theta)) \cup (\gamma_m^+(\theta), \infty), \quad \text{and} \quad \lambda^2(\varepsilon, \theta) < 0 \text{ for } \varepsilon \in (\gamma_m^-(\theta), \gamma_m^+(\theta)).$$

Moreover, we suppose in the following that the boundary curves  $\varepsilon = \gamma_m^\pm(\theta)$ ,  $\varepsilon = \gamma_M^\pm(\theta)$  are *continuously differentiable* and have the following properties:

$$\begin{aligned}\frac{d\gamma_M^+(\theta)}{d\theta} > 0, \quad \frac{d\gamma_M^-(\theta)}{d\theta} < 0, \quad \text{for } \theta \in (\theta_m, \theta_M); \quad \frac{d\gamma_m^+(\theta)}{d\theta} > 0, \quad \frac{d\gamma_m^-(\theta)}{d\theta} < 0, \quad \text{for } \theta < \theta_M \\ \gamma_M^+(\theta_m) = \gamma_M^-(\theta_m), \quad \gamma_m^-(\theta_M) = \gamma_M^-(\theta_M), \quad \gamma_m^+(\theta_M) = \gamma_M^+(\theta_M).\end{aligned} \quad (20)$$

If we denote  $\zeta_M^\pm(\theta) = \sigma_{eq}(\gamma_M^\pm(\theta), \theta)$  and  $\zeta_m^\pm(\theta) = \sigma_{eq}(\gamma_m^\pm(\theta), \theta)$  we remark that  $\zeta_M^+(\theta) < \sigma_M^+(\theta)$ ,  $\zeta_m^+(\theta) > \sigma_m^+(\theta)$ ,  $\zeta_M^-(\theta) > \sigma_M^-(\theta)$ ,  $\zeta_m^-(\theta) < \sigma_m^-(\theta)$  (Fig. 1).

Therefore, the functions  $\varepsilon = \varepsilon_m^\pm(\theta)$  and  $\varepsilon = \varepsilon_M^\pm(\theta)$  associated with the change of monotonicity of the isotherms  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  delimitate the *domains of thermodynamic stability* in the  $\varepsilon - \theta$  plane. On the other side, the constitutive functions  $\varepsilon = \gamma_m^\pm(\theta)$  and  $\varepsilon = \gamma_M^\pm(\theta)$  bound the *regions of hyperbolicity/ellipticity* of the adiabatic thermoelastic system in the same plane, i.e the *domains of dynamic stability* (Fig. 2). Indeed, it is known that if the initial boundary-value data belong to the domains of hyperbolicity of the adiabatic thermoelastic system the problems are well-posed and even more they are stable according to a linearized stability analysis. In the domains of ellipticity the initial-boundary data are ill-posed in the sense of Hadamard. Thus, possible solutions belonging to these regions will be dismissed in a pure thermoelastic approach of phase transitions.

We can identify the *stable phases* of the material, denoted by  $A$  phase and  $M^\pm$  phases, with the domains of hyperbolicity of the adiabatic system, while the so-called *unstable phases*, denoted by  $I^\pm$  phases, with the domains of ellipticity. For instance, in the case  $\theta \in [\theta_m, \theta_M]$ , we say that a particle  $X$  at a time  $t$  is in the austenitic phase  $A$  if the pair  $(\varepsilon, \theta)(X, t) \in A$ , where  $A = \{(\varepsilon, \theta) | \gamma_M^-(\theta) < \varepsilon < \gamma_M^+(\theta)\}$ . The other stable phases in which the material can exist are the martensitic phases  $M^+ = \{(\varepsilon, \theta) | \varepsilon > \gamma_m^+(\theta)\}$  and  $M^- = \{(\varepsilon, \theta) | \varepsilon < \gamma_m^-(\theta)\}$ , while  $I^+ = \{(\varepsilon, \theta) | \gamma_M^+(\theta) < \varepsilon < \gamma_m^+(\theta)\}$ ,  $I^- = \{(\varepsilon, \theta) | \gamma_m^-(\theta) < \varepsilon < \gamma_M^-(\theta)\}$  (Fig. 2).

### 3.4 Jump relations for thermoelastic materials

If  $\dot{S} > 0$  we call the material at the  $+$  side of the discontinuity to be *in front* of the wave, while the material at the  $-$  side to be *in back* of the wave. The wave discontinuity is said to be *compressive* if the deformation decreases after the passage of the wave ( $\varepsilon^- < \varepsilon^+$ ), and *expansive* if the deformation increases ( $\varepsilon^- > \varepsilon^+$ ). If  $\dot{S} < 0$  we have to change only  $+$  to  $-$  and correspondingly the terminology. In the present setting a strain discontinuity is called either a *thermoelastic shock wave*, or a *phase boundary*, according to whether the particles separated by the discontinuity are in the same phase, or in distinct phases. We only consider the adiabatic case when  $q^+ = q^- = 0$ . According to (2) and (3)<sub>2</sub> the relations between the front and back state read

$$v^- - v^+ = -\dot{S}(\varepsilon^- - \varepsilon^+), \quad \sigma_{eq}(\varepsilon^-, \theta^-) - \sigma_{eq}(\varepsilon^+, \theta^+) = \rho \dot{S}^2 (\varepsilon^- - \varepsilon^+), \quad (21)$$

$$\rho(e_{eq}(\varepsilon^-, \theta^-) - e_{eq}(\varepsilon^+, \theta^+)) = \frac{1}{2}(\sigma_{eq}(\varepsilon^-, \theta^-) + \sigma_{eq}(\varepsilon^+, \theta^+))(\varepsilon^- - \varepsilon^+), \quad (22)$$

$$\rho \dot{S}(\eta_{eq}(\varepsilon^-, \theta^-) - \eta_{eq}(\varepsilon^+, \theta^+)) \geq 0. \quad (23)$$

Relation (22) is known as the *Rankine-Hugoniot equation*. Relation (23) asserts that after the passage of a strong discontinuity the entropy of a particle will not decrease.

Let us suppose that the *front state*  $(\varepsilon^+, \theta^+, v^+)$  is known. Then, relations (21)-(22) represent an algebraic non-linear system for the unknown *back state*  $(\varepsilon^-, \theta^-, v^-)$  and the speed of the discontinuity  $\dot{S}$ . Depending on

the thermoelastic constitutive assumptions this system may generally be solved if one of these four quantities is prescribed. In addition, such a solution have to satisfy the entropy inequality (23). Let us note that, the Rankine-Hugoniot equation (22) provides only restrictions, on the back states  $(\varepsilon, \theta)$  which can be reached in a shock process which has  $(\varepsilon^+, \theta^+)$  as a front state. Moreover, this restriction does not depend on the shock speed  $\dot{S}$ . We denote by

$$H(\varepsilon, \theta; \varepsilon^+, \theta^+) = \rho e_{eq}(\varepsilon, \theta) - \rho e^+ - \frac{1}{2}(\sigma_{eq}(\varepsilon, \theta) + \sigma^+)(\varepsilon - \varepsilon^+) \quad (24)$$

the *Hugoniot function based at  $(\varepsilon^+, \theta^+)$*  where  $e^+ = e_{eq}(\varepsilon^+, \theta^+)$  and  $\sigma^+ = \sigma_{eq}(\varepsilon^+, \theta^+)$ . The set  $\{(\varepsilon, \theta) \mid H(\varepsilon, \theta; \varepsilon^+, \theta^+) = 0\}$  is called the *Hugoniot set (locus) based at  $(\varepsilon^+, \theta^+)$*  in the  $\varepsilon - \theta$  plane.

In the smooth case **S1**, the Hugoniot function is at least of  $C^1$  class. If  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  satisfies the weaker smoothness assumption **S2** then it is continuous, piecewise smooth, and

$$\frac{\partial H(\varepsilon, \theta)}{\partial \theta} = \rho C_{eq}(\varepsilon, \theta) - \frac{1}{2} \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} (\varepsilon - \varepsilon^+) > 0, \quad (25)$$

at the points where the derivative makes sense. The positivity is here an assumption justified by the fact that we do not consider shocks of arbitrary intensity, and in general, for real materials  $|\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta}| \ll \rho C_{eq}(\varepsilon, \theta)$ . Situations when the Hugoniot set is not curve-like and can bifurcate has been considered by Dunn and Fosdick [13]. According to (25) the implicit function theorem ensures that the equation  $H(\varepsilon, \theta; \varepsilon^+, \theta^+) = 0$  can be solved (at least locally) with respect to  $\theta$ . We suppose in the following that this unique solution

$$\theta = \Theta_H(\varepsilon; \varepsilon^+, \theta^+), \quad (26)$$

called the *temperature-strain Hugoniot curve (locus) based at  $(\varepsilon^+, \theta^+)$*  exists globally and has the properties that  $\theta^+ = \Theta_H(\varepsilon^+; \varepsilon^+, \theta^+)$  and  $H(\varepsilon, \Theta_H(\varepsilon; \varepsilon^+, \theta^+); \varepsilon^+, \theta^+) = 0$  on its domain of definition. If the smoothness assumption **S1** is satisfied, the function (26) is at least of  $C^1$  class, while if the smoothness assumption **S2** is fulfilled, it is continuous and piece-wise smooth. This function describes all those states in the  $\varepsilon - \theta$  plane that are potentially attainable as back states in a shock process which has  $(\varepsilon^+, \theta^+)$  as a front state.

The image of (26) through the function  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  in the  $\varepsilon - \sigma$  plane is

$$\sigma = \sigma_H(\varepsilon; \varepsilon^+, \theta^+) \stackrel{\text{def}}{=} \sigma_{eq}(\varepsilon, \Theta_H(\varepsilon; \varepsilon^+, \theta^+)), \quad (27)$$

and is called the *stress-strain Hugoniot curve (locus) based at  $(\varepsilon^+, \sigma^+)$* . This function describes all reachable  $(\varepsilon, \sigma)$  back states in a wave discontinuity which has  $(\varepsilon^+, \sigma^+)$  as a front state.

#### 4 A thermal Maxwellian rate-type approach to phase transitions

It is well known that initial-boundary value problems for the adiabatic thermoelastic system (17) can lead to non-unique discontinuous solutions even if the requirement that the entropy has to increase after the passage of the wave discontinuity is satisfied. We therefore need a *selection criterion* to identify meaningful physical solutions. We use in the following a standard procedure to establish such a criterion. This procedure asserts that: a propagating discontinuity, i.e. a thermoelastic shock wave or a phase boundary, is admissible within the thermoelastic theory if and only if the limit values  $(\varepsilon^\pm, \theta^\pm, v^\pm)$  on either side of the discontinuity can be connected by a traveling wave solution constructed within an *augmented theory*.

We introduce in the following an augmented theory whose dissipative mechanisms are described by regularizing terms characterizing stress relaxation and pseudo-creep processes toward equilibrium between phases and by axial heat conduction. Thus we consider in this paper the following Maxwellian rate-type constitutive relation

$$\frac{\partial \sigma}{\partial t} - E \frac{\partial \varepsilon}{\partial t} = -\frac{E}{\mu} (\sigma - \sigma_{eq}(\varepsilon, \theta)), \quad (28)$$

where  $E = \text{const.} > 0$  is called the *dynamic Young modulus*,  $\mu = \text{const.} > 0$  is a "viscosity" coefficient and  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is called the *equilibrium state equation* and satisfies assumptions **H1** - **H4** for the phase transforming thermoelastic material (4). Let us note that  $\tau = \frac{\mu}{E}$  is a *relaxation time*. When  $\mu \rightarrow 0$  (or,  $\tau \rightarrow 0$ ) this constitutive equation is seen as a rate-type approximation of the thermoelastic model.

The strain-rate effects and the stress-rate effects which intervene in the constitutive law (28) allow for describing the way a particle of the material can deviate and return to the thermoelastic equilibrium state equation. Consequently, the transition of a particle from one stable phase to another no longer occurs instantaneously, but it requires a finite phase transition time. The "viscosity" coefficient  $\mu$ , or equivalently the relaxation time  $\tau$ , characterizes how fast a perturbation of an "equilibrium state" decays, or grows in a stable, or unstable phase of the thermoelastic material. It is only for simplicity reasons that we have taken here the "viscosity" coefficient  $\mu$  as constant. This constitutive model has been successfully used to describe quasistatic strain-controlled austenitic-martensitic phase transformation in shape memory alloys in Făciu and Mihăilescu-Suliciu [20] and impact-induced phase transformation for the isothermal case in Făciu and Molinari [36].

The rate-type constitutive equation (28) includes as a limiting case for  $E \rightarrow \infty$  the Kelvin-Voigt model

$$\frac{\partial \varepsilon}{\partial t} = \frac{1}{\mu}(\sigma - \sigma_{eq}(\varepsilon, \theta)), \quad (29)$$

which has been used to describe quasistatic austenitic-martensitic phase transitions by Vainchtein [19] and to study the non-isothermal kinetics of a moving phase boundary by Vainchtein [23].

We assume here that the Fourier law of heat conduction  $q = -\kappa \frac{\partial \theta}{\partial X}$  holds, where  $\kappa = \text{const.} > 0$  is the heat conductivity coefficient.

#### 4.1 Thermodynamic considerations for the augmented theory.

By investigating the compatibility with the Clausius-Duhem inequality (7) of the Maxwellian rate-type material (28) endowed with Fourier heat conduction law one obtains the following results (see also [20]). The constitutive equation (28) admits a unique free energy function  $\psi = \psi_{Mxw}(\varepsilon, \sigma, \theta)$  (modulo an additive function of temperature) if and only if the slope of the straight line connecting any two points of an equilibrium isotherm is bounded from above by the instantaneous Young modulus  $E$ . Moreover, in what follows we suppose there are two positive constants  $E_*$  and  $E^*$  such that

$$-E_* \leq \frac{\sigma_{eq}(\varepsilon_1, \theta) - \sigma_{eq}(\varepsilon_2, \theta)}{\varepsilon_1 - \varepsilon_2} \leq E^* < E, \quad \text{for any } \varepsilon_1, \varepsilon_2 \text{ and any } \theta. \quad (30)$$

The free energy has to satisfy the following Cauchy problem for a first order PDE, i.e.

$$\frac{\partial \psi_{Mxw}}{\partial \varepsilon} + E \frac{\partial \psi_{Mxw}}{\partial \sigma} = \frac{\sigma}{\rho}, \quad \frac{\partial \psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma_{eq}(\varepsilon, \theta), \theta) = 0, \quad (31)$$

while the entropy, the intrinsic dissipation and the thermal dissipation are given, respectively by

$$\eta = -\frac{\partial \psi_{Mxw}}{\partial \theta}(\varepsilon, \sigma, \theta), \quad D_{Mxw} \equiv \frac{E}{\mu} \rho \frac{\partial \psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma, \theta)(\sigma - \sigma_{eq}(\varepsilon, \theta)) \geq 0, \quad D_{th} = \frac{\kappa}{\theta} \left( \frac{\partial \theta}{\partial X} \right)^2 \geq 0. \quad (32)$$

According to (31) the general form of the free energy function is

$$\rho \psi_{Mxw}(\varepsilon, \sigma, \theta) = \frac{\sigma^2}{2E} + \varphi(\sigma - E\varepsilon, \theta), \quad (33)$$

where  $\varphi = \varphi(\tau, \theta)$  satisfies relation

$$\frac{\partial \varphi}{\partial \tau}(\sigma_{eq}(\varepsilon, \theta) - E\varepsilon, \theta) = -\frac{\sigma_{eq}(\varepsilon, \theta)}{E}. \quad (34)$$

Let us denote by  $h(\varepsilon, \theta) = \sigma_{eq}(\varepsilon, \theta) - E\varepsilon$ . Condition (30) ensures that function  $h$  is invertible with respect to  $\varepsilon$  for any fixed  $\theta$ . We denote by  $h^{-1}(\cdot, \theta)$  this function. Therefore, for any triplet  $(\varepsilon, \sigma, \theta)$  there is a unique  $\tilde{\varepsilon} = \tilde{\varepsilon}(\varepsilon, \sigma, \theta) = h^{-1}(\sigma - E\varepsilon, \theta)$  such that

$$\sigma - E\varepsilon = h(\tilde{\varepsilon}, \theta) = \sigma_{eq}(\tilde{\varepsilon}, \theta) - E\tilde{\varepsilon}. \quad (35)$$

Thus, the free energy function of the Maxwellian rate-type constitutive equation (28) is explicitly determined (up to an additive function of  $\theta$ ) by the equilibrium relation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  and the Young modulus  $E$  through relation

$$\rho \psi_{Mxw}(\varepsilon, \sigma, \theta) = \frac{\sigma^2}{2E} - \frac{\sigma_{eq}^2(\tilde{\varepsilon}, \theta)}{2E} + \int_{\varepsilon_0}^{\tilde{\varepsilon}} \sigma_{eq}(s, \theta) ds + \rho \phi(\theta), \quad (36)$$

where  $\phi(\theta)$  is a smooth function. The entropy function is given by

$$\rho \eta_{Mxw}(\varepsilon, \sigma, \theta) = - \int_{\varepsilon_0}^{\tilde{\varepsilon}} \frac{\partial \sigma_{eq}(s, \theta)}{\partial \theta} ds - \rho \frac{d\phi(\theta)}{d\theta}, \quad (37)$$

and the specific heat by

$$C_{Mxw}(\varepsilon, \sigma, \theta) = \theta \frac{\partial \eta_{Mxw}}{\partial \theta} = - \frac{\theta}{\rho} \left( \int_{\varepsilon_0}^{\tilde{\varepsilon}} \frac{\partial^2 \sigma_{eq}(s, \theta)}{\partial \theta^2} ds + \frac{(\frac{\partial \sigma_{eq}(\tilde{\varepsilon}, \theta)}{\partial \theta})^2}{E - \frac{\partial \sigma_{eq}(\tilde{\varepsilon}, \theta)}{\partial \varepsilon}} + \rho \frac{d^2 \phi(\theta)}{d\theta^2} \right). \quad (38)$$

If the equilibrium relation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  satisfies the smoothness assumptions **S1** then the free energy  $\psi_{Mxw}(\varepsilon, \sigma, \theta)$  and the entropy  $\eta_{Mxw}(\varepsilon, \sigma, \theta)$  are at least of  $C^1$  class, while the specific heat  $C_{Mxw}(\varepsilon, \sigma, \theta)$  is at least of  $C^0$  class on the domain of definition. If the smoothness assumption **S2** is satisfied, i.e.  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  is continuous and piecewise smooth, then the free energy  $\psi_{Mxw}(\varepsilon, \sigma, \theta)$  is still of  $C^1$  class, the entropy is of  $C^0$  class and piecewise smooth, while the specific heat  $C_{Mxw}(\varepsilon, \sigma, \theta)$  is a discontinuous and piecewise smooth function.

One can show that the following two relations hold

$$\rho E \frac{\partial \psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma, \theta) = \sigma - \sigma_{eq}(\tilde{\varepsilon}, \theta) = E(\varepsilon - \tilde{\varepsilon}) = E(\varepsilon - h^{-1}(\sigma - E\varepsilon, \theta)), \quad (39)$$

$$\frac{E}{E + E_*} (\sigma - \sigma_{eq}(\varepsilon, \theta))^2 \leq E \rho \frac{\partial \psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma, \theta) (\sigma - \sigma_{eq}(\varepsilon, \theta)) \leq \frac{E}{E - E^*} (\sigma - \sigma_{eq}(\varepsilon, \theta))^2. \quad (40)$$

Thus, from (32)<sub>2</sub> one gets the following estimate on the intrinsic dissipation generated by the Maxwellian rate-type model

$$\frac{E}{\mu(E + E_*)} (\sigma - \sigma_{eq}(\varepsilon, \theta))^2 \leq D_{Mxw} \leq \frac{E}{\mu(E - E^*)} (\sigma - \sigma_{eq}(\varepsilon, \theta))^2. \quad (41)$$

Let us note that the free energy, entropy and internal energy of the Maxwellian model *at equilibrium* are just the free energy, entropy and internal energy of the thermoelastic model  $\sigma = \sigma_{eq}(\varepsilon, \sigma)$ , that is,  $\psi_{Mxw}(\varepsilon, \sigma_{eq}(\varepsilon, \theta), \theta) = \psi_{eq}(\varepsilon, \sigma)$ ,  $\eta_{Mxw}(\varepsilon, \sigma_{eq}(\varepsilon, \theta), \theta) = \eta_{eq}(\varepsilon, \sigma)$  and  $e_{Mxw}(\varepsilon, \sigma_{eq}(\varepsilon, \theta), \theta) = e_{eq}(\varepsilon, \sigma)$ . Indeed, from (35) we get that  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  involves  $\varepsilon = \tilde{\varepsilon}$ , wherefrom by using (36) and (37) we obtain relations (9). Concerning the relation between the specific heat of the Maxwellian model (38) at equilibrium and the specific heat of the thermoelastic model (10) we get by using notation (18)

$$C_{Mxw}(\varepsilon, \sigma_{eq}(\varepsilon, \theta), \theta) = C_{eq}(\varepsilon, \theta) - \frac{\theta}{\rho} \frac{(\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta})^2}{(E - \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon})} = C_{eq}(\varepsilon, \theta) \frac{E - \rho \lambda^2(\varepsilon, \theta)}{E - \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon}}. \quad (42)$$

Therefore, a necessary condition on the constitutive functions  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  and  $E$  to ensure the positiveness of the specific heat of the Maxwellian model is that the sound speed (18) satisfies

$$\rho \lambda^2(\varepsilon, \theta) = \frac{\partial \sigma_{eq}}{\partial \varepsilon} + \frac{\theta}{\rho C_{eq}(\varepsilon, \theta)} \left( \frac{\partial \sigma_{eq}}{\partial \theta} \right)^2 < E. \quad (43)$$

In order to determine the unknown function  $\phi(\theta)$  in (36) we suppose again that the specific heat of the thermoelastic model at a constant strain  $\varepsilon_0$  is known over an interval of temperature, i.e we may use again the equation (11).

By investigating the properties of the thermodynamic functions of the Maxwellian model when  $E \rightarrow \infty$  we obtain

$$\lim_{E \rightarrow \infty} \psi_{Mxw}(\varepsilon, \sigma, \theta) = \psi_{eq}(\varepsilon, \theta), \quad \lim_{E \rightarrow \infty} \eta_{Mxw}(\varepsilon, \sigma, \theta) = \eta_{eq}(\varepsilon, \theta), \quad \lim_{E \rightarrow \infty} C_{Mxw}(\varepsilon, \sigma, \theta) = C_{eq}(\varepsilon, \theta), \quad (44)$$



that means, the free energy, entropy, internal energy and specific heat of the Kelvin-Voigt model coincide with the free energy, entropy, internal energy and specific heat of the thermoelastic model (4).

Consequently, the internal dissipation generated in a smooth process by the Kelvin-Voigt model can be obtained from (41) and (29) as

$$D_{KV} = \lim_{E \rightarrow \infty} D_{Mxw} = \frac{1}{\mu} (\sigma - \sigma_{eq}(\varepsilon, \theta))^2 = \mu \frac{\partial \varepsilon^2}{\partial t}. \quad (45)$$

By using the balance laws (1), the constitutive equations (28) and relations (31)-(32) we can establish the following energy identities. For the Maxwellian rate-type material with Fourier heat conduction law the smooth solutions of the corresponding PDEqs system satisfy relations

$$\rho \frac{\partial e_{Mxw}(\varepsilon, \sigma, \theta)}{\partial t} = \sigma \frac{\partial \varepsilon}{\partial t} - \frac{E}{\mu} \rho \frac{\partial \psi_{Mxw}}{\partial \sigma} (\sigma - \sigma_{eq}(\varepsilon, \theta)) + \frac{E}{\mu} \rho \theta \frac{\partial^2 \psi_{Mxw}}{\partial \sigma \partial \theta} (\sigma - \sigma_{eq}(\varepsilon, \theta)) + \rho c_{Mxw} \frac{\partial \theta}{\partial t}, \quad (46)$$

$$\rho \frac{\partial \eta_{Mxw}(\varepsilon, \sigma, \theta)}{\partial t} + \frac{\partial}{\partial X} \left( \frac{q}{\theta} \right) = \frac{1}{\theta} (D_{Mxw} + D_{th}) \equiv P_{Mxw} \geq 0. \quad (47)$$

Let us note that in relation (46) the first right term with minus sign is the *rate of work*, while the second, the third, and the fourth right-terms represent the contribution to the *rate of heat* of the *internal dissipation*, of the *latent heat* and of the *specific heat*, respectively. Since, according to (37) we have

$$\rho \frac{\partial^2 \psi_{Mxw}}{\partial \sigma \partial \theta} (\varepsilon, \sigma, \theta) = - \frac{\partial \sigma_{eq}}{\partial \theta} (\tilde{\varepsilon}, \theta) \left( E - \frac{\partial \sigma_{eq}}{\partial \varepsilon} (\tilde{\varepsilon}, \theta) \right)^{-1}, \quad (48)$$

where  $\tilde{\varepsilon}$  is given by equation (35) it follows, as usually, that the latent heat released or absorbed by the rate-type material depends mainly on the variation of the equilibrium stress with respect to the temperature.

We also note that the right-hand term in (47) denoted by  $P_{Mxw}$  represents the *total entropy production* corresponding to a heat conducting smooth process of a Maxwellian material.

The system of equations (1) and (28), with  $e = e_{Mxw}(\varepsilon, \sigma, \theta)$ , describing the adiabatic motion ( $q = 0$ ) of an isolated ( $r = 0$ ) Maxwellian rate-type bar can be written as a *relaxation system* with stiff sources

$$\frac{\partial}{\partial t} \begin{pmatrix} v \\ \varepsilon \\ \theta \\ \sigma \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 1/\rho \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ E & 0 & 0 & 0 \end{pmatrix} \frac{\partial}{\partial X} \begin{pmatrix} v \\ \varepsilon \\ \theta \\ \sigma \end{pmatrix} = \frac{E}{\mu} (\sigma - \sigma_{eq}(\varepsilon, \theta)) \begin{pmatrix} 0 \\ 0 \\ \frac{1}{c_{Mxw}} \left( \frac{\partial \psi_{Mxw}}{\partial \sigma} - \theta \frac{\partial^2 \psi_{Mxw}}{\partial \sigma \partial \theta} \right) \\ -1 \end{pmatrix}. \quad (49)$$

This system is always hyperbolic semi-linear irrespective of the slope with respect to  $\varepsilon$  of the equilibrium curve  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  as long as the dynamic Young's modulus  $E$  is strictly positive and finite. Indeed, this system is semi-linear since all non-linear terms are included in the right part of (49) and the eigenvalues of the matrix are given by  $\lambda = \pm \sqrt{E/\rho}$  and  $\lambda = 0$  (twice). Therefore, initial-boundary value problems are now well-posed even in the unstable domains  $I^\pm$  where phase transformations occur. One expects that when  $\mu \rightarrow 0$  solutions of the rate-type system (49) "approach" solutions of the adiabatic thermoelastic system (17) in the sense that the stress  $\sigma$  is rapidly driven back to the equilibrium  $\sigma_{eq}(\varepsilon, \theta)$ , except perhaps in narrow phase transition time intervals where  $\sigma$ ,  $\varepsilon$ ,  $\theta$  and  $v$  have a very steep variation.

Let us note that while the information for the adiabatic thermo-viscoelastic system propagates with the characteristic speeds  $\pm \sqrt{E/\rho}$ , for the "approximated" adiabatic thermo-elastic system it propagates with the characteristic speeds  $\pm \lambda(\varepsilon, \theta)$  given by (18). Usually, for systems with relaxation one requires a priori that the characteristic speed of the reduced system cannot exceed the characteristic speed of the system with relaxation, i.e. condition (43) in our case. This condition is called *sub-characteristic condition* and was introduced by Liu in [39] for relaxation systems. For the Maxwellian thermo-viscoelastic system (49) the sub-characteristic condition appears naturally when studying the restrictions imposed by the second law of thermodynamics on the rate-type constitutive equation. In fact this is a necessary condition for the existence of a positive specific heat for the Maxwellian thermo-viscoelastic model and it implies condition (30) which ensures the existence of a free energy function.

The adiabatic Kelvin-Voigt rate-type system (1) and (29), where  $e = e_{eq}(\varepsilon, \theta)$ , can be viewed as a limiting case of the Maxwellian rate-type system for  $E \rightarrow \infty$ . In this case the characteristic directions of the hyperbolic system in the  $X - t$  plane tend to infinite, i.e. the hyperbolic system (49) transforms into a parabolic one.

## 5 Traveling wave solutions.

We seek steady wave solutions for the system of six equations composed by the balance laws (1), the Maxwellian rate-type constitutive equation (28), the corresponding internal energy law  $e = e_{Mxw}(\varepsilon, \sigma, \theta)$  and the Fourier law which satisfy the entropy inequality (3)<sub>1</sub> for  $r = 0$ . These solutions, sought in the form  $(\varepsilon, \sigma, \theta, v, q, e, \eta) = (\hat{\varepsilon}, \hat{\sigma}, \hat{\theta}, \hat{v}, \hat{q}, \hat{e}, \hat{\eta})(\xi)$ , where  $\xi = X - \hat{S}t$ ,  $\hat{S} = \text{const.}$  have to satisfy the boundary conditions

$$\lim_{\xi \rightarrow \pm\infty} (\hat{\varepsilon}, \hat{\sigma}, \hat{\theta}, \hat{v}, \hat{q}, \hat{e}, \hat{\eta})(\xi) = (\varepsilon^\pm, \sigma^\pm = \sigma_{eq}(\varepsilon^\pm, \theta^\pm), \theta^\pm, v^\pm, 0, e^\pm = e_{eq}(\varepsilon^\pm, \theta^\pm), \eta^\pm = \eta_{eq}(\varepsilon^\pm, \theta^\pm)), \quad (50)$$

where  $\varepsilon^\pm, v^\pm, \theta^\pm, \varepsilon^-, v^-, \theta^-$  are given values.

In general, such traveling wave solutions of the rate-type systems represent a profile layer which connects two thermomechanical equilibrium states of the material and approximates a strong discontinuity of the adiabatic thermoelastic system propagating with a constant velocity  $\hat{S}$ .

Let us look first *smooth* steady wave solutions. We denote by prime the derivative with respect to  $\xi$ . Independent of any constitutive assumption we get from balance laws (1) and entropy inequality (3)<sub>1</sub> relations

$$\hat{v}'(\xi) + \hat{S}\hat{\varepsilon}'(\xi) = 0, \quad \hat{\sigma}'(\xi) + \rho\hat{S}\hat{v}'(\xi) = 0, \quad \hat{S}(\rho\hat{e}'(\xi) - \hat{\sigma}(\xi)\hat{\varepsilon}'(\xi)) = \hat{q}'(\xi), \quad \rho\hat{S}\hat{\eta}' \leq \left(\frac{q}{\theta}\right)', \quad (51)$$

wherefrom, by using the boundary conditions (50) one gets

$$\begin{aligned} \hat{v}(\xi) &= v^+ - \hat{S}(\hat{\varepsilon}(\xi) - \varepsilon^+), \quad \hat{\sigma}(\xi) = \sigma_R(\hat{\varepsilon}(\xi)) \stackrel{\text{def}}{=} \sigma^+ + \rho\hat{S}^2(\hat{\varepsilon}(\xi) - \varepsilon^+), \\ \hat{q}(\xi) &= \hat{S}(\rho\hat{e}(\xi) - \rho e^+ - \frac{1}{2}(\hat{\varepsilon}(\xi) - \varepsilon^+)(\hat{\sigma}(\xi) + \sigma^+)), \quad \hat{q}(\xi) \leq \rho\hat{S}\hat{\theta}(\xi)(\hat{\eta}(\xi) - \eta^+). \end{aligned} \quad (52)$$

If we set  $\xi \rightarrow -\infty$  we recover the Rankine-Hugoniot relations (21)-(22) and the entropy jump inequality (23) for the adiabatic thermoelastic system. Therefore, if  $\hat{S} > 0$  and  $(\varepsilon^+, \theta^+)$  is a given front state of a wave discontinuity then the pair  $(\varepsilon^-, \theta^-)$  has to belong to the Hugoniot set based at  $(\varepsilon^+, \theta^+)$  given by (24), i.e.  $H(\varepsilon^-, \theta^-; \varepsilon^+, \theta^+) = 0$  or equivalently  $\theta^- = \Theta_H(\varepsilon^-; \varepsilon^+, \theta^+)$ . If  $\hat{S} < 0$  and  $(\varepsilon^-, \theta^-)$  is a given front state of a wave discontinuity then the pair  $(\varepsilon^+, \theta^+)$  has to belong to the Hugoniot set based at  $(\varepsilon^-, \theta^-)$ , i.e.  $H(\varepsilon^+, \theta^+; \varepsilon^-, \theta^-) = 0$  or equivalently  $\theta^+ = \Theta_H(\varepsilon^+; \varepsilon^-, \theta^-)$ . Moreover, the constant steady wave speed  $\hat{S}$  is determined by the equilibrium states to be connected through relation

$$\rho\hat{S}^2 = \frac{\sigma_{eq}(\varepsilon^+, \theta^+) - \sigma_{eq}(\varepsilon^-, \theta^-)}{\varepsilon^+ - \varepsilon^-} < E. \quad (53)$$

Let us note that relation (52)<sub>2</sub> asserts that in a steady structured wave the strain-stress pairs  $(\hat{\varepsilon}(\xi), \hat{\sigma}(\xi))$  belong to a straight line of slope  $\rho\hat{S}^2$  in the  $\varepsilon - \sigma$  plane. This is called the *Rayleigh line construction*. Therefore, the function  $\sigma = \sigma_R(\varepsilon)$  defined above is called the *Rayleigh line*.

By using the Maxwellian rate-type constitutive equation (28) and the Fourier law we get that  $\varepsilon = \hat{\varepsilon}(\xi)$  and  $\theta = \hat{\theta}(\xi)$  have to satisfy the non-linear autonomous system with boundary conditions

$$\begin{aligned} \hat{\varepsilon}' &= -\frac{E}{\mu\hat{S}(E - \rho\hat{S}^2)}R(\hat{\varepsilon}, \hat{\theta}), & \lim_{\xi \rightarrow \pm\infty} \hat{\varepsilon}(\xi) &= \varepsilon^\pm \\ \hat{\theta}' &= -\frac{\hat{S}}{K}H_{Mxw}(\hat{\varepsilon}, \hat{\theta}), & \lim_{\xi \rightarrow \pm\infty} \hat{\theta}(\xi) &= \theta^\pm, \end{aligned} \quad (54)$$

where, if  $\hat{S} > 0$ ,

$$R(\varepsilon, \theta; \varepsilon^+, \theta^+, \varepsilon^-) \equiv \sigma_R(\varepsilon) - \sigma_{eq}(\varepsilon, \theta) = \sigma^+ + \rho\hat{S}^2(\varepsilon - \varepsilon^+) - \sigma_{eq}(\varepsilon, \theta), \quad (55)$$

$$H_{Mxw}(\varepsilon, \theta; \varepsilon^+, \theta^+, \varepsilon^-) \equiv \rho e_{Mxw}(\varepsilon, \sigma_R(\varepsilon), \theta) - \rho e^+ - \frac{1}{2}(\varepsilon - \varepsilon^+)(\sigma_R(\varepsilon) + \sigma^+). \quad (56)$$

and  $(\varepsilon^+, \theta^+)$  represents the front state, while  $(\varepsilon^-, \theta^-)$  is the Hugoniot state, i.e.  $\theta^- = \Theta_H(\varepsilon^-; \varepsilon^+, \theta^+)$ .

If  $\hat{S} < 0$ , the initial front state is  $(\varepsilon^-, \theta^-)$  and  $(\varepsilon^+, \theta^+)$  is the Hugoniot state, i.e.  $\theta^+ = \Theta_H(\varepsilon^+; \varepsilon^-, \theta^-)$ , then the superscripts + and - have to be inverted in (56). For simplicity, when there are no ambiguities we will drop from the notations of  $R$  and  $H_{Mxw}$  their dependence on  $(\varepsilon^+, \theta^+)$ , and  $(\varepsilon^-, \theta^-)$ .

We note that the pairs  $(\varepsilon^\pm, \theta^\pm)$  are fixed points for the dynamical systems (54). Indeed, according to (53) we have  $R(\varepsilon^\pm, \theta^\pm) = 0$ . On the other side, since  $e_{Mxw}(\varepsilon^\pm, \sigma_{eq}(\varepsilon^\pm, \theta^\pm), \theta^\pm) = e_{eq}(\varepsilon^\pm, \theta^\pm)$  it follows  $H_{Mxw}(\varepsilon^\pm, \theta^\pm) = H(\varepsilon^\pm, \theta^\pm) = 0$ . In the  $\varepsilon - \sigma$  plane that means the pairs  $(\varepsilon^\pm, \sigma^\pm)$  represent the intersection of the Hugoniot locus (27) with the Rayleigh line.

*Remark 1* For future use it is important to note that function  $H_{M_{xw}}(\varepsilon, \theta; \varepsilon^+, \theta^+, \varepsilon^-)$  is related to the Hugoniot function  $H(\varepsilon, \theta; \varepsilon^+, \theta^+)$  through relation

$$H_{M_{xw}}(\varepsilon, \theta) = H(\varepsilon, \theta) + \rho e_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \theta) - \rho e_{eq}(\varepsilon, \theta) - \frac{1}{2}(\varepsilon - \varepsilon^+)R(\varepsilon, \theta). \quad (57)$$

*Remark 2* According to relation (44) we can obtain the autonomous system describing the traveling wave solutions for the Kelvin-Voigt model (29) with Fourier heat conduction law by making  $E \rightarrow \infty$  in the system (54). Moreover, from the results obtained below concerning traveling wave solutions for the Maxwellian rate-type model we can derive by the same limiting process the characterization of the traveling wave solutions for the Kelvin-Voigt model.

The question to be answered in the following concerns the conditions which ensure the existence and uniqueness of traveling wave solutions for the system (54). These conditions also provide a *selection criterion* for admissible discontinuous solutions of the adiabatic thermoelastic system (17).

## 5.1 Structuring mechanism: only Maxwellian rate-type effects without heat conduction

### 5.1.1 Admissibility condition: chord criterion with respect to the Hugoniot locus in the strain-stress plane

We say that an elastic shock wave or a phase boundary is an *admissible* weak solution for the adiabatic thermoelastic system if there exists a unique traveling wave  $(\varepsilon(\xi), \theta(\xi), v(\xi))$  provided by the augmented constitutive approach which connects the limit values  $(\varepsilon^\pm, \theta^\pm, v^\pm)$ . We say that the traveling wave describes a *shock layer* if  $(\varepsilon^\pm, \theta^\pm)$  are in the same phase, or an *interphase transition layer* if  $(\varepsilon^\pm, \theta^\pm)$  are in different phases. We designate them in a generic way as a *profile layer*.

In order to clarify our result we briefly *recall* the case of *isothermal elasticity* with non-monotone stress-strain relation. In this case the PDEs system is composed by equations (1)<sub>1-2</sub> and an *isothermal* equilibrium curve  $\sigma = \sigma_{eq}(\varepsilon)$ . We have shown in Făciu and Molinari [36, Part II] that by considering the Maxwellian rate-type approach as an augmented theory for the non-monotone elastic model we obtain the same viscosity admissibility criterion as that obtained by Pego [40] using Kelvin-Voigt isothermal viscoelastic constitutive equation (see also Slemrod [4]). According to the traveling wave analysis for the rate-type system one has shown that the *Maxwellian admissibility criterion* in the isothermal case is equivalent with a *chord criterion with respect to the elastic constitutive equation*  $\sigma = \sigma_{eq}(\varepsilon)$  which claims that: a *compressive wave discontinuity*, i.e.  $(\varepsilon^+ - \varepsilon^-)\dot{S} > 0$ , is admissible if and only if the chord which joins  $(\varepsilon^+, \sigma^+ = \sigma_{eq}(\varepsilon^+))$  to  $(\varepsilon^-, \sigma^- = \sigma_{eq}(\varepsilon^-))$  lies *below* the graph of the function  $\sigma = \sigma_{eq}(\varepsilon)$  for  $\varepsilon$  between  $\varepsilon^+$  and  $\varepsilon^-$ , while an *expansive wave discontinuity*, i.e.  $(\varepsilon^+ - \varepsilon^-)\dot{S} < 0$ , is admissible if and only if the chord lies *above* the graph in the same interval.

When we consider the *non-isothermal case* we extend this result and we derive as admissibility condition for shock waves and phase boundaries of the thermoelastic adiabatic system a *chord criterion with respect to the Hugoniot locus in the strain-stress plane*  $\sigma = \sigma_H(\varepsilon; \varepsilon^+, \theta^+)$  defined by (27).

**Proposition 1** *Let us suppose that the thermoelastic constitutive equation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  satisfies the general assumptions **H1-H4**, which includes the case of negative Grüneisen coefficients. If  $(\varepsilon^\pm, \theta^\pm)$  are the strain and temperature states across a propagating discontinuity such that at least one of the sound speed (18) at these states is different from the discontinuity speed  $\dot{S}$ , i.e.  $\lambda(\varepsilon^+, \theta^+) \neq \dot{S}$ , or  $\lambda(\varepsilon^-, \theta^-) \neq \dot{S}$ , then the admissibility criterion generated by the Maxwellian rate-type approach (28) when heat conduction is neglected is equivalent with the following selection criterion:*

*Chord criterion with respect to the Hugoniot locus in the strain-stress plane.*

If  $\dot{S} > 0$ , the front state is  $(\varepsilon^+, \theta^+)$  and the Hugoniot back state is  $(\varepsilon^-, \theta^-)$  then a *compressive wave discontinuity* is admissible if and only if the Rayleigh line lies *below* the Hugoniot locus, i.e.

$$\sigma_R(\varepsilon) = \sigma^+ + \rho \dot{S}^2(\varepsilon - \varepsilon^+) < \sigma_H(\varepsilon; \varepsilon^+, \theta^+), \text{ for any } \varepsilon \in (\varepsilon^-, \varepsilon^+), \quad (58)$$

and an *expansive wave discontinuity* is admissible if and only if the Rayleigh line lies *above* the Hugoniot locus, i.e.

$$\sigma_R(\varepsilon) = \sigma^+ + \rho \dot{S}^2(\varepsilon - \varepsilon^+) > \sigma_H(\varepsilon; \varepsilon^+, \theta^+), \text{ for any } \varepsilon \in (\varepsilon^+, \varepsilon^-). \quad (59)$$

If  $\dot{S} < 0$ , the front state is  $(\varepsilon^-, \theta^-)$  and the Hugoniot back state is  $(\varepsilon^+, \theta^+)$  then the above statement remains valid if we invert superscripts + with - in relations (58) and (59).

This result is related with the extended entropy condition for gas dynamic equations of Liu [3] (see also Pego [6]). We have to prove in the following that conditions (58)-(59) are necessary and sufficient for the existence of a unique profile layer connecting the limit values  $(\varepsilon^\pm, \theta^\pm)$ .

### 5.1.2 Traveling waves for the Maxwellian rate-type model (28) without heat conduction.

The only structuring parameters of these layers are the "viscosity"  $\mu$  and the dynamic Young's modulus  $E$ . Such traveling waves are solutions of the problem

$$\begin{aligned} \hat{\varepsilon}' &= -\frac{E}{\mu\dot{S}(E - \rho\dot{S}^2)}R(\hat{\varepsilon}, \hat{\theta}), \quad \lim_{\xi \rightarrow \pm\infty} \hat{\varepsilon}(\xi) = \varepsilon^\pm, \\ 0 &= H_{M_{xw}}(\hat{\varepsilon}, \hat{\theta}). \end{aligned} \quad (60)$$

Let us consider  $\dot{S} > 0$  and  $(\varepsilon^+, \theta^+)$  a fixed front state and  $(\varepsilon^-, \theta^-)$  a Hugoniot state, i.e.  $\theta^- = \Theta_H(\varepsilon^-; \varepsilon^+, \theta^+)$ . The strain-temperature pair  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi))$  has to satisfy the algebraic equation (60)<sub>2</sub> where function  $H_{M_{xw}}(\hat{\varepsilon}, \hat{\theta})$  is given by (56). The set  $\{(\varepsilon, \theta) \mid H_{M_{xw}}(\varepsilon, \theta; \varepsilon^+, \theta^+, \varepsilon^-) = 0\}$  describes the trajectory in the  $\varepsilon - \theta$  plane of a traveling wave governed by a Maxwellian rate-type dissipative mechanism in the absence of heat conduction. Let us note that  $H_{M_{xw}}(\varepsilon^\pm, \theta^\pm; \varepsilon^+, \theta^+, \varepsilon^-) = 0$ . The function  $H_{M_{xw}}(\varepsilon, \theta)$  is at least of  $C^1$  class if the smoothness assumption **S1** is satisfied and it is a continuous and piecewise  $C^1$  function on its domain of definition for the weaker assumption **S2**. Since  $\frac{\partial H_{M_{xw}}}{\partial \theta}(\varepsilon, \theta) = \rho \frac{\partial e_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \theta)}{\partial \theta} = \rho C_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \theta) > 0$  at the points where the derivative makes sense, by using the theorem of implicit function it can be shown that the equation  $H_{M_{xw}}(\varepsilon, \theta) = 0$  can be solved at least locally with respect to  $\varepsilon$ . In the following we suppose that it can be solved globally, that means, there exists a unique function

$$\theta = \Theta_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-), \quad (61)$$

with the property that  $H_{M_{xw}}(\varepsilon, \Theta_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)) = 0$  for  $\varepsilon$  belonging to an interval which contains  $\varepsilon^\pm$  and  $\Theta_{M_{xw}}(\varepsilon^\pm; \varepsilon^+, \theta^+, \varepsilon^-) = \theta^\pm$ . This function is at least of  $C^1$  class if assumption **S1** is satisfied and it is continuous and piecewise  $C^1$  for the weaker assumption **S2**. Its image through the function  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  in the  $\varepsilon - \sigma$  plane is given by

$$\sigma = \sigma_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-) \stackrel{\text{def}}{=} \sigma_{eq}(\varepsilon, \Theta_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)), \quad (62)$$

and connects the states  $(\varepsilon^\pm, \sigma^\pm)$ . It is useful to note that  $\sigma^\pm = \sigma_{M_{xw}}(\varepsilon^\pm) = \sigma_H(\varepsilon^\pm) = \sigma_{eq}(\varepsilon^\pm, \theta^\pm)$ .

By using the above notations we get from (60) that  $\varepsilon = \hat{\varepsilon}(\xi)$  has to be solution of the problem

$$\hat{\varepsilon}' = -\frac{E}{\mu\dot{S}(E - \rho\dot{S}^2)}(\sigma^+ + \rho\dot{S}^2(\hat{\varepsilon} - \varepsilon^+) - \sigma_{M_{xw}}(\hat{\varepsilon}; \varepsilon^+, \theta^+, \theta^-)), \quad \lim_{\xi \rightarrow \pm\infty} \hat{\varepsilon}(\xi) = \varepsilon^\pm \quad (63)$$

It is already known from the isothermal case of the Maxwellian rate-type model studied in [36, Part II] that a unique solution of the problem (63) exists if and only if a chord criterion with respect to the curve  $\sigma = \sigma_{M_{xw}}(\varepsilon)$  is fulfilled.

Thus, for a right-facing discontinuity  $\dot{S} > 0$ , in the *compressive* case ( $\varepsilon^- < \varepsilon^+$ ), the Rayleigh line has to lie *below* the curve  $\sigma_{M_{xw}}(\varepsilon)$ , i.e.  $\sigma_R(\varepsilon) = \sigma^+ + \rho\dot{S}^2(\varepsilon - \varepsilon^+) < \sigma_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$ , for any  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , while for the *expansive* case ( $\varepsilon^+ < \varepsilon^-$ ), the Rayleigh line has to lie *above*, i.e.  $\sigma_R(\varepsilon) = \sigma^+ + \rho\dot{S}^2(\varepsilon - \varepsilon^+) > \sigma_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$ , for any  $\varepsilon \in (\varepsilon^+, \varepsilon^-)$ .

For a left-facing wave  $\dot{S} < 0$ , when the front state is  $(\varepsilon^-, \theta^-)$  and the Hugoniot state is  $(\varepsilon^+, \theta^+)$  the admissibility condition is obtained by inverting the superscripts + and - in the above relations.

*Proof of Proposition 1.* Let us consider the *compressive* case of a forward propagating discontinuity, that is  $\dot{S} > 0$  and  $\varepsilon^- < \varepsilon^+$ . In this case the *chord criterion with respect to the curve*  $\sigma = \sigma_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  requires that

$$s(\varepsilon) \stackrel{\text{def}}{=} \sigma_R(\varepsilon) - \sigma_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-) < 0, \quad \text{for any } \varepsilon \in (\varepsilon^-, \varepsilon^+). \quad (64)$$

We first prove that, if the chord condition (64) is satisfied, then the Hugoniot curve  $\sigma = \sigma_H(\varepsilon)$  cannot intersect the Rayleigh line  $\sigma = \sigma_R(\varepsilon)$  for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . The proof is based by reduction to the absurd. Suppose

there is an  $\varepsilon^* \in (\varepsilon^-, \varepsilon^+)$  such that  $\sigma_R(\varepsilon^*) = \sigma_H(\varepsilon^*; \varepsilon^+, \theta^+)$ . We denote by  $\theta^* = \theta_H(\varepsilon^*; \varepsilon^+, \theta^+)$ . Therefore,  $H(\varepsilon^*, \theta^*; \varepsilon^+, \theta^+) = 0$  and  $\sigma_R(\varepsilon^*) = \sigma_H(\varepsilon^*; \varepsilon^+, \theta^+) \equiv \sigma_{eq}(\varepsilon^*, \theta_H(\varepsilon^*; \varepsilon^+, \theta^+)) = \sigma_{eq}(\varepsilon^*, \theta^*)$ . By using (57) and the fact that  $e_{M_{xw}}(\varepsilon, \sigma_{eq}(\varepsilon, \theta), \theta) = e_{eq}(\varepsilon, \theta)$  we get that  $H_{M_{xw}}(\varepsilon^*, \theta^*; \varepsilon^+, \theta^+) = 0$ . Therefore,  $\theta^* = \theta_{M_{xw}}(\varepsilon^*; \varepsilon^+, \theta^+)$ , which implies  $\sigma_{M_{xw}}(\varepsilon^*; \varepsilon^+, \theta^+) \equiv \sigma_{eq}(\varepsilon^*, \theta_{M_{xw}}(\varepsilon^*; \varepsilon^+, \theta^+)) = \sigma_{eq}(\varepsilon^*, \theta^*) = \sigma_R(\varepsilon^*)$ . Thus, it results a contradiction with assumption (64). In a similar way one shows that if the chord condition with respect to the Hugoniot curve (58) is satisfied then the curve  $\sigma = \sigma_{M_{xw}}(\varepsilon)$  can not intersect the Rayleigh line  $\sigma = \sigma_R(\varepsilon)$  for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . The proof is similar for the expansive case and for a back propagating discontinuity  $\dot{S} < 0$ .

To complete the proof we have to show that the curves  $\sigma = \sigma_{M_{xw}}(\varepsilon)$  and  $\sigma = \sigma_H(\varepsilon)$  are always on the same side of the Rayleigh line for  $\varepsilon$  between  $\varepsilon^-$  and  $\varepsilon^+$ .

We first establish some properties of the functions (61) and (62). By using the theorem of implicit functions and the thermodynamic properties established in Section 4.1 for the Maxwellian rate-type model we show that

$$\frac{d\Theta_{M_{xw}}(\varepsilon)}{d\varepsilon} = \frac{(E - \rho\dot{S}^2)}{C_{M_{xw}}} \left( \frac{\partial \Psi_{M_{xw}}}{\partial \sigma} - \Theta_{M_{xw}}(\varepsilon) \frac{\partial^2 \Psi_{M_{xw}}}{\partial \theta \partial \sigma} \right) (\varepsilon, \sigma_R(\varepsilon), \Theta_{M_{xw}}(\varepsilon)), \quad (65)$$

and using relations (39) and (48) we can rewrite (65) as

$$\frac{d\Theta_{M_{xw}}(\varepsilon)}{d\varepsilon} = \frac{(E - \rho\dot{S}^2)}{\rho C_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \Theta_{M_{xw}}(\varepsilon))} \left( \frac{\sigma_R(\varepsilon) - \sigma_{eq}(\cdot, \cdot)}{E} + \Theta_{M_{xw}}(\varepsilon) \frac{\frac{\partial \sigma_{eq}(\cdot, \cdot)}{\partial \theta}}{E - \frac{\partial \sigma_{eq}(\cdot, \cdot)}{\partial \varepsilon}} \right) \Big|_{(\tilde{\varepsilon}, \Theta_{M_{xw}}(\varepsilon))}, \quad (66)$$

where  $\tilde{\varepsilon} = \tilde{\varepsilon}(\varepsilon)$  is the unique solution of equation (35) for  $\sigma = \sigma_R(\varepsilon)$  and  $\theta = \theta_{M_{xw}}(\varepsilon)$ , i.e. it satisfies

$$\sigma_R(\varepsilon) - E\varepsilon = \sigma_{eq}(\tilde{\varepsilon}, \Theta_{M_{xw}}(\varepsilon)) - E\tilde{\varepsilon}. \quad (67)$$

Finally, one shows that at the critical points we have

$$\frac{d\Theta_{M_{xw}}(\varepsilon^\pm)}{d\varepsilon} = \frac{(E - \rho\dot{S}^2)\theta^\pm \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^\pm, \theta^\pm)}{\rho C_{M_{xw}}(\varepsilon^\pm, \sigma^\pm, \theta^\pm) \left( E - \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\varepsilon^\pm, \theta^\pm) \right)}. \quad (68)$$

Since  $\frac{d\sigma_{M_{xw}}(\varepsilon)}{d\varepsilon} = \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\varepsilon, \Theta_{M_{xw}}(\varepsilon)) + \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon, \Theta_{M_{xw}}(\varepsilon)) \frac{d\Theta_{M_{xw}}(\varepsilon)}{d\varepsilon}$ , by using (68) and (42) we get from (64) that

$$s'(\varepsilon^\pm) = \frac{d\sigma_R(\varepsilon^\pm)}{d\varepsilon} - \frac{d\sigma_{M_{xw}}(\varepsilon^\pm)}{d\varepsilon} = \frac{C_{eq}(\varepsilon^\pm, \theta^\pm)}{C_{M_{xw}}(\varepsilon^\pm, \sigma^\pm, \theta^\pm)} \rho (\dot{S}^2 - \lambda^2(\varepsilon^\pm, \theta^\pm)). \quad (69)$$

Because  $s(\varepsilon^\pm) = 0$ , a direct consequence of the condition (64) is  $s'(\varepsilon^-) \leq 0$  and  $s'(\varepsilon^+) \geq 0$ . Thus, by using (69) one obtains that *for the compressive case the chord criterion with respect to  $\sigma = \sigma_{M_{xw}}(\varepsilon)$  requires*

$$\dot{S}^2 - \lambda^2(\varepsilon^-, \theta^-) \leq 0, \quad \text{and} \quad \dot{S}^2 - \lambda^2(\varepsilon^+, \theta^+) \geq 0, \quad \varepsilon^- < \varepsilon^+. \quad (70)$$

That means that the chord criterion with respect to  $\sigma = \sigma_{M_{xw}}(\varepsilon)$  is consistent with the shock inequalities of Lax [33], which for a right-facing wave discontinuity read  $\lambda(\varepsilon^+, \theta^+) < \dot{S} < \lambda(\varepsilon^-, \theta^-)$ . **It is worth noting here that "viscosity-capillarity" augmented models (e.g. Slemrod [5], Ngan and Truskinovsky [7], [21]) can generate admissible nonclassical shock waves or subsonic propagating phase transitions which violate the Lax criterion.**

We also establish some properties of the Hugoniot curves (26) and (27). By using the theorem of implicit functions and the thermodynamic properties established in Section 3.2 for the thermoelastic model one gets

$$\frac{d\Theta_H(\varepsilon)}{d\varepsilon} = \frac{\frac{1}{2}(\sigma^+ - \sigma_H(\varepsilon)) + \frac{1}{2}(\varepsilon - \varepsilon^+) \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\varepsilon, \Theta_H(\varepsilon)) + \Theta_H(\varepsilon) \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon, \Theta_H(\varepsilon))}{\rho C_{eq}(\varepsilon, \Theta_H(\varepsilon)) - \frac{1}{2}(\varepsilon - \varepsilon^+) \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon, \Theta_H(\varepsilon))}, \quad (71)$$



wherefrom, after some computations one derives that

$$\begin{aligned} \frac{d\sigma_R(\varepsilon^+)}{d\varepsilon} - \frac{d\sigma_H(\varepsilon^+)}{d\varepsilon} &= \rho(\dot{S}^2 - \lambda^2(\varepsilon^+, \theta^+)), \\ \frac{d\sigma_R(\varepsilon^-)}{d\varepsilon} - \frac{d\sigma_H(\varepsilon^-)}{d\varepsilon} &= \frac{\rho^2 C_{eq}(\varepsilon^-, \theta^-)(\dot{S}^2 - \lambda^2(\varepsilon^-, \theta^-))}{\rho C_{eq}(\varepsilon^-, \theta^-) - \frac{1}{2}(\varepsilon^- - \varepsilon^+) \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^-, \theta^-)}, \end{aligned} \quad (72)$$

Using (25) one obtains  $\text{sgn}\left(\frac{d\sigma_R(\varepsilon^\pm)}{d\varepsilon} - \frac{d\sigma_{Mxw}(\varepsilon^\pm)}{d\varepsilon}\right) = \text{sgn}\left(\frac{d\sigma_R(\varepsilon^\pm)}{d\varepsilon} - \frac{d\sigma_H(\varepsilon^\pm)}{d\varepsilon}\right)$ . This implies that if the curve  $\sigma = \sigma_{Mxw}(\varepsilon)$  lies, in the interval  $(\varepsilon^-, \varepsilon^+)$ , above (or, below) the Rayleigh line  $\sigma = \sigma_R(\varepsilon)$  at least in a neighborhood of  $\varepsilon^+$ , or  $\varepsilon^-$ , then the Hugoniot curve  $\sigma = \sigma_H(\varepsilon)$  also lies above (or, below) the Rayleigh line in this neighborhood, and vice versa. Thus, both curves have to be on the same side of the Rayleigh line which proves the equivalence between the two chord criteria in the conditions of Proposition 1.

*Remark 3* In the degenerate case when  $\lambda(\varepsilon^\pm, \theta^\pm) = \dot{S}$  the chord criterion with respect to the curve  $\sigma = \sigma_{Mxw}(\varepsilon)$  ensures the existence of a unique "viscous", heat non-conducting profile layer, but we cannot prove from the above considerations that the Hugoniot curve  $\sigma = \sigma_H(\varepsilon)$  and  $\sigma = \sigma_{Mxw}(\varepsilon)$  lies on the same side of the Rayleigh line for  $\varepsilon$  between  $\varepsilon^-$  and  $\varepsilon^+$ .

*Remark 4* The equivalence between the two chord criteria transfers the admissibility condition from a relation which depends on the energetic properties of the rate-type dissipative model, namely  $\sigma = \sigma_{Mxw}(\varepsilon)$ , to a relation which depends only on the energetic properties of the thermoelastic constitutive model, namely  $\sigma = \sigma_H(\varepsilon)$ . That is why the chord criterion with respect to the Hugoniot locus is extremely useful in practice.

*The entropy production in a "viscous", thermally non-conducting profile layer.* Let us denote by  $\hat{\psi}(\varepsilon) \equiv \Psi_{Mxw}(\varepsilon, \sigma_R(\varepsilon), \Theta_{Mxw}(\varepsilon))$ ,  $\hat{\eta}(\varepsilon) \equiv \eta_{Mxw}(\varepsilon, \sigma_R(\varepsilon), \Theta_{Mxw}(\varepsilon))$  and  $\hat{e}(\varepsilon) \equiv e_{Mxw}(\varepsilon, \sigma_R(\varepsilon), \Theta_{Mxw}(\varepsilon))$  the free energy, entropy and internal energy along a "viscous", heat non-conducting profile layer. In these equations  $\varepsilon = \hat{e}(\xi)$  is solution of (63). By using relation (31) we get

$$\sigma_R(\varepsilon) = \rho \frac{d\hat{e}(\varepsilon)}{d\varepsilon} + (E - \rho \dot{S}^2) \rho \frac{\partial \Psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma_R(\varepsilon), \Theta_{Mxw}(\varepsilon)) - \rho \Theta_{Mxw}(\varepsilon) \frac{d\hat{\eta}(\varepsilon)}{d\varepsilon}. \quad (73)$$

Since  $H_{Mxw}(\varepsilon, \Theta_{Mxw}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)) = 0$  for any  $\varepsilon$  between  $\varepsilon^+$  and  $\varepsilon^-$  one obtains from (56) the following identities

$$\rho \hat{e}(\varepsilon) - \rho \varepsilon^+ = \frac{1}{2}(\varepsilon - \varepsilon^+)(\sigma^+ + \sigma_R(\varepsilon)), \quad \text{and} \quad \rho \frac{d\hat{e}(\varepsilon)}{d\varepsilon} = \sigma_R(\varepsilon). \quad (74)$$

From (73) and (74)<sub>2</sub> we derive

$$\rho \frac{d\hat{\eta}(\varepsilon)}{d\varepsilon} = \frac{E - \rho \dot{S}^2}{\Theta_{Mxw}(\varepsilon)} \rho \frac{\partial \Psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma_R(\varepsilon), \Theta_{Mxw}(\varepsilon)), \quad (75)$$

wherefrom, by integration, one obtains

$$\rho(\eta_{eq}(\varepsilon^+, \theta^+) - \eta_{eq}(\varepsilon^-, \theta^-)) = \rho(\hat{\eta}(\varepsilon^+) - \hat{\eta}(\varepsilon^-)) = \int_{\varepsilon^-}^{\varepsilon^+} \frac{E - \rho \dot{S}^2}{\Theta_{Mxw}(\varepsilon)} \rho \frac{\partial \Psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma_R(\varepsilon), \Theta_{Mxw}(\varepsilon)) d\varepsilon. \quad (76)$$

According to relations (32)<sub>2</sub>, (47), (63) and (76) the total entropy production induced by a traveling wave governed by a Maxwellian rate-type constitutive equation in the absence of heat conduction is given by

$$\begin{aligned} P_{Mxw}^{trav} &= \int_{-\infty}^{\infty} \frac{D_{Mxw}(\hat{e}, \hat{\sigma}, \hat{\theta})}{\Theta_{Mxw}(\hat{e})} d\xi = \int_{-\infty}^{\infty} \frac{E}{\mu} \frac{\rho}{\Theta_{Mxw}(\hat{e})} \frac{\partial \Psi_{Mxw}}{\partial \sigma}(\hat{e}, \sigma_R(\hat{e}), \Theta_{Mxw}(\hat{e})) (\sigma_R(\hat{e}) - \sigma_{Mxw}(\hat{e})) d\xi \\ &= -\dot{S} \int_{-\infty}^{\infty} \frac{(E - \rho \dot{S}^2)}{\Theta_{Mxw}(\hat{e})} \rho \frac{\partial \Psi_{Mxw}}{\partial \sigma}(\hat{e}, \sigma_R(\hat{e}), \Theta_{Mxw}(\hat{e})) \hat{e}' d\xi = -\dot{S} \rho (\eta_{eq}(\varepsilon^+, \theta^+) - \eta_{eq}(\varepsilon^-, \theta^-)) \geq 0. \end{aligned} \quad (77)$$

*Remark 5* Therefore, in a "viscous", thermally non-conducting profile layer, the entropy of the Hugoniot back state can not be lower than the entropy of the front state. Moreover, the total entropy production  $P_{Mxw}^{trav}$  of the traveling wave solution does not depend on the "viscosity" and is, according to (23), exactly the entropy production of a strong discontinuity compatible with the second law of thermodynamics for the associated thermoelastic constitutive equation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$ . Thus, a strong discontinuity which satisfies the "chord criterion" is compatible with the second law of thermodynamics

## 5.2 Structuring mechanisms: Maxwellian rate-type effects coupled with heat conduction.

We are now interested to investigate the existence and uniqueness of the solutions of the non-linear autonomous system (54). Following the method proposed by Gilbarg [9] we first analyze the system behavior near its critical points. The linearization of (54) in a neighborhood of  $(\varepsilon^\pm, \theta^\pm)$  leads to the system

$$\frac{d}{d\xi} \begin{pmatrix} \hat{\varepsilon} \\ \hat{\theta} \end{pmatrix} = J_{Mxw}(\varepsilon^\pm, \theta^\pm) \begin{pmatrix} \hat{\varepsilon} \\ \hat{\theta} \end{pmatrix}, \quad (78)$$

where

$$J_{Mxw}(\varepsilon, \theta) = - \begin{pmatrix} \frac{E}{\mu\dot{S}(E-\rho\dot{S}^2)} \frac{\partial R}{\partial \varepsilon} & \frac{E}{\mu\dot{S}(E-\rho\dot{S}^2)} \frac{\partial R}{\partial \theta} \\ \frac{\dot{S}}{\kappa} \frac{\partial H_{Mxw}}{\partial \varepsilon} & \frac{\dot{S}}{\kappa} \frac{\partial H_{Mxw}}{\partial \theta} \end{pmatrix}. \quad (79)$$

One shows that

$$\frac{\partial R}{\partial \varepsilon}(\varepsilon^\pm, \theta^\pm) = \rho\dot{S}^2 - \frac{\partial \sigma_{eq}}{\partial \varepsilon}, \quad \frac{\partial R}{\partial \theta}(\varepsilon^\pm, \theta^\pm) = -\frac{\partial \sigma_{eq}}{\partial \theta}, \quad (80)$$

$$\frac{\partial H_{Mxw}}{\partial \varepsilon}(\varepsilon^\pm, \theta^\pm) = -\theta^\pm \frac{(E-\rho\dot{S}^2) \frac{\partial \sigma_{eq}}{\partial \theta}}{(E-\frac{\partial \sigma_{eq}}{\partial \varepsilon})}, \quad \frac{\partial H_{Mxw}}{\partial \theta}(\varepsilon^\pm, \theta^\pm) = \rho \frac{\partial e_{eq}}{\partial \theta} - \theta^\pm \frac{\left(\frac{\partial \sigma_{eq}}{\partial \theta}\right)^2}{(E-\frac{\partial \sigma_{eq}}{\partial \varepsilon})}. \quad (81)$$

To prove relations (81) we have to use the properties of the free energy function  $\psi = \psi_{Mxw}(\varepsilon, \sigma, \theta)$  of the Maxwellian model from Section 4.1. Starting from (56), by using the properties (31)<sub>1</sub> and (32)<sub>1</sub> we get

$$\frac{\partial H_{Mxw}}{\partial \varepsilon}(\varepsilon, \theta) = -\rho(E-\rho\dot{S}^2) \left( \frac{\partial \psi_{Mxw}}{\partial \sigma}(\varepsilon, \sigma_R(\varepsilon), \theta) - \theta \frac{\partial^2 \psi_{Mxw}}{\partial \sigma \partial \theta}(\varepsilon, \sigma_R(\varepsilon), \theta) \right). \quad (82)$$

Relation (81)<sub>1</sub> is obtained by using (39) and (48) in (82) and taking into account that  $\tilde{\varepsilon}(\varepsilon^\pm, \sigma_{eq}(\varepsilon^\pm, \theta^\pm), \theta^\pm) = \varepsilon^\pm$ . Relation (81)<sub>2</sub> is obtained directly from (42).

The characteristic equation of the linearized system (78) at the critical points  $(\varepsilon^\pm, \theta^\pm)$  is

$$r^2 + r \left\{ \frac{E \left( \rho\dot{S}^2 - \frac{\partial \sigma_{eq}}{\partial \varepsilon} \right)}{\mu\dot{S}(E-\rho\dot{S}^2)} + \frac{\dot{S}}{\kappa} \left( \rho \frac{\partial e_{eq}}{\partial \theta} - \frac{\theta^\pm \left( \frac{\partial \sigma_{eq}}{\partial \theta} \right)^2}{(E-\frac{\partial \sigma_{eq}}{\partial \varepsilon})} \right) \right\} + \frac{E \left( \rho\dot{S}^2 - \frac{\partial \sigma_{eq}}{\partial \varepsilon} \right)}{\kappa\mu(E-\rho\dot{S}^2)} \left\{ \rho \frac{\partial e_{eq}}{\partial \theta} - \frac{\theta^\pm \left( \frac{\partial \sigma_{eq}}{\partial \theta} \right)^2}{\left( \rho\dot{S}^2 - \frac{\partial \sigma_{eq}}{\partial \varepsilon} \right)} \right\} = 0. \quad (83)$$

The discriminant of this equation

$$\Delta(\varepsilon^\pm, \theta^\pm) = \left\{ \frac{E \left( \rho\dot{S}^2 - \frac{\partial \sigma_{eq}}{\partial \varepsilon} \right)}{\mu\dot{S}(E-\rho\dot{S}^2)} - \frac{\dot{S}}{\kappa} \left( \rho \frac{\partial e_{eq}}{\partial \theta} - \frac{\theta^\pm \left( \frac{\partial \sigma_{eq}}{\partial \theta} \right)^2}{(E-\frac{\partial \sigma_{eq}}{\partial \varepsilon})} \right) \right\}^2 + \frac{4E\theta^\pm \left( \frac{\partial \sigma_{eq}}{\partial \theta} \right)^2}{\mu\kappa \left( E - \frac{\partial \sigma_{eq}}{\partial \varepsilon} \right)}, \quad (84)$$

is positive and then both eigenvalues  $r_{1,2}(\varepsilon^\pm, \theta^\pm)$  are real. Let us note that their product and their sum are

$$r_1 r_2 = \frac{\rho^2 E}{\mu\kappa(E-\rho\dot{S}^2)} \frac{\partial e_{eq}}{\partial \theta} (\dot{S}^2 - \lambda^2), \quad (85)$$

$$r_1 + r_2 = -\frac{1}{\dot{S}} \left[ \frac{\rho E (\dot{S}^2 - \lambda^2)}{\mu(E-\rho\dot{S}^2)} + \frac{E\theta^\pm \left( \frac{\partial \sigma_{eq}}{\partial \theta} \right)^2}{\mu(E-\rho\dot{S}^2)\rho \frac{\partial e_{eq}}{\partial \theta}} + \frac{\dot{S}^2}{\kappa} \rho \frac{\partial e_{eq}}{\partial \theta} \frac{(E-\rho\lambda^2)}{\left( E - \frac{\partial \sigma_{eq}}{\partial \varepsilon} \right)} \right], \quad (86)$$

where  $\lambda^2(\varepsilon^\pm, \theta^\pm)$  represents according to (18) the square of non-zero characteristic directions of the adiabatic thermoelastic system at the critical points. Let us note that the sign of the product of the eigenvalues is positive or negative according to whether the speed of the propagating discontinuity  $\dot{S}$  is larger or smaller than the adiabatic sound speed at the critical point.

If  $r_1 r_2 < 0$ , i.e.  $\dot{S}^2 < \lambda^2(\varepsilon, \theta)$ , (subsonic case) the eigenvalues have opposite signs and the critical point is a *saddle point*.

If  $r_1 r_2 > 0$ , i.e.  $\dot{S}^2 > \lambda^2(\varepsilon, \theta)$ , (supersonic case) the eigenvalues have the same sign. According to (30), (43) and (53) we have  $E > \frac{\partial \sigma_{eq}}{\partial \varepsilon}$ ,  $E > \rho \lambda^2(\varepsilon, \theta)$  and  $E > \rho \dot{S}^2$ , respectively. Therefore, the sign of  $r_1 + r_2$  is equal to the sign of  $-\dot{S}$ . Thus, if  $\dot{S} > 0$  then both eigenvalues are negative and the critical point is an *attractive node* while if  $\dot{S} < 0$  both eigenvalues are positive and the critical point is a *repulsive node*.

If  $r_1 = 0$ , i.e.  $\dot{S}^2 = \lambda^2(\varepsilon, \theta)$  then the sign of  $r_2$  is equal to the sign of  $-\dot{S}$ . In this case, in the neighborhood of the critical point the orbits are straight lines parallel with the eigenvector corresponding to the non-zero eigenvalue. The orientation being away ( $r_2 > 0$ ), or towards ( $r_2 < 0$ ) an axis of stationary points parallel with the eigenvector corresponding to the null eigenvalue.

### 5.2.1 Existence, uniqueness and structure of "viscous", heat conducting profile layers.

We assume that the thermoelastic constitutive equation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  satisfies assumptions **H1-H4** corresponding to a phase transforming material, the smoothness assumption **S1**, and the dynamic Young's modulus  $E$  satisfies the sub-characteristic condition (43).

Our goal is to investigate if *the chord criterion (58)-(59) with respect to the Hugoniot locus  $\sigma = \sigma_H(\varepsilon; \varepsilon^+, \theta^+)$*  is still a necessary and sufficient condition for the existence of a unique profile layer when the structuring mechanism is governed by the Maxwellian rate-type constitutive equation coupled with the Fourier law. In fact, we first investigate under what conditions *the chord criterion with respect to the stress-strain curve  $\sigma = \sigma_{Mxw}(\varepsilon)$* , defined in (62), ensures the existence and uniqueness of a "viscous", heat conducting profile layer for any given coefficients  $\mu > 0$  and  $\kappa > 0$ . Then, one gets by using the same proof like in Proposition 1, that this criterion is equivalent with the chord criterion with respect to the Hugoniot locus  $\sigma = \sigma_H(\varepsilon; \varepsilon^+, \theta^+)$ .

The study of the behavior of the solutions of the system (54) is based on the idea of Gilbarg [9] and used later by Pego [6] to exploit the topological properties of the curves  $H_{Mxw}(\varepsilon, \theta) = 0$  and  $R(\varepsilon, \theta) = 0$  along which  $\hat{\theta}'(\xi)$  and  $\hat{\varepsilon}'(\xi)$  vanishes.

*Remark 6* We have seen in Section 5.1.2 that the curve  $H_{Mxw}(\varepsilon, \theta) = 0$ , or equivalently  $\theta = \Theta_{Mxw}(\varepsilon)$ , represents the trajectory in the  $\theta - \varepsilon$  plane of a traveling wave solution governed by the Maxwellian rate-type constitutive equation in the absence of heat conduction. From thermodynamical point of view it is useful to note that relation (65) can be directly obtained by writing the energy identity (46) for the "viscous" traveling wave solution ( $\hat{\varepsilon}(\xi), \hat{\theta}(\xi) = \sigma_R(\hat{\varepsilon}(\xi)), \hat{\theta}(\xi) = \Theta_{Mxw}(\hat{\varepsilon}(\xi))$ ) described by (63) and then by using relation (74)<sub>2</sub>. One can give now a clear physical meaning to the right-terms in relation (65), or equivalently, in relation (66). The first right-term in the parenthesis is related to the contribution of the intrinsic dissipation, while the second one is related to the contribution of the latent heat, to the increase or decrease of the temperature in the "viscous", heat non-conducting profile layer. In other words, the slope of the curve  $\theta = \Theta_{Mxw}(\varepsilon)$  reflects a competition inside the profile layer between the heating due to the intrinsic dissipation and the heating, or cooling, due to the latent heat.

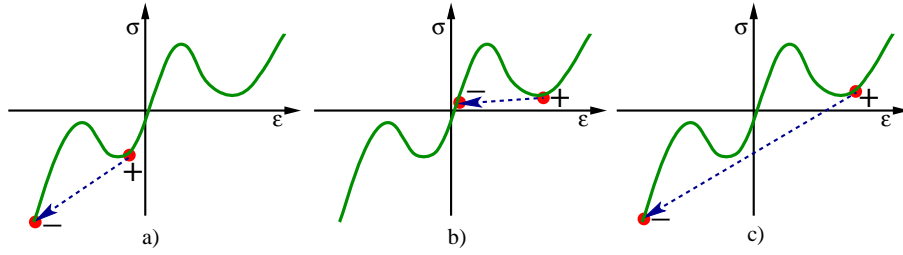
### C. The compressive case ( $\varepsilon^- < \varepsilon^+$ ).

We consider  $\dot{S} > 0$  and  $(\varepsilon^+, \theta^+)$  a front state and  $(\varepsilon^-, \theta^-)$  a Hugoniot back state of a wave discontinuity for the adiabatic thermoelastic system. One has seen in the proof of Proposition 1 that in the compressive case the *chord criterion (64) with respect to the curve  $\sigma = \sigma_{Mxw}(\varepsilon)$*  requires that the characteristic directions at the critical points  $\lambda(\varepsilon^\pm, \theta^\pm)$  satisfy the inequalities (70). Let us note that if these inequalities are strict, one gets from relations (85)-(86), that  $(\varepsilon^-, \theta^-)$  is a *saddle node (subsonic critical point)*, while  $(\varepsilon^+, \theta^+)$  is an *attractive node (supersonic critical point)* for the linearized system (78).

We distinguish several situations depending on the sign of  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^\pm, \theta^\pm)$ , i.e. on the sign of the Grüneisen coefficient (15) at the critical points. The *expansive case* when  $\varepsilon^+ < \varepsilon^-$  can be treated in a similar way.

*Case C1.*  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^\pm, \theta^\pm) < 0$ , i.e. positive Grüneisen coefficients (15) at the critical points.

That means  $(\varepsilon^\pm, \theta^\pm)$  belong to the region where  $\frac{\partial \sigma_{eq}}{\partial \theta} < 0$ , that is where  $\varepsilon < \varepsilon_t(\theta)$  (Fig. 2). According to assumption **H3-H4** the front state and the Hugoniot state  $(\varepsilon^\pm, \theta^\pm)$  lie in the austenitic phase  $A$  or in the martensitic variant  $M^-$ . A typical compressive jump discontinuity from  $A$  to  $M^-$  is illustrated in Fig. 3a.



**Fig. 3** Typical compressive jump discontinuities from state  $(\varepsilon^+, \theta^+)$  to  $(\varepsilon^-, \theta^-)$  satisfying the chord criterion with respect to the Hugoniot curve  $\sigma = \sigma_H(\varepsilon; \varepsilon^+, \theta^+)$ . Phase transformations: a) Case C1.  $A \rightarrow M^-$ ; b) Case C2.  $M^+ \rightarrow A$ ; c) Case C3.  $M^+ \rightarrow M^-$ .

Since  $\frac{\partial R(\varepsilon, \theta)}{\partial \theta} = -\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} > 0$  for  $\varepsilon < \varepsilon_t(\theta)$ , it follows that  $R(\varepsilon, \theta) = 0$  is locally uniquely representable as a single valued function of  $\varepsilon$ . We assume there exists a function denoted  $\theta = \Theta_R(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  for  $\varepsilon$  belonging to an interval which contains  $\varepsilon^\pm$  such that  $R(\varepsilon, \Theta_R(\varepsilon)) = 0$  and  $\theta^\pm = \Theta_R(\varepsilon^\pm; \varepsilon^+, \theta^+, \varepsilon^-)$ . Its image through the function  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  in the  $\varepsilon - \sigma$  plane is just the Rayleigh line, i.e.  $\sigma_R(\varepsilon) = \sigma_{eq}(\varepsilon, \Theta_R(\varepsilon))$ . Moreover, we have

$$\frac{d\Theta_R(\varepsilon)}{d\varepsilon} = \left( \rho \dot{S}^2 - \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\varepsilon, \Theta_R(\varepsilon)) \right) \left( \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon, \Theta_R(\varepsilon)) \right)^{-1}. \quad (87)$$

Let us introduce the function  $t(\varepsilon) \stackrel{\text{def}}{=} \Theta_R(\varepsilon) - \Theta_{M_{XW}}(\varepsilon)$  for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . We note that  $t(\varepsilon^\pm) = 0$ , and these are the only points where function  $t = t(\varepsilon)$  vanishes, or equivalently,  $(\varepsilon^\pm, \theta^\pm)$  are the only critical points of (54) in the interval  $(\varepsilon^-, \varepsilon^+)$ . Indeed, if we suppose there exists an  $\varepsilon^* \in (\varepsilon^-, \varepsilon^+)$  such that  $\Theta_R(\varepsilon^*) = \Theta_{M_{XW}}(\varepsilon^*)$  we get  $\sigma_R(\varepsilon^*) = \sigma_{eq}(\varepsilon^*, \Theta_R(\varepsilon^*)) = \sigma_{eq}(\varepsilon^*, \Theta_{M_{XW}}(\varepsilon^*)) = \sigma_{M_{XW}}(\varepsilon^*)$  which is in contradiction with our assumption that the chord condition (64) is satisfied. By using relations (66) and (87) we get that

$$t'(\varepsilon^\pm) = \frac{d\Theta_R(\varepsilon^\pm)}{d\varepsilon} - \frac{d\Theta_{M_{XW}}(\varepsilon^\pm)}{d\varepsilon} = s'(\varepsilon^\pm) \left( \rho \frac{\partial \sigma_{eq}(\varepsilon^\pm, \theta^\pm)}{\partial \theta} \right)^{-1}. \quad (88)$$

Since the chord criterion (64) requires  $s'(\varepsilon^-) \leq 0$  and  $s'(\varepsilon^+) \geq 0$  one gets that  $t'(\varepsilon^-) \geq 0$  and  $t'(\varepsilon^+) \leq 0$ . Thus, it follows that  $t(\varepsilon) = \Theta_R(\varepsilon) - \Theta_{M_{XW}}(\varepsilon) > 0$ , for any  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  (Fig. 4).

Let us note that in case C1 the function  $\theta = \Theta_{M_{XW}}(\varepsilon)$  is a *strictly decreasing* function of  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , and consequently, *the Hugoniot back state temperature has to be larger than the front state temperature*, i.e.  $\theta^- > \theta^+$ . Therefore, the corresponding *compressive discontinuity is of heating type*. The result is in agreement with the fact that the phase transformation  $A \rightarrow M^-$  is exothermic. This behavior is a consequence of the fact that both terms in the parenthesis of the right part of relation (66) are negative. From physical point of view that means, according to Remark 6, that *both the intrinsic dissipation and the latent heat* contribute to the increase of temperature in the "viscous", heat non-conducting profile layer.

To prove this assertion we have to note that  $\frac{\partial \sigma_{eq}}{\partial \theta}(\tilde{\varepsilon}(\varepsilon), \Theta_{M_{XW}}(\varepsilon)) < 0$ , and the chord condition (64) implies that  $\sigma_R(\varepsilon) - \sigma_{eq}(\tilde{\varepsilon}(\varepsilon), \Theta_{M_{XW}}(\varepsilon)) < 0$ , where  $\tilde{\varepsilon}(\varepsilon)$  is given by (67), for any  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . The last inequality follows from the identity  $(\sigma_R(\varepsilon) - \sigma_{eq}(\tilde{\varepsilon}, \Theta_{M_{XW}}(\varepsilon))) \left( E - \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\varepsilon^*, \Theta_{M_{XW}}(\varepsilon)) \right) = (\sigma_R(\varepsilon) - \sigma_{eq}(\varepsilon, \Theta_{M_{XW}}(\varepsilon))) E$ , where  $\varepsilon^*$  lies between  $\varepsilon$  and  $\tilde{\varepsilon}(\varepsilon)$ .

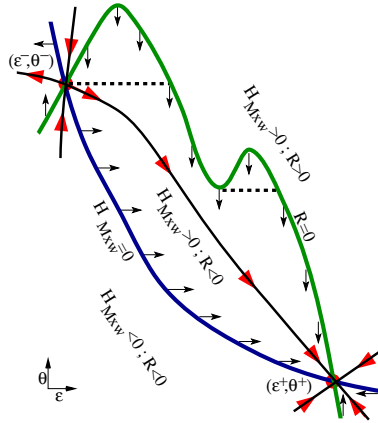
Concerning the function  $\theta = \Theta_R(\varepsilon)$ , we note that it can be monotone decreasing, but it can be non-monotone, too. Indeed, the inequalities  $\frac{d\Theta_R(\varepsilon^+)}{d\varepsilon} < \frac{d\Theta_{M_{XW}}(\varepsilon^+)}{d\varepsilon} < 0$  and  $\frac{d\Theta_R(\varepsilon^-)}{d\varepsilon} > \frac{d\Theta_{M_{XW}}(\varepsilon^-)}{d\varepsilon}$ , which follow from relation (88), require only that  $\theta = \Theta_R(\varepsilon)$  is a decreasing function of  $\varepsilon$  in the neighborhood of  $\varepsilon^\pm$  (Fig. 4).

The existence of a connecting orbit follows now from topological considerations similar with those used by Gilbarg [9]. The closed curve formed by  $\theta = \Theta_{M_{XW}}(\varepsilon)$  and  $\theta = \Theta_R(\varepsilon)$ , for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , bounds a simply connected region  $P$  of the  $\varepsilon - \theta$  plane. Since  $H_{M_{XW}} > 0$  on the curve  $R = 0$  and  $R < 0$  on the curve  $H_{M_{XW}} = 0$ , for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , one concludes that everywhere in  $P$ ,  $H_{M_{XW}} > 0$  and  $R < 0$ . Let us note that on the boundaries  $H_{M_{XW}} = 0$  and  $R = 0$  all vector fields of the flow induced by (54) point toward the region  $P$ , horizontally and vertically, respectively.

Let us first consider the case of strict inequalities, i.e.  $\dot{S}^2 > \lambda^2(\varepsilon^+, \theta^+)$  and  $\dot{S}^2 < \lambda^2(\varepsilon^-, \theta^-)$ . Since  $\frac{d\theta}{d\varepsilon} = \frac{\mu(E - \rho \dot{S}^2) \dot{S}^2}{\kappa E} \frac{H_{M_{XW}}}{R}$ , all integral curves of (54) must be monotone decreasing in  $P$ , and because they cannot leave  $P$  and there is no critical point in this region they must tend to the attractive point  $(\varepsilon^+, \theta^+)$  (Fig. 4). Taking into account that  $(\varepsilon^-, \theta^-)$  is a saddle point one obtains that a trajectory connecting  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$

exists and lies inside the region  $P$ . Moreover, the temperature and the deformation vary *monotonously* across this "viscous", *thermally conducting profile layer*.

When  $\dot{S}^2 = \lambda^2$  at a critical point, i.e. when one eigenvalue given by (83) is zero and the another one is negative, the two curves  $H_{M_{xw}} = 0$  and  $R = 0$  are tangent at this point. Moreover, they are tangent with the integral curve of (54) and with the isentrope (14) passing through this point. The direction of this common tangent coincides with the direction of the eigenvector corresponding to the eigenvalue zero. Similar topological arguments prove the existence of a trajectory connecting  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$ .



**Fig. 4** Case C1 - phase portrait of (54) for  $A \rightarrow M^-$  phase transformation illustrated in Fig. 3a.

Conversely, let us prove that the chord criterion is also a necessary condition for the existence of a profile layer. We suppose by absurd that a profile layer connecting  $(\varepsilon^\pm, \theta^\pm)$  exists, but the chord criterion is violated. Let us assume there exists at least one point  $\varepsilon^* \in (\varepsilon^-, \varepsilon^+)$  such that  $\sigma_R(\varepsilon^*) = \sigma_{M_{xw}}(\varepsilon^*; \varepsilon^+, \theta^+, \varepsilon^-)$ . According to relation

$$s(\varepsilon) = \sigma_R(\varepsilon) - \sigma_{M_{xw}}(\varepsilon) = \sigma_{eq}(\varepsilon, \Theta_R(\varepsilon)) - \sigma_{eq}(\varepsilon, \Theta_{M_{xw}}(\varepsilon)) = -\frac{\partial \sigma_{eq}(\varepsilon, \bar{\theta}(\varepsilon))}{\partial \theta} (\Theta_{M_{xw}}(\varepsilon) - \Theta_R(\varepsilon)), \quad (89)$$

where  $\bar{\theta}(\varepsilon)$  lies between  $\Theta_{M_{xw}}(\varepsilon)$  and  $\Theta_R(\varepsilon)$ , it follows that  $\Theta_{M_{xw}}(\varepsilon^*) = \Theta_R(\varepsilon^*) \equiv \theta^*$ , i.e.  $R(\varepsilon^*, \theta^*) = 0$  and  $H_{M_{xw}}(\varepsilon^*, \theta^*; \varepsilon^+, \theta^+, \varepsilon^-) = 0$ . Therefore,  $(\varepsilon^*, \theta^*)$  is a critical point of the system (54). On the other side, by using relation (57) we obtain  $H(\varepsilon^*, \theta^*; \varepsilon^+, \theta^+) = 0$ , that is  $(\varepsilon^*, \theta^*)$  is also a Hugoniot state. Therefore, the curves  $\theta = \Theta_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  and  $\theta = \Theta_R(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  pass through the critical points between  $\varepsilon^-$  and  $\varepsilon^+$ . We also note that the Rayleigh line provides a natural ordering for these points. Considering the position of  $\sigma = \sigma_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  with respect to the Rayleigh line one proves as before that these critical points alternate between being saddle points and attractive points. Because  $H_{M_{xw}} > 0$  above  $\theta = \Theta_{M_{xw}}(\varepsilon)$  and  $R < 0$  below  $\theta = \Theta_R(\varepsilon)$  one gets from a phase portrait diagram of type in Fig. 4 that  $(\varepsilon^+, \theta^+)$  can be connected by a trajectory only with the first critical point with smaller strain than  $\varepsilon^+$  and thus it is impossible to connect  $(\varepsilon^+, \theta^+)$  by a trajectory with  $(\varepsilon^-, \theta^-)$ . Contradiction.

The uniqueness of the profile layer is based on the fact that a trajectory connecting  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$  can not lie outside  $P$  (see also Pego [6]).

Thus, for any  $\mu > 0$  and  $\kappa > 0$  there exists a unique profile layer  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \kappa)$  joining  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$ . The limit behavior of such profile layer as  $\mu \rightarrow 0$  and  $\kappa \rightarrow 0$  can be studied in a similar way as was done by Gilbarg [9] for a viscous, thermally conducting fluid. One proves the existence of the iterated limits and their equality with the double limit. The limit is just a step wave discontinuity connecting  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$ . Moreover, Gilbarg [9] has put into evidence a basic difference in the effect of "viscosity" and of heat conduction on the structure of the profile layers which holds for the Maxwellian approach, too. Thus, if we consider a fixed "viscosity"  $\mu = \bar{\mu}$  and  $\kappa \rightarrow 0$ , the trajectories in  $\varepsilon - \theta$  plane of all profile layers  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \bar{\mu}, \kappa)$  are increasingly close to the decreasing curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$  and approach the solutions of the reduced system (60). This traveling wave solution is smooth with respect to  $\xi$  and describes a "viscous", *heat non-conducting profile layer*.



If  $\theta = \Theta_R(\varepsilon)$  is *monotone* decreasing and if we consider a fixed heat conductivity  $\kappa = \bar{\kappa}$  and  $\mu \rightarrow 0$ , all profile layers curves  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \bar{\kappa})$  are increasingly close to the curve  $\theta = \Theta_R(\varepsilon)$  and approach the solutions of the following reduced system

$$\begin{aligned} 0 &= R(\hat{\varepsilon}, \hat{\theta}), \\ \hat{\theta}' &= -\frac{\hat{\varepsilon}}{\bar{\kappa}} H_{M_{xw}}(\hat{\varepsilon}, \hat{\theta}), \quad \lim_{\xi \rightarrow \pm\infty} \hat{\theta}(\xi) = \theta^\pm, \end{aligned} \quad (90)$$

These solutions describe "non-viscous", *heat conducting profile layers*.

An important difference appears when  $\theta = \Theta_R(\varepsilon)$  is *non monotone*. Since all integral curves of the system (54) are strictly decreasing in  $P$  one shows that as  $\mu \rightarrow 0$  the trajectories in  $\varepsilon - \theta$  plane of the profile layers  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \bar{\kappa})$  are increasingly close to the monotone decreasing curve  $\theta = \bar{\Theta}_R(\varepsilon)$  defined by

$$\theta = \bar{\Theta}_R(\varepsilon) = \min_{\zeta \in [\varepsilon^-, \varepsilon^+]} \Theta_R(\zeta), \quad \text{for } \varepsilon \in [\varepsilon^-, \varepsilon^+]. \quad (91)$$

This function is the maximum among all monotone decreasing curves bounded from above by the curve  $\theta = \Theta_R(\varepsilon)$ . It is represented with dotted line on those parts which do not coincide with  $\theta = \Theta_R(\varepsilon)$  in Fig. 4. If  $\theta = \Theta_R(\varepsilon)$  has a finite number of minima then  $\theta = \bar{\Theta}_R(\varepsilon)$  has at most a finite number of intervals on which  $\theta$  is constant. They correspond to *isothermal jumps in strain inside the profile layer*. Therefore, in this case, as  $\mu \rightarrow 0$  the profile layers  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \bar{\kappa})$  approach a pair of functions denoted by  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu = 0, \bar{\kappa})$  with the property that  $\hat{\varepsilon}(\xi; \mu = 0, \bar{\kappa})$  is *discontinuous* and  $\hat{\theta}(\xi; \mu = 0, \bar{\kappa})$  is continuous and piecewise smooth. Thus, the notion of traveling wave solution must be enlarged in order to admit such discontinuous solutions for the reduced system (90).

*Case C2.*  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^\pm, \theta^\pm) > 0$ , i.e. negative Grüneisen coefficients at the critical points.

That means  $(\varepsilon^\pm, \theta^\pm)$  belong to the region where  $\frac{\partial \sigma_{eq}}{\partial \theta} > 0$ , that is where  $\varepsilon > \varepsilon_t(\theta)$  (Fig. 2). According to assumptions **H3-H4** the front state and the Hugoniot state  $(\varepsilon^\pm, \theta^\pm)$  lie in the austenitic phase  $A$  or in the martensitic variant  $M^+$ . A typical compressive jump discontinuity from  $M^+$  to  $A$  is illustrated in Fig. 3b.

Since  $\frac{\partial R(\varepsilon, \theta)}{\partial \theta} = -\frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} < 0$  for  $\varepsilon > \varepsilon_t(\theta)$ , it follows that  $R(\varepsilon, \theta) = 0$ , given by (55), is representable as a single valued function of  $\varepsilon$ . We suppose there exists a function  $\theta = \Theta_R(\varepsilon; \varepsilon^+, \theta^+, \theta^-)$ , which satisfies  $R(\varepsilon, \Theta_R(\varepsilon)) = 0$  and consequently,  $\sigma_R(\varepsilon) = \sigma_{eq}(\varepsilon, \Theta_R(\varepsilon))$ , for  $\varepsilon$  belonging to an interval which contains  $\varepsilon^-$  and  $\varepsilon^+$ . Moreover, relations (66) and (87) are still valid.

By defining the function  $t(\varepsilon) \stackrel{\text{def}}{=} \Theta_R(\varepsilon) - \Theta_{M_{xw}}(\varepsilon)$ , for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , taking into account that the Grüneisen coefficient is negative at the critical points, and using the same reasoning based on the chord condition (64) as in case C1 we obtain from (88) that  $t'(\varepsilon^-) \leq 0$  and  $t'(\varepsilon^+) \geq 0$ , which involves that  $t(\varepsilon) = \Theta_R(\varepsilon) - \Theta_{M_{xw}}(\varepsilon) < 0$ , for any  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  (Figs. 5-6).

From (68) one gets that  $\frac{d\Theta_{M_{xw}}(\varepsilon^\pm)}{d\varepsilon} \geq 0$ . Therefore,  $\theta = \Theta_{M_{xw}}(\varepsilon)$  is monotone increasing in the neighborhood of  $\varepsilon^\pm$ , but we cannot say anything, without additional constitutive assumptions, neither about its monotonicity, nor about the order relation between  $\theta^-$  and  $\theta^+$ . Indeed, in the present compressive case, the first term in the right part of relation (66) is always negative as a consequence of the chord criterion. That means the intrinsic dissipation always contributes to the increase of the temperature inside the "viscous", heat non-conducting profile layer. The second term is always positive, since the Grüneisen coefficient is negative. That means the latent heat contributes to the decrease of the temperature inside this layer. Therefore,  $\theta = \Theta_{M_{xw}}(\varepsilon)$  is monotone increasing on those intervals where the cooling due to latent heat dominates the heating due to intrinsic dissipation and it is monotone decreasing when the opposite case happens.

The following representative cases will be analyzed:

- a)  $\theta^- < \theta^+$  and  $\theta = \Theta_{M_{xw}}(\varepsilon)$  *monotone increasing* (Fig. 5a).
- b)  $\theta^- < \Theta_{M_{xw}}(\varepsilon) < \theta^+$ , but  $\theta = \Theta_{M_{xw}}(\varepsilon)$  is *non-monotone* (Fig. 5b).
- c)  $\theta^- > \theta^+$  (Figs. 6).

We consider as natural from physical point of view for phase transforming materials the case **a**) where the latent heat effect is more important than the dissipation effect.

*Example.* Let us consider a thermoelastic constitutive equation  $\sigma = \sigma_{eq}(\varepsilon, \theta)$  satisfying the conditions

$$\theta \left| \frac{\partial^2 \sigma_{eq}(\varepsilon, \theta)}{\partial \theta^2} \right| \ll \left| \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} \right|, \quad \left| \varepsilon \frac{\partial^2 \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon \partial \theta} \right| \ll \left| \frac{\partial \sigma_{eq}(\varepsilon, \theta)}{\partial \theta} \right|, \quad \left| \varepsilon \frac{\partial^2 \sigma_{eq}(\varepsilon, \theta)}{\partial \varepsilon^2} \right| \ll E. \quad (92)$$

Then one can show by using relation (66) that

$$\frac{d\Theta_{M_{XW}}(\varepsilon)}{d\varepsilon} \approx \frac{(E - \rho\zeta^2)\Theta_R(\varepsilon)}{\rho C_{M_{XW}}(\varepsilon, \sigma_R(\varepsilon), \Theta_{M_{XW}}(\varepsilon))(E - \frac{\partial\sigma_{eq}}{\partial\varepsilon}(\varepsilon, \Theta_{M_{XW}}(\varepsilon)))} \frac{\partial\sigma_{eq}(\varepsilon, \Theta_{M_{XW}}(\varepsilon))}{\partial\theta} > 0. \quad (93)$$

Consequently,  $\theta = \Theta_{M_{XW}}(\varepsilon)$  is a *strictly increasing* function of  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  and *the Hugoniot back state temperature has to be lower than the front state temperature*, i.e.  $\theta^- < \theta^+$ . Therefore, the corresponding *compressive wave discontinuity is of cooling type*. The result is in agreement with the fact that the reverse phase transformation  $M^+ \rightarrow A$  is endothermic.

Let us note that, since  $\theta \frac{\partial^2\sigma_{eq}(\varepsilon, \theta)}{\partial\theta^2} = -\rho \frac{\partial C_{eq}(\varepsilon, \theta)}{\partial\varepsilon}$ , condition (92)<sub>1</sub> requires in fact that the variation of the specific heat  $C_{eq}(\varepsilon, \theta)$  with respect to  $\varepsilon$  be negligible regarding the variation of  $\sigma_{eq}(\varepsilon, \theta)$  with respect to  $\theta$ . In Part II [35] an explicit piecewise linear thermoelastic model which describes phase transformation in a SMA alloy and fulfills conditions (92) is considered.

*Remark 7* Let us note that in the complementary *expansive case* ( $\varepsilon^+ < \varepsilon^-$ ) with *positive Grüneisen coefficients* at the critical points, i.e.  $\frac{\partial\sigma_{eq}}{\partial\theta}(\varepsilon^\pm, \theta^\pm) < 0$ , according to relation (66), the intrinsic dissipation and the latent heat act again in opposite sense. Indeed, this happens because the chord condition in the expansive case requires that  $\sigma_R(\varepsilon) - \sigma_{M_{XW}}(\varepsilon) > 0$  for any  $\varepsilon \in (\varepsilon^+, \varepsilon^-)$  and  $\frac{\partial\sigma_{eq}}{\partial\theta}$  is supposed negative along the "viscous" traveling wave solution. Restrictions (92), which lead to relation (93), imply that in this case  $\theta = \Theta_{M_{XW}}(\varepsilon)$  is a strictly decreasing function of  $\varepsilon$ , that is, the heating due to the intrinsic dissipation is dominated by the cooling due to latent heat inside the layer. Thus, the Hugoniot back state temperature has to be lower than the front state temperature, i.e.  $\theta^+ > \theta^-$ . Therefore, the corresponding *expansive wave discontinuity (rarefaction shock) is of cooling type*. Such behavior is natural and in agreement with the fact that the reverse phase transformation  $M^- \rightarrow A$  is also endothermic.

We can show now that for the phase diagrams illustrated in Figs. 5 and Fig. 6a, which correspond to **cases a), b) and c)**, respectively, the chord condition (64) is a necessary and sufficient requirement for the existence and uniqueness of a "viscous", heat conducting profile layer for any given coefficients  $\mu > 0$  and  $\kappa > 0$ . The proof, given below, is based on the properties of the vector field of the flow induced by (54) and topological considerations related to the corresponding figures.

On the other side, for the phase diagram illustrated by Fig. 6b, where the chord criterion is satisfied, but the curves  $\theta = \Theta_{M_{XW}}(\varepsilon; \varepsilon^+ \theta^+, \theta^-)$  and  $\theta = \Theta_R(\varepsilon; \varepsilon^+ \theta^+, \theta^-)$  meet again at a critical point  $(\varepsilon_0, \theta_0)$ , with the properties that  $\varepsilon_0 > \varepsilon^+$  and  $\theta_0 < \theta^-$ , a trajectory connecting  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$  no longer exists if the heat conduction dominates the "viscosity". This phase diagram corresponds to the example given by Pego [6] concerning the nonexistence of a shock layer in gas dynamics with a nonconvex equation of state.

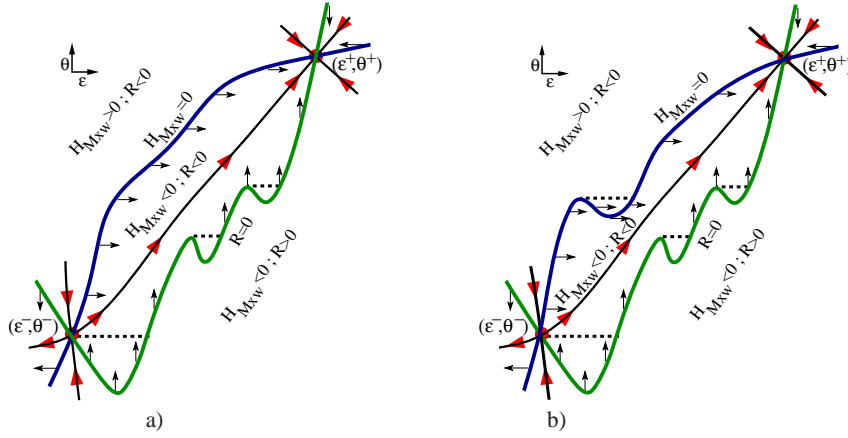
Let us consider, for example, **case b)** represented by Fig. 5b). We denote by  $P$  the simply connected region bounded by  $\theta = \Theta_{M_{XW}}(\varepsilon)$  and  $\theta = \Theta_R(\varepsilon)$  for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . Since  $H_{M_{XW}} < 0$  and  $R < 0$  in  $P$  any integral curves of (54) is monotone increasing inside  $P$ . On the boundary  $R = 0$  all vector fields of the flow induced by (54) point vertically toward the region  $P$  while on the boundary  $H_{M_{XW}} = 0$  all vector fields point horizontally right. Therefore, on the ascending branches of the curve  $\theta = \Theta_{M_{XW}}(\varepsilon)$  the vector fields point toward the region  $P$  while on the descending branches of the curve  $\theta = \Theta_{M_{XW}}(\varepsilon)$  they point horizontally outwards the region  $P$ . Let us note that if  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  and  $\theta > \Theta_{M_{XW}}(\varepsilon)$  we have  $H_{M_{XW}} > 0$  and  $R < 0$ . Consequently, any integral curve which leaves the domain  $P$  through the descending branches of the curve  $\theta = \Theta_{M_{XW}}(\varepsilon)$  is monotone decreasing and when it meets again an ascending branch of this curve it is directed inside the region  $P$ .

Let us introduce the continuous and monotonic function

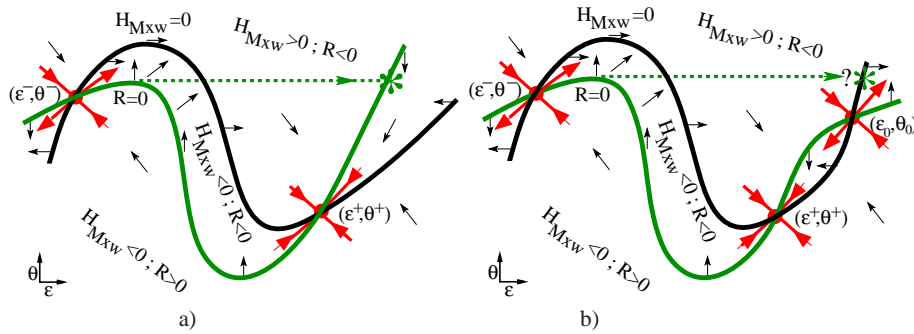
$$\theta = \bar{\Theta}_{M_{XW}}(\varepsilon) = \max_{\zeta \in [\varepsilon^-, \varepsilon]} \Theta_{M_{XW}}(\zeta), \quad \text{for } \varepsilon \in [\varepsilon^-, \varepsilon^+]. \quad (94)$$

This is the minimum among all monotone increasing curves bounded from below by the curve  $\theta = \Theta_{M_{XW}}(\varepsilon)$ . It is composed by ascending branches of  $\theta = \Theta_{M_{XW}}(\theta)$  and by the horizontal lines marked with dotted lines in Fig. 5b). Let us denote by  $\bar{P}$  the simply connected region bounded by  $\theta = \bar{\Theta}_{M_{XW}}(\varepsilon)$  and  $\theta = \Theta_R(\varepsilon)$ . According to the above said, any integral curve of (54) cannot leave  $\bar{P}$  and since there is no critical point in region  $\bar{P}$  they must tend to the attractive point  $(\varepsilon^+, \theta^+)$ . Because  $(\varepsilon^-, \theta^-)$  is a saddle point one obtains that a trajectory connecting  $(\varepsilon^+, \theta^+)$  and  $(\varepsilon^-, \theta^-)$  exists for any  $\mu > 0$  and  $\kappa > 0$  and lies inside  $\bar{P}$ .

The reverse implication can be proved in the same way as in case C1 using relation (89). The uniqueness of the connecting orbit is based on the fact that a trajectory connecting  $(\varepsilon^\pm, \theta^\pm)$  cannot lie outside  $\bar{P}$ .



**Fig. 5** Case C2 - phase portrait of (54) when: a)  $\theta^- < \theta^+$  and  $\theta = \Theta_{Mxw}(\varepsilon)$  monotone increasing; b)  $\theta^- < \Theta_{Mxw}(\varepsilon) < \theta^+$ , but  $\theta = \Theta_{Mxw}(\varepsilon)$  is non-monotone.



**Fig. 6** Case C2 - possible phase portraits of (54) when  $\theta^- > \theta^+$  and the chord criterion is satisfied: a) profile layers exists for any  $\mu > 0$  and  $\kappa > 0$ ; b) profile layers does not exists if heat conduction dominates the "viscosity".

Let us note that, for fixed "viscosity"  $\mu = \bar{\mu}$  and sufficiently small  $\kappa$ , the connecting orbit  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \bar{\mu}, \kappa)$  is close to the non-monotone curve  $\theta = \Theta_{Mxw}(\varepsilon)$ . In this case the smooth profile layer has the property that  $\varepsilon = \hat{\varepsilon}(\xi)$  is strictly monotone, but  $\theta = \hat{\theta}(\xi)$  may become non-monotone as it happens in Fig. 5b. On the other side, when the heat conduction dominates the "viscosity", the connecting orbit has to be close to the curve  $\theta = \Theta_R(\varepsilon)$  if this is monotone increasing or to the curve  $\theta = \bar{\Theta}_R(\varepsilon)$  defined by relation

$$\theta = \bar{\Theta}_R(\varepsilon) = \max_{\zeta \in [\varepsilon^-, \varepsilon^+]} \Theta_R(\zeta), \text{ for } \varepsilon \in [\varepsilon^-, \varepsilon^+], \quad (95)$$

if  $\theta = \Theta_R(\varepsilon)$  is non-monotone. In this second case the limit trajectory  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); 0, \bar{\kappa})$  has the property that  $\hat{\varepsilon}(\xi)$  is discontinuous (isothermal jumps inside the profile layer) and piecewise smooth, while  $\hat{\theta}(\xi)$  is continuous and piecewise smooth. Its trajectory in the  $\varepsilon - \theta$  plane is given by the ascending branches of  $\theta = \Theta_R(\varepsilon)$  and by the isothermal strain jumps represented by dotted lines in Fig. 5b.

The case when the *non-monotone* function  $\theta = \Theta_{Mxw}(\varepsilon)$  overcomes  $\theta^+$  can be treated as in **case c)** considered in the following.

Let us first consider the phase diagram in Fig. 6a. Since  $\theta^- > \theta^+$  and  $\frac{d\Theta_{Mxw}(\varepsilon^+)}{d\varepsilon} \geq 0$  it follows that  $\theta = \Theta_{Mxw}(\varepsilon)$  must necessarily be *non-monotone*. According to relation (88) we have  $\frac{d\Theta_R(\varepsilon^+)}{d\varepsilon} > \frac{d\Theta_{Mxw}(\varepsilon^+)}{d\varepsilon} > 0$  and  $\frac{d\Theta_R(\varepsilon^-)}{d\varepsilon} < \frac{d\Theta_{Mxw}(\varepsilon^-)}{d\varepsilon}$ . Consequently,  $\theta = \Theta_R(\varepsilon)$  has to be also a non-monotone function for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , but always ending with a positive slope in the neighborhood of  $\varepsilon^+$ . Since  $H_{Mxw} < 0$  and  $R < 0$  in the region  $P$  bounded by  $\theta = \Theta_{Mxw}(\varepsilon)$  and  $\theta = \Theta_R(\varepsilon)$ , for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  it follows that any integral curve of (54) is monotone increasing inside  $P$ . On the boundary  $R = 0$ , for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , all vector fields of the flow point vertically toward the region  $P$ , while on the curve  $\theta = \Theta_{Mxw}(\varepsilon)$  the vector fields point horizontally toward the region  $P$  on the ascending branches and point horizontally outwards  $P$  on the descending branches. In

the region above  $H_{M_{xw}} = 0$  for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  we have  $H_{M_{xw}} > 0$  and  $R < 0$ , and consequently the integral curves of (54) are monotone decreasing. Therefore, the integral curve starting from the saddle point  $(\varepsilon^-, \theta^-)$  towards  $P$  has to be monotone increasing until it meets the descending branch of the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$ . After traversing it, this integral curve is monotone descending. If the "viscosity" dominates the heat conduction then this integral curve is close to the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$ . It may happen that  $\hat{\theta}(\xi)$  descends below  $\theta^+$ . Then, this integral curve will meet the ascending branch of the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$  and will enter again inside  $P$  reaching the attractive point  $(\varepsilon^+, \theta^+)$  by an ascending curve.

A different situation appears when the "viscosity" is dominated by the heat conduction. In this case the strain  $\hat{\varepsilon}(\xi)$  may overcome  $\varepsilon^+$ . Thus, when  $\mu \rightarrow 0$  the profile layers  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \bar{\kappa})$  will approach a pair of functions denoted by  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu = 0, \bar{\kappa})$  with the property that  $\hat{\varepsilon}(\xi)$  is *discontinuous* while  $\hat{\theta}(\xi)$  is continuous and piecewise smooth. Let us denote by  $(\varepsilon^*, \theta^-)$  the unique point with the property that  $R(\varepsilon^*, \theta^-) = 0$ , where  $\varepsilon^* > \varepsilon^+$  (Fig. 6a). Due to the above topological considerations this discontinuous limit solution, which corresponds to a "non-viscous", heat conducting profile layer, is characterized by an isothermal jump from  $(\varepsilon^-, \theta^-)$  to  $(\varepsilon^*, \theta^-)$  and next is described by a pair of smooth functions  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi))$  which are solution of the reduced system (90) and connect the point  $(\varepsilon^*, \theta^-)$  with the attractive point  $(\varepsilon^+, \theta^+)$ .

The reverse implication that the chord criterion is also a necessary condition for the existence of a connecting orbit and its uniqueness can be also proved. We omit here the details.

Let us consider now the uncommon **case c**) illustrated in Fig. 6b. We denote again by  $(\varepsilon^*, \theta^-)$  the unique point with the property that  $R(\varepsilon^*, \theta^-) = 0$ , where  $\varepsilon^* > \varepsilon^+$ . Unlike the diagram in Fig. 6a, we suppose that between  $\varepsilon^-$  and  $\varepsilon^*$  there exists another critical point  $(\varepsilon_0, \theta_0)$  for the system (54), i.e. a point where the curves  $\theta = \Theta_{M_{xw}}(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  and  $\theta = \Theta_R(\varepsilon; \varepsilon^+, \theta^+, \varepsilon^-)$  intersect each other again. Let us note that this point has to be a saddle point like  $(\varepsilon^-, \theta^-)$ . The chord condition is satisfied for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$  and if the "viscosity" dominates heat conduction it is obvious that a shock layer connecting  $(\varepsilon^\pm, \theta^\pm)$  exists. Instead, if the "viscous" effects are negligible with respect to heat conduction effects, it is possible that there is no trajectory connecting  $(\varepsilon^-, \theta^-)$  with  $(\varepsilon^+, \theta^+)$ . Indeed, for fixed  $\kappa$  and  $\mu \rightarrow 0$ , the trajectory  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \bar{\kappa})$  leaving the saddle point  $(\varepsilon^-, \theta^-)$  is almost horizontal and must enter in the region between  $R(\varepsilon, \theta; \varepsilon^+, \theta^+, \varepsilon^-) = 0$  and  $H_{M_{xw}}(\varepsilon, \theta; \varepsilon^+, \theta^+, \varepsilon^-) = 0$ , for  $\varepsilon > \varepsilon_0$ . Since in this region  $H_{M_{xw}} > 0$  and  $R > 0$  the trajectory must be monotone increasing ( $\varepsilon$  increasing,  $\theta$  increasing). Consequently, the trajectory can not more reach the critical point  $(\varepsilon^+, \theta^+)$ . Such an explicit example has been constructed by Pego [6] for gas dynamics equations in order to exemplify that there may be a wave discontinuity which satisfies the chord criterion, but for which a profile layer does not exist if the heat conduction dominates the "viscosity".

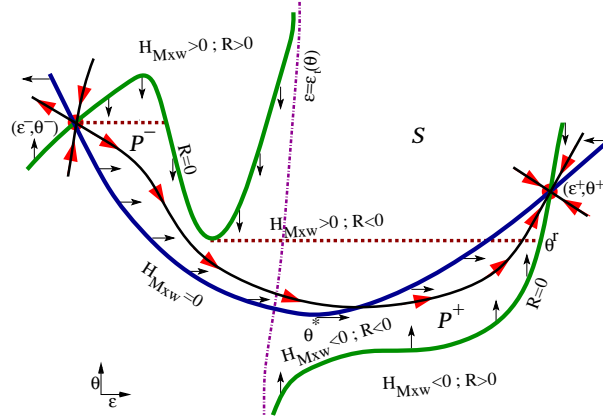
*Case C3.*  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^+, \theta^+) > 0$  and  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^-, \theta^-) < 0$ , i.e. different signs of the Grüneisen coefficient at the critical points.

That means,  $(\varepsilon^-, \theta^-)$  belongs to the region  $D^-$  where  $\frac{\partial \sigma_{eq}}{\partial \theta} < 0$ , that is, where  $\varepsilon < \varepsilon_t(\theta)$  and  $(\varepsilon^+, \theta^+)$  belongs to the region  $D^+$  where  $\frac{\partial \sigma_{eq}}{\partial \theta} > 0$ , that is, where  $\varepsilon > \varepsilon_t(\theta)$  (Fig. 2). A typical compressive jump discontinuity  $M^+ \rightarrow M^-$  is illustrated in Fig. 3c and Fig. 7.

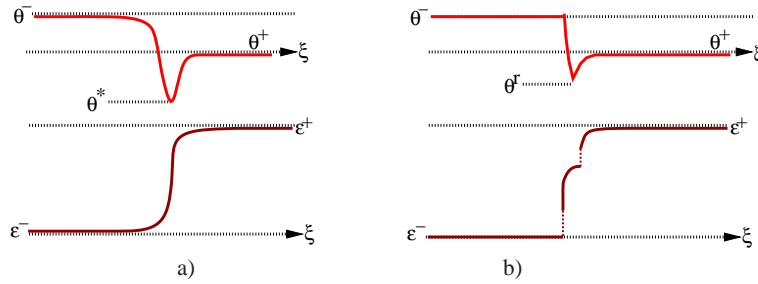
We **recall** that the chord condition (64) requires that the inequalities (70) be satisfied. We suppose first that the inequalities are strict. That means  $(\varepsilon^-, \theta^-)$  is a *saddle point* and  $(\varepsilon^+, \theta^+)$  is an *attractive point*.

By using relation (68) one gets that  $\frac{d\Theta_{M_{xw}}(\varepsilon^-)}{d\varepsilon} < 0$  and  $\frac{d\Theta_{M_{xw}}(\varepsilon^+)}{d\varepsilon} > 0$ . Therefore,  $\theta = \Theta_{M_{xw}}(\varepsilon)$  must necessarily be a *non-monotone* function. It is monotone decreasing in the neighborhood of  $\varepsilon^-$  and monotone increasing in the neighborhood of  $\varepsilon^+$ . Moreover, by using the chord condition (64) and relation (66) one gets that the branch of the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$  which lies in  $D^-$  is monotone decreasing. This reflects the fact that, on this part of the trajectory of a "viscous", heat non-conducting profile layer, both the intrinsic dissipation and the latent heat contribute to the heating process inside the layer. After the intersection with  $\varepsilon = \varepsilon_t(\theta)$ , the function  $\theta = \Theta_{M_{xw}}(\varepsilon)$  reaches a minimum point at  $(\varepsilon^*, \theta^*)$  and we suppose, that later on, it is monotone increasing as in Fig. 7. This situation always happens if the additional restrictions (92) are satisfied. On this part of the trajectory of the "viscous", heat non-conducting profile layer, the intrinsic dissipation contributes to the heating, while the latent heat contribute to the cooling process inside the layer. Let us note that we can not say anything about the order relation between  $\theta^+$  and  $\theta^-$ .

Since the Grüneisen coefficients have different signs at the critical points it follows that the implicit equation  $R(\varepsilon, \theta) = 0$ , given by (55), is representable, and we assume that globally, by two functions of  $\varepsilon$ . One branch  $\theta = \Theta_R^-(\varepsilon)$ , passing through  $(\varepsilon^-, \theta^-)$ , lies in the domain  $D^-$  and satisfies  $R(\varepsilon, \Theta_R^-(\varepsilon)) = 0$  and  $\sigma_R(\varepsilon) = \sigma_{eq}(\varepsilon, \Theta_R^-(\varepsilon))$  on the corresponding interval of definition. The second branch  $\theta = \Theta_R^+(\varepsilon)$ , passing



**Fig. 7** Case C3 - phase portrait of (54) for the  $M^+ \rightarrow M^-$  phase transformation illustrated in Fig. 3c.



**Fig. 8** Case C3 - temperature spike-layers and strain interphase transition layers corresponding to Fig. 7. a) "viscous" ( $\mu > 0$ ), heat non-conducting layer ( $\kappa = 0$ ); b) "non-viscous" ( $\mu = 0$ ), heat conducting ( $\kappa > 0$ ).

through  $(\varepsilon^+, \theta^+)$ , lies in the domain  $D^+$  and satisfies  $R(\varepsilon, \Theta_R^+(\varepsilon)) = 0$  and  $\sigma_R(\varepsilon) = \sigma_{eq}(\varepsilon, \Theta_R^+(\varepsilon))$  on the corresponding interval of existence. Relations (87) and (88) are still valid for each branch and we get that  $\frac{d\Theta_R^-(\varepsilon^-)}{d\varepsilon} > \frac{d\Theta_{Mxw}^-(\varepsilon^-)}{d\varepsilon}$  and  $\frac{d\Theta_R^+(\varepsilon^+)}{d\varepsilon} > \frac{d\Theta_{Mxw}^+(\varepsilon^+)}{d\varepsilon} > 0$ . Therefore,  $\theta = \Theta_R^+(\varepsilon)$  is an increasing function of  $\varepsilon$  in the neighborhood of  $\varepsilon^+$  and moreover  $\Theta_R^+(\varepsilon) < \Theta_{Mxw}(\varepsilon)$  in  $D^+$  for  $\varepsilon < \varepsilon^+$ . Indeed, this inequality can be proved by taking into account that it is satisfied in a neighborhood of  $\varepsilon^+$  and from the fact that  $\theta = \Theta_R^+(\varepsilon)$  (even non-monotone) cannot intersect  $\theta = \Theta_{Mxw}(\varepsilon)$  a second time without violating the chord condition (64). In a similar way one shows that  $\Theta_R^-(\varepsilon) > \Theta_{Mxw}(\varepsilon)$  in  $D^-$  for  $\varepsilon > \varepsilon^-$ .

Let us note that  $\theta = \Theta_R^-(\varepsilon)$  has to be a non monotone function. Indeed, when  $(\varepsilon, \Theta_R^-(\varepsilon)) \in I^- \subset D^-$  (see Fig. 2) we have  $\frac{\partial \sigma_{eq}(\varepsilon, \Theta_R^-(\varepsilon))}{\partial \varepsilon} < 0$  and we get from (87) that  $\theta = \Theta_R^-(\varepsilon)$  is monotone decreasing. When  $\theta = \Theta_R^-(\varepsilon)$  enters on that part of the austenitic domain  $A \subset D^-$ , it must end with a positive slope since otherwise would intersect the curve  $\theta = \Theta_{Mxw}(\varepsilon)$ , which would contradict the chord criterion. Therefore, there exists a point  $(\varepsilon^r, \theta^r) \in D^-$  where the branch  $\theta = \Theta_R^-(\varepsilon)$  reaches its minimum and for simplicity we assume that its form is as shown in Fig. 7. We suppose first that  $\theta^r < \theta^+$ .

The existence of a profile layer, follows now from the following topological considerations. We denote by  $P^-$  the simply connected region bounded from above by  $\theta = \Theta_R^-(\varepsilon)$ , from the right by  $\varepsilon = \varepsilon_t(\theta)$  and from below by  $\theta = \Theta_{Mxw}(\varepsilon)$ . We denote by  $P^+$  the simply connected region bounded from below by  $\theta = \Theta_R^+(\varepsilon)$ , from the left by  $\varepsilon = \varepsilon_t(\theta)$  and from above by  $\theta = \Theta_{Mxw}(\varepsilon)$ . We denote by  $S$  the simply connected region bounded from below by  $\theta = \Theta_{Mxw}(\varepsilon)$ , from the left by  $\varepsilon = \varepsilon_t(\theta)$  and from the right by  $\theta = \Theta_R^+(\varepsilon)$  for  $\varepsilon > \varepsilon^+$ . Let us note that  $H_{Mxw} > 0$  on the curve  $\theta = \Theta_R^-(\varepsilon)$  for  $\varepsilon > \varepsilon^-$  and  $H_{Mxw} < 0$  on the curve  $\theta = \Theta_R^+(\varepsilon)$  for  $\varepsilon < \varepsilon^+$ . On the other side,  $R < 0$  on the curve  $\theta = \Theta_{Mxw}(\varepsilon)$  for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . Therefore, on the curve  $H_{Mxw} = 0$  all vector fields of the flow induced by (54) point horizontally to the right, for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . On the curve  $\theta = \Theta_R^-(\varepsilon)$  the vector fields point vertically down, while on the curve  $\theta = \Theta_R^+(\varepsilon)$  they point vertically up (Fig. 7). The integral curves of (54), which satisfy  $\frac{d\theta}{d\varepsilon} = \frac{\mu(E - \rho \dot{S}^2) \dot{S}^2}{\kappa E} \frac{H_{Mxw}}{R}$ , have the following properties. For given  $\mu > 0$  and  $\kappa > 0$  they are monotone decreasing in  $P^- \cup S$  and are monotone increasing in  $P^+$ . Since  $(\varepsilon^-, \theta^-)$  is a saddle point, the trajectory starting from this point toward region  $P^-$  is monotone decreasing



and intersects the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$  at a point in the region  $D^+$ . At this point the temperature reaches a minimum value in the profile layer. After entering in the domain  $P^+$  the trajectory is monotone increasing and since it cannot leave this domain it must end at the attractive point  $(\varepsilon^+, \theta^+)$ .

Therefore, when the Grüneisen coefficient has different signs at the critical points the temperature variation inside a "viscous", heat conducting profile layer is *non-monotone*. Moreover, in the compressive case, the temperature reaches lower values than the front and back state temperature (Fig. 7), while in the expansive case it will reach higher values. Thus, the profile layer of the temperature displays a narrow peak (or, spike) pointing down as it is illustrated for instance in Fig. 8. At the point  $\xi_0$  where  $\frac{d\hat{\theta}}{d\xi} = 0$  the heat flux  $q$  changes the sign, that means the heat flux  $q$  changes the direction inside the profile layer. This behavior is in agreement with the fact that, a continuous transformation from variant  $M^+$  to variant  $M^-$  passes through the phase  $A$  and the transformation  $M^+ \rightarrow A$  is endothermic (cooling for  $\xi > \xi_0$ ) while the transformation  $A \rightarrow M^-$  is exothermic (heating for  $\xi < \xi_0$ ) (Fig. 8).

The limit behavior of the profile layers  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \kappa)$  as  $\mu \rightarrow 0$  and/or  $\kappa \rightarrow 0$  can be studied in the same way as in the previous compressive cases.

One observes that when the "viscosity" largely dominates the heat conduction, the trajectory of the connecting integral curve is closer to the curve  $H_{M_{xw}} = 0$ . Moreover, for fixed "viscosity"  $\mu = \bar{\mu}$  and  $\kappa = 0$  the connecting orbit  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \bar{\mu}, 0)$  is solution of the reduced system (60) and matches with the non-monotone curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$ . The corresponding "viscous", *heat non-conducting profile layer* is illustrated in Fig. 8a. It is worth to remark that when  $\mu \rightarrow 0$  the limit of the strain profile  $\hat{\varepsilon}(\xi; \mu, 0)$  is a step discontinuous function whose value is  $\varepsilon^-$  for  $\xi < \xi_0$  and  $\varepsilon^+$  for  $\xi > \xi_0$ . On the other side, due to the spike-layer form of the temperature profiles, the limit of  $\hat{\theta}(\xi; \mu, 0)$ , for  $\mu \rightarrow 0$ , is a discontinuous function whose value is  $\theta^-$  for  $\xi < \xi_0$ ,  $\theta^*$  at  $\xi = \xi_0$  and  $\theta^+$  for  $\xi > \xi_0$ , where  $\theta^*$  represents the minimum value of the function  $\theta = \Theta_{M_{xw}}(\varepsilon)$ , for  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ . For both strain and temperature profiles the convergence for  $\mu \rightarrow 0$  is uniform in  $\xi$  in any closed interval not containing the discontinuity point  $\xi_0$ .

We have to remark that the adiabatic thermoelastic temperature structure with sharp interface does not inherit the temperature structure of the augmented theory. Indeed, the minimum value  $\theta^*$  of  $\theta = \Theta_{M_{xw}}(\varepsilon)$  does not play any role in solving a Riemann problem involving a compressive shock induced  $M^- \rightarrow M^+$  phase transformation in the framework of the adiabatic thermoelastic wave theory. In this approach only the lateral limits  $\theta^\pm$  across the discontinuity are relevant. On the other side, for an adiabatic rate-type approach of the same problem, with small "viscosity"  $\mu$ , the minimum value  $\theta^*$  and the corresponding spike-layer temperature structure may become extremely important, specially when one describes wave interaction phenomena. The prediction of the augmented theory of larger values of the temperature inside the profile layer than the front state and back state temperatures could be extremely important from experimental point of view.

Let us consider the opposite case when the heat conduction largely dominates the "viscosity". In a similar way as in the previous cases one shows that for fixed  $\kappa = \bar{\kappa}$ , as  $\mu \rightarrow 0$ , the trajectories  $(\hat{\theta}(\xi), \hat{\varepsilon}(\xi); \mu, \bar{\kappa})$  of the integral curves of (54) in the region  $D^-$  tend to be closer to a monotone decreasing curve  $\theta = \bar{\Theta}_R^-(\varepsilon)$  of the type (91), while the trajectories of the integral curves in the region  $D^+$  tend to be closer to a monotone increasing curve  $\theta = \bar{\Theta}_R^+(\varepsilon)$  of the type (95). We also note that the intersection point between the trajectory of the profile layer  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); \mu, \bar{\kappa})$  with the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$  moves up as  $\mu \rightarrow 0$ . The corresponding limit value of the temperature is  $\theta^r$ , which is the minimum value of the function  $\theta = \bar{\Theta}_R^-(\varepsilon)$ .

Since the sign of the slope of these trajectories is negative in  $P^- \cup S$  and positive in  $P^+$  one gets that the limit trajectory  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); 0, \bar{\kappa})$  in the  $\varepsilon - \theta$  plane, for the phase portrait in Fig. 7, is composed by: a horizontal line starting at  $(\varepsilon^-, \theta^-)$  and ending at the intersection point with the curve  $\theta = \bar{\Theta}_R^-(\varepsilon)$  (dotted line in Fig. 7), then by the curve  $\theta = \bar{\Theta}_R^-(\varepsilon)$  until its minimum point having the temperature  $\theta^r$ , next by a horizontal line which ends at the intersection point with the curve  $\theta = \bar{\Theta}_R^+(\varepsilon)$  (dotted line in Fig. 7) and finally by the curve  $\theta = \bar{\Theta}_R^+(\varepsilon)$  until the point  $(\varepsilon^+, \theta^+)$ . Thus, for this "non-viscous", *heat conducting profile layer*, illustrated in Fig. 8b, the temperature is continuous, but the strain is discontinuous having isothermal jumps inside the profile layer.

The limit of the "non-viscous", heat conducting profile layer  $(\hat{\varepsilon}(\xi), \hat{\theta}(\xi); 0, \bar{\kappa})$ , as  $\kappa \rightarrow 0$ , has the following properties. The strain profile is a step discontinuous function whose value is  $\varepsilon^-$  for  $\xi < \xi_0$  and  $\varepsilon^+$  for  $\xi > \xi_0$ , while the temperature profile is a discontinuous function whose value is  $\theta^-$  for  $\xi < \xi_0$ ,  $\theta^r$  at  $\xi = \xi_0$  and  $\theta^+$  for  $\xi > \xi_0$  (Fig. 8b).

It should be noted that as  $\mu, \kappa \rightarrow 0$  the iterated limits coincide and are equal with the double limit for any  $\xi \neq \xi_0$ . The difference appears at  $\xi = \xi_0$  where the iterated limits do not coincide more.

The case  $\dot{S}^2 = \lambda^2(\varepsilon^+, \theta^+)$ , or  $\dot{S}^2 = \lambda^2(\varepsilon^-, \theta^-)$  can be treated as previously. The reverse implication that the chord criterion is also a necessary condition for the existence of a connecting orbit and its uniqueness can be also proved. We omit here the details.

When  $\theta^r > \theta^+$  in Fig. 7 two phase portraits similar with those illustrated in Figs. 6 are possible, but we disregard here their analysis.

### 5.2.2 The entropy production in a "viscous", thermally conducting profile layer.

Let the pair  $(\hat{\varepsilon}(\xi; \mu, \kappa), \hat{\theta}(\xi; \mu, \kappa))$  be a traveling wave solution of the system (54). According to the entropy identity (47) and the dissipation relations (32) established for the Maxwellian rate-type material coupled with the Fourier heat conduction law it follows that the total entropy production in a profile layer is given by

$$P_{M_{xw}}^{trav} = -\dot{S} \int_{\Gamma} \frac{(E - \rho \dot{S}^2)}{\theta} \rho \frac{\partial \psi_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \theta)}{\partial \sigma} d\varepsilon + \frac{1}{\theta^2} H_{M_{xw}}(\varepsilon, \theta) d\theta \geq 0, \quad (96)$$

where  $\Gamma = \{(\hat{\varepsilon}(\xi; \mu, \kappa), \hat{\theta}(\xi; \mu, \kappa)) \mid \xi \in (-\infty, \infty)\}$  is the continuous piece-wise smooth curve connecting  $(\varepsilon^-, \theta^-)$  and  $(\varepsilon^+, \theta^+)$  in the  $\varepsilon - \theta$  plane. Let us note that, by using relation (31)<sub>1</sub>, we can prove that the integrand is a total differential. Moreover, one can show that

$$P_{M_{xw}}^{trav} = -\dot{S} \int_{\Gamma} d\left(-\frac{H_{M_{xw}}(\varepsilon, \theta)}{\theta} + \rho \eta_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \theta)\right) = -\dot{S} \rho (\eta_{eq}(\varepsilon^+, \theta^+) - \eta_{eq}(\varepsilon^-, \theta^-)) \geq 0 \quad (97)$$

Therefore, the total entropy production in the profile layer does not depend on "viscosity" or heat conductivity. All the comments in Remark 5 remain valid.

### 5.2.3 The entropy variation inside a profile layer.

Let us denote by  $\theta = \hat{\theta}(\varepsilon; \mu, \kappa)$  the trajectory in the  $\varepsilon - \theta$  plane of the Maxwellian "viscous", heat conducting traveling wave solution of the problem (54). By using the thermodynamic properties established in Sect. 4.1 and relation (48) one gets that, if the strain profile  $\varepsilon = \hat{\varepsilon}(\xi; \mu, \kappa)$  is strictly monotone, the entropy along this trajectory, denoted by  $\eta = \hat{\eta}(\varepsilon; \mu, \kappa) \equiv \eta_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \hat{\theta}(\varepsilon; \mu, \kappa))$ , satisfies relation

$$\rho \frac{d\hat{\eta}(\varepsilon; \mu, \kappa)}{d\varepsilon} = \frac{\rho C_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \hat{\theta}(\varepsilon))}{\hat{\theta}(\varepsilon)} \frac{d\hat{\theta}(\varepsilon)}{d\varepsilon} - \frac{(E - \rho \dot{S}^2)}{(E - \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\tilde{\varepsilon}, \hat{\theta}(\varepsilon)))} \frac{\partial \sigma_{eq}}{\partial \theta}(\tilde{\varepsilon}, \hat{\theta}(\varepsilon)), \quad (98)$$

for  $\varepsilon$  between  $\varepsilon^-$  and  $\varepsilon^+$ , where  $\tilde{\varepsilon}(\varepsilon)$  is the unique solution of equation (67).

a) *Monotonous variation of the entropy inside a "viscous", heat non-conducting profile layer.* We have seen that for fixed  $\mu = \bar{\mu}$  and  $\kappa \rightarrow 0$ ,  $\hat{\varepsilon}(\xi; \bar{\mu}, \kappa)$  and  $\hat{\theta}(\xi; \bar{\mu}, \kappa)$  approach the solution of the reduced system (60) and the curves  $\theta = \hat{\theta}(\varepsilon; \bar{\mu}, \kappa)$  are increasingly close to the curve  $\theta = \Theta_{M_{xw}}(\varepsilon)$ . Therefore, by making  $\kappa \rightarrow 0$  in relation (98) and taking into account that  $\lim_{\kappa \rightarrow 0} \hat{\theta}(\varepsilon; \bar{\mu}, \kappa) = \Theta_{M_{xw}}(\varepsilon)$  and  $\lim_{\kappa \rightarrow 0} \frac{d\hat{\theta}(\varepsilon; \bar{\mu}, \kappa)}{d\varepsilon} = \frac{d\Theta_{M_{xw}}(\varepsilon)}{d\varepsilon}$ , at the points where the derivative makes sense, we obtain by using relation (66) that

$$\rho \frac{d\hat{\eta}(\varepsilon; \mu, 0)}{d\varepsilon} = \frac{(E - \rho \dot{S}^2)}{E} \frac{(\sigma_R(\varepsilon) - \sigma_{eq}(\tilde{\varepsilon}, \Theta_{M_{xw}}(\varepsilon)))}{\Theta_{M_{xw}}(\varepsilon)}, \quad (99)$$

where  $\tilde{\varepsilon}(\varepsilon)$  is given by relation (67). From (39) it results that this relation is just relation (75) already established when investigating the entropy production in a "viscous", heat non-conducting profile layer.

It is obvious now that for the compressive case, when  $\varepsilon^- < \varepsilon^+$ , the chord condition (64) requires that the entropy  $\eta = \hat{\eta}(\varepsilon; \bar{\mu}, 0)$  in a "viscous", heat non-conducting profile layer be a *strictly decreasing* function of  $\varepsilon$ , while for the expansive case,  $\varepsilon^+ < \varepsilon^-$ , it requires to be a *strictly increasing* function of  $\varepsilon$ .

By using continuity arguments, we expect that this property of monotonicity of the entropy inside a profile layer remains valid when the "viscosity" effect largely dominates the heat conductivity effect.

b) *Non-monotonous variation of the entropy inside a "non-viscous", heat conducting profile layer.* We show now that when the heat conductivity effect largely dominates the "viscosity" effect the variation of the entropy  $\eta = \hat{\eta}(\xi)$ , for  $\xi \in (-\infty, \infty)$ , is *non-monotone* and even more its value can become inside the profile layer lower than the front state value  $\eta^+$  and/or larger than Hugoniot back state value  $\eta^- > \eta^+$ . This phenomenon of entropy overshoot or undershoot has been mentioned for instance by Landau and Lifschitz [41, Chap. IX, §87] in gas dynamics and by Dunn and Fosdick [13] in thermoelastic materials.

We recall that for fixed  $\kappa = \bar{\kappa}$  and  $\mu \rightarrow 0$  the pair  $\hat{\varepsilon}(\xi; \mu, \bar{\kappa})$  and  $\hat{\theta}(\xi; \mu, \bar{\kappa})$  approach the solution of the reduced system (90), which describes a "non-viscous", heat conducting profile layer, and its trajectory in the  $\varepsilon - \theta$  plane,  $\theta = \hat{\theta}(\varepsilon; \bar{\mu}, \bar{\kappa})$  is increasingly close to the curve  $\theta = \bar{\Theta}_R(\varepsilon)$  defined by (91), or by (95), depending on the monotonicity of the function  $\theta = \Theta_R(\varepsilon)$ . Therefore, by making  $\mu \rightarrow 0$  in relation (98) and taking into account that  $\lim_{\mu \rightarrow 0} \hat{\theta}(\varepsilon; \mu, \bar{\kappa}) = \bar{\Theta}_R(\varepsilon)$ , and  $\lim_{\mu \rightarrow 0} \frac{d\hat{\theta}(\varepsilon; \mu, \bar{\kappa})}{d\varepsilon} = \frac{d\bar{\Theta}_R(\varepsilon)}{d\varepsilon}$ , at the points where the derivative makes sense, we obtain

$$\rho \frac{d\hat{\eta}(\varepsilon; 0, \bar{\kappa})}{d\varepsilon} = \frac{\rho C_{M_{xw}}(\varepsilon, \sigma_R(\varepsilon), \bar{\Theta}_R(\varepsilon))}{\bar{\Theta}_R(\varepsilon)} \frac{d\bar{\Theta}_R(\varepsilon)}{d\varepsilon} - \frac{(E - \rho \dot{S}^2) \frac{\partial \sigma_{eq}}{\partial \theta}(\tilde{\varepsilon}, \bar{\Theta}_R(\varepsilon))}{\left(E - \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\tilde{\varepsilon}, \bar{\Theta}_R(\varepsilon))\right)} \quad (100)$$

where  $\tilde{\varepsilon}(\varepsilon)$  is the unique solution of equation (35) for  $\sigma = \sigma_R(\varepsilon)$  and  $\theta = \bar{\Theta}_R(\varepsilon)$ .

Let us note that, according to the definition (91), or (95) of function  $\theta = \bar{\Theta}_R(\varepsilon)$ , the expression of  $\frac{d\bar{\Theta}_R(\varepsilon)}{d\varepsilon}$  is given by relation (87) on the open intervals on which  $\bar{\Theta}_R(\varepsilon) \equiv \Theta_R(\varepsilon)$ , or  $\frac{d\bar{\Theta}_R(\varepsilon)}{d\varepsilon} = 0$  on the open intervals on which  $\bar{\Theta}_R(\varepsilon) \neq \Theta_R(\varepsilon)$ , i.e. on the intervals on which  $\bar{\Theta}_R(\varepsilon)$  is constant.

We are interested to calculate the expression of (100) at  $\varepsilon = \varepsilon^\pm$ . By using relation (87) at the critical points  $(\varepsilon^\pm, \theta^\pm)$  one gets

$$\rho \frac{d\hat{\eta}(\varepsilon^\pm; 0, \bar{\kappa})}{d\varepsilon} = \begin{cases} \frac{\rho^2 C_{eq}(\varepsilon^\pm, \theta^\pm) (\dot{S}^2 - \lambda^2(\varepsilon^\pm, \theta^\pm))}{\theta^\pm \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^\pm, \theta^\pm)}, & \text{if } \frac{d\bar{\Theta}_R(\varepsilon^\pm)}{d\varepsilon} \neq 0, \\ -\frac{(E - \rho \dot{S}^2)}{\left(E - \frac{\partial \sigma_{eq}}{\partial \varepsilon}(\varepsilon^\pm, \theta^\pm)\right)} \frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^\pm, \theta^\pm), & \text{if } \frac{d\bar{\Theta}_R(\varepsilon^\pm)}{d\varepsilon} = 0. \end{cases} \quad (101)$$

where  $\lambda(\varepsilon, \theta)$  is according to (18) the sound speed of the adiabatic thermoelastic system.

Let us consider for illustration the case C3, when  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^+, \theta^+) > 0$ ,  $\frac{\partial \sigma_{eq}}{\partial \theta}(\varepsilon^-, \theta^-) < 0$  and the phase portrait is illustrated in Fig. 7. We have already established that in this case  $\frac{d\bar{\Theta}_R(\varepsilon^+)}{d\varepsilon} < 0$  and  $\dot{S}^2 - \lambda^2(\varepsilon^+, \theta^+) \geq 0$ , since  $(\varepsilon^+, \theta^+)$  is an attractive node. One gets from (101)<sub>1</sub> that  $\hat{\eta}'(\varepsilon^+; 0, \bar{\kappa}) > 0$ . At the critical point  $(\varepsilon^-, \theta^-)$  where  $\dot{S}^2 - \lambda^2(\varepsilon^-, \theta^-) \leq 0$  we have two possibilities concerning the value of  $\frac{d\bar{\Theta}_R(\varepsilon^-)}{d\varepsilon}$ . First, if  $\frac{d\bar{\Theta}_R(\varepsilon^-)}{d\varepsilon} > 0$ , like in Fig. 7, then  $\frac{d\bar{\Theta}_R(\varepsilon^-)}{d\varepsilon} = 0$  and according to (101)<sub>2</sub> it results that  $\hat{\eta}'(\varepsilon^-; 0, \bar{\kappa}) > 0$ . Second, if  $\frac{d\bar{\Theta}_R(\varepsilon^-)}{d\varepsilon} = \frac{d\bar{\Theta}_R(\varepsilon^-)}{d\varepsilon} < 0$ , then according to (101)<sub>1</sub> it follows that  $\hat{\eta}'(\varepsilon^-; 0, \bar{\kappa}) > 0$ .

Therefore, the entropy  $\eta = \hat{\eta}(\varepsilon; 0, \bar{\kappa})$ ,  $\varepsilon \in (\varepsilon^-, \varepsilon^+)$ , is an increasing function of  $\varepsilon$  in the neighborhoods of  $\varepsilon^-$  and  $\varepsilon^+$ ,  $\varepsilon^- < \varepsilon^+$ . Since  $\eta^- = \hat{\eta}(\varepsilon^-; 0, \bar{\kappa}) > \eta^+ = \hat{\eta}(\varepsilon^+; 0, \bar{\kappa})$  it results that the entropy in a neighborhood of  $\varepsilon^-$ , for  $\varepsilon > \varepsilon^-$  is larger than the back state entropy  $\eta^-$  and its value in the neighborhood of  $\varepsilon^+$ , for  $\varepsilon < \varepsilon^+$  is lower than the front state entropy  $\eta^+$ . As a result, the entropy has inside the profile layer an interior absolute maxima which overshoots the Hugoniot back state entropy  $\eta^-$  and an absolute minima which undershoots the front state entropy  $\eta^+$ .

In a similar way one shows that in case C1 the entropy inside a "non-viscous", heat conducting profile layer overshoots the back state entropy  $\eta^- > \eta^+$  and in case C2 the entropy undershoots the front state entropy  $\eta^+$ .

By using continuity arguments one gets that the non-monotonous variation of the entropy and the phenomena of entropy overshoot and entropy undershoot always occur when the heat conductivity effect dominates the "viscosity" effect.

## 6 Summary

We consider that knowledge of temperature variation is critical in studies of phase transition phenomena and that the transition from one stable phase to another does not occur instantaneously. For that reason we introduce a dissipative mechanism governed by a Maxwellian rate-type constitutive equation and by heat conduction. The equilibrium of this model is described by a thermoelastic relation with the typical feature that the Grüneisen coefficient changes its sign. The thermodynamic properties of the Maxwellian model are systematically used in investigating the existence, uniqueness and the structure of shock and interphase layers.

We show how steady wave profiles reflect, on one side, the exothermic or endothermic character of phase transitions, and on the other side, the effect of internal dissipative mechanism. It is emphasized that the variation of the temperature inside a "viscous", heat non-conducting profile layers results from the competition between the cooling/heating effect due to the latent heat, and the heating effect due to the intrinsic dissipation. Based on this observation additional constitutive assumptions are discussed for phase transforming materials.

For a  $M^+ \rightarrow M^-$  impact induced phase transformation, when the sign of the Grüneisen coefficient changes inside the layer, the temperature variation has a spike-layer form. Therefore, the experimental detection that a particle, during the passage of a wave, can experience lower or larger temperatures than that at its front state and back state could provide valuable information on the presence of an interphase layer and on the time of transition between phases.

We also discuss when the *chord criterion with respect to the Hugoniot locus in the strain-stress space* is a necessary and sufficient condition for the existence of a profile layer and its role as admissibility condition for discontinuous solutions of the adiabatic thermoelastic system.

The profound difference in the effect of "viscosity" and of heat conduction on the structure of the profile layers (possible existence of isothermal jumps inside a profile layer) and on the behavior of the entropy inside the profile layer (the phenomenon of entropy overshoot, or undershoot) have been discussed.

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