Shock-Induced Martensitic Phase Transitions I: Critical Stresses, Two-wave Structures, Riemann Problems
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Abstract

We consider a class of shock-loading experiments which, as a result of solid-to-solid phase transitions, give rise to certain characteristic patterns consisting of two shock-like waves. We show that the single assumption that stresses in a phase cannot lie beyond the transition boundaries leads to a complete description of the observed phenomena. The model presented here is different from others proposed in the literature: it does not make use of kinetic relations and it accounts for the observed wave histories without parameter fitting. The present paper focuses on the basic mathematical description of our model and it presents solutions to the complete set of Riemann problems which could arise as a result of dynamic interactions — including the basic two-wave structures mentioned above. In the companion paper, based on our Riemann solver and appropriate equations of state (EOS), we solve initial boundary value problems associated with a variety of experimental configurations. There we show that, in presence of well-accepted EOS for the pure phases, our model leads to close quantitative agreement with a wide range of experimental results.

1 Introduction

Ever since the famous 1956 experiments by Bancroft et al. leading to the discovery of the $\alpha$-\(\epsilon\) transition in iron (Bancroft et al., 1956), shock-induced polymorphic phase transitions in solids have received sustained attention in the literature. Shock waves in solids are often produced by the impact of a (planar) projectile which leads to (essentially planar) fronts propagating through a flat slab. The phase transitions we consider manifest themselves through a rather peculiar phenomenon: upon impact, not one but two parallel shock-fronts are induced in the slab. In this paper we show that a single, well-substantiated critical condition captures the essence of the phenomena under consideration. As shown in the companion paper (Part II), our model results in predictions in close quantitative agreement with a wide variety of experimental results and, unlike other models considered previously, it does not require use of fitting parameters.
In this paper we focus on the basic mathematical description of our model and we present solutions to the complete set of Riemann problems which could arise as a result of dynamic interactions — including the basic two-wave structures mentioned above. This Riemann solver will be used in Part II as a building block for solutions of the general initial and boundary value problems arising in experiment.

The main emphasis of previous analyses (Vlodarchik & Trebinski, 1997; Boettger & Wallace, 1997) lies on metastability and the kinetics of the transformation processes. The resulting models depend on a variety of material parameters and functions which are difficult to obtain. As we shall show, the major aspects of the shock-induced transition processes under consideration can in fact be captured without recourse to such detailed information. Secondary corrections to our model, including deviation from planarity — due to the influence of edges and the finite size of specimens — as well as effects associated with microstructure and partial transformation of the material, which are not discussed here, can also be incorporated.

As mentioned above, in the experiments under consideration phase transitions result from the impact of a planar projectile on the free surface of a flat slab. The impact occurs at the surface labeled ITI (Impactor-Target Interface); manifestations of the ensuing phenomena are recorded through the particle-velocity histories at the surface opposite to the ITI. Typical experimental particle-velocity histories are shown in the left portions of Figure 1; note the rather prominent two-wave structure manifested in these graphs. It is known that such two-wave structures are intimately related to phase transitions. As a characteristic feature of these waves we note their extremely short rise-times. Our description of the physics of such processes is based, in fact, on consideration of their fast dynamics, which has been recognized before as clear evidence of the martensitic nature of the shock-induced phase transition (Duvall & Graham, 1977; Al'tshuler, 1978; Davison & Graham, 1979; Brown & McQueen, 1986; Erskine & Nellis, 1992).

Martensitic transformations are non-diffusive: they arise as a result of transitions between two crystal structures. These transitions, which are characterized by cooperative motions of many atoms, lead to fast (and large) macroscopic shape changes. The transformation times are extremely small, as is apparent in the vertical portions of experimental curves such as those in Figure 1 (left). An idealized infinite transformation rate leads naturally to the critical stress condition which is the centerpiece of our theory. To introduce our postulate let us consider first a simplified context in which stresses are purely hydrostatic and phase transitions lead to purely dilatational, volume-decreasing shape-changes. In this context, infinite transformation rates imply that, at any given temperature, the pressure in the untransformed (austenitic) phase cannot exceed the pressure of transformation. Indeed, a pressure value above the transformation pressure would lead to immediate transformation to the lower-volume martensitic phase. This reduction of specific volume leads, in turn, to a corresponding immediate reduction in pressure. Our postulate thus follows: the pressure in the austenite cannot exceed a critical value which equals the (temperature dependent) transition pressure — compare the corresponding formulation given in (Bruno et al., 1995) for the low-stress case.

In the context of general stress states, infinite transformation rates imply that the austenitic
Figure 1: Graphite-diamond shock induced transformation experiments. Left: Experimental curves (Erskine & Nellis, 1992). Right: Predictions. Interface velocity profiles are presented for three experiments labeled according to (Erskine & Nellis, 1992). The corresponding impactor velocities are: gF, 2.60 km/s; gG, 3.12 km/s; gD, 3.47 km/s. As in (Erskine & Nellis, 1992), the curves are staggered horizontally on the graphs for clarity.

phase cannot be subject to stresses outside a certain critical surface. We thus postulate that

1. **The stress in the austenite cannot lie outside a (temperature dependent) critical-stress surface** $S_F$.

2. **The stress in the martensite cannot lie inside a (temperature dependent) critical-stress surface** $S_B$.

It should be noticed that this postulate does not require the critical surface $S_F$ for the forward austenite to martensite transition to coincide with the critical surface $S_B$ for the reverse transition from martensite to austenite. Thus the present framework is fully consistent with the well documented (Duvall & Graham, 1977) existence of pressure hysteresis. Also, for single crystals (or, indeed, highly oriented polycrystals) our postulate implies that the transformation is completed across an infinitely thin front, and no regions of mixed phases occur. In lower grade polycrystals and for certain ranges of stresses, however, a transition from austenite to an austenite-martensite mixture with various volume fractions is possible (Duvall & Graham, 1977; Al’tshuler, 1978; Erskine & Nellis, 1992). The relevant relationships between stresses and corresponding transformation patterns in a polycrystal can be obtained through rigorous homogenization procedures similar to those considered in (Bruno et al., 1996). A full investigation of the details of shock induced phase transitions under such general conditions will be left for future work.
This paper is organized as follows: after a qualitative description presented in Section 2, Section 3 introduces the necessary notations and formalisms. The discussion of wave curves of Section 4.2 constitutes the main portion of this paper, from which the Riemann solver of Section 5 follows directly. Solutions of a variety of initial boundary value problems and corresponding comparisons with experiment are presented in the companion paper II. Here we merely point out that the profiles resulting from our theory are in close quantitative agreement with those obtained experimentally (as illustrated in Figure 1), and that, as shown in part II, in some cases our model predicts sequences of events which differ from those generally accepted.

2 Plane Shock Configuration: Qualitative description

As we mentioned above, we consider shock-compression experiments which result from the the impact of a planar projectile on a planar slab; see Figure 2. Velocity measurements are taken in the central part of the face of the target opposite to the ITI. The ratio of the lateral to the transversal dimensions is always chosen so that all the measurements are completed before the arrival of any release wave originating at the lateral faces of the slab. This assumption allows us to assume the slab is of infinite lateral extent, and that the motion is one-dimensional — in the direction of the coordinate axis $x_1$ normal to the ITI.

The flyer-target impact results in a virtually discontinuous velocity increase of the impacted target boundary. To present our interpretation of the underlying physical processes and the origin of the two wave structure, however, we begin with a description of the initial stages of the experiment, when the velocity of the impactor-target interface (ITI) rises continuously from zero to a certain value $u^*$ in a very small but nonzero time interval $t^*$. (The $t^* = 0$ limit is, of course, completely appropriate in our context; corresponding explicit solutions are described in the latter portions of this paper.)

Initially the target is in the austenitic standard state — that is, the austenite at zero velocity $u = 0$, at zero normal stress, and with specific volume $v = v_r$ as measured at room temperature. (In this paper the negative of the normal stress is denoted by the symbol $q$; we are presently assuming that initially $q = 0$ in the target. Note that, for a hydrostatic stress $q$ equals the pressure $p$.) At $t = 0$ the flyer, which is traveling at speed $u_f$, hits the target. After this time the ITI is subject to a positive acceleration $\ddot{X}(t) > 0$ and, after a small time interval $t^*$, the target boundary travels at an essentially constant speed $u^* = \dot{X}(t^*)$. For sufficiently small values of $u_f$ the negative normal stress $q$ will remain below its critical value $q_{\text{crit}}$ throughout the sample and no transformation will occur. Thus, this case, which is mathematically equivalent to the classical problem of shock-wave generation resulting from the compressive motion of a piston (Courant & Friedrichs, 1948), leads to a single regular shock traveling through the target.

At a certain higher value of $u_f = u_{f,\text{crit}}$ the critical stress $q_{\text{crit}}$ will be attained at a single surface within the sample, namely the ITI, but a higher value of $q$ will not occur at any time within the target. According to our model, thus, no phase transitions are feasible in this case.
either, and a single shock configuration again results. Let us consider, then, a slightly higher value of $u_f$ for which such a single shock structure is no longer viable in our model. For such larger values of $u_f$ a single shock configuration would result in a growing layer of super-critical stress behind the first shock and adjacent to the ITI (Courant & Friedrichs, 1948). In this case, thus, the austenite at the ITI is eventually unable to sustain the stress imposed on it, and, therefore, the ITI acceleration must be accommodated through the volume-decreasing phase transition. That is, a thin layer in the target adjacent to the ITI transforms into martensite and the austenite-martensite interface moves into the material following the first shock. All of the material between the ITI and the moving transition front is in the martensite phase. The speed of this austenite-martensite interface is exactly the one needed in order to keep all austenite stresses $q$ at or below critical values; naturally, the speed of the transformation front increases with $u_f$.

The two-wave structure thus emerges directly from our main postulate. Now, taking the limit as $t^* \to 0$ we obtain the appropriate discontinuous description: the ITI velocity first jumps from 0 to $u^*$ instantaneously and, from then on, it remains equal to $u^*$. For $t > 0$ and before wave reflections and interactions occur, three alternatives are possible depending on the magnitude of $u_f$: there may be a single shock, a shock followed by a transition front (see Figure 2) or a single transition front. To visualize the occurrence of the latter case consider a sequence of two-wave experiments with subsequently increasing values of $u_f$. The speed of the transition front will increase accordingly and, at a certain value $u_f = u_{f,\text{doub}}$, it will equal the

Figure 2: Impact experiment: An illustration of the two-wave structure.
shock speed. (Note that the speed of the shock wave stays constant for \( u_{f, \text{crit}} \leq u_f \leq u_{f, \text{doub}} \) since the stress in the region between the shock and the transition front must necessarily assume its critical value, as explained below.) Clearly, a single transition front structure will occur for all higher values of \( u_f \).

Note that, in this \( t^* = 0 \) limit, all discontinuities are initiated at the origin \( x = 0 \) at time \( t = 0 \), and they move with constant speeds. The state of the material between any two discontinuities is uniform, and it is determined by a triple \((v, q, u)\) of values which does not vary with time. Consequently, to solve our problem in its initial stages we need to obtain the velocities of the discontinuities as well as the triples \((v, q, u)\) for the regions between discontinuities. Additional waves will arise as a result of interactions with material boundaries, and between previously formed waves; the rest of this paper provides a solutions to the Riemann problems associated with such initial boundary value problems.

3 Mathematical Formulation: Uniaxial Strain

Our description of basic nonlinear continuum dynamics follows (Truesdell & Noll, 1965; Marsden & Hughes, 1983; Hill, 1961). The Cartesian and reference coordinates of a point at time \( t \) are denoted by \( x_i = x_i(t) \) and \( X_i, i = 1, 2, 3 \), respectively. The deformation is given by \( x_i = \chi_i(X_1, X_2, X_3, t) \); if the configuration at \( t = t_0 \) is used for reference we then have \( X_i = \chi_i(X_1, X_2, X_3, t_0) \).

In the uniaxial case relevant to the configurations discussed in Section 2 the deformation takes the form

\[
x_1 = \chi_1(X_1, t), \quad x_2 = X_2, \quad x_3 = X_3,
\]

and all variables are independent of \( X_2 \) and \( X_3 \). Thus, we only need to consider the coordinates \( X = X_1, x = x_1 \) and the first component of the deformation vector, which we denote by and \( \chi = \chi_{, 1} \).

The particle velocity vector \( u_i = D\chi_i/Dt \) corresponding to the deformation (1) has only one non-zero component \( u = u_1 \equiv \chi_{, 1} \). The deformation gradient \( F_{ij} = \partial \chi_i / \partial X_j \) corresponding to the deformation (1) is diagonal with the components \( F = F_{11} \equiv \chi, \ F_{22} = F_{33} = 1 \). The material strain tensor corresponding to the deformation (1) has only one non-zero component \( E_{11} = \frac{1}{2}(F^2 - 1) \). The volumetric strain is \( J = F \), and the densities in the reference and the current configurations are related to the strain by the expression \( \rho_R / \rho = F \). The specific volume is defined as the inverse of the density \( v = 1 / \rho \).

The thermodynamic properties of a single-phase thermoelastic medium are completely determined by its specific internal energy \( U(E_{ij}, S) \) as a function of the strain \( E_{ij} \) and the specific entropy \( S \). Then the Cauchy stress tensor \( \tau_{ij} \) and the temperature \( \theta \) are expressed through the
first derivatives of $U$:

$$
\tau_{ij} = \rho F_{im} \frac{\partial U}{\partial E_{mn}} F_{jn}, \quad \theta = \frac{\partial U}{\partial S}.
$$

(2)

In particular, the Cauchy stress tensor corresponding to the deformation (1) is given by the following equations

$$
\tau_{11} = (\rho_R v) \frac{\partial (\rho_R U)}{\partial E_{11}}, \quad \tau_{ij} = (\rho_R v)^{-1} \frac{\partial (\rho_R U)}{\partial E_{ij}}, \quad \text{and} \quad \tau_{11} = \tau_{i1} = \frac{\partial (\rho_R U)}{\partial E_{11}},
$$

(3)

with $i, j = 1, 2$.

### 3.1 Dynamics

The evolution of the material is governed by the equations of conservation of mass, momentum and energy. Since the first derivatives of $\chi(X, t)$ are allowed to be piece-wise smooth functions, the conservation laws will take different forms in regions of smoothness and at discontinuity surfaces. (Across such a surface the derivatives of the deformation with respect to coordinates and time become discontinuous together with the components of the strain and stress tensors, while the deformations themselves remain continuous. We note that in the uniaxial strain case considered here any discontinuity surface is actually a discontinuity plane.)

In smooth regions the conservation laws are given by the partial differential equations

$$
\frac{D}{Dt} u = \frac{\partial u}{\partial \xi}, \quad \frac{D}{Dt} u = \frac{\partial u}{\partial \tau_{11}}, \quad \frac{D}{Dt} \left( U + \frac{1}{2} u^2 \right) = \frac{\partial}{\partial \xi} (\tau_{11} u)
$$

(4)

where $\xi = \rho_R X$ denotes Lagrangian mass coordinate; see (Courant & Friedrichs, 1948). At discontinuity surfaces the conservation laws take form of jump conditions

$$
\mathcal{M} [v] + [u] = 0, \quad \mathcal{M} [u] + [\tau_{11}] = 0, \quad \mathcal{M} \left[ U + \frac{1}{2} u^2 \right] + [u \tau_{11}] = 0.
$$

(5)

Here the jump $[Q]$ in a quantity $Q$ is defined by $[Q] = Q^b - Q^a$, where $Q^b$ and $Q^a$ are the limiting values of $Q$ behind and ahead of the discontinuity, respectively. (As usual, the side
of the discontinuity through which the material particles enter is called the side ahead of the discontinuity.) The quantity $\mathcal{M}$ equals the speed of propagation of the discontinuity surface with respect to the Lagrangian mass coordinates $\xi$; note that the (non-negative) mass flux across the discontinuity is given by

$$ M = |\mathcal{M}|. \quad (6) $$

The Eulerian speed of propagation of the discontinuity surface $s$ is related to $\mathcal{M}$ through the expression

$$ \mathcal{M} = (s - u^a) \rho^a = (s - u^b) \rho^b. \quad (7) $$

In the uniaxial strain case considered here the normal stress $\tau_{11}$ is distinguished from the other components of the stress tensor. Indeed, $\tau_{11}$ is the only component explicitly entering the equations of motion (4) and (5). Once $\tau_{11}$ is found from (4) and (5), the other components of the stress tensor can be obtained from equations (3)\_2, (3)\_3 and, thus, the single quantity $\tau_{11}$ determines the entire stress tensor. To streamline our presentation along the intuition familiar in inviscid gas dynamics, however, we shall use the negative normal stress

$$ q = -\tau_{11} \quad (8) $$

as the single stress variable. In the hydrostatic case $q$ is equal to the pressure, $p = - (\tau_{11} + \tau_{22} + \tau_{33})/3$; in the general case, however, $q = p + ((\tau_{22} - \tau_{11}) + (\tau_{33} - \tau_{11}))/3 \neq p$. Using the variable $q$ equations (4) and (5) become

$$ \frac{D}{Dt} v = \frac{\partial}{\partial \xi} u, \quad \frac{D}{Dt} u = - \frac{\partial}{\partial \xi} q, \quad \frac{D}{Dt} \left( U + \frac{1}{2} u^2 \right) = - \frac{\partial}{\partial \xi} (qu). \quad (9) $$

and

$$ \mathcal{M}[v] + [u] = 0, \quad \mathcal{M}[u] - [q] = 0, \quad \mathcal{M} \left[ U + \frac{1}{2} u^2 \right] - [uq] = 0. \quad (10) $$

respectively.

As in gas dynamics, the Riemann problem — for which the initial data $\Sigma = (v, q, u)$ consists of two distinct spatially constant states

$$ \Sigma(\xi, t = 0) = \begin{cases} \Sigma^L, & \text{if } \xi < \xi_0 \\
\Sigma^R, & \text{if } \xi > \xi_0 \end{cases} \quad (11) $$
on the sides of the jump discontinuity $\xi = \xi_0$ — plays a central role in the study of the dynamics of solids capable of phase transitions. In Section 5 we provide the general solution for such Riemann problems; in Part II, those results are used to construct solutions for the general piecewise constant initial value problems arising in applications.

### 3.2 Equation of State

As we have mentioned, our description of media capable of phase transitions requires introduction of certain critical surfaces $S_F$ and $S_B$ (in 7-dimensional stress-temperature space) in addition to the EOSs $U^A$ and $U^M$ for the pure austenite and pure martensite phases. The surfaces $S_F$ and $S_B$ characterize the domains beyond which each one of the phases may not exist; they are given by equations of the form

$$T_F(\tau_{ij}, \theta) = 0 \quad \text{and} \quad T_B(\tau_{ij}, \theta) = 0,$$

for certain experimentally determined functions $T_F$ and $T_B$.

The critical surfaces $S_F$ and $S_B$ assume a particularly simple form in the case of uniaxial strain. Indeed, using $(q, \theta)$ as primal thermodynamic variables we can regard equations (12) as curves in the $(q, \theta)$-plane

$$T_F(\tau_{ij}, \theta) = T_F(\tau_{ij}(q, \theta), \theta) = T_F(q, \theta) = 0,$$

$$T_B(\tau_{ij}, \theta) = T_B(\tau_{ij}(q, \theta), \theta) = T_B(q, \theta) = 0,$$

which can be solved for $q$ to obtain the critical stress relations

$$q = \bar{q}_F(\theta) \quad \text{and} \quad q = \bar{q}_B(\theta).$$

Combining critical stress relations and pure-phase EOSs we may write a single EOS for the material capable of phase transitions

$$U = \begin{cases} U^A, & \text{if } q < \bar{q}_F(\theta) \\ U^M, & \text{if } q > \bar{q}_B(\theta). \end{cases}$$

**Remark 1** We note that, when the inequalities $\bar{q}_B(\theta) < q < \bar{q}_F(\theta)$ hold, the two phases may coexist. Our postulate is meant to imply, however, that phase transitions only occur when needed to avoid supercritical stresses.

**Remark 2** The general description introduced in the present Part I of this work does not require explicit functional forms for the single-phase specific internal energies $U^A(v, \mathcal{S}, \ldots)$ and $U^M(v, \mathcal{S}, \ldots)$. Here we therefore assume a general thermodynamic description — and general form of the functions $U^A$ and $U^M$ — limited only by the well-accepted thermodynamic
constraints; see e.g. (Menikoff & Plohr, 1988). Specific forms of the well-known single-phase EOSs are reviewed and utilized in Part II of this work, where comparison of predictions with results of experiment are given.

In addition to \((q, \theta)\) we will also use \((v, q)\) as a primal pair. When using \((v, q)\) the equations defining the entropy and temperature will be denoted by

\[
S = \hat{S}(v, q) \quad \text{and} \quad \theta = \hat{\theta}(v, q).
\]

(16)

In these variables the critical stress relations (14) become

\[
q = \hat{q}_F(v) \quad \text{and} \quad q = \hat{q}_B(v),
\]

(17)

respectively.

A few comments are in order with regards to thermodynamic reversibility and entropy changes associated with the types of phase transitions we consider. According to our assumptions, for a mass element in an austenitic critical state \(\Sigma^A_{\text{crit}} = (v^A_{\text{crit}}, q^A_{\text{crit}}, u^A_{\text{crit}})\), any stress increase, whether fully dynamic or quasi-static, must necessarily lead to phase transition. When the transition occurs quasi-statically at constant stress, the new (martensitic) state of the mass element is \(\Sigma^M_{\text{stat}} = (v^M_{\text{stat}}, q^M_{\text{stat}}, u^M_{\text{stat}})\) with \(q^M_{\text{stat}} = q^A_{\text{crit}}, u^M_{\text{stat}} = u^A_{\text{crit}},\) and \(v^M_{\text{stat}}\) determined by the thermodynamics of the process. In case the process is adiabatic, for example, \(v^M_{\text{stat}}\) is determined from the equation \(\hat{H}^M_{\text{stat}}(v^M_{\text{stat}}, q^M_{\text{stat}}) = \hat{H}^A_{\text{crit}}(v^A_{\text{crit}}, q^A_{\text{crit}})\) where \(\hat{H}(v, q) \equiv \hat{U}(v, q) + qv\) denotes the specific enthalpy. If for such a quasi-static adiabatic process there is no dissipation associated with the phase transition, then the transition process is reversible (Duvall & Horie, 1965) and thus, isentropic: \(\hat{S}^M(v^M_{\text{stat}}, q^M_{\text{stat}}) = \hat{S}^A(v^A_{\text{crit}}, q^A_{\text{crit}})\). In case dissipation occurs, in turn, we must have \(\hat{S}^M(v^M_{\text{stat}}, q^M_{\text{stat}}) > \hat{S}^A(v^A_{\text{crit}}, q^A_{\text{crit}})\). In other words, the equations of state of the pure phases must necessarily satisfy the inequality

\[
\hat{S}^M(v^M_{\text{stat}}, q^M_{\text{stat}}) \geq \hat{S}^A(v^A_{\text{crit}}, q^A_{\text{crit}}).
\]

(18)

(We note that the existence of hysteresis between forward and backward phase transitions requires for the strict inequality to hold (Bruno et al., 1995; Leo et al., 1993).)

Similarly, for a mass element in a martensitic a critical state \(\Sigma^M_{\text{crit}} = (v^M_{\text{crit}}, q^M_{\text{crit}}, u^M_{\text{crit}})\), where \(q^M_{\text{crit}} = \hat{q}_B(v^M_{\text{crit}})\), any stress decrease must necessarily lead to phase transition. When the transition occurs quasi-statically at constant stress, the new (austenitic) state of the mass element is \(\Sigma^A_{\text{stat}} = (v^A_{\text{stat}}, q^A_{\text{stat}}, u^A_{\text{stat}})\) with \(q^A_{\text{stat}} = q^M_{\text{crit}}, u^A_{\text{stat}} = u^M_{\text{crit}},\) and \(v^A_{\text{stat}}\) determined by the thermodynamics of the process. The rational of the previous paragraph in this case leads to the inequality \(\hat{S}^A(v^A_{\text{stat}}, q^A_{\text{stat}}) \geq \hat{S}^M(v^M_{\text{crit}}, q^M_{\text{crit}})\).

4 Self-similar waves and wave curves

We begin by noting that, independently of whether stresses are hydrostatic \((q = p)\) or not, equations (9)–(10) are formally identical to the equations governing a one-dimensional flow in
inviscid gas dynamics; c.f. (Courant & Friedrichs, 1948). As a result, the system (9) has many properties in common with the equations governing a one-dimensional inviscid gas flow. (The differences in behavior between gas dynamics and the type of systems we consider presently stem mainly from the peculiar character of the critical-stress postulate described in Section 1, see also equation (15) and Remark 1.) In particular, at any state \( \Sigma = (v, q, u) \), whether austenitic or martensitic, equations (9) form a strictly hyperbolic system of conservation laws with three characteristic fields. The 1st and the 3rd characteristic fields are genuinely nonlinear; the 2nd characteristic field is linearly degenerate. The 1, 2, and 3-characteristic velocities (with respect to the Lagrangian mass coordinates \( \xi \)) are \(-C, 0, +C\) respectively; where \( C \), defined in (20) below, denotes the acoustic impedance. The 1- and 3-characteristics correspond to left- and right-facing sound waves, respectively; the 2-characteristics, in turn, correspond to particle paths.

Dimensional analysis shows that the simplest solutions arising in the configurations under consideration are self-similar, that is, they depend on \( \xi \) and \( t \) through the combination \( \xi /t \). More complex solutions, further, can be constructed or approximated by combinations of such self-similar waves (through solution of a sequence of Riemann-problems, as shown in Part II). This motivates our present focus on self-similar problems. We begin by considering elementary self-similar waves which can be identified with their gas-dynamics counterparts. Based on these results we then construct, in Section 4.2, certain classes of generalized self-similar waves which are specific to the kinds of materials we consider. Section 4.2 gives a detailed account of all types of wave curves that can arise from our model. In Section 5 we utilize these curves to construct our general Riemann solver.

### 4.1 Fan curves and front curves

There are two types of genuinely nonlinear elementary self-similar waves, namely, discontinuous fronts — which arise from the jump conditions (10) together with the EOS (15) — and fans — which are defined as self-similar solutions without discontinuities. For consistency with previous uses of the terms “ahead” and “behind” (see Section 3 where discontinuity fronts were considered), the side of a self-similar wave through which the material particles enter will be called the side ahead of the wave; the other side will be called the side behind the wave. Our notation uses superscripts \( b \) and \( a \) to denote the behind and ahead states, so that, for example, the symbols \( \Sigma^a = (v^a, q^a, u^a) \) and \( \Sigma^b = (v^b, q^b, u^b) \) denote the volume-stress-velocity states ahead and behind a wave.

1-fronts and 3-fronts are self-similar waves which satisfy the system (10). Simple manipulations transform this system into one in which the energy equation does not contain the velocity:

\[
M = \sqrt{-\frac{q}{v}}, \quad [q] = \mp M [u], \quad [U] = -\frac{q^a + q^b}{2} [v].
\]  

(19)
Here the minus and plus signs correspond to 1-fronts and 3-fronts respectively. Together with (15) and Remark 1, this system provides three algebraic relations for the seven unknowns \((M; v^a, q^a, u^a; v^b, q^b, u^b)\).

**Remark 3** The materials behind and ahead of a discontinuous front may either be in the same phase or in different phases. In the former case the discontinuity is a regular shock front analogous to those arising in gas dynamics and one and the same of the two branches of the EOS (15) must be used to compute \([U]\) in (19). In the latter case, on the other hand, the discontinuity is a transformation front and both branches of the EOS (15) must be used to compute \([U]\).

**Remark 4** 1-fronts are “left-facing”, that is, material particles cross the front from left to right; 3-fronts are “right-facing”, with material particles crossing from right to left.

1-fronts and 3-fronts are continuous self-similar solutions of the system (9). Again, this system can be transformed into one in which the energy equation contains only thermodynamic variables:

\[
C = \sqrt{-\frac{\partial q}{\partial v}} , \quad dq = \pm C du , \quad dU = -q dv . \tag{20}
\]

Here, the minus and plus signs correspond to 1- and 3-fronts respectively. Taking into account (15) and Remark 1, equations (20) form a system of three differential relations for the seven unknowns \((C; v^a, q^a, u^a; v^b, q^b, u^b)\) — details on how to obtain functional relations between these quantities are given at the end of this section.

**Remark 5** Since a fan is a continuous self-similar wave, the two states connected by a fan must necessarily belong to the same phase. That is, as in gas dynamics, fans are always rarefaction waves within a single phase.

**Remark 6** As in the case of fronts, 1-fronts are “left-facing”, with material particles entering the fan from the left; 3-fronts are “right-facing”, with material particles entering the fan from the right.

We have thus introduced the elementary self similar waves, fronts and fans, both of which are defined as solutions of systems of three equations and seven unknowns. For a given ahead-state \(\Sigma^a\), a front or fan is determined if the value of one of the behind-state variables, say the negative normal stress \(q^b\), is prescribed. Thus, the loci of states \(\Sigma^b \equiv (v^b, q^b, u^b)\) which can be connected to \(\Sigma^a\) by a 1-front, say, is a (one dimensional) curve. This leads to the notion (Menikoff & Plohr, 1988) of front curve and fan curve.
Front curves (or Hugoniots): A 1-front curve (resp. 3-front curve) is the loci of all states $\Sigma^b \equiv (v^b, q^b, u^b)$ which can be connected to $\Sigma^a$ by 1-fronts (resp. 3-fronts) having $\Sigma^a$ as the state ahead of the front and $\Sigma^b$ as the state behind the front.

Fan curves: A 1-fan curve (resp. 3-fan curve) is the loci of all states $\Sigma^b \equiv (v^b, q^b, u^b)$ which can be connected to $\Sigma^a$ by 1-fans (resp. 3-fans) having $\Sigma^a$ as the state ahead of the fan and $\Sigma^b$ as the state behind the fan.

(Types of self-similar waves more general than fronts and fans will be described in Section 4.2. The corresponding generalization of the notion of front curve and fan curve is the notion of wave-curve; see 4.2 for details.)

We shall always parameterize curves by the value of the negative normal stress $q^b$ behind the wave — so that $q^b > q^a$ corresponds to compressive waves and $q^b < q^a$ corresponds to expansive waves. We will utilize certain projections of the front and fan curves onto the $(v, q)$- and $(u, q)$-planes.

The projection of a front curve onto the $(v, q)$-plane is given by equation (19)$_3$, which we will assume can be solved for $v^b$:

$$v^b = \hat{v}_{\text{frt}}(q^b, v^a, q^a).$$  \hspace{1cm} (21)

The projection of a front curve onto the $(u, q)$-plane, in turn, can be obtained by substituting equation (21) into (19)$_1$

$$M = \hat{M}_{\text{frt}}(q^b, v^a, q^a) \equiv \sqrt{-\frac{q^b - q^a}{\hat{v}_{\text{frt}}(q^b, v^a, q^a) - v^a}},$$  \hspace{1cm} (22)

and using this result together with equation (19)$_2$ to produce the particle velocity as a function of $q$:

$$u^b = u^a \mp \frac{q^b - q^a}{M_{\text{frt}}(q^b, v^a, q^a)}. \hspace{1cm} (23)$$

To obtain projections for the fan curves, which in fact coincide with the integral curves of equations (20) in the $(v, q, u)$-space, we proceed as follows. Since according to (20)$_3$ the entropy is constant along the fan curves, all states $\Sigma^b$ must lie on the isentrope passing through state $\Sigma^a$, that is $\Sigma^b$ must satisfy the algebraic equation $\hat{S}(v^b, q^b) = \hat{S}(v^a, q^a)$, see (16). We assume this equation may be solved for $v^b$, so that the projection

$$v^b = \hat{v}_{\text{fan}}(q^b, v^a, q^a)$$  \hspace{1cm} (24)
of the fan curve onto the \((v, q)\)-plane results. To obtain the remaining projection of the fan curves onto the \((u, q)\)-plane we first substitute (24) into the expression (20)\(_1\) for the acoustic impedance which yields

\[
C = \hat{C}(q^b, v^a, q^a).
\]  

(25)

The particle velocity then follows by substitution of this relation into equation (20)\(_2\) and integration of the resulting expression along the isentrope passing through state \(\Sigma^a\):

\[
u^b = u^a \pm \int_{q^a}^{q^b} \frac{dq}{C} \bigg|_{S = \tilde{S}(v^a, q^a)}. 
\]

(26)

All of the desired projections of front and fan curves have now been constructed. For future use we introduce a positive function \(\hat{M}_{\text{fan}}\) which equals the mass flux \(M\) through a fan

\[
M = \hat{M}_{\text{fan}}(q^b, v^a, q^a) \equiv (q^b - q^a) \left/ \int_{q^a}^{q^b} \frac{dq}{C} \bigg|_{S = \tilde{S}(v^a, q^a)} \right. 
\]

(27)

so that

\[
u^b = u^a \pm \frac{q^b - q^a}{\hat{M}_{\text{fan}}(q^b, v^a, q^a)}. 
\]

(28)

As we shall show, there are pairs of states \(\Sigma^a\) and \(\Sigma^b\) which lead to compressive waves \((q^b > q^a)\), and which may not be connected by either a regular front or a transformation front. A similar comment applies to pairs of states connected by expansive waves. The wave curves introduced in the following section provide a necessary generalization of the front curves and fan curves, showing, in particular, that an arbitrary pair of states can always be connected by a self-similar wave.

### 4.2 Wave curves

A 1-wave curve (resp. 3-wave curve) is defined as the loci of all states \(\Sigma^b \equiv (v^b, q^b, u^b)\) which can be connected to a given state \(\Sigma^a\) by left-facing self-similar waves (resp. right-facing self-similar waves) having \(\Sigma^a\) as the state ahead of the wave and \(\Sigma^b\) as the state behind the wave.
The solution of the Riemann problem presented in Section 5 is based on the wave curves we construct here.

(As we mentioned, in our model there are states $\Sigma^a$ and $\Sigma^b$ which cannot be connected by either a single fan or a single front, and thus, more complex self-similar waves arise. Each one of such self-similar waves is characterized by a point in the wave curves which we construct in the present section. We point out that, in the case of gas-dynamics wave-curves are particularly simple: a wave-curve equals the front curve under compression and the fan curve under expansion. In view of the variety of self-similar waves that occur in connection with our problem — which are composed by groups of several fronts or fans that belong to the same characteristic family, — the (exhaustive) account of wave curves we present is necessarily lengthy.)

Note that the ahead-state $\Sigma^a$ may lie either in the austenitic phase or in the martensitic phase. The wave curves with austenitic ahead-states (also called “austenite centered”) are described in Section 4.2.1; those with martensitic ahead-states (or “martensite centered”) are given in Section 4.2.2. Like front and fan curves, wave curves will be parametrized by the value of the negative normal stress $q^b$ behind the wave — so that $q^b > q^a$ corresponds to compressive waves and $q^b < q^a$ corresponds to expansive waves. Because of Galilean and reflection invariance of equations (9) we may restrict attention to 3-wave curves: the 1-wave curve for an ahead-state $\Sigma^a$ is the reflection, through the plane $u = u^a$, of the corresponding 3-wave curve for the ahead-state $\Sigma^a$.

4.2.1 Austenitic Initial State

In this section we construct the wave-curve for an arbitrary austenitic initial state.

**Expansion branch.** The expansion branch of the wave curve, that is, the portion of the curve with $q^b < q^a$, is simply the fan curve in austenite centered at the austenitic state $\Sigma^a$. This fan curve was already constructed in Section 4.1 and needs not be discussed further here; see equations (24)–(28).

**Compression branch.** The compression branch $q^b > q^a$ is more complex: it consists of three different sub-branches which we construct in points 1 to 3, below. As part of that construction we identify a set of three pivotal states $\Sigma^A_{\text{crit}}$, $\Sigma^M_{\text{lim}}$, and $\Sigma^M_{\text{doub}}$; the three sub-branches we seek are determined as front curves (21)–(23) related to these states. These states carry physical significance, as they give rise to the three regimes described in Section 2: For $q^a < q^b < q^A_{\text{crit}}$ the wave curve is realized physically by regular shock fronts; For $q^A_{\text{crit}} = q^M_{\text{lim}} < q^b < q^M_{\text{doub}}$ in turn, the compression branch corresponds to two-wave structures; For $q^b > q^M_{\text{doub}}$, finally, the compression branch is associated with single transition fronts.

As described in point 1 below, the critical state $\Sigma^A_{\text{crit}}$ is defined by the intersection of a front curve and a critical curve. Clearly, one can conceive of degenerate cases in which these curves do not intersect; physically, these cases correspond to values of $\Sigma^a$ for which phase transitions
cannot be achieved through shock loading for any values of $\Sigma^b$, however compressive. In this case, as in gas-dynamics, the entire compression branch equals the front curve. In what follows, however, we assume the intersections defining $\Sigma^A_{\text{crit}}$ exist and, thus, the compression branch is composed of three sub-branches as mentioned above.

1. The first compression sub-branch. For values of $q^b$ close to $q^a$ the compression branch is the locus of austenitic states $\Sigma^b$ connected to the initial state $\Sigma^a$ through single shock fronts, see Figure 4(a). The Lagrangian speeds of the fronts are given by equation (19). Such shock fronts are indeed compatible with the critical-stress condition of point 1 in Section 1 as long as $\Sigma^b$ remains close to the austenitic initial state $\Sigma^a$. Thus, the first compression sub-branch lies on the shock-front curve centered at state $\Sigma^a$. (This front curve is labeled 1 in Figure 3 and is constructed in Section 4.1; see (21)–(23).) As assumed above, the projection of this front curve onto the $(v, q)$-plane intersects the critical curve (17) (thick dashed curve in Figure 3) at some point $q^b = q^A_{\text{crit}}$.

Evidently, the compression branch cannot be continued as an austenitic shock-front curve past the point $q^A_{\text{crit}}$—since otherwise the critical-stress condition would be violated. Thus, the state $\Sigma^A_{\text{crit}}$, which is defined as the austenitic state at which the first compression sub-branch terminates, is computed as follows. We first evaluate the point $(v^A_{\text{crit}}, q^A_{\text{crit}})$ giving the intersection of the $(v, q)$-projection of the $\Sigma^a$-centered shock-front curve with the critical curve (17) (the intersection point of curve 1 and the thick dashed curve in Figure 3(a)). This point is the solution of the system of two nonlinear algebraic equations $q^A_{\text{crit}} = \hat{q}^A(v^A_{\text{crit}})$ and $v^A_{\text{crit}} = \hat{v}^A_{\text{crit}}(q^A_{\text{crit}}, v^a, q^b)$. The particle velocity $v^A_{\text{crit}}$ is then trivially computed using (23) with state $\Sigma^A_{\text{crit}}$ substituted for state $\Sigma^b$.

2. The second compression sub-branch. For $q^b > q^A_{\text{crit}}$ and close to $q^A_{\text{crit}}$ the compression branch is continued by the locus of martensitic states $\Sigma^b$ connected to the initial state $\Sigma^a$ through split waves. Indeed, use of appropriate split waves allow us to construct self-similar solutions connecting $\Sigma^a$ and $\Sigma^b$ which comply with the critical-stress condition. Each split wave is made up of (i) a shock front in austenite, compressing austenite from the initial state $\Sigma^a$ to the intermediate (critical) state $\Sigma^A_{\text{crit}}$, (ii) a constant austenitic state $\Sigma^A_{\text{crit}}$, and (iii) a (compressive) transformation front, transforming austenite in the intermediate (critical) state $\Sigma^A_{\text{crit}}$ into martensite in the final state $\Sigma^b$, see Figure 4(b). The Lagrangian speed of the shock front is given by equation (19) with $\Sigma^b = \Sigma^A_{\text{crit}}$, while the Lagrangian speed of the transformation front is given by equation (19) with $\Sigma^a = \Sigma^A_{\text{crit}}$. The second compression sub-branch, therefore, lies on the transformation-front curve centered at state $\Sigma^A_{\text{crit}}$. (This front curve is labeled 2 in Figure 3 and is constructed following the standard procedure presented in Section 4.1 by using (21)–(23) with $\Sigma^a = \Sigma^A_{\text{crit}}$). To complete the present construction of the second sub-branch, it remains to detail the states at which the sub-branch begins and terminates.

As mentioned above, the second compression sub-branch starts at $q^b = q^A_{\text{crit}}$. More precisely, the initial state $\Sigma^M_{\text{lim}}$ of this sub-branch, which is different from the final state $\Sigma^A_{\text{crit}}$ of the first sub-branch, is defined as the state on the $\Sigma^A_{\text{crit}}$-centered transformation-front curve at which $q^M_{\text{lim}} = q^A_{\text{crit}}$. Equations (19) immediately imply that the speed of the front
Figure 3: The compression branch of the austenite-centered wave curve. (a) Projection onto the \((v, q)\)-plane. (b) Projection onto the \((u, q)\)-plane. The projections of the wave-curve are represented by thick curves. Numbers 1, 2, and 3 label the projections of the \(\Sigma^p\)-centered austenitic shock-front curve, the \(\Sigma^A_{\text{crit}}\)-centered martensitic transformation-front curve, and the \(\Sigma^p\)-centered martensitic transformation-front curve, respectively. The thick dashed curve represents the critical normal-stress curve \(q = \dot{q}_f(v)\). The thin dashed lines are Rayleigh lines.

connecting the states \(\Sigma^A_{\text{crit}}\) and \(\Sigma^M_{\text{lim}}\) is zero, that \(u^A_{\text{lim}} = u^A_{\text{crit}}\), and, defining the specific enthalpy by \(\dot{H}(v, q) \equiv \dot{U}(v, q) + qv\), that \(\dot{H}^M(v^M_{\text{lim}}, q^M_{\text{lim}}) = \dot{H}^A(v^A_{\text{crit}}, q^A_{\text{crit}})\). To complete the construction of the state \(\Sigma^M_{\text{lim}}\), the latter equation should be solved for \(v^M_{\text{lim}}\).

As \(q^b\) increases along the second compression sub-branch, the speed of the transformation front (the second wave in the split wave) increases; the speed of the shock front (the first wave in the split wave), on the other hand, does not depend on \(q^b\) at all. Eventually, at some value \(q^b = q^M_{\text{doub}}\), the speed of the transformation front becomes equal to the speed of the shock front so that the shock front and the transformation front coincide. Clearly, the compression branch cannot be continued with the split-waves beyond the point \(q^M_{\text{doub}}\).

The limiting discontinuity is itself a transformation front, connecting directly the initial state \(\Sigma^a\) with the final state \(\Sigma^b = \Sigma^M_{\text{doub}}\) at which the second compression sub-branch terminates. (This can be easily shown by adding up appropriate jump conditions.) This means that the state \(\Sigma^M_{\text{doub}}\) lies on the intersection of the transformation-front curve centered at the austenitic intermediate state \(\Sigma^A_{\text{crit}}\) (labeled 2 in Figure 3) with the transformation-front curve centered at the austenitic initial state \(\Sigma^a\) (labeled 3 in Figure 3). Thus, the state \(\Sigma^M_{\text{doub}}\) at which the second sub-branch terminates is computed as follows: First, a pair \((v^M_{\text{doub}}, q^M_{\text{doub}})\) is found by solving the system of two nonlinear algebraic equations

\[
v^M_{\text{doub}} = \dot{u}^M_{\text{brt}}(q^M_{\text{doub}}, v^a, q^a) \quad \text{and} \quad v^M_{\text{doub}} = \dot{u}^M_{\text{brt}}(q^M_{\text{doub}}, v^A_{\text{crit}}, q^A_{\text{crit}}).
\]

The particle velocity \(v^M_{\text{doub}}\) is then trivially computed using equation (23) with \(\Sigma^a = \Sigma^A_{\text{crit}}\) and \(\Sigma^b = \Sigma^M_{\text{doub}}\).

3. **The third compression sub-branch** The third compression sub-branch spans the semi-infinite interval \(q^M_{\text{doub}} < q^b < \infty\). It is the locus of martensitic states \(\Sigma^b\) connected directly
Figure 4: $(\xi, t)$-plane representations of 3-waves connecting the initial state $\Sigma^a$ with states $\Sigma^b$ from the compression branch of the austenite-centered 3-wave curve. The state $\Sigma^b$ belongs to (a) the first compression sub-branch, (b) the second compression sub-branch, and (c) the third compression sub-branch. Trajectories of discontinuity fronts are represented by thick lines, 3-characteristics are represented by thin lines.

to the initial austenitic state $\Sigma^a$ by single transformation fronts, see Figure 4(c). The Lagrangian speeds of the fronts are given by equation (19). Hence, this sub-branch lies on the transformation-front curve centered at state $\Sigma^a$. (This front curve is labeled 3 in Figure 3 and is constructed following the standard procedure presented in Section 4.1; see equations (21)–(23)). This concludes the construction of the compression branch of the austenite-centered wave curve.

Remark 7 We note that the phase transformation from austenite to martensite is generally accompanied by either heat release or absorption. As a result, the temperature $\theta^b$ of the martensite behind the front is different from the temperature $\theta^a_{\text{crit}}$ of the austenite ahead of the front. It is therefore conceivable that, for materials for which the hysteresis $\bar{q}_F(\theta^b) - \bar{q}_B(\theta^b)$ is sufficiently low and for normal stresses $q^b$ sufficiently close to $q^a_{\text{crit}}$, the calculated value $\theta^b$ of the temperature in the martensite makes the martensite unstable: $q^b < \bar{q}_B(\theta^b)$. Most generally such situations do not arise, and therefore we always assume hysteresis is sufficiently large so that $q^b \geq \bar{q}_B(\theta^b)$. A treatment of the alternate case requires knowledge of the physical mechanisms arising under such circumstances in the particular system at hand, and cannot therefore be discussed in the present general framework.

Remark 8 (Entropy Inequality) Here we show that all solutions associated with the austenite-centered wave curve constructed in this section satisfy the entropy inequality $\mathcal{S}^b \geq \mathcal{S}^a$. Since the first compression sub-branch is associated with regular shock-fronts, the proof that entropy inequality is satisfied for all solutions in this sub-branch is classical (Courant & Friedrichs, 1948, pp. 141-146). Analogously, well known calculations (Courant & Friedrichs, 1948, pp. 211-218) show that the entropy $\mathcal{S}^b$ of a solution in the second and third sub-branches increases with $q$ (or, equivalently, it decreases with $v$). Thus, in order to establish the entropy-increase inequality it suffices to show that the inequality $\mathcal{S}^M_{\text{lim}} \geq \mathcal{S}^A_{\text{crit}}$ holds, see Figure 3(a). In detail, we have (i) $\mathcal{S}^A_{\text{crit}} = \mathcal{S}^A(\nu^A_{\text{crit}}, \nu^A_{\text{crit}})$, the entropy function for the austenitic EOS evaluated at the
state \( \Sigma_{\text{crit}}^{A} \), and (ii) \( S_{\text{lim}}^{M} = \hat{S}^{M}(\rho_{\text{lim}}^{M}, q_{\text{lim}}^{M}) \), the entropy function for the martensitic EOS evaluated at the state \( \Sigma_{\text{lim}}^{M} \). As discussed in point 2 above, \( q_{\text{lim}}^{M} = q_{\text{crit}}^{A} \), \( H_{\text{lim}}^{M} = H_{\text{crit}}^{A} \), and the speed of the transformation front connecting the states \( \Sigma_{\text{crit}}^{A} \) and \( \Sigma_{\text{lim}}^{M} \) is zero. Such transformation front can be thought of as a limiting point of a sequence of transformation fronts (each with a finite speed) such that the sequence of the corresponding front-speeds converges to zero. (In the analogy of Remark 9 between the transformation fronts and the weak deflagration fronts, this limit corresponds to the constant pressure deflagration.) Thus, the states \( \Sigma_{\text{crit}}^{A} \) and \( \Sigma_{\text{lim}}^{M} \) are the initial and final states of a mass element which undergoes a phase transition as it crosses a transformation front moving at a vanishingly small speed. This is precisely the type of quasi-static transition process which was discussed at the end of Section 3.2; the state \( \Sigma_{\text{lim}}^{M} \) is therefore equal to the state \( \Sigma_{\text{stat}}^{A} \) and the inequality \( S_{\text{lim}}^{M} \geq S_{\text{crit}}^{A} \) follows immediately from equation (18).

Remark 9 The transformation fronts of the second compression sub-branch are similar to weak deflagration fronts (and different from regular shocks) in the following sense: they are subsonic relative to both the states ahead and behind them. (Geometrically, when drawn in the \((\xi, t)\)-plane, the characteristic curves of the same family as the front go through the front trajectory, entering it from behind and leaving it from ahead; see Figure 4(b).) There is one degree of indeterminacy for such type of discontinuity; a single quantity can and must be prescribed to determine the solution (Courant & Friedrichs, 1948). The critical stress condition provides the necessary prescription. Indeed, in this sub-branch the critical stress condition is effectively equivalent to requiring the negative normal stress in front of the discontinuity to exactly equal \( q_{\text{crit}}^{A} \). The transformation fronts for the third compression sub-branch, in contrast, are similar to regular shocks (or strong detonation fronts): they propagate supersonically with respect to the material in front of them and subsonically with respect to the material behind them. (When drawn in the \((\xi, t)\)-plane, the characteristic curves of the same family as the front impinge on the front trajectory from both sides; see Figure 4(c).) The degree of indeterminacy for such kind of discontinuity is zero (Courant & Friedrichs, 1948).

4.2.2 Martensitic Initial State

In this section we construct the wave-curve for an arbitrary martensitic initial state. The constructions given in this section parallel those of Section 4.2.1, but are sufficiently different to warrant an independent description.

Compression branch. Like the expansion branch in austenite described in Section 4.2.1, the compression branch described here — that is the portion of the martensite-centered wave curve with \( q^{b} > q^{a} \) — is quite simple. Indeed, this compression branch is just the shock-front curve in martensite centered at the martensitic state \( \Sigma^{a} \). This front curve was already constructed in Section 4.1 and needs not be discussed here; see equations (21)–(23).
Expansion branch. The expansion branch $q^b > q^a$ is more complex: it consists of three different sub-branches which we construct in points 1 to 3 below. As part of that construction we identify a set of three pivotal states $\Sigma_{\text{crit}}^M, \Sigma_{\text{in}}^A, \Sigma_{\text{son}}^A$; the three sub-branches we seek are determined as fan and front curves (24)–(28) and (21)–(23) related to these states. These states carry physical significance — as they give rise to three different regimes. For $q^a > q^b > q_{\text{crit}}^M$ the wave curve is realized physically by single rarefaction fans; For $q_{\text{crit}}^M = q_{\text{in}}^A > q^b > q_{\text{son}}^A$, in turn, the expansion branch corresponds to certain types of split waves: a rarefaction fan in martensite followed by a transformation front; For $q^b < q_{\text{son}}^A$, finally, the expansion branch is associated with more complex self-similar waves (so called “composite” split waves).

As described in point 1 below, the critical state $\Sigma_{\text{crit}}^M$ is defined by the intersection of a fan curve and a critical curve. Again, one can think of degenerate cases in which these curves do not intersect; physically, these cases are associated with values of $\Sigma^a$ for which phase transitions cannot be achieved through adiabatic unloading for any values of $\Sigma^b$, however expansive. In this case, as in gas-dynamics, the entire expansion branch equals the fan curve. In what follows, however, we assume the intersections defining $\Sigma_{\text{crit}}^M$ exist and, thus, the expansion branch is made up of three sub-branches as mentioned above.

1. The first expansion sub-branch. For values of $q^b$ close to $q^a$ the expansion branch is the locus of martensitic states $\Sigma^b$ connected to the initial state $\Sigma^a$ through single rarefaction fans, see Figure 6(a). The Lagrangian speeds of the heads and the tails of the fans are given by equation (20) evaluated at the states $\Sigma^a$ and $\Sigma^b$, respectively. Such fans are indeed compatible with the critical-stress condition of point 2 in Section 1 as long as $\Sigma^b$ remains close to the martensitic initial state $\Sigma^a$. Thus, the first expansion sub-branch lies on the fan curve centered at state $\Sigma^a$. (This fan curve is labeled 1 in Figure 5 and is constructed in Section 4.1; see (24)–(28).) As assumed above, the projection of this fan curve onto the $(v, q)$-plane intersects the critical curve (17) (thick dashed curve in Figure 5) at some point $q^b = q_{\text{crit}}^M$.

Clearly, the expansion branch cannot be continued as a martensitic fan curve beyond the point $q_{\text{crit}}^M$ — since otherwise the critical-stress condition would be violated. Thus, the state $\Sigma_{\text{crit}}^M$, which is defined as the martensitic state at which the first expansion sub-branch terminates, is computed as follows. We first evaluate the point $(v_{\text{crit}}^M, q_{\text{crit}}^M)$ giving the intersection of the $(v, q)$-projection of the $\Sigma^a$-centered fan curve with the critical curve (17) (the intersection point of curve 1 and the thick dashed curve in Figure 5(a)). This point is the solution of the system of two nonlinear algebraic equations $q_{\text{crit}}^M = \hat{q}_B(v_{\text{crit}}^M)$ and $v_{\text{crit}}^M = \hat{v}_{\text{in}}^M(q_{\text{crit}}^M, v^a, q^a)$. The particle velocity $u_{\text{crit}}^M$ is then trivially computed using (28) with $\Sigma^b = \Sigma_{\text{crit}}^M$.

2. The second expansion sub-branch For $q^b < q_{\text{crit}}^M$ and close to $q_{\text{crit}}^M$ the expansion branch is continued by the locus of austenitic states $\Sigma^b$ connected to the initial state $\Sigma^a$ through split waves. Indeed, use of appropriate split waves allows us to construct self-similar solutions connecting $\Sigma^a$ and $\Sigma^b$ which comply with the critical-stress condition. Such a split wave comprises (i) a fan in martensite, rarefying martensite from the initial state $\Sigma^a$ to the intermediate (critical) state $\Sigma_{\text{crit}}^M$, (ii) a constant martensitic state $\Sigma_{\text{crit}}^M$,
Figure 5: The expansion branch of the martensite-centered wave curve. (a) Projection onto the $(v, q)$-plane. (b) Projection onto the $(u, q)$-plane. The projections of the wave-curve are represented by thick curves. Numbers 1, 2, and 3 label the projections of the $\Sigma^a$-centered martensitic fan curve, the $\Sigma^M_{\text{crit}}$-centered transformation-front curve, and the $\Sigma^A_{\text{son}}$-centered austenitic fan curve, respectively. The thick dashed curve represents the critical normal-stress curve $q = \hat{q}_B(v)$. The thin dashed lines are Rayleigh lines.

Figure 6: $(\xi, t)$-plane representations of 3-waves connecting the initial state $\Sigma^a$ with states $\Sigma^b$ from the expansion branch of the martensite-centered 3-wave curve. The state $\Sigma^b$ belongs to (a) the first expansion sub-branch, (b) the second expansion sub-branch, and (c) the third expansion sub-branch. Trajectories of discontinuity fronts are represented by thick lines. 3-characteristics are represented by thin lines.
and (iii) an (expansive) transformation front, transforming martensite in the intermediate (critical) state $\Sigma_{\text{crit}}^{M}$ into austenite in the final state $\Sigma^{b}$, see Figure 6(b). The Lagrangian speeds of the head and the tail of the fan are given by equation (20) evaluated at the states $\Sigma^{a}$ and $\Sigma_{\text{crit}}^{M}$ respectively; the Lagrangian speed of the front, in turn, is given by equation (19)' with $\Sigma^{a} = \Sigma_{\text{crit}}^{M}$. The second expansion sub-branch, therefore, lies on the transformation-front curve centered at state $\Sigma_{\text{crit}}^{M}$. (This front curve is labeled 2 in Figure 5 and is constructed following the standard procedure presented in Section 4.1 by using (21)–(23) with $\Sigma^{a} = \Sigma_{\text{crit}}^{M}$.) To complete the present construction of the second sub-branch, it remains to specify the states at which the sub-branch begins and ends.

As mentioned above, the second expansion sub-branch starts at $q^{b} = q_{\text{crit}}^{M}$. More precisely, the initial state $\Sigma_{\text{lim}}^{A}$ of this sub-branch, which is different from the final state $\Sigma_{\text{crit}}^{M}$ of the first sub-branch, is defined as the state on the $\Sigma_{\text{crit}}^{M}$-centered transformation-front curve at which $q_{\text{lim}}^{A} = q_{\text{crit}}^{M}$. Equations (19) immediately imply that the speed of the front connecting the states $\Sigma_{\text{crit}}^{M}$ and $\Sigma_{\text{lim}}^{A}$ is zero, that $u_{\text{lim}}^{A} = u_{\text{crit}}^{M}$, and that $\dot{H}^{A}(u_{\text{lim}}^{A}, q_{\text{lim}}^{A}) = \hat{H}^{A}(u_{\text{crit}}^{M}, q_{\text{crit}}^{M})$. To complete the construction of the state $\Sigma_{\text{lim}}^{A}$, the latter equation should be solved for $u_{\text{lim}}^{A}$.

As $q^{b}$ decreases along the second expansion sub-branch, the speed of the transformation front increases, starting from its zero value at $q_{\text{crit}}^{M}$; the rarefaction fan, on the other hand, does not depend on $q^{b}$ at all. Evidently, the speed of the transformation front cannot increase further when it becomes sonic with respect to either austenite (the material behind the front) or martensite (the material ahead of the front). Beyond a sonic point the expansion branch cannot be continued with the types of split waves considered thus far and, therefore, the second sub-branch must terminate at one of the two sonic points — whichever is reached first. The case when the front becomes sonic with respect to the material behind the front is the most common; only this case will be considered here. The alternative case, when the front becomes sonic with respect to the material ahead of the front, can be treated similarly.

Thus, we consider the state $\Sigma_{\text{son}}^{A}$ at which the second expansion sub-branch terminates as the corresponding front becomes sonic with respect to the material behind the front — $C_{\text{son}}^{A} = M_{\text{son}}^{A} = M_{\text{crit}}^{A}(q_{\text{son}}^{A}, u_{\text{son}}^{M}, q_{\text{crit}}^{M})$ — while remaining subsonic with respect to the material in front of it. This equation together with $C_{\text{son}}^{A} = \dot{C}^{A}(q_{\text{son}}^{A}, u_{\text{son}}^{A}, q_{\text{son}}^{A})$ and $v_{\text{son}}^{A} = \dot{v}_{\text{son}}^{A}(q_{\text{son}}^{A}, u_{\text{son}}^{M}, q_{\text{crit}}^{M})$ (which follow from (25) and (21) respectively) constitute an algebraic system of three equations with three unknowns $u_{\text{son}}^{A}$, $q_{\text{son}}^{A}$, and $C_{\text{son}}^{A}$. The particle velocity $v_{\text{son}}^{A}$ is then easily computed using (23) with $\Sigma^{a} = \Sigma_{\text{crit}}^{M}$ and $\Sigma^{b} = \Sigma_{\text{son}}^{A}$.

(Geometrically the $\Sigma_{\text{crit}}^{M}$-to-$\Sigma_{\text{son}}^{A}$ transformation front is represented in the $(v, q)$-plane by the Rayleigh line centered at the point $(u_{\text{crit}}^{M}, q_{\text{crit}}^{M})$ and tangent to the $(v, q)$-projection of the $\Sigma_{\text{crit}}^{M}$-centered transformation front curve; see Figure 5(a). The slope of this Rayleigh line is $-(M_{\text{son}}^{A})^{2}$. The slope of the $(v, q)$-projection of the $\Sigma^{a}$-centered fan curve at its rightmost point is $-(C_{\text{crit}}^{M})^{2}$, where $C_{\text{crit}}^{M} = \dot{C}^{M}(q_{\text{crit}}^{M}, u_{\text{crit}}^{M}, q_{\text{crit}}^{M})$. Which one of the two possible modes of termination of the second sub-branch occurs depends on which of the two lines, the Rayleigh line or the tangent line to the projection of the $\Sigma^{a}$-centered fan curve at its rightmost point, is the steeper. The sonic-behind case (the case treated here) corresponds
to \( M^A_{\text{son}} < C^M_{\text{crit}} \), the sonic-ahead case corresponds to \( M^A_{\text{son}} > C^M_{\text{crit}} \).)

3. The third expansion sub-branch The third expansion sub-branch spans the semi-infinite interval \(-\infty < q^b < q^A_{\text{son}}\). This sub-branch is, again, the locus of austenitic states \( \Sigma^b \) connected to the initial state \( \Sigma^a \) by split waves — whose structure is somewhat more complex than those arising in point 2 above. The split waves associated with the third expansion sub-branch consist of: (i) A rarefaction fan connecting two martensitic states \( \Sigma^a \) and \( \Sigma^M_{\text{crit}} \), (ii) A constant martensitic state \( \Sigma^M_{\text{crit}} \), (iii) An (expansive) transformation front, transforming martensite in state \( \Sigma^M_{\text{crit}} \) into austenitic in state \( \Sigma^A_{\text{son}} \), and (iv) A rarefaction fan connecting two austenitic states \( \Sigma^A_{\text{son}} \) and \( \Sigma^b \), see Figure 6(c). The Lagrangian speeds of the head and the tail of the martensitic fan are given by equation (20)$_1$ evaluated at the states \( \Sigma^a \) and \( \Sigma^M_{\text{crit}} \) respectively; the Lagrangian speed of the front, in turn, is given by equation (19)$_1$ with \( \Sigma^a = \Sigma^M_{\text{crit}} \) and \( \Sigma^b = \Sigma^A_{\text{son}} \); and, finally, the Lagrangian speeds of the head and the tail of the austenitic fan are given by equation (20)$_1$ evaluated at the states \( \Sigma^A_{\text{son}} \) and \( \Sigma^b \) respectively. The construction of the third expansion sub-branch is thus completed by means of the fan curve centered at state \( \Sigma^A_{\text{son}} \). This fan curve, which is labeled 3 in Figure 5, can be constructed following the standard procedure presented in Section 4.1 (using equations (24)–(28) with \( \Sigma^a = \Sigma^A_{\text{son}} \)).

Remark 10 In parallel with Remark 7, we always assume the hysteresis to be sufficiently large so that when phase transformation from martensite to austenite takes place the austenite behind the front is stable: \( q^b \leq q_f(\theta^b) \).

Remark 11 (Entropy Inequality) The entropy inequality \( \mathcal{S}^0 \geq \mathcal{S}^a \) for the solutions associated with the martensite-centered wave curve constructed in this section can be established in a manner analogous to that of Remark 8.

Remark 12 The transformation fronts of the second expansion sub-branch are subsonic relative to both the states ahead and behind them. Thus, the considerations presented in Remark 9 apply to the present case; the depiction relevant here is given in Figure 6(b). The transformation fronts of the third expansion sub-branch, in turn, are sonic with respect to the states behind them and subsonic with respect to the states ahead of them. Geometrically the sonic condition implies that the Rayleigh line of the transformation front (the thin dashed line in Figure 5(a)) is tangent to the \((v, q)\)-projection of the fan curve centered at state \( \Sigma^A_{\text{son}} \) (curve 3 in Figure 5(a)); the tangency point equals \((v^A_{\text{son}}, q^A_{\text{son}})\). The sonic condition guarantees that the transformation front and the second rarefaction wave constitute a composite wave: they propagate together as a single entity.

5 Riemann Problem

Using the wave curves constructed in Section 4.2 it is now an easy matter to construct solutions for the general Riemann problem (11) for the system of conservation laws (9) with the EOS (15):
the procedure parallels the one used in gas dynamics to obtain solutions to Riemann problems from wave curves.

The solution of the Riemann problem consists of four constant states separated by three self-similar waves; see Figure 7(a). (In the case of spallation the structure is different; see Remark 14 below.) From left to right, these three waves are a 1-wave, a 2-wave, and a 3-wave; the four corresponding constant states will be denoted by $\Sigma^{L,a}$ (left-ahead), $\Sigma^{L,b}$ (left-behind), $\Sigma^{R,b}$ (right-behind) and $\Sigma^{R,a}$ (right-ahead). The 2-wave is always a contact discontinuity. The 1- and 3-waves, in turn, may be single rarefaction fans or single shock fronts, but they may also be self-similar waves of more general types — as described in Section 4.2. The occurrence of such self-similar waves distinguishes the Riemann problem for a material with an EOS (15) from the Riemann problem in gas dynamics — where the 1- and 3-waves can only be rarefaction fans or shock fronts.

To obtain these states and waves we first note that $\Sigma^{L,a}$ and $\Sigma^{R,a}$ must equal the initial left and the right states $\Sigma^L$ and $\Sigma^R$ of equation (11), so that the quantities $v^{L,a}$, $q^{L,a}$, $u^{L,a}$ and $v^{R,a}$, $q^{R,a}$, $u^{R,a}$ are known from the initial data. The values of the states $\Sigma^{L,b}$ and $\Sigma^{R,b}$ and the structures of the 1- and 3-waves, in turn, must be found. In short: given $\Sigma^{L,a}$ and $\Sigma^{R,a}$, two intermediate states $\Sigma^{L,b}$ and $\Sigma^{R,b}$ must be determined in such a way that $\Sigma^{L,a}$ and $\Sigma^{L,b}$ are connected by a 1-wave, $\Sigma^{L,b}$ and $\Sigma^{R,b}$ are connected by a 2-wave, and $\Sigma^{R,b}$ and $\Sigma^{R,a}$ are connected by a 3-wave.

To determine these intermediate states we make use of the fact that, as shown below, the projections of the 1-wave-curve centered the state $\Sigma^{L,a}$ and the 3-wave-curve centered the state $\Sigma^{R,a}$ onto the $(q, u)$-plane intersect at a single point $(q_s, u_s)$; see Figure 7(b). This intersection point provides the solution we seek. Indeed, calling $\Sigma'_s$ and $\Sigma''_s$ the states in the 1- and 3-wave curves which project onto $(q_s, u_s)$, we note that $\Sigma'_s$ can be connected to $\Sigma^{L,a}$ through a 1-wave.
(since $\Sigma'_m$ lies on the 1-wave-curve centered at the state $\Sigma^{L,a}$). Analogously, $\Sigma'_p$ is connected to $\Sigma^{R,a}$ through a 3-wave (since $\Sigma'_p$ lies on the 3-wave-curve centered at the state $\Sigma^{R,a}$). Further, the states $\Sigma'_m$ and $\Sigma'_p$ can be connected by a 2-wave (contact discontinuity), since these states project onto the same point in the $(q,u)$-plane (normal stresses and velocities are continuous across contact discontinuities). Thus, setting $\Sigma^{R,b} = \Sigma'_m$ and $\Sigma^{L,b} = \Sigma'_p$, we have verified all the necessary conditions for the states $\Sigma^{L,a}$, $\Sigma^{L,b}$, $\Sigma^{R,b}$, $\Sigma^{R,a}$ and the intervening waves to make up the solution of the Riemann problem under consideration.

The existence and uniqueness of the intersection point $(q_s, u_s)$ of the projections of 1- and 3-wave curves follow immediately — since such projections are continuous functions $q = q^1(u)$ and $q = q^3(u)$ of the variable $u$ for $u \in (-\infty, +\infty)$, with $q^1(u)$ monotonically decreasing and $q^3(u)$ monotonically increasing; see Section 4. (We note that, although the 1- and 3-wave curves are themselves discontinuous — since $q$ jumps at $q = q^A_{\text{crit}}$ on an austenite centered wave curve and at $q = q^M_{\text{crit}}$ on a martensite centered wave curve; see Figures 3(a) and 5(a) — the projections of these wave curves are indeed continuous functions. The continuity of these projections follows directly from the constructions in Sections 4.2.1 and 4.2.2, which show that $q^A_{\text{crit}} = q^M_{\text{lim}}$, $u^A_{\text{crit}} = u^M_{\text{lim}}$ and $q^M_{\text{crit}} = q^A_{\text{lim}}$, $u^M_{\text{crit}} = u^A_{\text{lim}}$, respectively; see Figures 3(b) and 5(b).)

**Remark 13** Unlike the wave curves arising in gas dynamics, the wave curves constructed in Section 4.2 consist of several sub-branches; the same is true, naturally, of the corresponding $(q,u)$-projections needed in the present context. Each one of the sub-branches of these projections is given by some instance of either equation (23) or equation (28). The particular instance of these equations needed in a given sub-branch is determined in accordance with the procedures given in Section 4.2 for the determination of the sub-branches of the various wave curves. Once the $(q,u)$-projections of the relevant wave curves have been obtained, their intersection point $(q_s, u_s)$ can be efficiently determined by means of a Newton-Raphson-type method similar to the one described in (van Leer, 1979) for the case of gas dynamics.

**Remark 14** The constructions of solutions of the Riemann problem described in this section do not apply to problems involving spallation. Spall arises as large tensile stresses exceed the strength of the austenite leading to rupture and appearance of an intervening vacuum state. To incorporate this phenomenon into our model, the EOS (15) should be modified as follows

$$U = \begin{cases} U^A, & \text{if } \bar{q}_S(\theta) < q < \bar{q}_F(\theta) \\ U^M, & \text{if } q > \bar{q}_B(\theta), \end{cases} \quad (29)$$

where $\bar{q}_S(\theta)$ is the strength of the austenite. The existence of such critical stress $\bar{q}_S(\theta)$ leads to a critical state $\Sigma^A_{\text{spall}} = (u^A_{\text{spall}}, q^A_{\text{spall}})$ at which a wave curve — and thus its $(q,u)$ projection — terminates. As a result, the functions $q = q^1(u)$ and $q = q^3(u)$ are defined in semi-infinite intervals and the intersection $(q_s, u_s)$ of the corresponding curves may not exist. When these curves do not intersect, the solution to the Riemann problem describes a process of spallation. The constructions above may easily be modified to accommodate cases for which
spall occurs (van Leer, 1979; Miller & Puckett, 1996). Indeed, the \((q, u)\)-projections of the 1- and the 3-wave curves must intersect the \((q, u)\)-projection of the wave curve of the intervening vacuum state \(q = 0\) at certain points \((q^L_*, u^L_*)\) and \((q^R_*, u^R_*)\). (Clearly, \(q^L_* = q^R_* = 0\) and \(u^L_* < u^R_*\) are the escape speeds (Courant & Friedrichs, 1948) associated with the states \(\Sigma^{L,*}\) and \(\Sigma^{R,*}\), respectively.) The solution, thus, consists of 1- and 3-waves separating the states \(\Sigma^{L,*}\) and \(\Sigma^{R,*}\) from the single middle vacuum state \(\Sigma^b = \Sigma^V\), in which \(q^V = 0\), \(\rho^V = 0\), and \(u^V\) is undefined.

**References**


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