Solid-solid Phase Transformations: Non-existence of One-dimensional Stress Problems, Model Equation and Uniqueness Conditions

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Abstract

In the literature, many people have used *pure* one-dimensional theories to study boundary-value and/or initial-value problems of phase-transforming materials. In this paper, we shall show that these *pure* one-dimensional theories have some essential defects. More specifically, we reveal that for these materials there do not exist one-dimensional stress problems (at least in the continuum scale). Thus, to model phase-transforming materials physically and mathematically, it is essential to consider the influence from the other dimension(s). For a slender circular cylinder, by taking into account the effects due to the radial deformation, we establish the proper model equation, which shows that the problem is a singular perturbation one. The model equations used in the literature are only the leading order equations valid in the outer regions. The lack of uniqueness of solutions in the *pure* one-dimensional theories (both static and dynamical) is well-known (the author thinks that it is due to the above-mentioned defects). In the literature, the kinetic relation, which is regarded as *an extra constitutive relation* for the material to be determined experimentally, is proposed to give an additional condition (besides the two jump conditions across the phase boundary) to obtain unique solutions. Here, by using our model equation and matching its traveling wave solution to those in the outer regions, we obtain three relations for three unknowns, which provide the uniqueness conditions for solutions. Also, these three conditions are given in terms of the stress function (i.e., the usual strain-stress relation) alone, independent of the notion of the kinetic relation. Our results seem to resolve the long outstanding issue of nonuniqueness of solutions in modeling dynamical problems of phase-transforming materials.

PACS: 81.30.Kf, 64.70.Kd, 64.60.Ht, 02.30.Jr, 62.30.+d

1 Introduction

Phase-transforming materials (e.g., shape memory alloys and shape memory polymers) have many applications. For example, they have been used to design dampers for satellite applications, rotary actuators, snake-like robots and delicated medical devices. Many authors have studied various aspects of these types of materials (e.g., Boullay et al. 2002, Ahluwalia and Ananthakrishna 2001, Barsch and Krumhansl 1984, Bales and Gooding 1991, Kartha et al. 1995). On the physical and mathematical modeling of these materials, one important and difficult issue is the nonuniqueness of solutions. In a recent article by Abeyaratne et al (2001), an elegent review was given based on the papers by Abeyaratne and Knowles (1991, 1993 and 2000). They considered the impact-induced phase transition problem in a semi-infinite slab with a given velocity $-V$ at the end. The governing equations (in a Lagrangian description) used by them were pure one-dimensional dynamical equations

$$\rho\frac{\partial v}{\partial t}=\frac{\partial \sigma}{\partial x}=\sigma'(\gamma)\frac{\partial \gamma}{\partial x}, \tag{1.1}$$

$$\frac{\partial \gamma}{\partial t}=\frac{\partial v}{\partial x}, \tag{1.2}$$

where x and t are respectively the spatial and temporal variables, $\gamma = w_x$ (a subscript is used to denote the derivative, whenever suitable) is the axial strain and $v = w_t$ is the velocity (w is the axial displacement), σ is the stress and ρ is the density. The system (1.1) and (1.2) is hyperbolic for a standard material for which $\sigma'(\gamma) > 0$ and is hyperbolic-elliptic for a typical phase-transforming material for which $\sigma'(\gamma)$ changes signs (usually the strain-stress curve has a peak-valley combination). For a phase-transforming material, when the given velocity V is within a certain interval, the phase boundary is induced. Abeyaratne et al. (2001) gave the solution in the $x-t$ plane, which has the structures of one shock wave and a phase boundary. More recently, Knowles (2002) considered the case where $\sigma'(\gamma) > 0$ but $\sigma(\gamma)$ has an inflection point. He showed that when the phase boundary is induced, there is also a rarefaction wave; see Figure 1. The appearence of the rarefaction wave seems to be natural (and probably should also be present in the case where $\sigma'(\gamma)$ changes signs). (**Remark:** For the purpose of the present paper , whether the $x-t$ plane has a structure shown in Abeyaratne at al (2001) or Knowles (2002) makes no difference.)

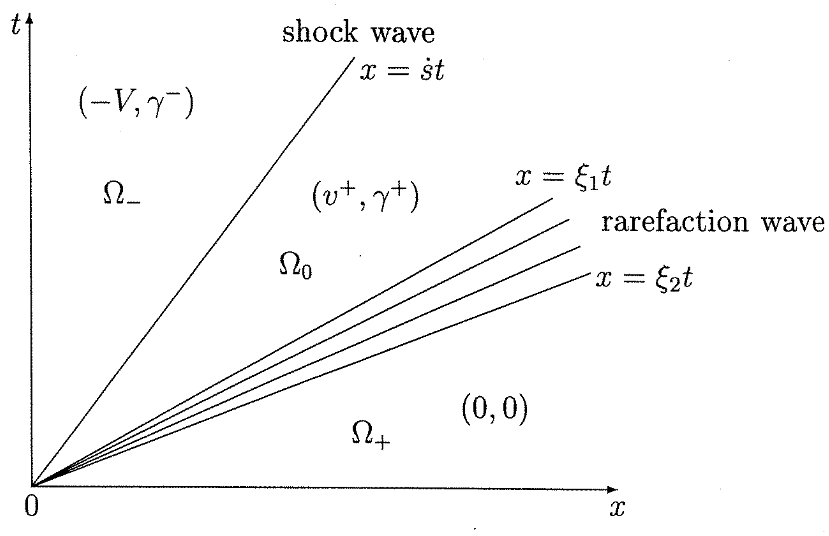

Figure 1: Impact-induced tensile wave with a similarity form $(v(x/t), \gamma(x/t))$

Across the phase boundary, there are the usual two jump conditions (see Knowles 2002):

$$(\gamma^+ - \gamma^-)\dot{s} + (v^+ + V) = 0, \tag{1.3}$$

$$\sigma(\gamma^+) - \sigma(\gamma^-) + \rho\dot{s}(v^+ + V) = 0, \tag{1.4}$$

where $\dot{s}$ is the speed of the phase boundary. In the above two equations, v^+ can be related to γ^+ through the stress function $\sigma(\gamma)$ but they only provide two relations for three unknowns γ^+, γ^- and $\dot{s}$. Thus, the solution is not unique and actually there is a one-parameter family of solutions. Abeyaratne and Knowles (1991, 1993 and 2000) introduced the concept of driving force $g(t)$, which is defined via the dissipation rate $D(t)$ as

$$D(t) = g(t)\dot{s} \tag{1.5}$$

and can be expressed as

$$g(t) = \int_{\gamma^-}^{\gamma^+} \sigma(\gamma)d\gamma - \frac{\sigma(\gamma^+) + \sigma(\gamma^-)}{2}(\gamma^+ - \gamma^-). \tag{1.6}$$

To determine the solution uniquely, they introduced the kinetic relation which means that the driving force is a function of the speed $\dot{s}$ (i.e., $g(t) = \phi(\dot{s})$). It was stated in Abeyaratne et al (2001) that this relation "is part of the charaterization of the material and needs to be determined through a combination of lattice-scale modeling and laboratory experiments".

However, as far as the author knows, such a function has never been provided in the literature. Since $\phi(\dot{s})$ is not known, in the literature people have used some hypotheses, such as maximally dissipative kinetics or dissipation-free kinetics. However, as pointed out in Knowles (2002, p.1173), there is "$\cdots$ the lack of a physical basis for choosing any *particular* kinetic relation or regularizing augmentation to complete the model $\cdots$". Also, no mathematical justifications have been provided for these hypotheses. Rather, they were used *artificially* to just single out the solutions. Certainly, for a given material, not all of these hypotheses can be valid.

Many authors have used these concepts proposed by Abeyaratne and Knowles (e.g., Truskinovsky and Vainchtein 2003, Bruno et al 1995, Levitas and Preston 2002, Shenoy et al. 1999). However, for a standard material, once the constitutive relation (i.e., the strain-stress relation) is given, usually one can determine everything in principle. It seems natural to ask the question: can we also determine everything for a phase-transforming material for which the only essential difference between it and a standard one is that its constitutive relation has a different character? One purpose of the present paper is to derive the uniqueness conditions for solutions based on the given strain-stress relation alone.

As noted by many people in the past, the lack of uniqueness of solutions is usually because some important physical effects are neglected in the model. So, for a phase-transforming material, what effects are neglected in the *pure* one-dimensional model (1.1) and (1.2)? In the next section, we shall show that to model phase transition problems one should consider the influence from other dimension rather than only considering the effects in the axial dimension. Then, we shall establish the proper model equation in section 3 through an approach in nonlinear wave theory. Based on this model equation, by using the matched asymptotics, three conditions will be derived which provide the uniqueness conditions for solutions.

2 Non-existence of One-dimensional Stress Problems

Consider the axial equilibrium equation in an axially symmetrical static problem

$$\frac{\partial S_{zZ}}{\partial Z} + \frac{\partial S_{zR}}{\partial R} + \frac{S_{zR}}{R} = 0, \tag{2.1}$$

where S_{zZ} and S_{zR} are the components of the first Piolar-Kirchhoff stress tensor, and (r, θ, z) and (R, Θ, Z) are the current and reference cylindrical coordinates, respectively (for convenience, we use Z as the axial spatial variable instead of x). For a thin bar (in experiments, the ratio of the radius and length is about $\frac{1}{60}$), one might think that the last two terms in (2.1) (representing the influence of the radial deformation in the axial direction) are very small and can be neglected. For standard elastic materials, indeed such an approximation is valid (actually, $\frac{\partial S_{zR}}{\partial R}$ and $\frac{S_{zR}}{R}$ are exponentially small for a neo-Hookean material; cf. Dai and Bi (2001)). However, for a phase-transforming material, the strain-stress curve typically has a peak-valley combination. In the loading process, as the external stress approaches the peak value σ_p, say, it is equal to σ_p^-. In this case, $\frac{\partial S_{zZ}}{\partial Z} = \frac{\partial S_{zZ}}{\partial \gamma}\gamma_Z$ is exactly equal to zero. Then, the terms, $\frac{\partial S_{zR}}{\partial R}$ and $\frac{S_{zR}}{R}$, no matter how small they are, are dominant terms and cannot be neglected! This implies there must be a radial deformation in the process of phase transformation. Thus, to model phase transitions, the influence of the radial deformation should be taken into account.

Phase transitions are also found in materials whose strain-stress curves are strictly increasing but have an inflection point (see Knowles 2002 and Favier et al. 2001). In this case, we differentiate (2.1) with respect to Z to obtain

$$\frac{\partial^2 S_{zZ}}{\partial Z^2} + \frac{\partial^2 S_{zR}}{\partial Z \partial R} + \frac{1}{R}\frac{\partial S_{zR}}{\partial Z} = 0. \tag{2.2}$$

In the loading process, as the external stress approaches the value (say, σ_i^-) at the inflection point, $\frac{\partial^2 S_{zZ}}{\partial Z^2} = \frac{\partial^2 S_{zZ}}{\partial \gamma^2}\gamma_Z + \frac{\partial S_{zZ}}{\partial \gamma}\gamma_{ZZ} = \frac{\partial S_{zZ}}{\partial \gamma}\gamma_{ZZ}$ since $\frac{\partial^2 S_{zZ}}{\partial \gamma^2}\gamma_Z = 0$ exactly. On the other hand, $\frac{\partial^2 S_{zR}}{\partial Z \partial R}$ and $\frac{1}{R}\frac{\partial S_{zR}}{\partial Z}$ are of the same order as $\frac{\partial S_{zZ}}{\partial \gamma}\gamma_{ZZ}$ (cf. the results for a neo-Hookean material (Dai and Bi 2001)). As a result, the influence of the radial deformation should not be neglected. In this case, the radial deformation is induced as the external stress tends to σ_i^- and the phase transformation begins.

According to the above analysis, it can be seen that in both cases when the phase transformation takes place the radial deformation must be present and is a domiant factor (or at least one of the dominant factors). Although our discussions hold for static problems, naturally any effects which are important in static problems should also be important in dynamical problems. Thus, we draw the following conclusion:

For phase-transforming materials whose strain energy functions are not strictly convex (equivalently, the strain-stress curves have a peak-valley combination or have an inflection point), there do not exist one-dimensional stress problems in phase transitions.

3 Model Equations

Based on the results given in section 2, it can be seen that to model phase transition problems, it is essential to take into account the influence of the radial deformation. Here, we shall establish the proper model equation by considering which terms should be present and then combining them together.

First, when the phase transformation has not started, the model equation should be able to yield the correct result for a uniform state for which the equation has the form

$$\sigma_Z = 0. \tag{3.1}$$

Thus, the term σ_Z should be present.

The linearization of σ_Z gives the term Ew_{ZZ}, where E is the Young's modulus and w is the axial displacement. The simplest model for linear waves propagating in a bar (rod) is the classical wave equation

$$\rho w_{tt} - Ew_{ZZ} = 0. \tag{3.2}$$

Thus, ρw_{tt} should be present in the model equation so that $\rho w_{tt} - \sigma_Z$ can yield $\rho w_{tt} - Ew_{ZZ}$ when the latter is linearized.

As discussed in section 2, to model phase transitions, one should take into account the radial deformation. For linear waves, when the lateral movement is present, they are dispersive. Linear dispersive terms are w_{ZZZZ}, w_{ZZtt} and w_{tttt} (dispersive terms with sixth-order or higher even-order derivatives, representing higher-order effects, will be neglected in our model). Then, combining these terms together, we have the model equation

$$\rho w_{tt} - \sigma_Z + A\mu w_{ZZZZ} + B\rho w_{ZZtt} + C\mu^{-1}\rho^2 w_{tttt} = 0 \tag{3.3}$$

with three undertermined constants A, B and C, where μ is the shear modulus.

To determine these constants, the idea is to match the dispersion relation of this model equation to the exact dispersion relation based on the three-dimensional field equations up to a certain asymptotic order (cf. Whitham 1974). The exact dispersion relation for linear waves in a circular cylinder is the so-called Pochhammer frequency equation, which takes the form (see Achenbach 1990)

$$\frac{2p}{a}(q^2 + k^2)J_1(pa)J_1(qa) - (q^2 - k^2)^2 J_0(pa)J_1(qa) - 4k^2 pq J_1(pa)J_0(qa) = 0, \tag{3.4}$$

where a is the radius, k is the wave number, $J_0(\cdot)$ and $J_1(\cdot)$ represent the Bessel functions, and

$$p^2 = \frac{\omega^2}{c_L^2} - k^2, \qquad q^2 = \frac{\omega^2}{c_T^2} - k^2. \tag{3.5}$$

Here, c_L and c_T are the longitudinal-wave speed and shear-wave speed, respectively.

For linear waves in a slender circular cylinder, the first mode is dominant. Thus, we require that the dispersion relation of the model equation matches that of the three-dimensional field equations up to $O(a^2)$ as $k \to 0$ (at $O(1)$ they are automatically matched since the linearized version of (3.3) contains $\rho w_{tt} - E w_{ZZ}$ and the wave propagates with the bar-wave speed $c_b = \sqrt{E/\rho}$). On the other hand, the effect of the radial deformation comes into the axial equation through the shear strain. Thus, we require that the dispersion relation of (3.3) matches that of the three-dimensional field equations at $O(1)$ for the second mode as $k \to \infty$ (i.e., in this case the phase velocity should match the shear-wave speed c_T).

From (3.4), we find for the first mode as $k \to 0$ that

$$\frac{\omega}{k} = c_b\left(1 - \frac{\nu^2}{4} a^2 k^2 + \cdots\right), \tag{3.6}$$

where ω is the frequency and ν is the Poisson's ratio. For the second mode, as $k \to \infty$ we have

$$\frac{\omega}{k} = c_T. \tag{3.7}$$

The matching of the dispersion relation of (3.3) to (3.7) yields two relations: $2A = 2C = -B$. Then, the matching to (3.6) determines B completely. As a result, we obtain

$$w_{tt} - \rho^{-1}\sigma_Z + m_1 a^2 w_{ZZZZ} - 2m_1 a^2 c_T^{-2} w_{ZZtt} + m_1 a^2 c_T^{-4} w_{tttt} = 0 \tag{3.8}$$

or

$$w_{tt} - \rho^{-1}\sigma_Z + m_1 a^2 c_T^{-4}[(w_{tt} - c_T^2 w_{ZZ})_{tt} - c_T^2 (w_{tt} - c_T^2 w_{ZZ})_{ZZ}] = 0, \tag{3.9}$$

where

$$m_1 = \frac{1}{3} \frac{\nu c_T^2 c_b^2}{(c_b^2 - c_T^2)^2}. \tag{3.10}$$

Equation (3.8) or (3.9) is the model equation for phase transitions in a slender circular cylinder, which has taken into account the effects due to the radial deformation. It can be seen from (3.9) that the waves exhibit clearly two-wave structures, one with the bar-wave speed c_b and the other with the shear-wave speed c_T.

Equation (3.8) can also be derived from the three-dimensional field equations together with the traction free boundary conditions in the lateral surface by a consistent asymptotic approach as we (Dai and Huo 2002 and Dai and Fan 2004) have carried out for nonlinear waves in slender circular cylinders composed of standard elastic materials. It should be noted that for an initial-value problem we require four initial conditions. One can impose the standrad conditions on the axial displacement and velocity. The other two conditions should be on w_{tt} and w_{ttt}. In the asymptotic approach, they can be related to the axial and radial displacements and the axial and radial velocities. Thus, to use this model equation for initial-value problems, one can further impose the initial conditions on the radial displacement and velocity. The results based on the asymptotic approach (very lengthy) will be reported elsewhere. Here, one of the main purposes is to establish the uniqueness conditions for solutions, for which to have the correct model equation is sufficient.

4 Uniqueness Conditions

From the model equation (3.8), it is easy to see the defects of the pure one-dimensional model (1.1) and (1.2). For small a, (3.8) represents a singular perturbation problem (where in front of the highest-derivative terms there is a small parameter). According to the standard singular perturbation theory, there should be outer and inner (boundary layer) regions. Only in the outer regions, at the leading order ($O(1)$) one has

$$w_{tt} - \rho^{-1}\sigma_Z = 0, \tag{4.1}$$

which is just the one-dimensional model (1.1) and (1.2) in a different form. Thus, the solutions which were constructed based on the pure one-dimensional model in the literature are only valid to the leading order in the outer regions. In the inner region, the higher-order derivatives come into play, and one should use the full equation (alternatively, one may introduce proper scalings to use the boundary layer equation. However, the full equation is valid everywhere and using it has the advantage that it is more flexible in choosing the points to do the matching to the outer regions). We rewrite (3.8) as

$$v_t - \rho^{-1}\sigma'(\gamma)\gamma_Z + m_1 a^2 \gamma_{ZZZ} - 2m_1 c_T^{-2} a^2 v_{ZZt} + m_1 c_T^{-4} a^2 v_{ttt} = 0, \tag{4.2}$$

$$v_Z = \gamma_t. \tag{4.3}$$

The reason is that the axial strain and velocity, but not the axial displacement, vary rapidly in the inner region.

The solution shown in Figure 1 is valid in the outer regions. Roughly speaking, one outer region (denoted by R_1) is a region, with the rarefaction wave and the undisturbed region included, some distance away from the phase boundary to the right, and another outer region (denoted by R_2) is some distance away from the phase boundary to the left. For a sub-region of R_1, to the left of the rarefaction wave, the strain is in a traveling wave state as time increases (along the line $\frac{Z}{t} = \dot{s}$, the strain is always constant). The same conclusion holds for a sub-region in R_2. The inner region (denoted by I) is in between R_1 and R_2. As in the overlapping region of R_1 and I and that of R_2 and I the strain is in a traveling wave state with propagating speed $\dot{s}$, the strain in the whole domain of I should also be in a traveling wave state with the same propagating speed. Thus, we seek the traveling wave solution of (4.2) and (4.3) and let

$$\gamma = f(\xi), \qquad \xi = Z - \dot{s}t. \tag{4.4}$$

Integrating the above equation with respect to Z once, we obtain

$$w = \int_{Z_0}^{Z} f(x - \dot{s}t)dx - Vt, \tag{4.5}$$

where Z_0 is a point in the overlapping region of R_2 and I and $-Vt$ appears in the left hand side in order to match the velocity at Z_0. Then, we have

$$v = -\dot{s}f(Z - \dot{s}t) + \dot{s}f(Z_0 - \dot{s}t) - V = -\dot{s}f(\xi) + \dot{s}\gamma^- - V. \tag{4.6}$$

Here, use has been made of $f(Z_0 - \dot{s}t) = \gamma|_{Z_0} = \gamma^-$. Matching the above relation to the velocity at a point Z_1 in the overlapping region of I and R_1, we have

$$(\gamma^+ - \gamma^-)\dot{s} + (v^+ + V) = 0. \tag{4.7}$$

Here, use has been made of the fact that at Z_1 the strain is γ^+. Equation (4.7) is just the jump condition (1.3)! This is understandable: If one has used the full equation correctly, one should be able to recover the results based on the correct degenerated equation. However, when a is nonzero, γ^+ and γ^- should be understood to be the strains at Z_1 and Z_0 respectively, not the strains just across the phase boundary (which has a structure, not a simple jump, in the case of non-zero a).

Substituting (4.4) and (4.6) into (4.2) and integrating once, we obtain

$$\dot{s}^2 f - \rho^{-1}\sigma(f) + m_1 a^2(1 - \dot{s}/c_T)^2 f'' = c_1, \tag{4.8}$$

where c_1 is an integration constant. By using the velocity and strain values at Z_0 and Z_1, we find that

$$c_1 = \dot{s}^2\gamma^- - \rho^{-1}\sigma(\gamma^-) = \dot{s}^2\gamma^+ - \rho^{-1}\sigma(\gamma^+). \tag{4.9}$$

By further using (4.7) in the above equation, we obtain

$$\sigma(\gamma^+) - \sigma(\gamma^-) + \dot{s}(v^+ + V) = 0. \tag{4.10}$$

This is just the second jump condition (1.4)!

Multiplying (4.8) by f' and integrating once more, we obtain

$$\frac{1}{2}\dot{s}^2 f^2 - \rho^{-1}\int_{\gamma^+}^{f}\sigma(\gamma)d\gamma + \frac{1}{2}m_1 a^2(1 - \dot{s}/c_T)^2(f')^2 = c_1 f + c_2, \tag{4.11}$$

where c_2 is another integration constant. By using the velocity and strain values at Z_0 and Z_1, we find that

$$c_2 = \rho^{-1}\gamma^+\sigma(\gamma^+) - \frac{1}{2}(\dot{s}\gamma^+)^2 = \rho^{-1}\gamma^-\sigma(\gamma^-) - \frac{1}{2}(\dot{s}\gamma^-)^2 - \rho^{-1}\int_{\gamma^+}^{\gamma^-}\sigma(\gamma)d\gamma. \tag{4.12}$$

After some rearrangement, we have

$$\int_{\gamma^+}^{\gamma^-}\sigma(\gamma)d\gamma = \gamma^-\sigma(\gamma^-) - \gamma^+\sigma(\gamma^+) - \frac{\rho}{2}\dot{s}^2({\gamma^-}^2 - {\gamma^+}^2). \tag{4.13}$$

Equations (4.7), (4.9) and (4.13) provide three equations for three unknowns γ^+, γ^- and $\dot{s}$, and these are the uniqueness conditions for the solution. We point out that these three conditions are derived without using any notion of the kinetic relation.

In the literature, it is stated that the kinetic relation (i.e., the specific form of the driving force in terms of $\dot{s}$) has to be determined from the lattice model and extra experiments, independently from the usual constitutive relation between the stress and strain. Here, we have actually derived the uniqueness conditions based on the given stress function $\sigma(\gamma)$ alone. Many people have also used hypotheses, such as dissipation-free kinetics and maximally dissipative kinetics, in order to determine the solution uniquely. It seems that these hypotheses are not necessary and incorrect for isothermal materials.

Using quadrature on (4.11) will give the detailed structure of the phase boundary. This and other issues, such as the asymptotic structure of the phase boundary for small a, the calculations of the dissipation rate and driving force for a nonzero a (it should be noted that the expression (1.6) does not stand for the driving force for nonzero a) and the nucleation condition, will be addressed and reported in the near future.

5 Conclusions

Important contributions have been made towards the understanding of dynamical phase transition problems in the work of Abeyaratne and Knowles and others; see the references cited in Abeyaratne et al. 2001. Solutions obtained by them are valid in the outer regions and the driving force (a quantity associated with dissipation rate and named by them) is also an important concept. Here, we have shown that for phase-transforming materials, there do not exist one-dimensional stress problems. Thus, it is essential to consider the influence of the radial deformation for phase transition problems in a circular rod (bar). We have adopted an approach similar to one used for nonlinear waves in fluids to obtain the model equation which takes into account the effect of the radial deformation. It turns out that the model equation represents a singular perturbation problem and the pure one-dimensional model is only the leading order equation at the outer regions. Then, by matching the traveling wave solution in the inner (boundary layer) region to the solutions in the two outer regions, we have obtained three equations for three unknowns across the phase boundary, which provide the uniqueness conditions for the solution. Our results seem to resolve the long outstanding issue of nonuniqueness of solutions in dynamical problems for phase-transforming materials. It should be emphasized that, although the uniqueness conditions obtained are for a particular physical problem, it seems that these conditions may apply to other physical problems which are modeled by the hyperbolic-elliptic equations (1.1) and (1.2) (the Lax entropy condition was obtained for gas dynamical equations but it also applies to other hyperbolic equations). Finally, we point out that our conclusion on the non-existence of one-dimensional stress problems for phase-transforming materials is purely based on the fact that there is a maximum/minimum in the constitutive strain-stress curve. It seems that for other physical problems if the constitutive relations have the same critical feature, the non-existence of one-dimensional problems might also hold.

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