Instability of equilibrium of evolving laminates in pseudo-elastic solids*

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Abstract

This study is concerned with isothermal stability of equilibrium of evolving laminated microstructures in pseudo-elastic solids with a multi-well free energy function. Several possible modes of instability associated with phase transition between energy wells are analysed. The related rate-independent dissipation is included by imposing a threshold value on the thermodynamic driving force. For a homogenized phase-transforming laminate with no length scale it is shown that localization instability is a rule in case of a nonzero interfacial jump of a directional nominal stress, irrespectively of actual boundary conditions. A stabilizing effect of elastic micro-strain energy at the boundary of the localization zone is demonstrated for laminates of finite spacing. Illustrative numerical examples are given for an evolving austenite-martensite laminate in a crystal of CuZnAl shape memory alloy.

Keywords: Microstructures; Phase transformation; Laminates; Energy methods; Stability

1 Introduction

Laminated microstructures are typical in pseudo-elastic solids with a multi-well free energy function, in particular in shape memory alloys under stress [1]. The term pseudo-elasticity is used here in relation to stress-induced phase transition between different energy wells; another meaning of pseudo-elasticity related to changes in the strain-energy function associated with damage [2] is not addressed here. Formation of fine laminates is explained by the tendency of the material to minimize its free energy [3, 1]. The respective mathematical theory and computational techniques of energy relaxation have been developed, e.g., in [4, 5, 6, 7, 8, 9]. Finite spacing of laminates and related size effects can be predicted by including interfacial energy of sharp or microstructured interfaces [10, 3, 11, 8, 12, 13]. Alternatively, strain-gradient or non-local effects in diffuse interface layers [14, 15, 16, 17, 18] can also be used to introduce length scales, although the material parameters involved in such modelling are not easily determined in advance.

Evolution of a laminate due to phase transition and interface propagation is associated with local jumps of the deformation gradient from one energy well to another. From a physical point of view, this is inevitably related to energy dissipation, no matter how slowly the macroscopic quantities vary in time. It follows that at least a part of dissipation must be treated as

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rate-independent in the *macroscopic* modelling. Therefore, although absolute minimization of free energy can correctly predict observable microstructures, it does not provide a complete description of their evolution under slowly applied loading. The simplest way to account for the rate-independent dissipation due to phase transformation is to impose a constant threshold value on the Eshelby driving force [19] acting on a moving phase transformation front. This yields a rate-independent constitutive law of macroscopic evolution of a phase-transforming laminate, whose explicit form, in case of fixed orientation of the *reference* traces of moving interfaces, was derived in [20]. It fits Rice's general internal-variable framework that includes both rate-independent and time-dependent dissipation and exhibits the 'normality structure' [21, 22]. At a finite macroscopic speed of evolution with respect to a natural time, the rate-independent dissipation is accompanied by time-dependent dissipation, for instance, due to viscous effects or to the transformation heat generated locally and next transported to the surrounding material and environment [23, 24, 25].

The presence of even small rate-independent dissipation has far-reaching consequences for the stability analysis. Absolute minimum of free energy at stable equilibrium is not required, rather, the sign of the total incremental energy supply including rate-independent dissipation on a path of departure from equilibrium is to be examined. This is an effect of treating micro-scale instabilities not as genuine instabilities at the macroscopic level, rather, as the source of the rate-independent dissipation itself, cf. [26] for a general discussion. The dissipation is path-dependent in general, which is evident for a closed cycle of deformation with or without phase transformation. For pseudo-elastic laminates, it may eliminate certain instability modes. In particular, uniform rotation of planar interfaces in an infinite continuum would enforce at infinity an infinite speed of phase transition fronts intersecting existing product phase layers and associated thus with infinitely many forward/reverse phase transitions. In the presence of dissipation, whatever small, this is not possible; this provides a motivation for the choice made in this paper to restrict attention to laminate interfaces that do not rotate in the reference configuration.

Quasi-static evolution of phase-transforming laminates in pseudo-elastic solids has been modelled, with particular reference to single crystals of shape memory alloys, e.g., in [27, 28, 29, 30, 31, 32, 33]. Although such laminates are commonly observed in experiments, a possible instability of a laminate model could rise questions about applicability of the results of calculations. In contrast to a well-developed theory of minimization of elastic strain energy and to related aspects of elastic stability, the problem of incremental stability of evolving laminates has attracted little attention so far. Available studies concern particular cases, e.g., [34], or are limited to laminates that are not undergoing phase transition, e.g., [35, 36]. No comprehensive analysis of stability of slowly evolving laminated microstructures undergoing phase transition with rate-independent dissipation has been found in the literature.

In this paper an attempt is made to fill this gap by systematic analysis of several possible modes of instability of equilibrium in evolving pseudo-elastic laminates and of respective stability criteria, under isothermal conditions. For this purpose, a general energy criterion of stability of equilibrium is applied which was earlier derived from the energy balance [37, 38], and more recently, from thermodynamic considerations [39]. In the criterion, it is the rate-independent part of dissipation which affects the thermodynamic criterion of stability of equilibrium, and not a rate-dependent part. In Section 4, the effect of flexibility of environment of a laminated domain on stability of equilibrium is investigated. In Section 5 we will show that specification of the stability criterion for a homogenized phase-transforming laminate with no length scale leads to the conclusion that intrinsic instability is a rule in case of a nonzero interfacial jump in a directional nominal stress, irrespectively of the stiffness of the loading device. A spontaneous localization of further phase transition is predicted, in relation to loss of rank-one convexity of a homogenized incremental potential at zero velocity gradient. This can lead to formation of laminates of a higher rank. The question whether instability persists for laminates of finite spacing within a bounded domain is addressed in Section 6 where a stabilizing effect of elastic micro-strain energy at the boundary of the localization zone is studied quantitatively. Illustrative numerical examples are given for an evolving austenite-martensite laminate in a crystal of CuZnAl shape memory alloy.

In the notation used below, bold-face letters denote vectors (in $\mathbf{R}^3$) or tensors, direct juxtaposition of two tensors or of a tensor and a vector in any order denotes simple contraction, a central dot means double contraction of tensors or a scalar product of vectors, and the symbol $\otimes$ denotes a tensor product.

2 Governing equations for an evolving laminate

Consider a laminate in which the material properties and deformation in a quasi-static process are uniform on every material plane orthogonal to a fixed unit vector $\mathbf{m}$ in the reference configuration. During the deformation, position vectors $\mathbf{X}$ of material points in the reference configuration do not vary, however, the reference traces of moving interfaces in an evolving laminate do. In the reference configuration, consider a representative volume element $\mathcal{R}$ such that the area A of a cross-section of $\mathcal{R}$ by any plane normal to $\mathbf{m}$ is independent of $\zeta_{\mathrm{m}} = \mathbf{X}\cdot\mathbf{m}$. In particular, in a periodic laminate we take $\mathcal{R}$ as a skew cylinder of a finite base at $\zeta_{\mathrm{m}} = 0$ and of a height equal to the laminate period $H > 0$ in the direction of $\mathbf{m}$. In a deformed configuration with position vectors $\mathbf{x}$, the boundary of $\mathcal{R}$ is, of course, corrugate (Fig. 1). The exposition in this section follows closely that in [20].

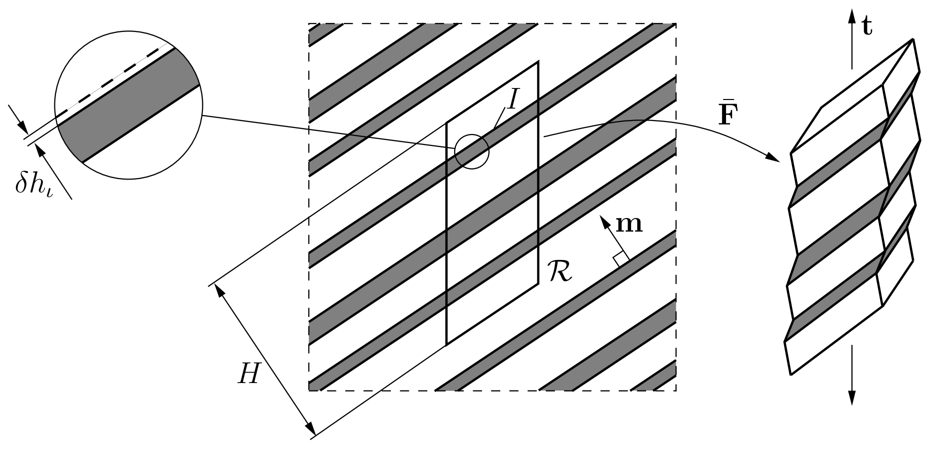


Figure 1: Laminated microstructure.

Denote by $\mathbf{F}$ the local deformation gradient, $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$, $\det\mathbf{F} > 0$, and by $\mathbf{S}$ the first (unsymmetric) Piola-Kirchhoff stress. No body forces or interface stresses are considered. The displacement continuity and stress equilibrium inside $\mathcal{R}$, assumed throughout the paper, require that

$$(\mathbf{F} - \{\mathbf{F}\})\mathbf{t} = \mathbf{0} \quad \text{if } \mathbf{t}\cdot\mathbf{m} = 0, \qquad (\mathbf{S} - \{\mathbf{S}\})\mathbf{m} = \mathbf{0}, \tag{1}$$

where, for ψ denoting any quantity and ':=' indicating a definition,

$$\{\psi\} := \frac{1}{H}\int_0^H \psi \,\mathrm{d}\zeta_{\mathrm{m}}\,, \qquad \zeta_{\mathrm{m}} := \mathbf{X}\cdot\mathbf{m}\,, \qquad \mathbf{X}\in\mathcal{R}. \tag{2}$$

The identity that follows,

$$(\mathbf{S}-\{\mathbf{S}\})\cdot(\mathbf{F}-\{\mathbf{F}\})=0, \tag{3}$$

upon averaging implies fulfillment of the Hill condition [40]

$$\{\mathbf{S}\cdot\mathbf{F}\}=\{\mathbf{S}\}\cdot\{\mathbf{F}\}. \tag{4}$$

Denote by a superimposed dot the forward rate, defined at a given $\zeta_{\rm m}$ as the *one-sided* derivative in the right-hand sense with respect to a time-like parameter θ, $\dot{\psi}=\mathrm{d}\psi/\mathrm{d}\theta^{+}$. By taking the rates of the equalities in (1) at fixed $\mathbf{m}$ and $\mathbf{t}$, and subtracting the averaged counterparts, we obtain

$$(\dot{\mathbf{F}}-\{\dot{\mathbf{F}}\})\mathbf{t}=\mathbf{0}\quad\text{if}\;\;\mathbf{t}\cdot\mathbf{m}=0,\qquad(\dot{\mathbf{S}}-\{\dot{\mathbf{S}}\})\mathbf{m}=\mathbf{0}. \tag{5}$$

This implies the rate analogs of Hill's condition (4),

$$\{\dot{\mathbf{S}}\}\cdot\{\mathbf{F}\}=\{\dot{\mathbf{S}}\cdot\mathbf{F}\},\qquad\{\mathbf{S}\}\cdot\{\dot{\mathbf{F}}\}=\{\mathbf{S}\cdot\dot{\mathbf{F}}\},\qquad\{\dot{\mathbf{S}}\}\cdot\{\dot{\mathbf{F}}\}=\{\dot{\mathbf{S}}\cdot\dot{\mathbf{F}}\}. \tag{6}$$

Note that if $\mathbf{m}$ were not fixed then (6) would not be a consequence of (4), in spite of validity of the latter at any instant.

We will assume that temperature has a given constant value and that the bulk material (outside the interfaces) obeys a local hyperelastic law,

$$\mathbf{S}=\frac{\partial\phi(\mathbf{F},\zeta_{\rm m})}{\partial\mathbf{F}}=\frac{\partial\dot{\phi}}{\partial\dot{\mathbf{F}}},\qquad\dot{\mathbf{S}}=\mathbf{C}\cdot\dot{\mathbf{F}},\qquad\mathbf{C}=\mathbf{C}(\mathbf{F},\zeta_{\rm m}):=\frac{\partial\dot{\mathbf{S}}}{\partial\dot{\mathbf{F}}}=\frac{\partial^2\phi}{\partial\mathbf{F}\partial\mathbf{F}}, \tag{7}$$

where ϕ is a non-convex, *multi-well* free energy density function. In particular, we will refer to shape memory alloys undergoing martensitic phase transformation (cf. [1]), with a finite number of phases indexed by ι, of deformation gradients $\mathbf{F}^{\rm t}_{\iota}$ in stress-free states,

$$\phi=\min_{\iota}\phi_{\iota}(\mathbf{F}^{\rm e}_{\iota}),\qquad\mathbf{F}^{\rm e}_{\iota}=\mathbf{F}(\mathbf{F}^{\rm t}_{\iota})^{-1}. \tag{8}$$

Of course, ϕ and ϕ_{ι} must satisfy the usual condition of frame-indifference, cf. [41]. In a special case within a geometrically linear framework, ϕ_{ι}'s may be quadratic functions so that ϕ is a piecewise quadratic function. However, in all theoretical considerations below, the actual form of ϕ is arbitrary except that it cannot be a rank-one convex function of $\mathbf{F}$.

Consider a given equilibrium state of the laminate, i.e. a given distribution of $\mathbf{F}(\zeta_{\rm m})$, $\mathbf{S}(\zeta_{\rm m})$ and phase index $\iota(\zeta_{\rm m})$ in $\mathcal{R}$. For a given $\{\dot{\mathbf{F}}\}$, the set of linear rate-equations in (5) and (7) defines the *elastic* response of the laminate and is assumed to have a unique solution in $\mathcal{R}$. Consequently, the local constitutive relationship (7) in the linear rate-form has a counterpart in the averaged variables:

$$\{\dot{\mathbf{S}}\}=\hat{\mathbf{C}}\cdot\{\dot{\mathbf{F}}\},\qquad\hat{\mathbf{C}}:=\frac{\partial\{\dot{\mathbf{S}}\}}{\partial\{\dot{\mathbf{F}}\}}=\frac{\partial^2\{\phi\}}{\partial\{\mathbf{F}\}\partial\{\mathbf{F}\}}, \tag{9}$$

with $\hat{\mathbf{C}}$ diagonally symmetric.

The macroscopic quantities, like deformation gradient $\bar{\mathbf{F}}$, first Piola-Kirchhoff stress $\bar{\mathbf{S}}$, and bulk free energy density $\bar{\phi}_V$ per unit reference volume, are defined as unweighted averages over $\mathcal{R}$ in the reference configuration of their local counterparts [40], viz.

$$\bar{\mathbf{F}}:=\{\mathbf{F}\},\qquad\bar{\mathbf{S}}:=\{\mathbf{S}\},\qquad\bar{\phi}_V:=\{\phi\}, \tag{10}$$

at each instant. Consider an evolving laminate where at one side of an interface I_ι a certain parent phase is transformed into a thin layer of a product phase (ι) that is growing with thickness $\delta h_\iota = \dot{h}_\iota \delta\theta + o(\delta\theta) > 0$ increasing continuously from zero at instant θ. Then, in contrast to (10), a macroscopic *rate*-variable $(\dot{\bar{\psi}})$ for an evolving laminate *differs* from the reference average of corresponding local rate-variable $\dot{\psi}$, viz.

$$\dot{\bar{\psi}} = \{\dot{\psi}\} + \frac{1}{H}\sum_\iota \dot{h}_\iota\, \Delta_\iota \psi, \qquad \dot{\bar{\mathbf{F}}} = \{\dot{\mathbf{F}}\} + \frac{1}{H}\sum_\iota \dot{h}_\iota\, \Delta_\iota \mathbf{F}, \qquad \dot{\bar{\mathbf{S}}} = \{\dot{\mathbf{S}}\} + \frac{1}{H}\sum_\iota \dot{h}_\iota\, \Delta_\iota \mathbf{S}, \tag{11}$$

where the sum is taken over all laminate interfaces within $\mathcal{R}$, although for convenience a product phase index ι is only displayed, and Δ_ι denote the interfacial jumps defined in Appendix A.

Consider now the particular case of a laminate formed by phase transition from an initially homogeneous parent phase, labeled by $\iota = 0$, say. Then, eqs. (1) have a solution such that all the parent phase layers are in the same current state. Consequently, in that state a single product phase is selected, in the manner to be discussed in Section 4, so that the jumps $\Delta_\iota \mathbf{F}$, $\Delta_\iota \mathbf{S}$ and $\Delta_\iota \phi$ do not vary within $\mathcal{R}$. Irrespectively of the number of active phase transformation fronts in $\mathcal{R}$, we can replace them by a single moving phase interface I that carries a jump $\Delta_I \psi$ in each relevant quantity ψ, and associate with it the rate $\dot{\eta} = \sum \dot{h}_\iota / H$ of the reference volume fraction of the currently produced product phase.

It is essential that (9) retains its validity also when phase interfaces are moving since the set of equations (5) and (7) is still to be satisfied in that case. On substituting (9) and eliminating $\{\dot{\mathbf{F}}\}$ between the last two equations in (11), for the laminate with a homogeneous parent phase we arrive at a particular form of plasticity-like macroscopic constitutive framework, viz.

$$\dot{\bar{\mathbf{S}}} = \hat{\mathbf{C}} \cdot \dot{\bar{\mathbf{F}}} - \dot{\eta}\, \mathbf{\Lambda}, \qquad \mathbf{\Lambda} := \hat{\mathbf{C}} \cdot \Delta_I \mathbf{F} - \Delta_I \mathbf{S}. \tag{12}$$

In a given state of $\mathcal{R}$, the driving force acting on the representative phase interface I is

$$f_I = \mathbf{S}_0 \cdot \Delta_I \mathbf{F} - \Delta_I \phi = -\frac{\partial \dot{\bar{\phi}}_V(\dot{\bar{\mathbf{F}}}, \dot{\eta})}{\partial \dot{\eta}} \tag{13}$$

at the current uniform stress $\mathbf{S}_0$ in the parent phase, cf. formula (A.7) in Appendix A. This formula remains valid also when product phase layers are *created* inside the parent phase. The well-known formula [19] for the Eshelby driving force acting on an *existing* phase transformation front is recovered in the particular case when (A.4) holds.

It has been shown [20] that

$$\overset{\circ}{f}_I = \mathbf{\Lambda} \cdot \{\dot{\mathbf{F}}\} = \mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} - g\dot{\eta}, \qquad g := \Delta_I \mathbf{F} \cdot \hat{\mathbf{C}} \cdot \Delta_I \mathbf{F}, \tag{14}$$

where the 'time' derivative $\overset{\circ}{f}_I$ of f_I is not taken at a material point, rather, it follows the normal trajectory of an evolving interface I in the reference configuration (the Thomas time derivative). Note that $g > 0$ if $\hat{\mathbf{C}}$ is strongly elliptic. We have

$$\dot{\eta} = \frac{1}{g}(\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} - \overset{\circ}{f}_I) \quad \text{if } g \neq 0. \tag{15}$$

On substituting equation (15) into (12), we obtain

$$\dot{\bar{\mathbf{S}}} = \hat{\mathbf{C}} \cdot \dot{\bar{\mathbf{F}}} - \frac{1}{g}(\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} - \overset{\circ}{f}_I)\mathbf{\Lambda} \quad \text{if } g \neq 0. \tag{16}$$

At the moment we have not postulated yet any constitutive relationship for $\overset{\circ}{f}_I$ or $\dot{\eta}$. The case of rate-independent phase transition that proceeds at $f_I = \text{const}$ on the time-scale of θ will be of particular interest below.

3 Energy criterion for stability of equilibrium

Let $\mathcal{G}$ denote symbolically the state of a material body within a certain domain $\mathcal{M}$ in the reference configuration. We restrict attention to the isothermal case. Then, $\mathcal{G}$ can be identified with a pair $(\tilde{\mathbf{u}}, \tilde{\iota})$, where $\mathbf{u} = \mathbf{x} - \mathbf{X}$ is a displacement, ι is a phase index as above, and a tilde denotes a field over $\mathcal{M}$. Consider an equilibrium state $\mathcal{G}^0$ which, by definition, may remain unchanged when a loading parameter λ is kept fixed. The energy condition for stability of an equilibrium state $\mathcal{G}^0$ at constant temperature reads

$$\Delta E > 0 \qquad \forall \mathcal{G} \neq \mathcal{G}^0 \quad \text{at fixed } \lambda, \tag{17}$$

which means that ΔE is positive for every admissible path from $\mathcal{G}^0$ to every accessible neighbouring state $\mathcal{G} \neq \mathcal{G}^0$ at a fixed value of a loading parameter λ. ΔE denotes here the energy to be supplied by a disturbing agency to the isolated thermodynamic system: material body + loading device + heat reservoir. It is essential that ΔE does not include a possible rate-dependent dissipation, whose assumed non-negativeness implies that $\Delta V = \Delta E + \Delta K$ has the usual properties of a Lyapunov functional [39], with $\Delta K \geq 0$ being the kinetic energy not included in ΔE. The condition (17) can also be derived from the energy balance [37, 38]. In accord with the classical thermodynamics, ΔE is specified as follows

$$\Delta E = \Delta W^{\text{in}} + \Delta \Omega = \Delta \Phi + \Delta \mathcal{D}^{\text{in}} + \Delta \Omega \tag{18}$$

in terms of the increments: ΔW of work supplied to the material, $\Delta \Phi$ of the total Helmholtz free energy of the material, $\Delta \mathcal{D}$ of the total dissipated energy, and $\Delta \Omega$ of the potential energy of the loading device (assumed conservative). Label 'in' means that only rate-independent part of dissipation is included. ΔE is to be calculated along a *virtual*, isothermal and quasi-static path of departure from a given equilibrium state $\mathcal{G}^0$. Φ includes a bulk free energy Φ_V and may also include energy of boundaries or interfaces, cf. [42] and Section 6 below.

The condition (17) is exploited by developing ΔE along a path of departure from $\mathcal{G}_0$ into the Taylor series, $\Delta E = \dot{E}\Delta\theta + \frac{1}{2}\ddot{E}(\Delta\theta)^2 + \ldots$, with respect to θ treated as a path-length parameter and not as a natural time. Fulfillment of (17) requires that

$$\dot{E} \geq 0 \qquad \text{and} \qquad \ddot{E} \geq 0 \quad \text{if} \quad \dot{E} = 0 \qquad \text{in } \mathcal{G}^0 \quad \text{at fixed } \lambda. \tag{19}$$

In contrast to (17), the conditions in (19) are regarded here as *necessary* for stability of equilibrium. A justification will be provided in the particular cases examined in next sections.

The dissipation in (18) is a *virtual rate-independent dissipation* that is defined, for the representative volume element $\mathcal{R}$ of a laminate, in the simplest form as follows,

$$\Delta \mathcal{D}^{\text{in}}_R := A \int_{\theta}^{\theta+\Delta\theta} D \, \mathrm{d}\theta', \qquad D = \sum_{\iota} f_c \dot{h}_\iota, \qquad f_c = \text{const} \geq 0, \qquad \dot{h}_\iota \geq 0, \tag{20}$$

where D is the dissipation function. If $f_c = 0$ then the stability condition (17) reduces to the classical condition of the minimum of the total potential energy of the system with path-independent ΔE.

The potential energy Ω of the loading device has to be included in the stability considerations, unless its value is insensitive to virtual deformations as in the case of purely kinematic control. In the assumed absence of body forces, Ω is taken to be a given function of a displacement field $\tilde{\mathbf{u}}$ restricted to $\partial\mathcal{M}$ and of a loading parameter λ, $\Omega = \Omega(\tilde{\mathbf{u}}, \lambda)$. In a special case examined below, $\tilde{\mathbf{u}}$ over $\partial\mathcal{M}$ will be generated by the overall deformation gradient.

4 Instability at uniform macroscopic strain

Throughout this section the deformation of a laminate domain $\mathcal{M}$ is assumed to be macroscopically uniform, so that the macroscopic deformation gradient is the same in every $\mathcal{R} \subset \mathcal{M}$; this special assumption will be relaxed in Section 5. We will examine stability of equilibrium of $\mathcal{M}$ placed in a flexible loading device, represented for instance by a surrounding elastic medium. We stick to the assumptions from Section 2, in particular of uniformity of the deformation within any material plane normal to a fixed $\mathbf{m}$ in the reference configuration. On a path of departure from equilibrium, the laminate can evolve smoothly by creation and propagation of phase interfaces in addition to elastic deformation.

4.1 First-order condition for stability

No interfacial or boundary energy is considered until Section 6. Accordingly, the work supplied to $\mathcal{M}$, identified with ΔW^{in} that appears in (18), per unit reference volume of $\mathcal{M}$ is specified as follows:

$$\Delta w^{\text{in}} := \frac{\Delta W_R^{\text{in}}}{|\mathcal{R}|} = \frac{\Delta W^{\text{in}}}{|\mathcal{M}|} = \Delta\bar{\phi}_V + \frac{1}{H}\int_{\theta}^{\theta+\Delta\theta} \sum_{\iota} f_c \dot{h}_{\iota}\,\mathrm{d}\theta'. \tag{21}$$

Since $\dot{\bar{\phi}}_V$ as a function of $\dot{\bar{\mathbf{F}}}$ and $\dot{h}_\iota$'s, treated as independent rate-variables, is homogeneous of degree one, on using Euler's theorem and eqs. (A.6) from Appendix A, we obtain

$$\dot{\bar{\phi}}_V = \frac{\partial \dot{\bar{\phi}}_V}{\partial \dot{\bar{\mathbf{F}}}} \cdot \dot{\bar{\mathbf{F}}} + \sum_{\iota} \frac{\partial \dot{\bar{\phi}}_V}{\partial \dot{h}_\iota} \dot{h}_\iota = \bar{\mathbf{S}} \cdot \dot{\bar{\mathbf{F}}} - \frac{1}{H}\sum_{\iota} f_\iota \dot{h}_\iota. \tag{22}$$

Hence,

$$\dot{w}^{\text{in}} = \bar{\mathbf{S}} \cdot \dot{\bar{\mathbf{F}}} + \frac{1}{H}\sum_{\iota}(f_c - f_\iota)\dot{h}_\iota. \tag{23}$$

The *first-order* stability condition $(19)_1$ in the special case $\dot{\bar{\mathbf{F}}} = \mathbf{0}$ yields

$$\dot{w}^{\text{in}}\Big|_{\dot{\bar{\mathbf{F}}}=\mathbf{0}} \geq 0 \quad \Longleftrightarrow \quad f_\iota \leq f_c \quad \forall \iota \qquad \text{in stable } \mathcal{G}^0, \tag{24}$$

which will be discussed below.

To study stability at $\dot{\bar{\mathbf{F}}} \neq \mathbf{0}$, consider $\mathcal{M}$ to be surrounded by an elastic medium; this may correspond to $\mathcal{M}$ viewed as a grain within a matrix representing, for instance, a polycrystalline aggregate. As we have assumed that $\bar{\mathbf{F}}$ is and remains uniform in $\mathcal{M}$, the surface displacement field over $\partial\mathcal{M}$ is generated by $\bar{\mathbf{F}}$. Accordingly, the potential energy of the environment of $\mathcal{M}$ is taken as a function $\Omega_M = \Omega_M(\bar{\mathbf{F}}, \lambda)$, so that

$$\frac{\dot{\Omega}_M}{|\mathcal{M}|} = -\mathbf{S}^{\text{ext}} \cdot \dot{\bar{\mathbf{F}}} + \frac{1}{|\mathcal{M}|}\frac{\partial \Omega_M(\bar{\mathbf{F}}, \lambda)}{\partial \lambda}\dot{\lambda}, \qquad \mathbf{S}^{\text{ext}} := -\frac{1}{|\mathcal{M}|}\frac{\partial \Omega_M(\bar{\mathbf{F}}, \lambda)}{\partial \bar{\mathbf{F}}}. \tag{25}$$

Displacement fluctuations over the boundary $\partial\mathcal{M}$ are not included in Ω_M being a function of a macroscopic quantity $\bar{\mathbf{F}}$ only. However, such fluctuations can be taken into account by introducing a boundary energy Φ_S, cf. Section 6. Time differentiation of the external stress $\mathbf{S}^{\text{ext}}$ (cf. [43] for a discussion of that concept) yields

$$\dot{\mathbf{S}}^{\text{ext}} = -\mathbf{C}^* \cdot \dot{\bar{\mathbf{F}}} - \frac{1}{|\mathcal{M}|}\frac{\partial^2 \Omega_M(\bar{\mathbf{F}}, \lambda)}{\partial \bar{\mathbf{F}}\partial \lambda}\dot{\lambda}, \qquad \mathbf{C}^* = \frac{1}{|\mathcal{M}|}\frac{\partial^2 \Omega_M(\bar{\mathbf{F}}, \lambda)}{\partial \bar{\mathbf{F}}\partial \bar{\mathbf{F}}}, \tag{26}$$

with $\mathbf{C}^*$ diagonally symmetric.

On combining equations (23) and (25), we obtain

$$\dot{e} := \frac{\dot{E}}{|\mathcal{M}|} = (\bar{\mathbf{S}} - \mathbf{S}^{\mathrm{ext}}) \cdot \dot{\bar{\mathbf{F}}} + \frac{1}{H} \sum_{\iota} (f_c - f_\iota) \dot{h}_\iota + \frac{1}{|\mathcal{M}|} \frac{\partial \Omega_M(\bar{\mathbf{F}}, \lambda)}{\partial \lambda} \dot{\lambda}. \tag{27}$$

In an equilibrium state the first term on the right-hand side vanishes by the principle of virtual work, while the last term vanishes at fixed λ. The remaining central term is to be nonnegative in a stable equilibrium state; it reduces to the first-order condition for stability of equilibrium (24) obtained for $\dot{\bar{\mathbf{F}}} = \mathbf{0}$.

The condition $\dot{e} > 0$ reduced to (24) is interpreted as necessary for stability of equilibrium in the following sense. Let the kinetic law for a phase transformation front moving with a *true* normal speed $v_\iota = \mathrm{d}h_\iota/\mathrm{d}t$, taken with respect to a *natural* time t rather than a time-like parameter θ, be of the form, cf. [21, 23, 25],

$$v_\iota = v_\iota(f_\iota) \quad \text{continuous}, \qquad v_\iota = 0 \quad \text{if} \ |f_\iota| \leq f_c, \qquad \frac{\mathrm{d}v_\iota}{\mathrm{d}f_\iota^+} > 0 \quad \text{if} \ f_\iota \geq f_c. \tag{28}$$

Then, in the state of mechanical equilibrium in which (24) is violated, a phase transition front can be created, or already exists in case of (A.4), that can start to move spontaneously with a normal speed $v_\iota > 0$, implying the possibility of quasi-static departure from equilibrium. If inertia effects are included during the departure then the definition of f_ι is to be modified [44].

The rate-independent analog of the kinetic law (28) reads [21, 22]

$$\dot{h}_\iota > 0 \quad \Longrightarrow \quad f_\iota = f_c, \qquad f_c = \text{const} \geq 0. \tag{29}$$

It may be interpreted as the condition of compatibility of the actual dissipation rate $f_\iota \dot{h}_\iota$ with the virtual rate-independent dissipation rate $f_c \dot{h}_\iota$. Jointly with (24) and positiveness of δh_ι, it yields the thermodynamic criterion of phase transformation in the rate-independent form

$$\dot{h}_\iota \geq 0, \qquad f_\iota - f_c \leq 0, \qquad (f_\iota - f_c)\dot{h}_\iota = 0. \tag{30}$$

It has the interpretation as the Kuhn-Tucker conditions for minimization of the supplied work-rate $\dot{w}^{\mathrm{in}}$ defined by (23) in a stable equilibrium state at given $\dot{\bar{\mathbf{F}}}$. Note that the minimization is performed with respect to all transformation modes, also those associated with creation of a new product phase layer. In particular, instability of equilibrium of a homogeneous parent phase can be concluded although no phase interface exists in that state; cf. the interpretation of f_ι that follows its definition (A.7). A recent extension of (30) accounting for interfacial energy contributions is given in [42].

4.2 Illustrative example

From now on we restrict attention to the particular case of an initially homogeneous parent phase ($\iota = 0$). Let $f_\iota < f_c$ initially for all $\iota \neq 0$ and for all laminate orientations $\mathbf{m}$. As an overall stress level increases, a critical state is reached when $f_\iota = f_c$ for some ι while (24) still holds. Then, a laminate can start to form by phase transition from the homogeneous parent phase to that phase ι, with the laminate orientation $\mathbf{m}$ found by maximizing f_ι with respect to $\mathbf{m}$. If the solution is not unique then the respective laminates are typically symmetry-related, and just one of them is selected for further study.

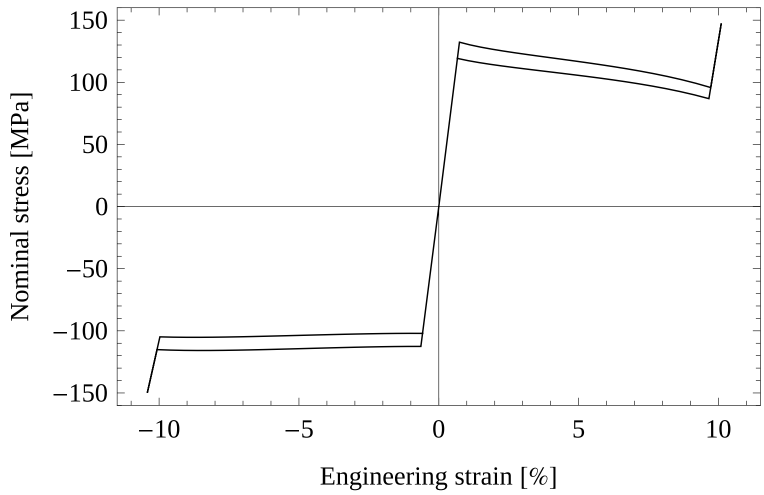


Figure 2: Pseudo-elastic response of a single crystal of CuZnAl shape memory alloy in uniaxial tension and compression.

As an illustration, we consider uniaxial tension or compression of a single crystal of CuZnAl shape memory alloy undergoing the cubic-to-monoclinic martensitic phase transformation. Stress-induced transformation in a pseudo-elastic regime is studied, hence austenite is the initial homogeneous parent phase, and evolution of a two-phase austenite-martensite laminate under controlled elongation in the direction of uniaxial stress is examined. The selected martensite variant (ι) and orientation $\mathbf{m}$ of the martensite layers are calculated by maximixing f_ι as discussed above, separately for tension and compression. Figure 2 shows the macroscopic response with the characteristic pseudo-elastic hysteresis loops upon unloading. In particular, the elastic loading is followed by a plateau that corresponds to the stress-induced transformation and a varying volume fraction of martensite. The loading scheme and the material parameters are here the same as in [30], and the loading axis orientation is specified by the unit vector $\mathbf{t} = (0.994, 0.099, 0.050)$ that corresponds to direction A in [30].

This numerical example is used throughout this work to illustrate the theoretical developments. In particular, macroscopically homogeneous equilibrium states of the evolving laminate, reached at an increasing absolute value of axial strain and parameterized by the volume fraction η of martensite increasing from 0 to 1, will be examined from the point of view of their resistance to different instability modes.

4.3 Second-order conditions for stability

In the case of a homogeneous parent phase discussed in Section 2 and illustrated by the example, a single representative phase interface I of normal $\mathbf{m}$ in the reference configuration is considered, with a jump $\Delta_I \psi$ in each relevant quantity ψ associated with the rate $\dot{\eta}$ of the reference volume fraction of the selected product phase; possible decomposition of the latter into a number of layers within $\mathcal{R}$ is inessential as long as interfacial and boundary energy is disregarded. Consider an equilibrium state $\mathcal{G}^0$ on a phase transformation path, such that $f_I = f_c$. Then $\dot{e} = 0$ in $\mathcal{G}^0$ at fixed λ since transformation modes other than that related to propagation of I are no longer considered. Consequently, the second stability condition in (19) is to be examined. A derivative of (27) with respect to θ, evaluated in an equilibrium state $\mathcal{G}^0$ at $f_I = f_c$ and at fixed

λ, leads to the following *second-order* condition for stability of equilibrium

$$\ddot{e} = (\dot{\bar{\mathbf{S}}} - \dot{\mathbf{S}}^{\mathrm{ext}}) \cdot \dot{\bar{\mathbf{F}}} - \overset{\circ}{f}_I \dot{\eta} \geq 0 \qquad \text{in } \mathcal{G}^0 \quad \text{if } \dot{e} = 0 \quad \text{(at fixed } \lambda).8 \tag{31}$$

On using equalities $(12)_1$ and $(26)_1$, the left-hand expression in (31) becomes

$$\ddot{e} = \dot{\bar{\mathbf{F}}} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*) \cdot \dot{\bar{\mathbf{F}}} - (\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} + \overset{\circ}{f}_I)\dot{\eta}. \tag{32}$$

On account of (32) and (14), the stability condition (31) is transformed to the form

$$\ddot{e} = \dot{\bar{\mathbf{F}}} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*) \cdot \dot{\bar{\mathbf{F}}} + (g\dot{\eta} - 2\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}})\dot{\eta} \geq 0 \qquad \text{in } \mathcal{G}^0 \quad \text{if } \dot{e} = 0 \quad \text{(at fixed } \lambda). \tag{33}$$

Let us analyze this condition in more detail under the assumption $f_I = f_c$. First, it is observed that

$$g > 0 \tag{34}$$

is necessary for fulfillment of (33) for a finite $\dot{\eta} > 0$ at $\dot{\bar{\mathbf{F}}} = \mathbf{0}$ (or at $\dot{\bar{\mathbf{F}}}$ small enough), as preventing uncontrolled phase transition at (almost) constant macroscopic deformation gradient $\bar{\mathbf{F}}$. The consistency conditions associated with the rate-independent transformation criterion (30) for the representative phase interface are

$$\overset{\circ}{f}_I \leq 0 \quad \text{if } f_I = f_c, \qquad \overset{\circ}{f}_I \dot{\eta} = 0. \tag{35}$$

If $g > 0$ then the value of $\dot{\eta}$ is uniquely determined from (15) and (35), viz.

$$\dot{\eta} = \frac{1}{g} \max\left(\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}}, 0\right), \tag{36}$$

and the expression (16) can be reformulated as follows:

$$\dot{\bar{\mathbf{S}}} = \frac{\partial \bar{U}}{\partial \dot{\bar{\mathbf{F}}}}, \qquad 2\bar{U}(\dot{\bar{\mathbf{F}}}) = \begin{cases} \dot{\bar{\mathbf{F}}} \cdot \hat{\mathbf{C}} \cdot \dot{\bar{\mathbf{F}}} - \dfrac{1}{g}(\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}})^2 & \text{if } \mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} > 0, \\ \dot{\bar{\mathbf{F}}} \cdot \hat{\mathbf{C}} \cdot \dot{\bar{\mathbf{F}}} & \text{if } \mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} \leq 0. \end{cases} \tag{37}$$

Moreover, the instantaneous stiffness moduli $\bar{\mathbf{C}}$ corresponding to $\dot{\eta} > 0$ read

$$\bar{\mathbf{C}} = \hat{\mathbf{C}} - \frac{1}{g}\mathbf{\Lambda} \otimes \mathbf{\Lambda}, \qquad \dot{\bar{\mathbf{S}}} = \bar{\mathbf{C}} \cdot \dot{\bar{\mathbf{F}}} \qquad \text{if } \mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} > 0. \tag{38}$$

It can be seen that there is a remarkable analogy to the constitutive rate equations of classical elastoplasticity at finite strain, with the normality flow rule relative to a smooth yield surface in strain space, cf. [37, 45].

Second, the condition for elastic stability (at $\dot{\eta} = 0$) is

$$\dot{\bar{\mathbf{F}}} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*) \cdot \dot{\bar{\mathbf{F}}} > 0 \qquad \text{for all } \dot{\bar{\mathbf{F}}} \neq 0, \tag{39}$$

i.e., that the fourth-order tensor $(\hat{\mathbf{C}} + \mathbf{C}^*)$ be positive definite. Clearly, for (33) it is necessary that $(\hat{\mathbf{C}} + \mathbf{C}^*)$ be positive semi-definite. If $g > 0$ then the fulfillment of (39) is necessary for (33) unless the left-hand expression in (39) happens to vanish only for some eigenmode $\dot{\bar{\mathbf{F}}}$ being precisely orthogonal to $\mathbf{\Lambda}$. Usually, the condition of elastic stability is examined in detail in the case of dead loading where $\mathbf{C}^* = \mathbf{0}$, cf. [41]. The reasons for including a stiffness $\mathbf{C}^*$ of the environment of a material element have been discussed in [45].

Third, if both conditions (34) and (39) are satisfied then constrained minimization of the left-hand expression in (33) with respect to $\dot{\bar{\mathbf{F}}}$ at any given $\dot{\eta}$ yields (cf. Appendix B)

$$\ddot{e}^{\min} := \min_{\dot{\bar{\mathbf{F}}}} \ddot{e}(\dot{\bar{\mathbf{F}}}, \dot{\eta}) = (g - \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \cdot \mathbf{\Lambda})\dot{\eta}^2. \tag{40}$$

The stability condition in (33), under assumptions (34) and (39), is thus reduced to

$$g^* := g - \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \cdot \mathbf{\Lambda} \geq 0, \tag{41}$$

where the left-hand expression contains no unknowns and can be calculated directly. This represents a special case of the stability condition derived in [26] for multiple internal mechanisms of inelastic deformation.

Instability related to failure of (41) can be given the following interpretation. With the reference to formulae given in Appendix B, the deformation mode defined at $f_I = f_c$ by (B.2) satisfies the condition (B.3) of continuing equilibrium and corresponds through (B.4) to $\overset{\circ}{f}_I > 0$. If a kinetic law (28) is used then this is associated with a non-zero *acceleration* $\dot{v}_\iota$ of phase interfaces represented by I, which implies instability of equilibrium. The acceleration with respect to a natural time must be sufficiently small initially to allow inertia effects to be neglected, in accord with (B.3). In brief, failure of (41) allows for spontaneous phase transformation in $\mathcal{M}$ under flexible external constraints.

As shown in Appendix B, if $\hat{\mathbf{C}}$ is positive definite then, in the limit case of dead loading, i.e. when $\mathbf{C}^* = \mathbf{0}$, we obtain

$$\lim_{\|\mathbf{C}^*\| \to 0} g^* = -\Delta_I \mathbf{S} \cdot (\hat{\mathbf{C}})^{-1} \cdot \Delta_I \mathbf{S} < 0 \qquad \text{if } \Delta_I \mathbf{S} \neq \mathbf{0}. \tag{42}$$

It follows that in a homogeneous equilibrium state of a laminate domain $\mathcal{M}$ under dead loading over $\partial\mathcal{M}$, in which $f_I = f_c$ and $\Delta_I \mathbf{S} \neq \mathbf{0}$, either the condition of elastic stability fails or $g^* < 0$. Except an uncertainty case where $\hat{\mathbf{C}}$ is just positive semidefinite (for instance, due to presence of a rotational symmetry axis), and in agreement with the conclusion in [26] derived on a different route, we arrive at the following general conclusion. Any equilibrium state of a phase-transforming laminate in $\mathcal{M}$ at $f_I = f_c$ is unstable under all-round dead loading in the presence of an interfacial jump in stress, $\Delta_I \mathbf{S} \neq \mathbf{0}$. The instability is understood in the sense described above when interpreting failure of (41).

Condition (41) with $\mathbf{C}^*$ calculated with the help of the Eshelby solution for an ellipsoidal inclusion in an infinite elastic matrix will be used in Section 6 in an extended version that will include the boundary energy effect.

5 Intrinsic instability in a homogenized laminate

In contrast to the preceding Section 4, macroscopic uniformity of deformation of the laminate is no longer assumed. To concentrate on intrinsic stability of the laminate irrespectively of the stiffness of a loading device, we regard here the boundary $\partial\mathcal{M}$ of a laminate domain $\mathcal{M}$ at fixed λ as rigidly constrained, so that $\Delta\Omega \equiv 0$. The attention is focused on stability against a spontaneous progress of phase transformation and deformation localized within a narrow subdomain $\mathcal{B}$ of $\mathcal{M}$, compensated by elastic unloading in $\mathcal{M} \setminus \mathcal{B}$. We adopt the assumptions under which the homogenized constitutive law in the potential form (37) can be applied pointwise. This is acceptable provided the lowest dimension of $\mathcal{B}$ is much greater than a laminate period H (arbitrarily small here), and the conditions (24) and (34) are satisfied to avoid instabilities of the type already discussed in Section 4.

5.1 Exploitation of macroscopic rate-potential

If the consistency condition (35) is enforced then the condition $(19)_2$ for stability of equilibrium takes an integral form over the reference volume of $\mathcal{M}$ in terms of the constitutive rate-potential $\bar{U}$ defined by (37), cf. [37, 46],

$$\ddot{W}^{\mathrm{in}} = 2\int_{\mathcal{M}} \bar{U}(\nabla\mathbf{v})\mathrm{d}V \geq 0 \quad \text{in } \mathcal{G}^0 \quad \forall \mathbf{v}:\ \mathbf{v}=\mathbf{0} \text{ on } \partial\mathcal{M}. \tag{43}$$

Here, $\mathbf{v}$ is a vector field $\mathcal{M} \to \mathbf{R}^3$ from the Sobolev space $H_0^1(\mathcal{M})$ (or simpler, a continuous and piecewise continuously differentiable field), interpreted as a virtual *macroscopic* velocity field, and the gradient $\nabla\mathbf{v}$ is taken in the reference configuration.

The condition (43) refers to a homogeneous continuous body. If the continuum were inhomogeneous then the condition (43) would also appear at a material point level as the condition of *quasiconvexity*[1] *of* $\bar{U}$ *at* $\nabla\mathbf{v}=\mathbf{0}$, necessary for $(19)_2$.

Point-wise conditions related to (43) are obtained by using the theorems of the calculus of variations and the special form of $\bar{U}$ [46]. Recall that a condition necessary for (43) (by the Graves theorem) is that $\bar{U}$ is *rank-one convex at* $\nabla\mathbf{v}=\mathbf{0}$, viz.

$$\bar{U}(\mathbf{c}\otimes\mathbf{n}) \geq 0 \qquad \forall\, \mathbf{c},\mathbf{n} \in \mathbf{R}^3. \tag{44}$$

Due to the special structure of $\bar{U}$ that is quadratic in each halfspace of $\nabla\mathbf{v}$-space corresponding to opposite signs of $\boldsymbol{\Lambda}\cdot\dot{\bar{\mathbf{F}}}$ (at assumed $g>0$), the stability condition (44) is *equivalent* (by van Hove's theorem and Hill's relative convexity property) both to (43) and to the Legendre-Hadamard condition for the moduli $\bar{\mathbf{C}}$ in the phase transition branch as defined by (38), viz.

$$(\mathbf{c}\otimes\mathbf{n})\cdot\hat{\mathbf{C}}\cdot(\mathbf{c}\otimes\mathbf{n}) - \frac{1}{g}(\mathbf{c}\boldsymbol{\Lambda}\mathbf{n})^2 \geq 0 \qquad \forall\, \mathbf{c},\mathbf{n}. \tag{45}$$

A prerequisite for (45) is that the elastic acoustic tensor is positive definite for every $\mathbf{n}\neq\mathbf{0}$ (or that $\hat{\mathbf{C}}$ is strongly elliptic), viz.

$$\mathbf{c}\hat{\mathbf{Q}}_{\mathrm{n}}\mathbf{c} > 0 \quad \forall\, \mathbf{c},\mathbf{n}\neq\mathbf{0}, \qquad (\hat{\mathbf{Q}}_{\mathrm{n}})_{pk} := \hat{C}_{prkl}n_r n_l, \tag{46}$$

except when the expression $\mathbf{c}\hat{\mathbf{Q}}_{\mathrm{n}}\mathbf{c}$ is nonnegative and happens to vanish only simultaneously with $(\mathbf{c}\boldsymbol{\Lambda}\mathbf{n})$ (the usual indicial notation with the summation convention is used above to define $\hat{\mathbf{Q}}_{\mathrm{n}}$).

Under the assumption (46) it can be shown that (45), and hence (44) and (43), all become equivalent to

$$g_{\mathrm{n}} := g - (\boldsymbol{\Lambda}\mathbf{n})(\hat{\mathbf{Q}}_{\mathrm{n}})^{-1}(\boldsymbol{\Lambda}\mathbf{n}) \geq 0 \qquad \forall\, \mathbf{n}. \tag{47}$$

With strict inequality, this condition is known as excluding *bifurcation* within a band, cf. [48, 49]. It represents also a special case of the condition for uniqueness and stability of equilibrium against spontaneous formation of deformation bands in an incrementally piecewise-linear continuum [43, 26]. The present proof given in Appendix C provides a direct energy interpretation of g_{n} as being proportional to the second-order energy input to a band $\mathcal{B}$, of a reference normal $\mathbf{n}$, that deforms with a velocity gradient $\dot{\bar{\mathbf{F}}} = \mathbf{c}\otimes\mathbf{n}$ compatible with rigid-body motion outside $\mathcal{B}$. Namely, is it shown that constrained minimization of that second-order energy input, per unit reference volume of $\mathcal{B}$, with respect to $\mathbf{c}$ at given $\mathbf{n}$ yields

$$\ddot{e}_{\mathrm{n}}^{\min} = g_{\mathrm{n}}\xi\dot{\eta}^2 \qquad \text{for } \mathbf{c}=\mathbf{c}_{\mathrm{n}} := \xi\dot{\eta}(\hat{\mathbf{Q}}_{\mathrm{n}})^{-1}\boldsymbol{\Lambda}\mathbf{n}, \tag{48}$$

[1] In the sense of Morrey [47].

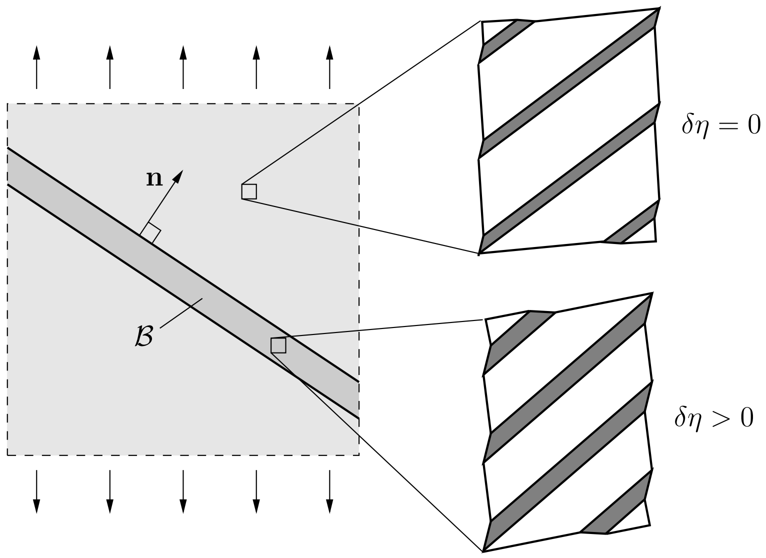


Figure 3: Intrinsic instability of equilibrium in a homogenized laminate.

where either $\xi = 1$ or $\xi = \xi_{\rm n}$ given by formula (C.9) is substituted depending on whether the minimization is performed at fixed $\dot\eta$ or at the side constraint $\overset{\circ}{f}_I = 0$, respectively. The latter case corresponds to the use of the constitutive rate-potential $\bar U$ defined by (37) while the former is useful in the interpretation below of the instability related to failure of (47).

Consider first an unbounded $\mathcal{M}$; then condition (47) is necessary for stability of equilibrium in the following sense. Failure of (47), and hence of (43), (44) and (45) simultaneously, implies through (48) that further transformation restricted to band $\mathcal{B}$ as above with $\dot{\bar{\mathbf{F}}} = \mathbf{c}\otimes\mathbf{n}$ at $\dot\eta > 0$ is associated with energy release from the material. In a time scale such that the kinetic law (28) for a moving phase transformation front is applicable but inertia effects can still be disregarded, that instability mode, visualized in Fig. 3, is indeed realizable. Namely, on substituting $\xi = 1$ into $(48)_2$ and the resulting $\dot{\bar{\mathbf{F}}} = \mathbf{c}_{\rm n}\otimes\mathbf{n}$ into (15) and (16), we obtain, cf. (C.4) and (C.6),

$$\xi = 1 \qquad \Longrightarrow \qquad \overset{\circ}{f}_I = -g_{\rm n}\dot\eta \quad \text{and} \quad \dot{\bar{\mathbf{S}}}\mathbf{n} = \mathbf{0}. \tag{49}$$

If $g_{\rm n} < 0$ then $\overset{\circ}{f}_I > 0$. It follows, according to (28), that phase transformation fronts represented by interface I within $\mathcal{B}$ can start to move spontaneously with the speed v_ι growing from zero with acceleration $\dot v_\iota > 0$, implying instability of equilibrium, in analogy to the interpretation of (41).

The same conclusion is obtained for a sufficiently thin disk $\mathcal{B}$ in a finite domain $\mathcal{M}$ by using the construction given in [46].

It is worth mentioning that another condition equivalent to (45) is

$$g_{\rm c} := g - (\mathbf{c}\mathbf{\Lambda})(\hat{\mathbf{R}}_{\rm c})^{-1}(\mathbf{c}\mathbf{\Lambda}) \geq 0, \qquad (\hat{\mathbf{R}}_{\rm c})_{rl} \equiv \hat C_{prkl}c_p c_k. \tag{50}$$

This is obtained analogously as (47) but physical interpretation is less clear.

5.2 Persisting instability of evolving laminates

Now we exploit the specific expressions $(12)_2$ for $\mathbf{\Lambda}$ and $(14)_2$ for g. For convenience, they are recalled here

$$\mathbf{\Lambda} := \hat{\mathbf{C}}\cdot\Delta_I\mathbf{F} - \Delta_I\mathbf{S}\,, \qquad g := \Delta_I\mathbf{F}\cdot\hat{\mathbf{C}}\cdot\Delta_I\mathbf{F}, \tag{51}$$

where, for some vector $\mathbf{b} \neq \mathbf{0}$, cf. (A.2),

$$\Delta_I \mathbf{F} = \mathbf{b} \otimes \mathbf{m}, \qquad \Delta_I \mathbf{S}\mathbf{m} = \mathbf{0}, \qquad \Delta_I \mathbf{S} \cdot \Delta_I \mathbf{F} = 0. \tag{52}$$

From $(51)_1$ and (52) it follows that

$$g_{\mathrm{n}} = (\mathbf{\Lambda m})(\hat{\mathbf{Q}}_{\mathrm{m}})^{-1}(\mathbf{\Lambda m}) - (\mathbf{\Lambda n})(\hat{\mathbf{Q}}_{\mathrm{n}})^{-1}(\mathbf{\Lambda n}). \tag{53}$$

Hence, g_{n} vanishes for $\mathbf{n} = \mathbf{m}$, so that the moduli $\bar{\mathbf{C}}$ in the phase transition branch, cf. (38) and (45), are never strongly elliptic. This is not surprising since there is a trivial indeterminacy in distribution of active transformation fronts in the direction of $\mathbf{m}$. This indeterminacy does not decide whether equilibrium is stable or not.

The proposition that follows shows that stability of equilibrium in the homogenized laminate under consideration is an exception rather than a rule.

Proposition 1. *Let $\bar{U}$ be defined by* (37) *along with* (51) *and* (52)*. Suppose that* (46) *holds true. Then the stability condition* (44) *is satisfied if* $\Delta_I \mathbf{S} = \mathbf{0}$ *and only if* $\mathbf{b}\Delta_I \mathbf{S} = \mathbf{0}$.

The *proof* is given in Appendix C.

The condition $\Delta_I \mathbf{S} = \mathbf{0}$ in Proposition 1 is practically always violated in the finite strain framework due to the difference of instantaneous elastic moduli of the phases under stress.

The meaning of the condition $\mathbf{b}\Delta_I \mathbf{S} = \mathbf{0}$ in Proposition 1 can be clarified by noting that, from (13),

$$\mathbf{b}\Delta_I \mathbf{S} = -\mathbf{b}\frac{\partial f_I}{\partial \Delta_I \mathbf{F}} = -\frac{\partial f_I}{\partial \mathbf{m}} \qquad \text{and} \qquad \frac{\partial f_I}{\partial \mathbf{m}} \cdot \mathbf{m} = -\mathbf{b}\Delta_I \mathbf{S}\mathbf{m} = 0. \tag{54}$$

Hence, if $\mathbf{b}\Delta_I \mathbf{S} \neq \mathbf{0}$ then the driving force f_I is not maximized with respect to the orientation $\mathbf{m}$, $|\mathbf{m}| = 1$, of the phase interface. It follows that the failure of the second-order stability condition due to $\mathbf{b}\Delta_I \mathbf{S} \neq \mathbf{0}$ is associated (and typically preceded) by failure of the first-order stability condition (24) inside the parent phase, for f_ι corresponding to a phase transformation front orientation different from the assumed $\mathbf{m}$.

As an illustration, the calculated dependence of g_{n} on $\mathbf{n}$ is visualized in Fig. 4 at the strain of 4% during uniaxial tension of a CuZnAl crystal, cf. Fig. 2. Two local minima of $g_{\mathrm{n}}(\mathbf{n})$ are found essential: one for $\mathbf{n}$ close to the direction of $\mathbf{m}$ and another one for $\mathbf{n}$ close to a direction of $\mathbf{b}$; this can be explained analytically within the linear (small strain) theory of martensite, not discussed here. The former minimum is never positive on account of (53) and reaches zero at $\mathbf{n} = \mathbf{m}$ only if $f_\iota(\mathbf{n})$ reaches its local maximum precisely at $\mathbf{m}$. The value of the second local minimum for $\mathbf{n}$ near a direction of $\mathbf{b}$ can be of either sign in general. This is demonstrated in Fig. 5, where the values of g_{n} at the two local minima are shown as functions of the increasing martensite volume fraction η during tension or compression. It has been verified that the local minima of $g_{\mathrm{n}}(\mathbf{n})$ are indeed located close to $\mathbf{m}$ and $\mathbf{b}$ in the whole range of η; the maximum deviation of the corresponding orientations is less than 6°.

As $\mathbf{m}$ in the present example is found by maximizing f_ι at the current stress at the first initial instant of martensitic phase transition, at this instant we have $\mathbf{b}\Delta_I \mathbf{S} = \mathbf{0}$ by (54) and $g_{\mathrm{n}}(\mathbf{n})$ reaches a local zero minimum at $\mathbf{n} = \mathbf{m}$. It is found that the second local minimum of $g_{\mathrm{n}}(\mathbf{n})$ at $\sim\mathbf{n}\|\mathbf{b}$ (denoting $\mathbf{n}$ nearly parallel to $\mathbf{b}$) can be negative at this instant, as shown in Fig. 5(b). This proves by a counterexample that the condition $\mathbf{b}\Delta_I \mathbf{S} = \mathbf{0}$ in Proposition 1 is not sufficient for fulfillment of (44). As mentioned in Section 4.2, evolution of the two-phase austenite-martensite laminate with increasing η has been calculated at fixed $\mathbf{m}$ during the

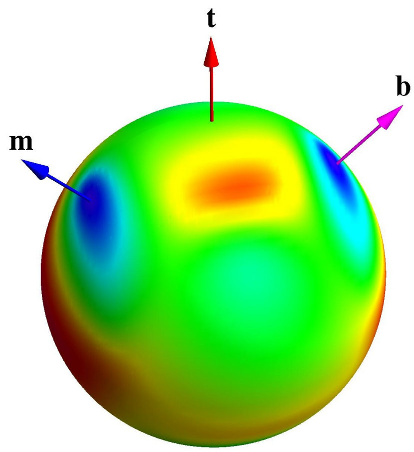


Figure 4: Dependence of the value of stability parameter g_{n} on the band normal $\mathbf{n}$. The minima (in blue) are located in the vicinity of $\mathbf{m}$ and $\mathbf{b}/|\mathbf{b}|$.

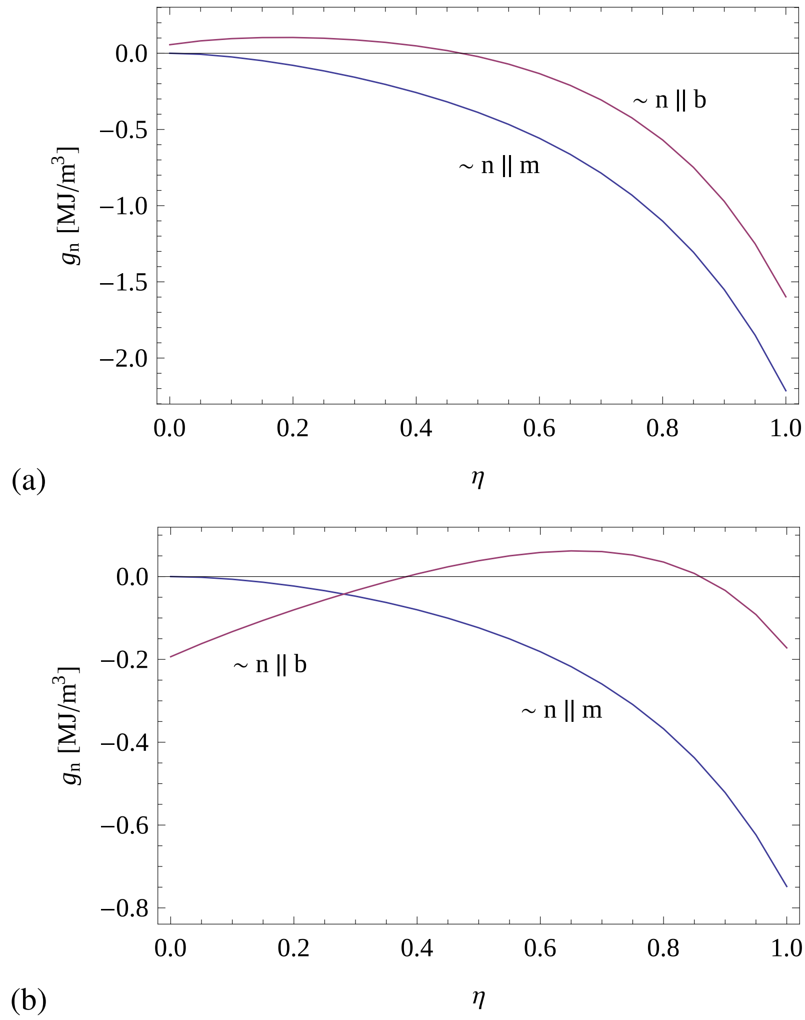


Figure 5: Intrinsic instability of equilibrium in a homogenized laminate: minimum values of g_{n} for (a) tension and (b) compression.

macroscopically uniform uniaxial tension or compression under elongation control.[2] It is found that $\mathbf{b}\Delta_I\mathbf{S}$ diverges from zero at increasing η, and g_n corresponding to a local minimum with respect to $\mathbf{n}$ close to $\mathbf{m}$ decreases monotonically below zero (Fig. 5), which implies failure of the stability condition (44) in the whole range of $0 < \eta < 1$.

Clearly, the above conclusion about instability is limited to inifinitely fine laminates in a bounded domain $\mathcal{M}$, or to laminates of a finite period H in an unbounded continuum. In the next section, we introduce scale effects for an evolving laminate of a finite period H by including the elastic micro-strain energy at boundary $\partial\mathcal{B}$ of the localization zone $\mathcal{B}$ being bounded first in one specific direction and next in all directions.

6 Instability and size effects

6.1 Laminated layer

We begin with a study of size effects in the stability analysis of a laminated layer. A periodic laminate is investigated, of a *finite* period H in the normal direction $\mathbf{m}$ in the reference configuration, and formed by phase transition from an initially homogeneous parent phase.

Consider a localization band $\mathcal{B}$ of normal $\mathbf{n}$ and finite thickness $B \gg H$ in the reference configuration, with $\mathbf{n}$ inclined to the laminate interfaces at an angle α, $0 \leq \sin\alpha = \mathbf{n}\cdot\mathbf{m} < 1$ (Fig. 6). Let the macroscopic velocity gradient in the reference configuration be equal to $\dot{\bar{\mathbf{F}}} = \mathbf{c}_\mathrm{n} \otimes \mathbf{n}$ for every $\mathcal{R} \in \mathcal{B}$. Along with $\dot{\bar{\mathbf{F}}} = \mathbf{0}$ for $\mathcal{R} \cap \mathcal{B} = \emptyset$, this defines the instability mode for an infinite laminate as discussed above.

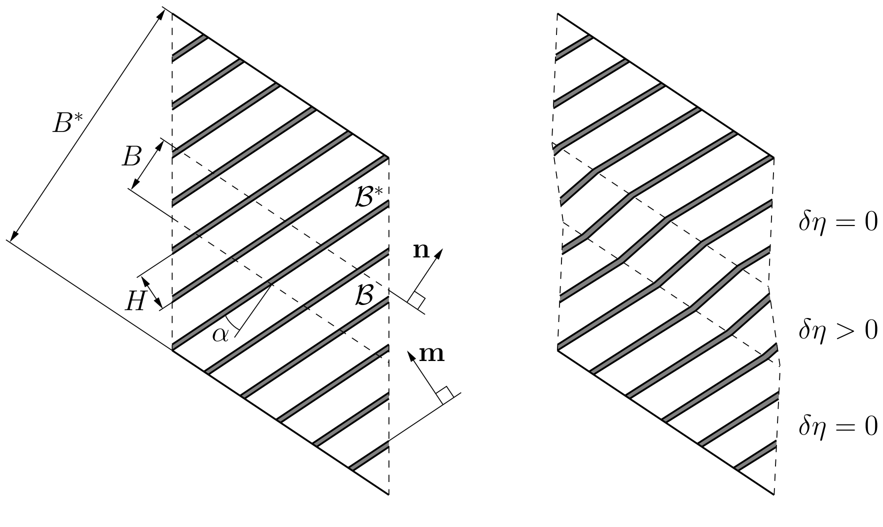


Figure 6: Intrinsic instability of equilibrium in a laminated layer.

Suppose for simplicity that at the local scale of the laminate, an infinitesimal increment $\delta\bar{\mathbf{F}} = \dot{\bar{\mathbf{F}}}\delta\theta$ of the macroscopic deformation gradient within $\mathcal{B}$ is associated with creation of just one product phase layer of infinitesimal thickness $\delta h = H\dot{\eta}\delta\theta$ per period H, both taken in the reference configuration. If $\dot{\bar{\mathbf{F}}} \cdot \mathbf{\Lambda} \leq 0$ for $\mathcal{R} \cap \mathcal{B} = \emptyset$ then the formation of those layers of infinitesimal thickness induces a local incompatibility of transformation strains across $\partial\mathcal{B}$, or in vicinity of $\partial\mathcal{B}$ if the transition between the transforming and non-transforming zones is smooth. In any case, there is an incompatibility of eigenstrains which must be accommodated by elastic

[2]Under nominal stress control equilibrium would be immediately unstable, cf. the discussion of condition (42).

micro-strains in vicinity of $\partial\mathcal{B}$. The associated increase in the resulting elastic strain energy with respect to that for the analogously deformed but homogenized laminate, when referred to the unit reference area of $\partial\mathcal{B}$, defines the *elastic micro-strain energy* density $\gamma^{\rm e}$ interpreted as boundary energy of $\partial\mathcal{B}$, cf. [11, 50, 51, 42, 13]. No development of macroscopic interface stresses within $\partial\mathcal{B}$ is considered.

Irrespectively of the reference thickness h of product phase layers formed before reaching the examined equilibrium state, its increment δh is regarded here as arbitrarily small. Following previous related studies [11, 12, 51, 13], the associated elastic micro-strain energy density $\gamma^{\rm e}$ is taken to be proportional to $(\delta h)^2$ for vanishingly small δh. Accordingly,

$$\delta\gamma^{\rm e} = \frac{\Gamma_0}{H}(\delta h)^2 + o((\delta h)^2), \qquad \ddot{\gamma}^{\rm e}|_{\delta h=0} = 2\Gamma_0 H\dot{\eta}^2, \tag{55}$$

where $\Gamma_0 > 0$ of dimension J/m^3 is a size-independent proportionality factor.

There may be another interfacial energy part on phase interfaces in the laminate itself. However, that energy is assumed to be proportional to the *reference* area of phase interfaces with a constant proportionality factor. As the instability mode under consideration leaves this area unchanged, the interfacial energy of phase interfaces in the laminate is inessential for the incremental energy balance that follows.

The area of $\partial\mathcal{B}$ in the reference configuration per unit reference volume of $\mathcal{B}$ is $2/B$. On combining (48) and (55), the second time derivative of the energy supply to $\mathcal{B}$ and $\partial\mathcal{B}$ jointly, taken per unit reference volume of $\mathcal{B}$, reads

$$\ddot{e}_B := \ddot{e}_{\rm n}^{\rm min} + \frac{2}{B}\ddot{\gamma}^{\rm e} = \left(g_{\rm n}\xi + 4\frac{\Gamma_0 H}{B}\right)\dot{\eta}^2. \tag{56}$$

In an unbounded laminate we can take $\dot{\mathbf{F}} = \mathbf{0}$ for $\mathcal{R}\cap\mathcal{B} = \emptyset$, and then there is no energy contribution other than (56). Moreover, B in an unbounded laminate can be taken arbitrarily large, so that the corresponding stability condition $\ddot{e}_B \geq 0$ reduces to (47) in the limit as $H/B \to 0$, which is an expected result.

The situation becomes different if the continuum is bounded in the direction of $\mathbf{n}$, or perhaps more appealing physically, if finite periodicity is enforced in the direction of $\mathbf{n}$. As an illustration, suppose that $\mathcal{B}\subset\mathcal{B}^*$ where $\mathcal{B}^*$ is an infinite laminated layer, of the same reference normal $\mathbf{n}$ but larger thickness $B^* > B$ (Fig. 6), such that $\mathbf{v} = \mathbf{0}$ over $\partial\mathcal{B}^*$. Then the velocity gradient $\dot{\mathbf{F}} = \mathbf{c}_{\rm n}\otimes\mathbf{n}$ corresponding to $\dot{\eta} > 0$ in $\mathcal{B}$ must be compensated by a nonzero velocity gradient $\dot{\mathbf{F}}^*$ corresponding to $\dot{\eta} = 0$ in $\mathcal{B}^*\setminus\mathcal{B}$, associated with the second-order rate of elastic energy density $\ddot{\phi}^*$ there, i.e.

$$\dot{\mathbf{F}}^* = -\frac{B}{B^*-B}\mathbf{c}_{\rm n}\otimes\mathbf{n} \quad \text{and} \quad \ddot{\phi}^* = \left(\frac{B}{B^*-B}\right)^2 \mathbf{c}_{\rm n}\hat{\mathbf{Q}}_{\rm n}\mathbf{c}_{\rm n} \qquad \text{for } \mathcal{R}\subset\mathcal{B}^*\setminus\mathcal{B}. \tag{57}$$

The second-order rate of elastic energy in $\mathcal{B}^*\setminus\mathcal{B}$ corresponding to unit reference volume of $\mathcal{B}$ is $\ddot{\phi}^*_B := \ddot{\phi}^*(B^*-B)/B$. On summing up $\ddot{e}_B$ and $\ddot{\phi}^*_B$ and rearranging with the help of (C.11) and (C.9), we obtain the following expression for the second-order rate of the total energy supply per unit reference volume of $\mathcal{B}$:

$$\ddot{e}^*_B := \ddot{e}_B + \ddot{\phi}^*_B = \left(g_{\rm n}\xi + \frac{B}{B^*-B}\frac{g\xi^2}{\xi_{\rm n}} + 4\frac{\Gamma_0 H}{B}\right)\dot{\eta}^2. \tag{58}$$

B is still a free parameter. The above expression is readily minimized by $B = B_{\rm n}$ that satisfies

$$\frac{B^*}{B_{\rm n}} = 1 + \frac{\xi}{2}\left(\frac{gB^*}{\xi_{\rm n}\Gamma_0 H}\right)^{\frac{1}{2}}. \tag{59}$$

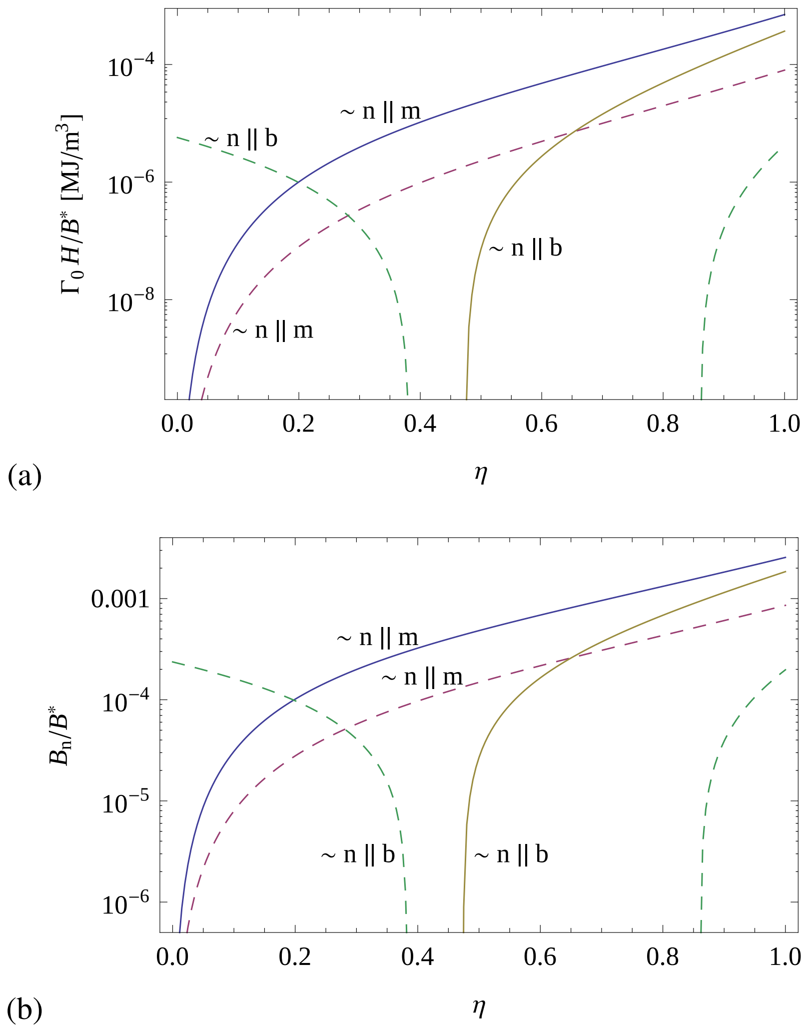


Figure 7: Laminated layer: critical values of parameters (a) $\Gamma_0 H/B^*$ and (b) $B_{\rm n}/B^*$ at the stability limit $g_{\rm n} + g^*_{\rm n} = 0$ (solid lines – tension, dashed lines – compression).

On using the above relationship, the stability condition $\ddot{E} \geq 0$ reduced to $\ddot{e}^*_B \geq 0$ can be written down in the following final form

$$g_{\rm n} + g^*_{\rm n} \geq 0, \qquad g^*_{\rm n} := \frac{4}{\xi}\frac{\Gamma_0 H}{B^*} + 4\left((\mathbf{\Lambda n})(\hat{\mathbf{Q}}_{\rm n})^{-1}(\mathbf{\Lambda n})\,\frac{\Gamma_0 H}{B^*}\right)^{\frac{1}{2}}. \tag{60}$$

Again, if $B^* \to \infty$ then (60) reduces to (47) as expected, but for any positive value of the ratio H/B^* the associated critical value of $g_{\rm n}$ is less than zero. It depends only slightly on whether $\xi = \xi_{\rm n}$ or $\xi = 1$ is substituted, that is, whether the constraint $\mathring{f}_I = 0$ is imposed or not, respectively. The latter case is more convincing since, first, it gives a lower value of $\ddot{e}^*_B$, and second, it provides the interpretation of instability analogous to that demonstrated in Section 5.

The critical value of $g_{\rm n}$, for which the left-hand expression in (60) vanishes, depends on parameter $\Gamma_0 H/B^*$. That relationship has been calculated using $\xi = 1$. By combining it with the result illustrated in Fig. 5, we obtain for the CuZnAl example the graphs presented in Fig. 7 that show the influence of increasing η of the critical value of the parameter $\Gamma_0 H/B^*$ and of the associated value $B_{\rm n}/B^*$ corresponding to equality sign in (60). Above the curves plotted in Fig. 7(a), the stability condition (60) is satisfied with strict inequality.

It is of prime interest to estimate the order of magnitude of realistic values of the parameter $\Gamma_0 H/B^*$. This is deferred to the next subsection where an example of a laminate domain bounded in all directions is analysed.

6.2 Laminated inclusion

Consider now the case when a laminate is evolving within a spherical inclusion (grain) $\mathcal{B}^*$ of a given size. Our aim is to examine the circumstances in which stability of equilibrium of the laminated inclusion is lost, taking into account size effects due to the elastic micro-strain energy. The analysis runs on similar lines as for the laminated layer above, however, with essential changes due to another geometry of the problem. In particular, a localized instability mode is considered where phase transition in the laminate is limited to a narrow zone modelled as an oblate spheroid $\mathcal{B}$ inscribed in a spherical domain $\mathcal{B}^*$ (Fig. 8). To emphasize analogies to the analysis in Subsection 6.1, the same symbols are given now a somewhat different but related meaning.

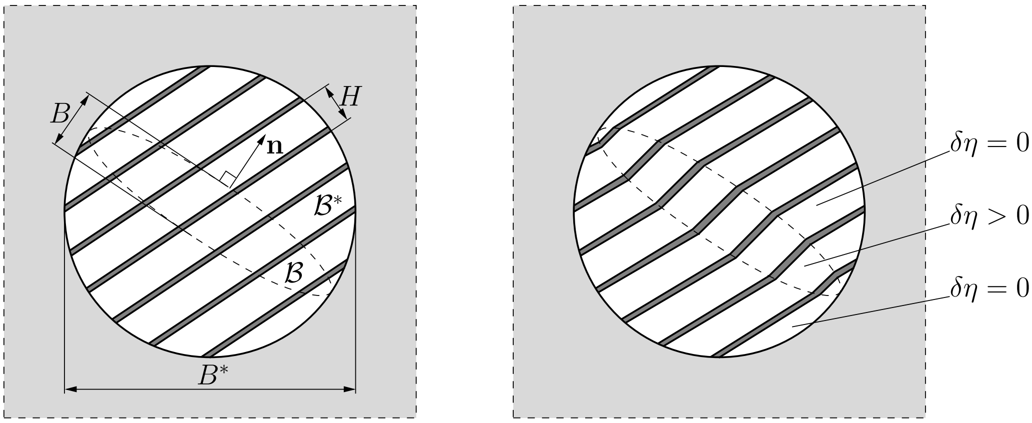


Figure 8: Instability of equilibrium in a laminated inclusion.

Several special cases of stability loss relevant to the present problem have already be examined in the preceding sections. Our aim is to extend the analysis to the case of instability associated with spontaneous evolution of the laminate within an ellipsoidal localization zone $\mathcal{B}$ with boundary energy of $\partial\mathcal{B}$ and flexibility of environment of $\mathcal{B}$ taken into account.

Locally at $\partial\mathcal{B}$, the elastic micro-strain energy density is governed by (55) with uniform H and $\dot\eta$. The growth of the total boundary energy Φ_S of $\partial\mathcal{B}$ is thus also quadratic in $\dot\eta$, viz.

$$\ddot\Phi_S = 2H\dot\eta^2 \int_{\partial\mathcal{B}} \Gamma_0 \mathrm{d}S = \pi(B^*)^2\hat\Gamma_0 H\dot\eta^2, \qquad \hat\Gamma_0 := \frac{2}{\pi(B^*)^2}\int_{\partial\mathcal{B}} \Gamma_0 \mathrm{d}S, \tag{61}$$

where the energy factor Γ_0 may in general vary on $\partial\mathcal{B}$, and the average energy factor $\hat\Gamma_0$ is introduced with respect to double area of the great circle of $\mathcal{B}$. The density of the second-order rate of the boundary energy per unit reference volume of $\mathcal{B}$ is

$$\ddot\phi_S := \frac{\ddot\Phi_S}{|\mathcal{B}|} = 6\frac{\hat\Gamma_0 H}{B}\dot\eta^2. \tag{62}$$

It remains to sum up $\ddot e_B^{\min}$ and $\ddot\phi_S$, defined by (40) with $\mathcal{B}$ replacing $\mathcal{M}$ and by (62), respectively, to obtain the second-order rate of the total energy supply to the whole system, per unit reference volume of $\mathcal{B}$. The outcome is

$$\ddot{e}_B^* := \ddot{e}_B^{\min} + \ddot{\phi}_S = g_B^* \dot{\eta}^2 + 6\frac{\hat{\Gamma}_0 H}{B}\dot{\eta}^2, \tag{63}$$

where

$$g_B^* := g - \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}_B^*)^{-1} \cdot \mathbf{\Lambda}, \tag{64}$$

and $\mathbf{C}_B^*$ characterizes the stiffness of the elastic environment of $\mathcal{B}$, including both the region $\mathcal{B}^* \setminus \mathcal{B}$ and the medium surrounding $\mathcal{B}^*$. Positiveness of $\ddot{e}_B^*$ above at $\dot{\eta} > 0$ is ensured if $g_B^* \geq 0$, thus the case $g_B^* < 0$ remains to be examined in the present stability analysis.

Finally, we arrive at the following stability condition equivalent to $\ddot{e}_B^* \geq 0$,

$$g_B^* + g_S := (g - \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}_B^*)^{-1} \cdot \mathbf{\Lambda}) + 6\frac{\hat{\Gamma}_0 H}{B} \geq 0. \tag{65}$$

In order to illustrate the stability condition (65), the stiffness $\mathbf{C}_B^*$ is approximated using the classical Eshelby solution of the linear elasticity. Specifically, the oblate spheroid $\mathcal{B}$ is considered as an inclusion in an infinite and homogeneous elastic medium of isotropic properties, i.e. the elastic anisotropy of $\mathcal{B}^* \setminus \mathcal{B}$ and the difference of elastic properties of $\mathcal{B}^*$ and the surrounding medium are neglected. The overall constraint tensor $\mathbf{L}^*$, introduced by Hill [52] and specified in terms of the respective Eshelby tensor, is then assumed to relate the stress and strain rates in the current configuration. The corresponding tensor $\mathbf{C}_B^*$ is obtained by applying appropriate transformation rules to $\mathbf{L}^*$, cf. [43]. The details are omitted here.

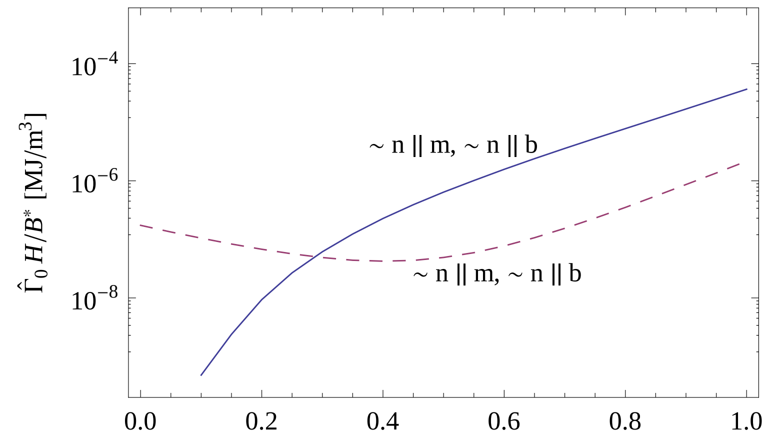
As a result, the left-hand side of the inequality in (65) can be expressed as a function of the aspect ratio B/B^* and orientation $\mathbf{n}$ of the oblate spheroid $\mathcal{B}$, and of parameter $\hat{\Gamma}_0 H/B^*$. The left-hand expression is then minimized with respect to B/B^* and $\mathbf{n}$, and the critical value of parameter $\hat{\Gamma}_0 H/B^*$ is determined at which this minimum is equal to zero.

The results of computations are provided in Fig. 9. The elastic properties of the isotropic matrix (shear modulus $\mu = 61$ GPa, Poisson's ratio $\nu = 0.3$) have been determined by adjusting the corresponding elastic moduli tensor to that of the cubic austenite, so that the norm of the difference of the two tensors is minimized. Two local minima of identical value have been found which correspond to the orientation $\mathbf{n}$ of the disk-shaped localization zone $\mathcal{B}$ that is close either to $\mathbf{m}$ or to $\mathbf{b}$. As in the case of the laminated layer, the aspect ratio B/B^* is small (below 0.001). In the case of tension, for $\eta \approx 0.1$ the aspect ratio B/B^* is of order of 10^{-6} and the obtained numerical results for still smaller values of η are not fully reliable. As in the case of a laminated layer, above the curves plotted in Fig. 9(a) the stability condition (65) is satisfied with strict inequality.

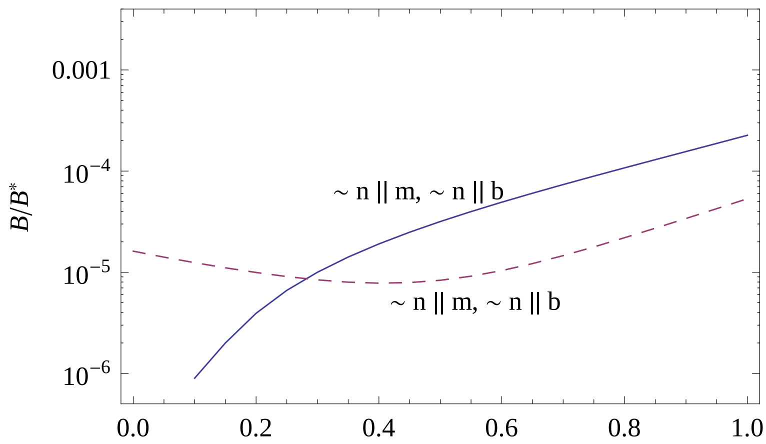
All the calculations reported on so far did not require any knowledge of the value of the elastic micro-strain energy factor $\hat{\Gamma}_0$ as it appeared together with the dimension ratio H/B^*. However, to conclude whether realistic values of H/B^* lie in the domain of stability or instability, an estimate for $\hat{\Gamma}_0$ is needed. Taking into account that the ratio B/B^* is estimated above as very small, the average energy factor $\hat{\Gamma}_0$ can be approximated by the recently derived formula [13] for elastic micro-strain energy at a planar boundary of a laminate with eigenstrains,

$$\hat{\Gamma}_0 \approx \Gamma_0(\alpha, \beta), \qquad \Gamma_0(\alpha, \beta) = 0.197\mu b^2 \cos\alpha \,\frac{1 - \nu \sin^2\beta}{1 - \nu}, \tag{66}$$

where $\Gamma_0(\alpha, \beta)$ has been determined for the case of elastic isotropy, and $b := |\mathbf{b}|$. Angles α and β correspond here to the nominal orientation $\mathbf{n}$ of the disk-shaped inclusion; α denotes the inclination of $\mathbf{n}$ with respect to laminate layers, and β denotes the out-of-plane inclination of $\mathbf{b}$.



(a)



(b)

Figure 9: Laminated inclusion: critical values of parameters (a) $\hat{\Gamma}_0 H/B^*$ and (b) B/B^* at the stability limit $g_B^* + g_S = 0$ (solid lines – tension, dashed lines – compression).

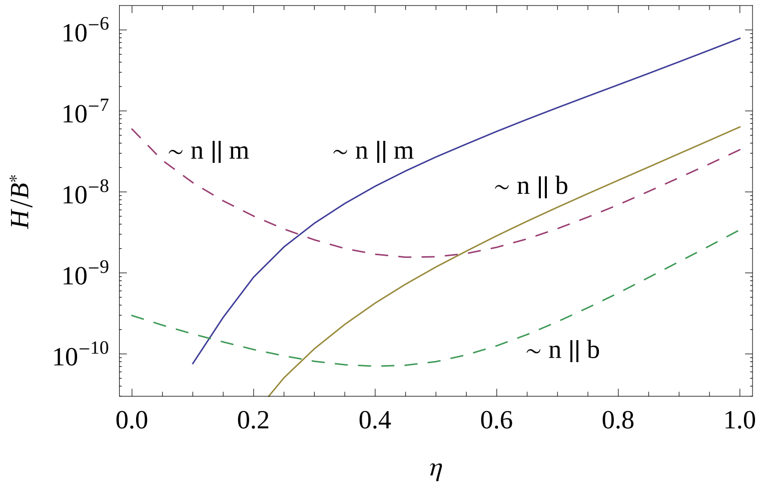


Figure 10: Laminated inclusion: critical values of the ratio H/B^* at the stability limit $g_B^* + g_S = 0$ for $\hat{\Gamma}_0$ estimated from (66) (solid lines – tension, dashed lines – compression).

Figure 10 shows the values of H/B^* corresponding to Fig. 9(a) and obtained using the estimate (66) of $\hat{\Gamma}_0$. The upper curves plotted in Fig. 10 define the upper limit of the instability region (separately for tension and compression), and the corresponding values of H/B^* turn out to be very small (below 10^{-6}).

The final conclusion is that the examined kind of instability is not expected to occur for physically realistic values of H/B^*, interpreted as the ratio of the laminate spacing to laminate external dimension (e.g., the grain size), which are at least 2–3 orders of magnitude above the instability domain in Fig . 10.

7 Conclusion

We have examined isothermal stability of equilibrium of evolving laminates in pseudo-elastic solids with a multi-well free energy function. Rate-independent dissipation associated with phase transition between energy wells has been included in the analysis by imposing a constant threshold value on the thermodynamic driving force acting on phase interfaces. Several conditions necessary for stability of equilibrium of a laminate, associated with distinct instability modes, have been derived from a general energy criterion. Their formulation and interpretation in the context of phase-transforming laminates is a novel feature of this study. For convenience of the reader, the conditions sufficient for instability of equilibrium of a pseudo-elastic laminate occupying a reference domain $\mathcal{M}$ are briefly summarized as follows:

(i) $f > f_c$ violating (24) is associated with a sudden phase transition in $\mathcal{M}$ placed in an arbitrarily rigid environment;

(ii) $g < 0$ violating (34) is associated with smooth but uncontrolled and macroscopically uniform phase transition in $\mathcal{M}$ placed in an arbitrarily rigid environment;

(iii) $g^* < 0$ violating (41) is associated with uncontrolled and macroscopically uniform phase transition in $\mathcal{M}$ placed in a sufficiently flexible environment;

(iv) $\mathbf{c}\hat{\mathbf{Q}}_{\mathrm{n}}\mathbf{c} < 0$ violating (46) has the usual interpretations of ellipticity loss in a homogenized elastic continuum;

(v) $g_{\rm n} < 0 \Leftrightarrow \bar{U}(\mathbf{c} \otimes \mathbf{n}) < 0$ violating (47) and (44) is associated with uncontrolled phase transition within a localized zone $\mathcal{B}$ in $\mathcal{M}$ placed in an arbitrarily rigid environment, with boundary energy of $\mathcal{B}$ neglected;

(vi) $g_{\rm n} + g_{\rm n}^* < 0$ violating (60) is associated with uncontrolled phase transition within layers $\mathcal{B}$ forming a higher-rank laminate of a finite period B^*, with boundary energy of $\mathcal{B}$ included;

(vii) $g_B^* + g_S < 0$ violating (65) is associated with uncontrolled phase transition in a narrow ellipsoidal zone $\mathcal{B}$ placed in a flexible environment, with boundary energy of $\mathcal{B}$ included.

The central role is played by the instability condition (v). New Proposition 1 has revealed that instability is a rule for *any* phase-transforming laminate under consideration, except in the special case when the interfacial jump in the specified directional stress happens to vanish ($\mathbf{b}\Delta_I \mathbf{S} = \mathbf{0}$). In the illustrative example of an evolving austenite-martensite laminate of a CuZnAl shape memory alloy in uniaxial tension or compression, the instability is predicted in the whole range $0 < \eta < 1$ of the volume fraction of martensite.

The analysis presented in Section 6 has shown quantitatively the stabilizing effect of elastic micro-strain energy at the boundary of the localized instability zone. The final conclusion, based on estimation of the boundary energy factor, is that the instability conditions (vi) and (vii) are *not* expected to be met for laminates of reasonable values of the ratio of laminate spacing to dimensions of laminate domain, at least not in the calculated example. However, stiffness of the environment of the laminate domain should be sufficient to avoid instability predicted by condition (iii) in the case of dead loading.

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Appendix A

In the extended transport theorem used to derive eq. (11), the interfacial jumps, denoted by Δ_ι, are taken with respect to a time-like variable and averaged over a growing layer thickness [20], viz.

$$\Delta_\iota \psi := \lim_{\delta\theta \to 0^+} \frac{1}{\delta h_\iota} \int_0^{\delta h_\iota} \Delta_\theta \psi(\mathbf{X} + \zeta_{\rm m}\mathbf{m})\, {\rm d}\zeta_{\rm m}, \qquad \mathbf{X} \in I_\iota, \qquad \Delta_\theta \psi = \psi|_{\theta+\delta\theta} - \psi|_\theta. \quad \text{(A.1)}$$

It is assumed here that at one side of an interface I_ι a thin layer of a product phase (ι) is growing with local thickness $\delta h_\iota = \dot{h}_\iota \delta\theta + o(\delta\theta) > 0$ increasing continuously from zero starting from a value θ of a time-like variable. The following compatibility conditions are satisfied (no implicit sum over ι)

$$\dot{h}_\iota \Delta_\iota \mathbf{F} = [\mathbf{v}]_\iota \otimes \mathbf{m} \quad \text{on } I_\iota, \qquad \dot{h}_\iota \Delta_\iota \mathbf{S}\,\mathbf{m} = \mathbf{0}, \qquad \dot{h}_\iota \Delta_\iota \mathbf{S} \cdot \Delta_\iota \mathbf{F} = 0, \qquad \text{(A.2)}$$

where

$$[\psi]_\iota = \lim_{\zeta_{\rm m} \to 0^+} (\psi(\mathbf{X} + \zeta_{\rm m}\mathbf{m}) - \psi(\mathbf{X} - \zeta_{\rm m}\mathbf{m})), \qquad \mathbf{X} \in I_\iota \qquad \text{(A.3)}$$

and $\mathbf{v}$ denotes the material velocity taken with respect to θ as a time-like variable.

The value of $\dot{h}_\iota$ at instant θ is arbitrary and may be equal to zero. The above formalism includes the case when a product phase layer is created *inside* the parent phase, so that $[\mathbf{F}] = \mathbf{0}$

and $[\mathbf{S}] = \mathbf{0}$ at instant θ. In that case, the standard formulation of the transport theorem would fail, as based on the assumption of existence of a single regular hypersurface of discontinuity in the four-dimensional time-space, in a neighborhood of I_ι. The latter assumption can be satisfied when a product phase layer is growing by smooth propagation of an already existing phase front I_ι. In this particular case, when the front is moving with a normal speed v_ι (positive if in the sense of $\mathbf{m}$) in the reference configuration, there is

$$\Delta_\iota \psi = \mp[\psi] \qquad \text{and} \qquad \Delta_\iota \mathbf{F} = \mp[\mathbf{F}], \quad \Delta_\iota \mathbf{S} = \mp[\mathbf{S}] \qquad \text{for } \operatorname{sign} v_\iota = \pm 1. \tag{A.4}$$

Examine now the rate of averaged bulk free energy $\bar{\phi}_V = \{\phi\}$. From the transport formula (11) and Hill's condition $(6)_2$, we obtain

$$\dot{\bar{\phi}}_V = \{\dot{\phi}\} + \frac{1}{H}\sum_\iota \dot{h}_\iota \, \Delta_\iota \phi, \qquad \{\dot{\phi}\} = \{\mathbf{S}\} \cdot \{\dot{\mathbf{F}}\} = \{\mathbf{S}\} \cdot (\dot{\bar{\mathbf{F}}} - \frac{1}{H}\sum_\iota \dot{h}_\iota \, \Delta_\iota \mathbf{F}) \tag{A.5}$$

and

$$\frac{\partial \dot{\bar{\phi}}_V}{\partial \dot{\bar{\mathbf{F}}}} = \bar{\mathbf{S}}, \qquad \left. \frac{\partial \dot{\bar{\phi}}_V}{\partial \dot{h}_\iota} \right|_{\dot{\bar{\mathbf{F}}}} = \frac{1}{H}(\Delta_\iota \phi - \{\mathbf{S}\} \cdot \Delta_\iota \mathbf{F}). \tag{A.6}$$

for a selected product phase layer. Note that on account of (1) and (A.2), the local stress on either side of I_ι can be substituted in place of $\{\mathbf{S}\}$ in the right-hand expression. We choose the side (+) of I_ι occupied by the parent phase being transformed to the product phase (ι). When multiplied by reference volume of $\mathcal{R}$, area A of the interface appears in place of $1/H$ in (A.6). Hence,

$$f_\iota = \mathbf{S}_\iota^+ \cdot \Delta_\iota \mathbf{F} - \Delta_\iota \phi \tag{A.7}$$

is the local thermodynamic driving force (per unit reference area) for *creation* of an incipient product phase layer associated with the jumps involved, irrespectively of existence or not of the product phase in vicinity of that layer. In case of (A.4), formula (A.7) is equivalent to the well-known Eshelby formula [19] for the driving force acting on an *existing* phase transformation front. If the parent phase is homogeneous and uniformly stressed to $\mathbf{S}_0$ and all I_ι are represented by a single discontinuity surface I with the jumps denoted by Δ_I then (A.7) can be written down in the form (13).

Appendix B

Consider the left-hand expression in (33) which is recalled here for convenience

$$\ddot{e} = \dot{\bar{\mathbf{F}}} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*) \cdot \dot{\bar{\mathbf{F}}} + (g\dot{\eta} - 2\boldsymbol{\Lambda} \cdot \dot{\bar{\mathbf{F}}})\dot{\eta}. \tag{B.1}$$

For any given $\dot{\eta}$, if $(\hat{\mathbf{C}} + \mathbf{C}^*)$ is positive definite then $\ddot{e}$ attains a minimum with respect to $\dot{\bar{\mathbf{F}}}$ at

$$\dot{\bar{\mathbf{F}}} = \dot{\eta}(\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \cdot \boldsymbol{\Lambda} \tag{B.2}$$

which satisfies, on account of (12) and (26) at $\dot{\lambda} = 0$, the condition of continuing equilibrium,

$$\dot{\bar{\mathbf{S}}} - \dot{\mathbf{S}}^{\text{ext}} = (\hat{\mathbf{C}} + \mathbf{C}^*) \cdot \dot{\bar{\mathbf{F}}} - \dot{\eta}\boldsymbol{\Lambda} = \mathbf{0}, \tag{B.3}$$

and corresponds, through (14), to

$$\overset{\circ}{f}_I = \boldsymbol{\Lambda} \cdot \dot{\bar{\mathbf{F}}} - g\dot{\eta} = -g^*\dot{\eta}, \tag{B.4}$$

where

$$g^* := g - \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \cdot \mathbf{\Lambda}. \tag{B.5}$$

On substituting (B.2) into (B.1) and rearranging, it follows that

$$\min_{\dot{\bar{\mathbf{F}}}} \ddot{e}(\dot{\bar{\mathbf{F}}}, \dot{\eta}) = g^* \dot{\eta}^2. \tag{B.6}$$

Hence, if $g^* < 0$ then $\dot{\bar{\mathbf{F}}}$ given by (B.2) defines a quasi-static instability mode which corresponds to $\overset{\circ}{f}_I > 0$ at $\dot{\eta} > 0$ at fixed λ.

With the help of $(A.2)_3$ and $(12)_2$, using diagonal symmetry of $\hat{\mathbf{C}}$ and $\mathbf{C}^*$, and introducing an auxiliary variable

$$\mathbf{\Lambda}^* := \mathbf{C}^* \cdot \Delta_I \mathbf{F} + \Delta_I \mathbf{S}, \tag{B.7}$$

the expression for g^* can be rearranged as follows

$$\begin{aligned} g^* &= g - \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \cdot ((\hat{\mathbf{C}} + \mathbf{C}^*) \cdot \Delta_I \mathbf{F} - \mathbf{C}^* \cdot \Delta_I \mathbf{F} - \Delta_I \mathbf{S}) \\ &= g - \Delta_I \mathbf{F} \cdot \hat{\mathbf{C}} \cdot \Delta_I \mathbf{F} + \mathbf{\Lambda} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \mathbf{\Lambda}^* \\ &= (\Delta_I \mathbf{F} \cdot (\hat{\mathbf{C}} + \mathbf{C}^*) - \mathbf{\Lambda}^*) \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \mathbf{\Lambda}^* \\ &= \Delta_I \mathbf{F} \cdot \mathbf{C}^* \cdot \Delta_I \mathbf{F} - \mathbf{\Lambda}^* \cdot (\hat{\mathbf{C}} + \mathbf{C}^*)^{-1} \mathbf{\Lambda}^*. \end{aligned} \tag{B.8}$$

The structure of the final expression above is fully analogous to the original expression (B.5), with $\hat{\mathbf{C}}$ interchanged with $\mathbf{C}^*$ and $\mathbf{\Lambda}^*$ with $\mathbf{\Lambda}$.

Consider the effect of decreasing a norm $\|\mathbf{C}^*\|$ of $\mathbf{C}^*$ to zero, i.e. when stiffness of the material surrounding $\mathcal{M}$ decreases towards the limit case of dead loading where $\mathbf{C}^* = \mathbf{0}$. Suppose that $(\hat{\mathbf{C}} + \mathbf{C}^*)$ satisfies the condition (39) of elastic stability in the limit $\mathbf{C}^* = \mathbf{0}$. Note that this is only possible in a state of predominantly tensile stress [53]. Then, at a positive definite $\hat{\mathbf{C}}$, from (B.8) we obtain

$$\lim_{\|\mathbf{C}^*\| \to 0} g^* = -\Delta_I \mathbf{S} \cdot (\hat{\mathbf{C}})^{-1} \cdot \Delta_I \mathbf{S} < 0 \qquad \text{if} \qquad \Delta_I \mathbf{S} \neq \mathbf{0}. \tag{B.9}$$

We conclude that in a homogeneous equilibrium state of a laminate domain $\mathcal{M}$ under all-round dead loading over $\partial\mathcal{M}$, in which $f_I = f_c$ and $\Delta_I \mathbf{S} \neq \mathbf{0}$, either the condition of elastic stability fails or $g^* < 0$. The latter case is interpreted as instability of equilibrium against spontaneous phase transformation under dead loading, cf. the interpretation of failure of (41).

Appendix C

Consider a planar band $\mathcal{B}$ of normal $\mathbf{n}$ and thickness B in the reference configuration of a homogenized continuum under uniform macroscopic stress $\bar{\mathbf{S}}$. A material point in $\mathcal{B}$ is identified with a representative volume element $\mathcal{R}$ of a laminate with a homogeneous parent phase, so that only one phase transition mode is considered. A possible instability mode is defined by $\dot{\bar{\mathbf{F}}} = \mathbf{c} \otimes \mathbf{n}$ within $\mathcal{B}$ for some vector $\mathbf{c} \neq \mathbf{0}$ and $\dot{\bar{\mathbf{F}}} = \mathbf{0}$ outside $\mathcal{B}$, which corresponds to a continuous velocity field in an infinite continuum. Alternatively, $\mathcal{B}$ may be considered as a disk-like domain of thickness B in a bounded finite domain $\mathcal{M}$, in the limit as $B \to 0$, cf. e.g. the construction in the Appendix in [46]. At a fixed value of λ as an external loading parameter, the first-order energy supply to $\mathcal{B}$ per unit reference volume of $\mathcal{B}$, as a specialized version of (27), reads

$$\dot{e} = \mathbf{c}(\bar{\mathbf{S}} - \mathbf{S}^{\text{ext}})\mathbf{n} + (f_c - f_I)\dot{\eta}, \tag{C.1}$$

where f_I is the driving force defined by (13) and $\dot{\eta} \geq 0$ is the rate of volume fraction of the selected product phase in the reference configuration.

We examine stability of an equilibrium state $\mathcal{G}^0$ in which $(\bar{\mathbf{S}} - \mathbf{S}^{\text{ext}})\mathbf{n} = \mathbf{0}$ necessarily and $f_I = f_c$ by assumption. We thus have $\dot{e} = 0$ in $\mathcal{G}^0$, and the sign of $\ddot{e}$ is to be examined, in $\mathcal{G}^0$ at fixed λ. Since we have assumed that $\dot{\bar{\mathbf{F}}} = \mathbf{0}$ outside $\mathcal{B}$, we have $\dot{\mathbf{S}}^{\text{ext}} = \mathbf{0}$, while $\dot{\bar{\mathbf{S}}}$ is expressed by (12) and $\overset{\circ}{f}_I$ by (14). It follows that the second-order energy input to $\mathcal{B}$, per unit reference volume, reads

$$\ddot{e} = \mathbf{c}\hat{\mathbf{Q}}_{\text{n}}\mathbf{c} + (g\dot{\eta} - 2\mathbf{c}\mathbf{\Lambda}\mathbf{n})\dot{\eta}. \tag{C.2}$$

This can be regarded as a specialized version of (B.1).

We assume below that $\hat{\mathbf{Q}}_{\text{n}}$ is positive definite for every $\mathbf{n} \neq \mathbf{0}$, which implies $g > 0$. Then, analogously as in Appendix B, for any given $\dot{\eta} > 0$, $\ddot{e}$ attains a minimum with respect to $\mathbf{c}$ at

$$\mathbf{c} = \mathbf{c}_{\text{n}} := \dot{\eta}(\hat{\mathbf{Q}}_{\text{n}})^{-1}\mathbf{\Lambda}\mathbf{n}, \tag{C.3}$$

which satisfies the condition of continuing equilibrium,

$$\dot{\bar{\mathbf{S}}}\mathbf{n} = \hat{\mathbf{Q}}_{\text{n}}\mathbf{c} - \dot{\eta}\mathbf{\Lambda}\mathbf{n} = \mathbf{0}, \tag{C.4}$$

the loading condition

$$\mathbf{\Lambda} \cdot \dot{\bar{\mathbf{F}}} = \mathbf{c}_{\text{n}}\mathbf{\Lambda}\mathbf{n} > 0 \tag{C.5}$$

and corresponds to

$$\overset{\circ}{f}_I = \mathbf{c}_{\text{n}}\mathbf{\Lambda}\mathbf{n} - g\dot{\eta} = -g_{\text{n}}\dot{\eta}, \tag{C.6}$$

where g_{n} is defined by (47). On substituting (C.3) into (C.2) and rearranging, it follows that

$$\min_{\mathbf{c}} \ddot{e}(\mathbf{c}, \mathbf{n}, \dot{\eta}) = g_{\text{n}}\dot{\eta}^2. \tag{C.7}$$

Hence, if $g_{\text{n}} < 0$ then $\dot{\bar{\mathbf{F}}} = \mathbf{c}_{\text{n}} \otimes \mathbf{n}$ defines a quasi-static instability mode in $\mathcal{B}$ that corresponds to $\overset{\circ}{f}_I > 0$ at $\dot{\eta} > 0$.

The stability condition (44) has been derived in the case when the consistency condition (35) holds true. The above proof of (C.7) shows that fulfillment of (44), equivalent to (47), is necessary and sufficient for non-negativeness of $\ddot{e}$ in (C.2) without restriction to (35).

The condition (44) has a direct energy interpretation since the expression (C.2) on substituting the consistency condition $\overset{\circ}{f}_I = \mathbf{c}\mathbf{\Lambda}\mathbf{n} - g\dot{\eta} = 0$ reduces simply to $2\bar{U}(\mathbf{c} \otimes \mathbf{n})$. To provide a direct energy interpretation to (47) at $\dot{\eta} > 0$ subject to the side constraint $(35)_2$, i.e. to $\mathbf{c}\mathbf{\Lambda}\mathbf{n} = g\dot{\eta}$, we minimize the respective Lagrangian. Straightforward calculations show that the minimum is attained at

$$\mathbf{c} = \mathbf{c}_{\text{n}} := \xi_{\text{n}}\dot{\eta}(\hat{\mathbf{Q}}_{\text{n}})^{-1}\mathbf{\Lambda}\mathbf{n}, \tag{C.8}$$

where

$$\xi_{\text{n}} := \frac{g}{(\mathbf{\Lambda}\mathbf{n})(\hat{\mathbf{Q}}_{\text{n}})^{-1}(\mathbf{\Lambda}\mathbf{n})} > 0, \tag{C.9}$$

implying (C.5) but not (C.4). It readily follows that

$$\min_{\mathbf{c}} \ddot{e}(\mathbf{c}, \mathbf{n}, \dot{\eta})\Big|_{\mathbf{c}\mathbf{\Lambda}\mathbf{n} = g\dot{\eta}} = 2\bar{U}(\mathbf{c}_{\text{n}} \otimes \mathbf{n}) = g_{\text{n}}\xi_{\text{n}}\dot{\eta}^2. \tag{C.10}$$

The above two versions of constrained minimization of $\ddot{e}$ taken jointly lead to the conclusion that the minimum second-order energy input to $\mathcal{B}$, per unit reference volume of $\mathcal{B}$, is

$$\ddot{e}^{\min}_{\text{n}} = g_{\text{n}}\xi\dot{\eta}^2 \qquad \text{for } \mathbf{c} = \mathbf{c}_{\text{n}} := \xi\dot{\eta}(\hat{\mathbf{Q}}_{\text{n}})^{-1}\mathbf{\Lambda}\mathbf{n}, \tag{C.11}$$

where $\xi = 1$ or $\xi = \xi_{\rm n}$ depending on whether the minimization is performed at fixed $\dot\eta$ or at the side constraint $\overset{\circ}{f}_I = 0$, respectively. It is easy to check that $g_{\rm n}\xi_{\rm n} \geq g_{\rm n}$ so that the latter estimate of $\ddot e_{\rm n}^{\rm min}$ is not lower than the former as expected, with equality only if $g_{\rm n} = 0$.

Proof of Proposition 1. *Sufficiency*. Suppose that $\Delta_I\mathbf{S} = \mathbf{0}$. In the space of rank-one tensors $(\mathbf{c}\otimes\mathbf{n})$, introduce a scalar product denoted by a central circle and the related norm $\|\mathbf{c}\otimes\mathbf{n}\|_{\hat{\mathbf{C}}}$, defined by

$$(\mathbf{c}_1\otimes\mathbf{n}_1)\circ(\mathbf{c}_2\otimes\mathbf{n}_2) := (\mathbf{c}_1\otimes\mathbf{n}_1)\cdot\hat{\mathbf{C}}\cdot(\mathbf{c}_2\otimes\mathbf{n}_2), \quad \|\mathbf{c}\otimes\mathbf{n}\|^2_{\hat{\mathbf{C}}} := (\mathbf{c}\otimes\mathbf{n})\circ(\mathbf{c}\otimes\mathbf{n}). \tag{C.12}$$

It can easily be shown, using the strong ellipticity assumption (46) and diagonal symmetry of $\hat{\mathbf{C}}$, that the definition (C.12) gives all the required properties of a scalar product and a norm. Thus, by the Schwarz inequality,

$$\|\mathbf{b}\otimes\mathbf{m}\|^2_{\hat{\mathbf{C}}}\,\|\mathbf{c}\otimes\mathbf{n}\|^2_{\hat{\mathbf{C}}} \geq ((\mathbf{b}\otimes\mathbf{m})\circ(\mathbf{c}\otimes\mathbf{n}))^2, \qquad \forall\,\mathbf{c},\mathbf{n}. \tag{C.13}$$

From $(52)_1$ and (51) it follows that

$$g = \|\mathbf{b}\otimes\mathbf{m}\|^2_{\hat{\mathbf{C}}}, \qquad \mathbf{\Lambda}\cdot(\mathbf{c}\otimes\mathbf{n}) = (\mathbf{b}\otimes\mathbf{m})\circ(\mathbf{c}\otimes\mathbf{n}) \quad \text{if } \ \Delta_I\mathbf{S} = \mathbf{0}\,. \tag{C.14}$$

Hence, from (37) and (C.13),

$$2g\bar U(\mathbf{c}\otimes\mathbf{n}) = \|\mathbf{b}\otimes\mathbf{m}\|^2_{\hat{\mathbf{C}}}\,\|\mathbf{c}\otimes\mathbf{m}\|^2_{\hat{\mathbf{C}}} - ((\mathbf{b}\otimes\mathbf{m})\circ(\mathbf{c}\otimes\mathbf{n}))^2 \geq 0 \qquad \forall\,\mathbf{c},\mathbf{n}, \tag{C.15}$$

which completes the proof of (44).

Necessity. Suppose that (44) holds. By (37), (51) and (52), we have

$$\mathbf{b\Lambda m} = g \qquad \text{and} \qquad \bar U(\mathbf{b}\otimes\mathbf{m}) = g - \frac{1}{g}g^2 = 0. \tag{C.16}$$

The partial derivative of $\bar U(\mathbf{c}\otimes\mathbf{n})$ with respect to $\mathbf{n}$, on using (51) and diagonal symmetry of $\hat{\mathbf{C}}$, reads

$$\frac{\partial\bar U(\mathbf{c}\otimes\mathbf{n})}{\partial\mathbf{n}} = \mathbf{c}\hat{\mathbf{C}}\cdot(\mathbf{c}\otimes\mathbf{n}) - \frac{\mathbf{c\Lambda n}}{g}\,(\mathbf{c}\hat{\mathbf{C}}\cdot(\mathbf{b}\otimes\mathbf{m}) - \mathbf{c}\Delta_I\mathbf{S}). \tag{C.17}$$

It must vanish at a minimum point of $\bar U(\mathbf{c}\otimes\mathbf{n})$, so that, by (C.16),

$$\left.\frac{\partial\bar U(\mathbf{c}\otimes\mathbf{n})}{\partial\mathbf{n}}\right|_{\mathbf{c}\otimes\mathbf{n}=\mathbf{b}\otimes\mathbf{m}} = \mathbf{b}\Delta_I\mathbf{S} = \mathbf{0}. \tag{C.18}$$

This completes the proof of Proposition 1.

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