NAMT
93-072

Dynamic Solid-Solid Transitions with Phase Characterized by an Order Parameter

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Research Report No. 93-NA-022

July 1993

Sponsors

U.S. Army Research Office
Research Triangle Park
NC 27709

National Science Foundation
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Washington, DC 20550

associated with heat and mass transport.[1] For (pure) martensitic transitions, in which the lattice undergoes a mechanical strain but for which there are no rearrangements of atoms within cells, the order parameter might be viewed as an artifice that yields a regularization of the mechanical equations, a regularization that models surface energy and stress as well as transition kinetics.[2] There are important situations, however, in which order parameters have a well-defined physical interpretation. Ginzburg-Landau order-parameter equations *alone* are used to describe interface kinetics for ordering transitions in which atoms undergo rearrangements within cells *(cf., e.g.,* Lai [13]). In similar situations, but with the added complexity of non-negligible transition (misfit) strains between phases *(cf., e.g.,* Lipman and Roitburd [14]), we expect the corresponding bulk stress to effect growth kinetics and microstructural morphology; such processes, involving a coupling between deformation and Ginzburg-Landau kinetics, should be described within the general framework developed here.

Our approach follows closely that taken in [lj. To account for situations involving a multiplicity of phases and/or phase variants, we introduce a vector order-parameter. We also introduce forces that work against the rate at which the order parameter changes and thereby characterize accretion (the growth of one phase at the expense of another). These configurational forces—which are distinct from the standard forces associated with momenta—are presumed consistent with their own force balance *(cf.* Gurtin [15, 16, 17], Gurtin and Struthers [17], Pried and Gurtin [1, 12]).[3]

We organize the paper as follows. In Section 2 we introduce the basic balance laws and a suitable version of the second law. In Section 3 we consider constitutive equations involving dependencies of the free energy, Piola-Kirchhoff stress, configurational stress, and internal configurational force on the deformation gradient, the order parameter, the order-parameter gradient, and the order-parameter rate. We then deduce restrictions placed on these constitutive equations by the second law. In conjunction with the local balance statements the restricted constitutive equations lead to field equations that we present in Section 4, where we also discuss boundary conditions and a Lyapunov relation. In Section 5 we propose possible simple forms for the free energy and discuss material symmetry. A theory appropriate to infinitesimal deformations is given in Section 6. Finally, in Section 7, we study the manner in which transition kinetics and interfacial structure are generated within our theory. We find that the theory allows for a full range of transition kinetics of the type discussed by Abeyaratne and Knowles [19], Truskinovsky [20], Gurtin and Struthers [18],

[1] In [2] we extend the theory presented here to include heat and mass transport.

[3] In contrast to regularizations that rely on strain gradients *(cf., e.g.,* Fàlk [3, 4], Miiller and Wilmanski [5], Achenbach and Müller [6], Barsch and Kromhansl [7, 8], Colli, Fréinond and Visintin [9], Hoffman, Niezg6dka and Songmu (10]), the regularization provided by our theory results, as in [1], from a constitutive dependence on the order-parameter gradient (see also [11, 12]).

[8] In (1] we use the adjective *accretive* instead of *configvrrUional.*

and Gurtin [17]. Further, granted certain simple constitutive assumptions, our theory leads to interfacial structure equivalent to that which arises in the sharp-interface theory of [16,17] for an interfacial energy that is isotropic and independent of interfacial strain.[4] In the Appendix we examine certain aspects of the configurational force system and balance from a fundamental perspective and determine a connection between our configurational stress and the capillarity vector of Cahn and Hof&nan [22].

2 Basic physical quantities. Balance laws. Dissipation inequality

2.1 Kinematics. Momentum

We consider a homogeneous body B, identified with the region of R^8 it occupies in a fixed uniform reference configuration with mass density Q. A motion of B is a mapping y of material points x and times t into points of space

$$y(x,t) = s + u(x,t) \tag{1}$$

in R^9. Here u is the *displacement* and

$$F = 1 + \nabla u \tag{2}$$

(with detJF> 0) is the *deformation gradient.* An appropriate measure of strain is the *right stretch tensor U* defined by the polar decomposition F= *RU* of F into a symmetric, positive definite tensor U and a rotation R; U may also be defined through the relation

$$U=y/F^{*}¥. \tag{3}$$

We associate with each motion a *(first Piola-Kirchhoff) stress tensor S* and an external *body force b.* Letting V denote an arbitrary subregion of B, with n the unit outward normal to dV> the balance laws for linear and angular momentum take the form

$$\left.\begin{array}{l} / \; Snda + fbdv = \overline{f\ giidv}, \\ \partial P \qquad V \qquad V \\ / \; yxSnda\text{-}r\ Jyxbdv = \overline{fyxgudv}, \\ aV \qquad\quad V \qquad\quad V \end{array}\right\} \tag{4}$$

for all V and all time; or equivalently,

$$\left.\begin{array}{l} \mathrm{div}S+\& = ,\rho\ddot{u}, \\ SF^{T} = FS^{T}. \end{array}\right\} \tag{5}$$

[4] In [21] it Is shown that, under slightly more general constitutive assumptions, our theory generates anlsotopic interfacial energy and interfacial stress consistent with the general framework of [16, 17].

2.2 Vector order-parameters. Configurational force balance

Throughout the paper we use lists $TJ = (i^{\wedge}, tfe, ..., iy_A) \in R^A$; we write

$$\langle \mu, \eta \rangle := \mu_1 \eta_1 + \mu_2 \eta_2 + \cdots + \mu_A \eta_A \tag{6}$$

for the inner product of such lists to differentiate it from the inner product on R^s, which we denote by a dot. We also use this notation for the inner product of lists $£ = (^{\wedge}iCaj\text{-}.\text{-}tO \ldots (^{RS})^A$ of vectors $£_a$ in R^3: given two such lists £ andC

$$\langle ,C\rangle := {}^{\wedge}C_1 + {}^{\wedge}C_2 + \text{---} + €_A\text{-}C_A. \tag{7}$$

Finally, given £ in $(R^3)^A$ and c in R^3,

$$C\text{-}c := ({}^{\wedge}c, {}^{\wedge}c, \ldots, \{_A.c) € R^A. \tag{8}$$

We consider materials whose phase is characterized by a list $<p = fa, <p_2, \ldots, (p_A)$ of scalar order-parameters tp_m. The *vector order-parameter (p* will generally be constrained; entries of *(p* may, for example, satisfy a constraint of the form

$$p. \in [0,1] \quad \text{for each a,} \qquad \overset{A}{£}{}^*>. = *\bullet \tag{9}$$

We allow for the possibility of more general constraints by restricting attention to *(p* that lie in the closure *$* of a relatively open subset of an affine set *H* in R^A. (Extension of the theory to the case where *H* is a smooth manifold is straightforward.) We write *T(H)* for the subspace of R^A consisting of vectors tangent to *H* and *P(H)* for the projection onto *T(H)* with the understanding that *P(H)* denotes the identity on R^A if *T(H)* = R^A. *T(H)* generates a corresponding space *V(H)* contained in $(R^3)^A$ consisting of all (in $(R^S)^A$ such that, for each c in R^s, $^{\wedge}c$ is an element of T(W).

When the dimension of *H* is *A* - 1, the elements IJ of *H* are consistent with an equation of the form (d, *rf)* = *6,* with *d* in R^A and *6* in R prescribed, and *T{H)* is the set of all *fi* with (d, *fi)* = 0. If each entry of d is 1, and if £ = 1, then we recover $(9)_2$.

During an evolution of *B* the order parameter will be a field $<p$ on *B* for all time. We associate with each such evolution an *configurational force system* that acts in response to changes in $<p$. This force system consists of a *stress* £ with values in V(H),[5] an *internal force n* with values in T(W), and an *external force* 7 with values in T(W); most importantly, this system is presumed consistent with the *force balance*

$$\int_{\partial V} Z\text{-}n da + \int_V (\mathrm{tr} + 7) <^* t; = O \tag{10}$$

[6]Thus, the stress £ is a list of vectors; in the Appendix £ Is related to the more conventional tensorial notion of stress.

for all V *(cf.* (8)), where we have chosen to neglect microstructural inertia. Thus

$$\text{div}^* + \text{ir} + {}_7 = \text{O}, \quad \text{div}\pounds = (\text{div}\$_1, \text{div}\epsilon_{21}\ldots, \text{div}\pounds_l), \tag{11}$$

or equivalently,

$$\text{di}\langle + *. + 7. = 0, \tag{12}$$

for a = 1,2,..., A; because of the underlying constraint, the equations (12) are generally *not* independent.

It is difficult at this stage in the development to give precise physical interpretations to the stress £ and the internal force TT, but some preliminary remarks of an intuitive nature might be helpful. Consider the special case of a single scalar order-parameter $\langle p$. Across a transition layer between phases, tp should vary rapidly in the direction m = $-V\langle p/|V\langle p|$ and, for an isotropic material, (should be parallel to m; in this case our intuitive expectation is that (*m represents surface tension within the layer. For an anisotropic material, £ • v would not generally vanish for v orthogonal to m; we believe that £ • v would in this case account for microstructural shearing, across the layer, induced by anisotropy. For a scalar order-parameter $(p$, we view the scalar force TT as a microstructural tension representing both configurational forces of the type discussed by Eshelby [23] and dissipative forces within transition zones associated, for example, with the rearrangement of atoms. These intuitive remarks are justified by the discussion of the Appendix, the asymptotic analysis of Section 7.2 (in particular (117)), and the analysis presented in [21].

2.3 Dissipation inequality

When thermal effects are suppressed the second law is the assertion that the rate of energy increase cannot exceed the total expended power. Letting $|p$ denote the *free energy,* we write the second law in the form of a dissipation inequality to be satisfied for all time and all V:

$$\int_{\dot{P}} (\psi + \tfrac{1}{2}\rho|\dot{u}|^2)\,dv \leq \int_{\partial V} Snu\,da + \int_V fbu\,dv + \int_{\partial V} J\{Z,\langle p)da + \int_V j\{\%\$)dv, \tag{13}$$

which makes precise our assertion that configurational forces act in response to changes in the order parameter. We do not include the force TT in (13) as it acts internally to V. In this sense n has a role analogous to that of the internal forces G^1 and g^1 in Ericksen's theory of liquid crystals [24], since TT enters a balance equation but does not contribute to the working.[6]

If we use $(5)_t$ and $(11)_x$ to eliminate the external forces 6 and 7 from the local form of (13), we arrive at the local dissipation inequality

$$\wedge - S\,.\,\dot{F} - \langle t\,p \rangle + \langle *, \pounds \rangle \leq 0, \tag{14}$$

[6] *Cf.* (3.4M3.7)of[24].

where p, with values in V(W), is defined by

$$\boldsymbol{p} := \nabla\boldsymbol{\varphi} := (\nabla\boldsymbol{\varphi}_1, \nabla\boldsymbol{\varphi}_2, \ldots, \nabla\boldsymbol{\varphi}_A). \tag{15}$$

3 Constitutive equations. Compatibility with the dissipation inequality

We consider constitutive equations in which the independent variables are the deformation gradient *F* and the configurational variables <f>; p, and <£;

$$\psi = \hat{\psi}(\boldsymbol{F}, \boldsymbol{\varphi}, \boldsymbol{p}, \dot{\boldsymbol{\varphi}}), \quad \boldsymbol{S} = \hat{\boldsymbol{S}}(\boldsymbol{F}, \boldsymbol{\varphi}, \boldsymbol{p}, \dot{\boldsymbol{\varphi}}), \quad \boldsymbol{\xi} = \hat{\boldsymbol{\xi}}(\boldsymbol{F}, \boldsymbol{\varphi}, \boldsymbol{p}, \dot{\boldsymbol{\varphi}}), \quad \boldsymbol{\pi} = \hat{\boldsymbol{\pi}}(\boldsymbol{F}, \boldsymbol{\varphi}, \boldsymbol{p}, \dot{\boldsymbol{\varphi}}). \tag{16}$$

We assume that, under observer changes, <*p*, p, £, £, and 7r are ṫnwriant, and that the remaining fields transform in the standard manner, so that, for example,

$$\hat{*}(\mathrm{F},\mathrm{v},\mathrm{P},*) = \dot{}\mathrm{tev.P,V}), \tag{17}$$

with *U* the right stretch tensor (3). (We also require that $\hat{5}$ be consistent with $(5)_2$, but this is of no concern, since it will satisfied automatically by virtue of (17) and $(20)_x$.) We do not provide constitutive equations for the external forces 6 and 7, but instead allow them to be assigned in any way compatible with the balance laws for linear momentum and configurational force.

Given a displacement field *u* and an order-parameter field <*p*, the constitutive equations (16) can be used to compute a constitutive process consisting of u, <p, and the fields *ij*>, 5, £, and TT; the balances $(5)_1$ and $(11)_1$ for linear momentum and configurational force can then be used to determine the external forces 6 and 7 needed to support this process. The second law remains to be satisfied in all such constitutive processes, a requirement that we use to restrict the constitutive equations. Specifically, we assume that *the local dissipation inequality* (14) *is satisfied in all constitutive processes.*

Writing *h* == *(p* and £ = (F,^,p,h), we see that, granted (16), (14) is equivalent to the inequality

$$(\hat{\psi}_{\boldsymbol{F}}(\zeta) - \hat{\boldsymbol{S}}(\zeta))\cdot\dot{\boldsymbol{F}} + \langle\hat{\psi}_{\boldsymbol{\varphi}}(\zeta) + \hat{\boldsymbol{\pi}}(\zeta), \boldsymbol{h}\rangle + \langle\wedge\ (\zeta) - \hat{\boldsymbol{\xi}}(\zeta), \dot{\boldsymbol{p}}\rangle + \langle\wedge(\mathrm{C}), \dot{*}\rangle \leq \mathrm{o_f} \tag{18}$$

with subscripts indicating partial differentiation, so that

$$\dot{\psi}\mathrm{U}\zeta) \in \mathcal{T}(\mathcal{H}), \quad \wedge\ (\zeta) \in \mathcal{T}(\mathcal{H}), \quad \hat{\psi}_{\boldsymbol{p}}(\zeta) \in \mathcal{V}(\mathcal{H}). \tag{19}$$

Since we can always find fields *u* and *(p* such that F, $\dot{\mathrm{F}}$, p, $\dot{\mathrm{p}}$, h, and $\dot{h}$ have arbitrarily prescribed values (consistent with the constraint) at some chosen point and time, we must have $\hat{if}>_h = 0$, $\hat{ip}_F = \hat{\mathrm{S}}$, and $\hat{\wedge}_p = \hat{\pounds}$.

The free energy, stress, and configurational stress are therefore independent of *(p* and related through

$$\boldsymbol{S} = \hat{\psi}_{\boldsymbol{F}}(\boldsymbol{F}, \varphi>, \mathrm{p}), \quad * = \wedge_{\underline{\mathrm{p}}}(\mathrm{F},*>,\mathrm{p}), \tag{20}$$

and the internal configurational force admits the representation

$$\pi = -\hat{\psi}_{\varphi}(F, \varphi, p) - B(F, \varphi, p, \dot{\varphi})\dot{\varphi}, \tag{21}$$

where the *kinetic coefficient* B(F, ^, p, <p) = $B(U_y<p,p_y(\dot{p})$ is, for each value of its argument, a linear transformation from *T(H)* into itself consistent with

$$\mathcal{D} := (\dot{\varphi}, B(F, \varphi, p, \dot{\varphi})\dot{\varphi}) \geq 0. \tag{22}$$

In view of (20) and (21), a complete constitutive specification of the material consists of prescription of the free energy *fp* and kinetic coeflScient *B* as functions of (F,^>,p,h).

The relations (20)-(21) yield the dissipation balance

$$ij, \_ S\text{-}\dot{F}\text{-} \ (£,\dot{p}) + (*r, \dot{\gamma}(f) = -V \leq 0, \tag{23}$$

identifying *V* and hence transformation kinetics as the sole source of dissipation in the theory.

4 Field equations. Boundary conditions. Lyapunov relation

Using (20)-(21) in the local balances (5), and (11), yields

$$\begin{aligned} &\operatorname{div}(\hat{\psi}_{F}(F, \varphi, p>)) + 6 = £\dot{t}i, \\ &\operatorname{div}(\hat{\psi}_{p}(F, \varphi, p)) - \hat{\psi}_{\varphi}(F, \varphi, p) + \gamma = \{ «**» \bullet * \} \end{aligned} \tag{24}$$

While the configurational force balance (11)^ involves no time derivatives, rate terms enter the final equation $(24)_2$ through the constitutive equation for the internal force *n.* For that reason we do not view $(24)_2$ as a transport equation for *(f,* but rather as a balance law for force in which a rate term arises as a consequence of the dissipative nature of the internal configurational force. We assume, for the remainder of the paper, that the external forces vanish:

$$6 = 0, \qquad 7 = 0. \tag{25}$$

Note that, by (24) and (9), writing *B* = JB(F, <p,p, <p), we have

$$\mathrm{dj}_{v}((V> - x£|u|^2)l - F^T S - \overset{a=1}{S} P « ® € «) + QF^T ii - \overset{a=1}{\underset{b=1}{\Sigma}} B_{mh}<p_b p_a = 0, \tag{26}$$

a balance that involves a generalization

$$(\psi - \tfrac{1}{2}\rho|\dot{u}|^2)_1 - F^T S - £P.®£. \tag{27}$$

of the *Eshetby tensor* appropriate to our theory (c/. [23]).

Appropriate boundary conditions for the general equations (24) might consist of classical conditions prescribing *Sn* on a portion *C* of *dB* and *u* on *dB \C* in conjunction with the prescription of (n on a portion *C* of *8B* and *(p* on *8B\C.*

In the case of an order parameter with two components tp_x and $(p_2$, constrained via $d_l(p_l + d_2tp_2 = £$ with d_n d_3, and *6* nonzero, only one of the scalar order-parameters is independent. Writing $(f = d_l<p_l = 6\text{-}\ d_2tp_2$, and expressing the free energy as a function of F, y>, and p := *V<p* through

$$\hat{\psi}(F, \varphi, p) = \hat{\psi}(F, \varphi_1, \varphi_2, \nabla\varphi_1, \nabla\varphi_2), \tag{28}$$

(24) reduces to

$$\left.\begin{aligned} &\operatorname{div}\left(\hat{\psi}_F(F, \varphi, p)\right) \\ &\operatorname{div}\left(\hat{\psi}_p(\mathrm{F}, \mathrm{v?}, \mathrm{p})\right) - \%\{F, ip, p) = /?(\mathrm{F}, \mathrm{v?}, \mathrm{p}, \text{^})\text{^},\ \mathrm{J} \end{aligned}\right\} \tag{29}$$

with

$$fi := \mathrm{Bu/rff} - 2B_{l\%}/d_l d_2 + \mathrm{B_M/d_2^{\,2}} \geq 0 \tag{30}$$

a 5oa/ar kinetic coefficient. Equations (29) are identical to the specialization of (24) that arises when the order parameter is a scalar.

Returning to the general equations (24), our development ensures consistency with (14) and hence yields the growth relation

$$\overline{\int_V (\psi + \tfrac{1}{2}\varrho|\dot{u}|^2)\, dv} - \int_{dB} Snuda - \int_{dB} I(£,(f)da < \_ - \int_B Vdv. \tag{31}$$

If Sn = *S.n* on *dC* with S. constant, if u ≐ 0 on 3iB \ C, and if ((-n, <*j*>) = 0 on dB, then (31) reduces to the Lyapunov relation

$$\overline{\int_5 t(tl> - S.\text{-}Vu + y|\dot{u}|^2)dv} = - \int_B fvdv \leq 0. \tag{32}$$

5 Free energies

5.1 A model with separable free energy

We now describe a simple model that should yield many of the qualitative features of displacive phase transitions. We assume that the order parameter *cp* is constrained as in (9) and consider free energies *i*> that are *separable* in the sense of the decomposition

$$\left.\begin{aligned} &\hat{\psi}(F, \varphi, p) = W(F, \varphi) + f(\varphi) + g(p), \\ &W(F, \varphi) = \sum_{\alpha=1}^{A} \varphi_\alpha W_\alpha(F). \end{aligned}\right\} \tag{33}$$

Writing

$$M.:=(O,O,...,O,1,O,...,O), \qquad gentry=1), \tag{34}$$

we assume that / and g comply with the normalization

$$/(fij = 0 \quad \text{for each a,} \qquad g\{0) = 0. \tag{35}$$

For this model there are A phases, labeled $a = 1,2,\ldots,A$, and phase a may be identified with the particular value $<p = /i_{\#}$ of the order parameter. The function $W(F_y <p)$ represents the *strain energy*, with $WJ^F)$ the *strain energy* of phase a. $W_m(F)$ should be of the type usually considered for single-phase materials; in particular, we assume that $W_a(F)$ is rank-one convex (or even quasiconvex) and that $W^*(U)$ restricted to right stretch tensors U (c/. (17)), has a strict global minimimum L£,

$$W_m\{U) \leq W_m(U) \quad \text{for} \quad U^*U \tag{36}$$

with l£ the *natural stmin* for phase *a.*

While the individual strain energies display the energetic preference—within each phase—of the natural strain for that phase, the *exchange energy f((p)* should characterize the energetic favorability of the individual phases. We therefore require that the JA_O form the complete set of global minima for /(<p); thus, by (35), assuming the minima are strict,

$$/(/O = 0, \quad f(<p)>0 \quad \text{for} \quad {}_V?p_m. \tag{37}$$

Finally, the structure of transition layers is characterized by the dependence of the free energy on p, while the bulk material should correspond to states with $p = 0$. Further, the *gradient energy g(p)* should, in some sense, regularize the system. With this in mind, we assume that *g(p)* is strictly convex with a minimum at $p = 0$.

When viewing this model as a *regxdarizaUon* of a more standard theory in which phase transitions are the result of a lack of rank-one-convexity in the underlying strain energy $W(F) = W(l/)$, one might choose the energy $W_U\{U)$ as an approximation of $W(U)$ near the well describing phase *a* (c/., *e.g.,* Grinfeld [25], FWed and Gurtin [11]).

A standard gradient energy is

$$*(p) = i<p,4p), \tag{38}.$$

with A a (constant) symmetric, positive-definite linear transformation from V(H) into itself; the isotropic version of this relation has the simple form $\backslash A|p|^2$.

A standard exchange energy, for a system constrained by $(9)_2$, is

$$f(\varphi) = \tfrac{1}{2}\nu \prod_{o=1}^{A} (1 - \varphi_o)^2, \tag{39}$$

with *(p** the a-th component of <*p.*

The constitutive equations appropriate to a separable free energy have the form

$$\left.\begin{aligned} \hat{S}(F,\varphi) &= \sum_{a=1}^{A} \varphi_a S_a(F), \quad S.(F) = \tfrac{\partial}{\partial F} W_a(F), \\ \hat{\xi}(p) &= g_p(p), \\ \hat{\pi}(F,\varphi,p,\dot{\varphi}) &= -w(F) - f_\varphi(\varphi) - B(F,\varphi,p,\dot{\varphi})\dot{\varphi}, \end{aligned}\right\} \qquad (40)$$

with S_a(F) the partta/ atress in phase a, and ti>(F) := P(W)(W^ (F), W£ (F), . . . , W_A (F)), where P(W) is the projection onto T(W); and in the absence of external forces, the governing equations (24) reduce to

$$\begin{aligned} &\operatorname{div}\hat{S}(F,\varphi) = \varrho\ddot{u}, \\ &\operatorname{div}\left(g_p(p)\right) - w(F) - f_\varphi(\varphi) \text{ « C F . . . . . } \end{aligned} \qquad \text{<4I>}$$

Thus far we have not distinguished between *pure phases* and *phase variants.* To do so requires a discussion of material symmetry, which is the subject of the next section.

5.2 General theory. Coarse-grain free energy. Material symmetry

We now return to the theory described by a *general* free energy V̂>(F, *(p,p).* Here bulk phases are associated with properties of the *coarse-grain free energy*

$$\#(\mathrm{F}, if) = \wedge(\mathrm{F}, tf)\,0), \qquad (42)$$

while the structure of transition layers is characterized by the dependence of the *gradient energy*

$$g(F, <p,p) = tj,(F, <p,p) - 4>\hat{}(F, <p, 0) \qquad (43)$$

on p. We now focus on ideas of material symmetry for individual phases using the coarse-grain free energy as basis. Symmetry considerations for the gradient energy should, in some sense, entail the interaction between phases *(cf.* Lai [13]).

Using separable free energies as motivation, we assume that there are *K* phases, labeled *k* = 1,2,..., *K,* and we associate with each phase *k* a unique value *(p_k* in * of the order parameter, with *(p_k*^<p_t* for *k* ^ /. Focusing on the dependence of #(F, *(p)* = #(17, *(p)* on the stretch tensor *U,* we assume that, for each phase fc, *&{U, (p_h)* has a strict global minimum at U_k, that is

$$w_h = *(U_k, ip_h) < *(U, <p_h) \quad \text{for} \quad U \pm U_k. \qquad (44)$$

Then

$$W_k(F) = \#(\mathrm{F}, \mathrm{v}>\mathrm{J} \qquad (45)$$

is the strain energy of phase *, while U_k is the natural state for k; by (44),

$$_{Wk} = W_h(U_k) < W_k(U) \quad \text{for} \quad U?U_k. \tag{46}$$

We define the *symmetry group* for phase k to be the group Q_k of unimodular tensors H (tensors H with detH = 1) such that

$$W_k(F) = W_k(FH) \tag{47}$$

for all F.[7] This relation restricts the natural strains U_k, since (47) with F= t/$_{fc}$, (17) with F= U_kH> (3), and (46) yield

$$Ul = ITUIH \tag{48}$$

for all Hin Q_k.

The definition (47) describes symmetry within a given phase; *variants* are described by symmetry transformations between phases. Precisely, phases k and / are *equivalent* if there is a unimodular tensor JJ, called a *symmetry transformation* from k to /, such that

$$*(F,<p_k) = *(FH,_{Vl}) \tag{49}$$

for all F. This defines an equivalence relation on the set of all phases; the corresponding equivalence classes are called *pure phases.* If a pure phase C has more than one member, then its members are called variants of £ (or of / € £).

Let k and / be variants of a pure phase and let if be a symmetry transformation from k *to* L Then

$$G_k = \quad ^{-} \qquad \text{ff'ftff} \tag{50}$$

and

$$W_i(F) = W_h(FH), \quad w_h = w_i, \quad U_i^2 = H^T U_h^2 H. \tag{51}$$

We will verify only (50); the proof of (51) is similar to that of (48). Choose F and A € Q_k arbitrarily and let $G = FIT^1$. Then

$$9\{GAH, *>,) = \#(O4, ip_k) = \#(G, y>J = \wedge(GH, _{Vl}); \tag{52}$$

thus !P^r(Fff"^{1}AHT,Vi) = $9\{F_f ip_l)$ and IT^1AH is an element of ft; hence $H\sim^l G_k H$ C Gi. A similar argument yields $H'^l GM$ D Gi-

Since the material under consideration is solid, it seems reasonable to assume that, given a phase k there is a choice of reference configuration such that all symmetry transformations in ft, as well as all symmetry transformations to variants of k are orthogonal. Granted this, (47) and (48) imply that, for any Q

$$W_h(U) = W_h(Q^T UQ), \quad U_k = Q^T U_k Q, \tag{53}$$

[7] *Cf.* Truesdell and Noll [26] and Gurtin [27] for discussions of material symmetry.

while (51) yield the relations

$$W_h(U) = W_t(Q^T U Q), \qquad \text{Ui} = \text{Q}^{\text{T}}\text{C7}_{\text{fc}}\text{Q}, \tag{54}$$

for any symmetry transformation Q from k to /.

Phases k and I are *kinematically compatible* if there are orthogonal tensors Q_k and Q_l such that

$$Q_k U_h - QiUi \qquad \text{is a tensor of rank one;} \tag{55}$$

in which case it is kinematically possible for a coherent sharp interface—involving a jump in the deformation gradient F—to form between phases k and / at the stretches U_h and L£. Condition (55) is most often satisfied when k and / are variants of martensite, but not generally between austenitic and martensitic phases (c/, *e.g.,* [28, 29]). Conditions of the form (55) are important in equilibrium theories, since they allow for the possibility of layering between k and /.

6 Linearly elastic phases

To model situations in which the displacement gradient is small, it might be appropriate to reconsider the theory assuming, from the outset, that both strains and rotations are infinitesimal. To set our theory within that framework we redefine F to be Vu and replace $(5)_2$ by $S = 5^{\text{T}}$; the steps leading to (20)-(21) and (24) then remain unchanged, as do these relations. Further, invariance of the constitutive equations under infinitesimal rotations (t.e., replacement of Vu by Vu + W with W skew) implies that the constitutive hinctions can depend on F only through the infinitesimal strain

$$\boldsymbol{E} := \tfrac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\text{T}}). \tag{56}$$

Again we consider free energies that are separable:

$$\begin{aligned} \hat{\psi}(\boldsymbol{E}, \varphi, p) &= \text{W(£,¥>)} + /(\text{V}) + \$(\text{P})> \\ W(\boldsymbol{E}, \varphi) &= \sum_{0=1}^{A} \varphi_{\text{a}} W_{*}(\boldsymbol{E}) \end{aligned} \tag{57}$$

with / and g as defined in Section 5.1 and <p constrained as in (9). Consistent with our assumption of infinitesimal deformations, we require that the individual energies *WJJ2)* be quadratic functions of the infinitesimal strain:

$$W_{\text{a}}(\boldsymbol{E}) = w_{\text{a}} + \tfrac{1}{2}(\boldsymbol{E} - \boldsymbol{E}_{\text{a}}) \cdot \mathbf{C}_{\text{a}}[\boldsymbol{E} - \boldsymbol{E}_{\text{a}}], \tag{58}$$

with E_m the natural strain of phase o and C.[•]—a symmetric, positive-definite linear transformation from the space of symmetric tensors into itself—the *elasticity tensor* of phase o. The stress $S = \hat{S}(E, <p)$ is then given by

$$\hat{\boldsymbol{S}}(\boldsymbol{E}, \varphi) = \sum_{\text{a}=1}^{\text{A}} \varphi_{\text{a}} \boldsymbol{S}_{\text{a}}(\boldsymbol{E}), \qquad \text{S.(E)} = \text{C.[£-JE.]}, \tag{59}$$

with $S_m(E)$ the partial stress for phase a.

For a separable free energy such as $(57)_1$, $(40)_{28}$ remain valid, and, ignoring external forces, the governing equations are

$$\left.\begin{array}{ll} \operatorname{div}\hat{S}(E,\varphi) = \varrho\ddot{u}, & \\ \operatorname{div}(g_p(p)) & I_{\varphi}(\varphi) = \Xi(E,\varphi,p,\varphi)\varphi, \end{array}\right\} \tag{60}$$

where $w(E)$ ** P(H)(H^(£?), $W_a(25),\ldots,W_A\{B))$.

An alternate free energy that might be useful in describing ordering transitions has the separable form of (57^ with the strain energy given by[8]

$$W(E,\varphi) = w(<p) + \{E-E\{\hat{<}p))-C\{<p)\E -E\hat{\}<p\% \tag{61}$$

where $<p$ is constrained in a manner consistent with the particular transition under consideration.

7 Comparison with sharp interface theory

We now investigate the formal consistency of our theory with the sharp interface approach. As a basis for this, we list the governing equations derived by Gurtin and Struthers [18] and Gurtin [17] specialized to the case of an isotropic interfacial energy that is independent of the deformation gradient. Neglecting body forces, the bulk equations consist of the momentum balance

$$\operatorname{div}S = g\ddot{u}, \tag{62}$$

supplemented, in each phase $q = 0,1$, by constitutive equations

$$W = \hat{W}_q(F), \quad S = \frac{\partial}{\partial F}\hat{W}_q(F). \tag{63}$$

The equations that hold across a phase interface, represented by a smoothly evolving surface E with orientation m and normal velocity V, consist of the compatibility condition

$$M=0, \tag{64}$$

expressing the requirement of coherence, the momentum balance

$$[S]m = -\varrho V[\dot{u}]_v \tag{65}$$

and the normal configurations! force balance

$$W\ \sim\ <S>\cdot\{F\ + wK = bV. \tag{66}$$

Here $[4>\$ and {<£) denote the jump and average of a bulk field $<j>$ at the interface,

$$[W] - (5)\cdot[F] = m\cdot[Wl - F^TS + \_eV^iF^TF]m \tag{67}$$

[e] *Cf.* Libman and Roitburd (14).

is the Eshelby (or *"driving")* traction, *w* is the interfacial energy (per unit area), *K* is twice the mean curvature of 27, and $6 \geq 0$ is the kinetic coefficient.

Consistent with (62)-(67), we focus on situations local to a single interface separating two phases. (We recall that such an interface may represent, depending on the constitutive details, a boundary separating either two variants of a pure phase or two distinct phases.) Specifically, we consider situations described by a single unconstrained order parameter *(p* (c/. the paragraph following (25)) and, hence, restrict attention to the system (29).

7.1 Relation between Eshelby traction and interfacial velocity

Let *B* occupy all of space, and consider a longitudinal motion described by the axial coordinate x. In this setting the displacement and order parameter are functions of *x* and t, and the displacement may be identified with a scalar-valued function *u.* Therefore, letting

$$e := tx_x, \quad p := <p_x, \tag{68}$$

we may consider the response functions \j) and /? of the general theory as functions of (e,<p,p) and (e,y?,p,<£), respectively, and, in the absence of external forces, reduce the governing equations (24) to

$$\left.\begin{aligned} s_x &= \varrho \ddot{u}, \\ \xi_x - \hat{\psi}_\varphi(e,\varphi,p) &= \beta(e,\varphi,p,\dot{\varphi})\dot{\varphi}, \end{aligned}\right\} \tag{69}$$

where

$$s = \hat{\psi}_e(e,\varphi,p), \quad \xi = \hat{\psi}_p(e,\varphi,p). \tag{70}$$

We seek a solution of (69) of the form

$$ti(x,t) = tl(y), \quad <p(M) = £(y), \quad y = x - V t, \quad V \geq 0, \tag{71}$$

subject to the far-field conditions

$$\bar{e}(\pm oo) = e\pm, \quad \bar{<}f(\pm oo) = v^*, \quad r(\pm oo) = \bar{p}(\pm oo) = \wedge(\pm oo) = 0, \tag{72}$$

where $\bar{c} = €'$, $\bar{p} = <p'$. A solution of this type represents a traveling wave with velocity *V* connecting the states (e~,yr) and $(c^+,\wedge>^+)$.

Substituting (71) into (69), we obtain the following system of ordinary differential equations

$$\hat{\psi}_\varphi(e,\varphi,p) - \xi' = V\beta(e,\varphi,p,-Vp)\varphi', \tag{73}$$

where for convenience we have suppressed the overbars. We now investigate properties of solutions of (73) that are consistent with (72).

First, by (72) and $(73)_a$,

$$\wedge(e^*, V^*, 0) = 0, \tag{74}$$

so that the energy of states connected by a traveling wave is stationary with respect to the order parameter. Next, letting

$$**:\!\!\ll \&e^*_{tV}\!>\!*,0), \quad **:=tf.(e^*.**.O), \quad [a] := o^+\text{-}a", \quad fa) := \wedge+a\sim), \tag{75}$$

we note that (73), can be integrated to give

$$s\text{-}O) = {}_eV"(e\text{-}(e\!\!\ll \tag{76}$$

and the *Rankine-Hugoniot* relation

$$W = *VM\!\!\ll 1\text{-} \tag{77}$$

Further, multiplying both sides of (73), by p and using (77), we obtain

$$(fa, \langle P, P) \sim \ll \text{-}J^* + *\underline{\ }\langle ?VV)' = VP(e, \langle p, p, -Vp)p\rangle, \tag{78}$$

which, when integrated from $y = -\infty$ to $y = +00$, yields, with the aid of (75)-(76),

$$M\text{-}\{*)M = \dot{T}V, \tag{79}$$

where

$$r := \overset{+00}{\underset{-\infty}{I}} P(e(y)My), P(v), -Vp(y))p^2(y)dy. \tag{80}$$

FVom (74) and (76) one might expect that—granted suitable constitutive hypotheses—*if*$^{\pm}$ and the functions c(«) and *tp{)* are uniquely determined by the limiting values e* of the strain; in this case r = r(e~, e+, *V)*.

Recognizing that the geometry of the problem at hand obscures potential sources of interfacial structure and disregarding the finite thickness of the phase interface, we see that (79) is the one-dimensional counterpart of the normal configurational force balance (66). Our theory therefore contains an implicit *"kinetic relation"* between the Eshelby traction and the interfacial velocity of the type introduced by Abeyaratne and Knowles [19] and TVuskinovsky [20]. Since the function *0* is restricted by thermodynamics only in sign, the kinetics of our theory is more general than that based on viscosity-capillarity or maximum-dissipation criteria (c/. Abeyaratne and Knowles [30, 31] and the references therein).

To identify sources of interfacial structure in our theory, we turn next to a problem that allows for the study of curved interfaces.

7.2 Formal asymptotics of a transition layer. Interfacial tension

In our theory phase interfaces are modeled by thin transition layers in which the order parameter suffers large gradients. We now study the behavior of the basic fields across such a layer assuming that /? is constant and that the free energy has the form

$$\hat{\psi}(F,\varphi,p) = W(F,\varphi) + f(\varphi) + \tfrac{1}{2}\lambda|p|^2, \tag{81}$$

in which case the basic equations (24) become

$$\left.\begin{aligned} &\operatorname{div}(W_F(F,\varphi)) = \rho\ddot{u}, \\ &AAy> - V^*i,(iS<f) - f_v\backslash ip) = p<f- \end{aligned}\right\} \tag{82}$$

Regarding the strain energy $W(F, <p)>$ we require only that the constitutive equation for the stress,

$$S = \hat{S}(F,\varphi) = W_F(F,\varphi), \tag{83}$$

satisfy

$$\backslash\hat{S}\{F_f<p)\backslash\text{-}+oo \text{ as } |F|\text{-}oo, \tag{84}$$

uniformly for $<p$ in any bounded set.[9] Further, we suppose that the exchange energy is a double-well potential with minima at $(p = 0$ and $(p = 1$, so that (c/. (37))

$$/(0) = /(I) < /(¥>) \quad \text{for} \quad v/0,1, \tag{85}$$

with / strictly convex except for a *"spinodal"* interval $[g_0, q_x)$ contained in (0,1). We then identify the two phases, *"phase zero[1]"* and *"phase one,"* with the intervals $(-oo,g_0)$ and $(^,-foo)$, respectively. A standard example of such an energy is

$$f(\varphi) = M\,\varphi(1)-\varphi)' \ . \tag{86}$$

We allow the body to occupy all of space, and consider a process in which one phase, say phase zero, occupies a bounded region. We write *I* for a characteristic length associated with this region during the time-interval under consideration; we let /i and *v* denote scale factors for *W* and / (for example, the maximum of $|\hat{S}_F(1/_o,0)|$ and $|^_F(1/_{1t}1)|$ and the maximum value of $|/^|$ in (0,1)); we introduce dimensionless variables $\bar{x} := x/l$, $i := ct/C$, $\bar{u}(\bar{x},t) := u(x,t)/£$, with $c := y/\overline{l^*/Q}$, as well as dimensionless constitutive functions $\bar{W} := W//i$, $S := S/ii$, $f^- := ffv\backslash$ and we assume that the dimensionless moduli $/3c/i/£$, $\lambda/\nu f$, and /x/i/ scale according to $c^a/3$, $c^2\bar{A}$, and c, respectively, with $c > 0$ small

[9] In particular, we do *not* require that the strain energy have a specific form such as that specified in $(33)_2$, $(57)_2$, or (61).

and *W*, 5, /, 0, and A of O(1). With this scaling (82) become, upon suppressing the overbars,

$$\begin{aligned} &\operatorname{div}\left(W_F(F,\varphi)\right) = \ddot{u}, \\ &\epsilon^2\lambda\Delta\varphi - \epsilon W_\varphi(F,\varphi) - f_\varphi(\varphi) = \epsilon^2\beta\dot{\varphi}. \end{aligned} \qquad (87)$$

We now perform a formal asymptotic analysis for e small, assuming that the thickness of the transition layer is O(e). We choose a value *q* in the spinodal interval (g_0, q_x) and identify the phase interface with the set

$$\pounds(*,*) = \{x:*>(x,M) = 9\}, \qquad (88)$$

which we assume to be a smoothly evolving surface. We write d(x,t, e) for the signed distance between x and *E(t,e)* with *d(x,t,t)* < 0 in the phase-zero region and d(x, t, *e)* > 0 in the phase-one region. We focus attention on an arbitrary but sufficiently small open subset *S(t,* c) of $E(t_y$ e) and define a function C(x,t,e) with values in R^2 such that (d(x,t,e),C(x,M)) provides a local orthogonal coordinate field near 5(t,e). In the transition layer we stretch the coordinate normal to S(t, c) by letting

$$r(*,t,e) := €\text{-}'(*(*,*,€). \qquad (89)$$

For each field r?(x,t,c) of interest, in particular, for t; = *u* and *tj* = ^>, we introduce an *outer expansion*

$$\eta(x,t,\epsilon) = \tilde{\eta}_0\big(d(x,t,\epsilon),\zeta(x,t,\epsilon),t\big) + \epsilon\tilde{\eta}_1\big(d(x,t,\epsilon),\zeta(x,t,\epsilon),t\big) + O(e^3), \qquad (90)$$

that we assume to be valid away from the layer, and an *inner expansion*

$$\eta(x,t,\epsilon) = \eta_0\big(r(x,t,\epsilon),\zeta(x,t,\epsilon),t\big) + \epsilon\eta_1\big(r(x,t,\epsilon),\zeta(x,t,\epsilon),t\big) + O(\epsilon^2), \qquad (91)$$

that we assume to be valid within the layer. The inner expansion at r = ±00 is related to the outer expansion at *d* = 0±; in particular, writing

$$\begin{aligned} &\eta_k^{\pm}(\zeta,t) = \eta_k(\pm\infty,\zeta,t), \quad \tilde{\eta}_k^{\pm}(\zeta,t) = \tilde{\eta}_k(0\pm,\zeta,t), \quad k = 0,1, \\ &[\![\cdot]\!] := (\cdot)^+ - (\cdot)^-, \quad \langle\!\langle\cdot\rangle\!\rangle := \tfrac{1}{2}\big((\cdot)^+ + (\cdot)^-\big), \end{aligned} \qquad (92)$$

we have the O(l) matching conditions (see, for example, Caginalp and Fife [32])

$$\eta_0^{\pm} = \tilde{\eta}_0^{\pm}, \quad [\![\eta_0]\!] = [\![\tilde{\eta}_0]\!], \quad \langle\!\langle\eta_0\rangle\!\rangle = \langle\!\langle\tilde{\eta}_0\rangle\!\rangle. \qquad (93)$$

We consider first the outer expansions of *u(x,t,e)* and ^>(x,t,c). By $(87)_2$, *ftpi&o)* = 0, so that $\tilde{p}_Q$ is constant in each of the two regions separated by the layer; assuming that these constant values lie outside the spinodal, we conclude that $\tilde{p}_0$ = 0 or $\tilde{p}_0$ = 1. Thus, by $(87)_x$, at O(l),

$$\begin{aligned} &\text{iiv}\tilde{S}_0 = \ddot{i}_0, \\ &\tilde{S}> = \text{Wi-}^\text{o}.\,0) \quad \text{»" Phase zero,} \quad \tilde{S}_o = W_p(F_0,1) \quad \text{in phase one,} \end{aligned} \qquad (94)$$

with $F_o = 1 + Vu_0$, so that, away from the interface,

$$\left.\begin{aligned} &\text{divS} = \text{ti} + O(e), \\ &S = W_F(F, 0) + O(e) \text{ in phase zero}, \quad S = W^{\wedge}(F, 1) + O(c) \text{ in phase one.} \end{aligned}\right\} \tag{95}$$

We will show further, as a consequence of the matching condition, that $[\tilde{u}_0] = 0$ and hence

$$[u] = O(e). \tag{96}$$

We next examine behavior within the transition layer. Considering C(-,*, c) as a coordinate field on 5(t,c), let m(C,M), V(CM), and £«,t,e) denote, respectively, the unit normal to S(t, c), the normal velocity of $S(t,$ c), and twice the mean curvature of 5(t, c) (taken as positive whenever the osculating sphere lies in the phase zero region). Then, assuming that these fields have inner expansions of the form (91), it follows (c/ Evans and Spruck [33]) that

$$\left.\begin{aligned} Vd(x, t, e) &= m_o(C(\ldots) + O(e), \\ \dot{d}(x, t, \epsilon) &= V_0(\zeta(x, \ldots), t) + O(e), \\ \Delta d(x, t, \epsilon) &= K_0(\zeta(x, t, e), t) + O(e). \end{aligned}\right\} \tag{97}$$

We assume that within the transition layer the stress $S(x,t,e)$ is bounded in e; in fact, we assume that S has an inner expansion of the form (91) (as do **u** and $<p)$. Expanding the deformation gradient F= 1 + **Vti,** we see that

$$F = \epsilon^{-1} u_0' \otimes m_0 + O(1), \tag{98}$$

where a prime indicates differentiation with respect to r, and consistency of this estimate with (93) and the inner expansions for S and $(p$ yields $u'_o = 0$, so that u_0 *is independent of the normal coordinate* r. Therefore $[u_0] = 0$ and the conclusion $[\tilde{u}_0] = 0$, and hence (96), follows from (93). Further,

$$\left.\begin{aligned} F &= \underbrace{1 + Vu_0 + u_1' \otimes m_0}_{F_0} + O(\epsilon), \\ F' &= tt;'\circledR m_0 + O(e), \\ &\quad \overbrace{}^{F_0'} \\ \dot{u} &= \dot{u}_0 - V_0 u_1' + O(\epsilon), \\ \epsilon\tilde{u} &= V_0^2 u_1'' + O(\epsilon), \\ \epsilon\dot{\varphi} &= -V_0 \varphi_0' + O(\epsilon), \\ &\varphi_0'' + \epsilon(\varphi_1'' - K_0\varphi_0') + O(\epsilon^2). \end{aligned}\right\} \tag{99}$$

Note also that $(99)_{lfS}$ yield

$$V[F] + [\dot{u}] \otimes m = O(\epsilon), \tag{100}$$

a kinematic condition consistent with (96).

Next, (87), gives

$$\text{Atf} = /\!>.)\bullet \tag{101}$$

By (93), to match conditions in the far field requires a solution of this equation satisfying $(p_0 = 0$ at r = —oo and $tp_x = 1$ at r = +00. We assume that such a solution $<p_0$ exists and is unique, so that, necessarily, $<p_0$ depends only on r; when the unsealed exchange energy has the form (86) such a solution is furnished by

$$\varphi_0(r) = \tfrac{1}{2}(1 + \tanh(r/\sqrt{\lambda})). \tag{102}$$

Our next step is to consider the lowest-order terms in (87),. Since $S_c = \hat{S}(F_0, \varphi_0)$,

$$S' = \hat{S}_F(F, \varphi)[F] + \hat{S}_\varphi(F, M = \$ + \text{O(e)}, \tag{103}$$

and

$$\text{div } 5 = t\text{-}'S'Vd + \text{O(l)} = \text{c-}'\wedge\text{m}, + 0(1), \tag{104}$$

so that, by (101), (87)j yields $V_*^* u_i'' = 5\dot{o}''^{m}{}_0$; we therefore have the relations

$$(\text{S}, - \{So))m_o = \text{V?}(\text{«}; - (\text{u};\text{»}, \qquad [\$,]\text{m}_0 = \text{V}_o^{a}[\text{u'J}. \tag{105}$$

At O(e), $(87)_a$ has the form

$$L(\varphi_0)\varphi_1 := \lambda\varphi_1'' - f_{\varphi\varphi}(\varphi_0)\varphi_1 = (\lambda\mathcal{K}_0 - \beta V_0)\varphi_0' + W_v(F_0, <p_0) =: z. \tag{106}$$

Differentiating (101) with respect to r shows that $(p'_o$ is a solution of the equation $L(<p_o)ip'_o = 0$; hence tp'_o and z satisfy the orthogonality condition

$$\int_{-00}^{+0} ti(r)z\{r)dr = 0. \tag{107}$$

Next, by (99) and $(105)_a$,

$$W_\varphi(F_0, \varphi_0)\varphi_0' = (W(F_0, \varphi_0) - \langle S_0 \rangle \cdot F_0 - V_0^2(\tfrac{1}{2}\bullet \text{KI-}(\text{«;w},))', \tag{108}$$

so that, if we introduce the material constants

$$a := y/2\overline{/X} \;/\; y/\overline{f(<P)}\,\&P, \quad \circ \bullet = \wedge\text{a}, \quad \text{r} := 0a, \tag{109}$$

(101) gives

$$\text{a} = j\&\{r)^{\%}dr, \tag{110}$$

and, since K_o and V_o are independent of r, (107)-(110) yield

$$m\&<p.)\ \text{-}\ (\text{flLl-Kl} + \wedge_0 = rv.. \qquad \text{(in)}$$

Finally, by (99), $(105)_2$, and (111), we have the formal estimates

$$[S]m + V[\dot{u}]\wedge O(e\backslash \quad [W] - (S)\cdot[F] + {}^*K = rV + O(e). \qquad (112)$$

In conclusion, as c —> 0 the system (87) is formally asymptotic to

$$\mathrm{div}5 = \mathrm{ti} \qquad (113)$$

away from phase interfaces, with

$$S = W\wedge(F,0) \quad \text{in phase zero,} \quad S = W\dot{p}(F,l) \quad \text{in phase one,} \qquad (114)$$

in conjunction with the jump conditions

$$[u] = 0, \quad [S]m = -V[ti], \quad lW]\text{-}(S).[F\backslash + a)C = TV \qquad (115)$$

across phase interfaces. Equations (114)—(115) are, modulo the underlying non-dimensionalization, equivalent to (62)-(66).

We emphasize that, while $(115)_s$, like (79), relates the Eshelby traction and the interfacial velocity, unlike (79), it also includes a term a/C, allowing us to identify a oc $\sqrt{A}$, appropriately rescaled, with interfacial tension. Thus for free energies of the form (81), the gradient term models the effect of a constant interfacial tension.

Next, using the inner expansions, we find that the scaled configurational stress £ and internal force 7r have the forms

$$\left.\begin{aligned} \xi &= \epsilon\lambda\varphi_0' m_0 + O(\epsilon^2), \\ \pi &= -f_\varphi(\varphi_0) - \epsilon(f_{\varphi\varphi}(\varphi_0)\varphi_1 + W_\varphi(F_0,\varphi_0) - \beta V_0) + O(\epsilon^2); \end{aligned}\right\} \qquad (116)$$

thus, since /(0) = /(I) = 0, we have, formally,

$$\left.\begin{aligned} &\lim_{\epsilon\to 0}(\epsilon^{-1} \int_{-\infty} \wedge i(r)\{(r,\cdot)\,dr) = am, \\ &\lim_{\epsilon\to 0}(\wedge T^0 \int_{-\infty} \wedge(r) w(r_9 -)dr) = [W\backslash - \{5>\text{-}[F] - TV. \end{aligned}\right\} \qquad (117)$$

This allows us to identify £ with a vector whose magnitude is the interfacial tension and whose action is normal to the transition layer, and to identify n as the sum of the Eshelby traction $[W]$ - (S>[-FJ and a drag force - T V .

It is interesting to note that, granted the scaling used above, the particular form of $f(ip)$ effects the limiting equations (114)—(115) only through the integral of $y/\sqrt{f(<p)}$ from well to well across the spinodal. Inspection of (109) reveals,

father, that at most two of the constants a, A, and *0* are independent. The asymptotic correspondence of (82) to (62)-(66) is, in this sense, insensitive to the particular features of the exchange energy, gradient energy, and kinetic coefficient. We view this flexibility, which allows the portions of the constitutive description associated with the order parameter to be selected based on practical considerations (associated, for example, with the desire for computational simplicity), to be a major strength of the theory.

Acknowledgement

We thank J.K. Knowles, M.T. Lusk, G.B. McFadden, P. Rosakis, AX. Roytburd, and P.W. Voorhees for valuable discussions. This work was supported by the Army Research Office and by the National Science Foundation.

A Appendix

To simplify the presentation, we restrict attention to the case of a scalar order-parameter *ip.*

This parameter is a field that describes the state—in the sense of phase—of points of the body. We now identify states with possible values of <*p,* and write $E_e(t)$ for the set of points *x* for which <*p(x,t)* = c. We assume that these sets $E_c\{t)$ describe smoothly evolving surfaces, called *state surfaces,* in the body *B.* The fields

$$\frac{\nabla\varphi}{|\nabla\varphi|}, \qquad \frac{\dot{\varphi}}{|\nabla\varphi|}, \tag{118}$$

then define a unit normal and corresponding normal velocity on each state surface. Given a local parameterization *x* = r(C, *t)* for $£_e(t)$, v(x, *t)* = *(d/dt)r(C t)* satisfies

$$\mathbf{V} = \mathbf{v}\cdot\mathbf{m}\,; \tag{119}$$

we will refer to fields *v* consistent with (119) as *admissible velocity fields* (for the family of state surfaces). Different admissible velocity fields correspond to different choices of time-dependent parameterization for the state surfaces. Each admissible velocity field admits the representation

$$v = Vm + (1 - m\otimes m)w, \tag{120}$$

with *w* an arbitrary vector field, and conversely.

We now consider a somewhat different treatment of forces in which the configurational system consists of a stress tensor C, an internal force TT, and an external force 7, which enter the theory through an configurational force balance

$$\int_{\partial V} Cnda + \int_V (\mathbf{r} + 7)dv = 0 \tag{121}$$

for all P, or equivalently,

$$\mathrm{div}C+7r + 7 = 0. \tag{122}$$

We assume that configurational forces work to change the state of points of the body by expending power over the velocity of state surfaces. Precisely, we assume that the configurational power expended on a part *V* is given by

$$P(\mathcal{P}) = \int_{\partial rp} Jcnvda + \int_{V} fr\wedge dv. \tag{123}$$

A basic stipulation of our theory is that *P(V) is independent of the choice of velocity field v used to describe the motion of the state surfaces.* Writing $C_{Xma} := (1 - m\langle g\rangle m)C$ and $7_{tan} := (1 - m \otimes m)7$, it follows that

$$\int_{\partial BV} C_{tmn}nwda + \int_{V} 1_{\%mn}wdv = 0 \tag{124}$$

for all vector fields it?, which yields

$$(\mathrm{div}C_{tM\rangle} + \%J\text{-}w + C_{tmn} \cdot Vw = 0 \tag{125}$$

for all such to. Thus $C_{tmn} = 0$ and $7_{taa} = 0$, so that *C* and 7 admit the representations

$$C=m\langle g\rangle c, \quad 7 = \$m. \tag{126}$$

Therefore (123 has the *intrinsic form:*

$$P(\mathcal{P}) = \int_{BV} cnVda + \int_{V} JgVdv. \tag{127}$$

Hence, given a part *V* of B, the power expended on *V* by the configurational stress is computed by integrating the measure c • *nVda* over *dV.* Consider a state surface *E(t)* that intersects *dV* in a smoothly evolving closed curve *C(t).* Let i/(x, t), a vector in the tangent space to *E(t)* at x, denote the outward unit normal to *C(t).* Then the vectors m, n, and 1/ are coplanar, and the intrinsic velocity of *C* has two components: Vm, which is normal to *E;* and v_{tan}i/, which is tangent to *E* but normal to *C.* Let 1? denote the angle between *m* and n, and assume that t9 ^ O,TT. Then n = (cost?)m + (sini9)i/, v_{tmn} = Vcott?, and

$$cnVda = (c\text{-}mv\wedge\wedge \; ci/FJsintf \; da. \tag{128}$$

The tangential velocity v_{tmn} represents the rate at which the area enclosed by *C* is increasing, per unit length of *C.* Thus *c* • m works to increase the area of state surfaces, and hence represents a "surface tension." Similarly, *eu* represents a "surface shear." (In fact, the vector c is a counterpart for state surfaces of the *"capillarity vector"* of Cahn and Hoffman [22] for sharp interfaces.) Finally,

sintf transforms the area measure *da* on *8V* to its projection sin t? *da* on the plane perpendicular to i/.

Next, writing $7r_{iMI} := (1 - mg>m)7r$, and substituting (126) into (122), we find that

$$(\text{dive} + w\text{-m} + \mathbf{7\text{-}m)m} + w_{tM} + (Vm)c = 0. \tag{129}$$

At each (x, t), **Vm(x,** t) maps vectors into vectors tangent to the state surface through x; thus (129) yields a normal oonfigurational balance

$$\text{dive} + t\text{r}\,m + 7\text{-}m = 0 \tag{130}$$

and a tangential balance $n_{tmn} = —(Vm)c$. The normal balance governs the motion of state surfaces. The intrinsic velocity of such surfaces is normal; tangential motion is irrelevant; for that reason we take ic_{tmn} to be indeterminate (not specified by a constitutive equation, but rather, *defined* by the tangential balance).

Next, we introduce £, 7r, and 7 through the relations

$$c = \backslash V<p\backslash\& \quad *m = |V<P|TT - £\cdot V|Vy>|, \quad *y\ m = |V\wedge 7; \tag{131}$$

the normal balance (130) then takes the form

$$\text{div}£ + 7r + 7 = 0, \tag{132}$$

and the power becomes

$$\boldsymbol{P(P) = \int_{dr} <pSnda + \int_{v} <rfdv.} \tag{133}$$

These are consistent with the local configurational balance $(11)_x$ and the configurational contribution to the working in (10) for the case of a scalar order-parameter.

Finally, we emphasize that the assumption V<p ^ 0 is crucial to the foregoing discussion, and note that, using (118)^ (130), and the tangential balance, the decompositions of C, TT, and 7 simplify to:

$$C = -VV®£ \quad it = -7rV\wedge> + (VV\wedge>)£, \quad 7 = -7V<p, \tag{134}$$

which can be used to obtain (132)-(133) directly from (122)-(123).

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