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On the Kinematics of Incoherent Phase Transitions

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b. Two-phase deformations

A two-phase deformation is described by a pair y_n (Tt«oc,p) of deformations: y_n associates with each material point X in a closed region B_n a point $x^*y_n(X)$ of space. The points X of B_n are then the material points of phase n, S^^y^tB^) is the region of space occupied by phase it.

$$B = B_a \cup B$$
 . (2.2)

is the *deformed body*, and

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$$Z * S^n S^n \tag{2.3}$$

is the deformed interface (Figure 1). We write Y_n for the inverse deformation:

$$X * Y^{x}$$
 «* x « y^X). (2.4)

We assume that Z is a smooth (possibly unbounded) surface; the surface S_n in B[^] that deforms to Z,

$$\mathbf{S}_{n} * Y_{n}(\mathbf{Z}), \tag{2.5}$$

is the *undeformed phase n interface*, it being tacit that the phases not separate at the interface. We emphasize that — to allow for incoherency — we do not require coincidence of the undeformed interfaces S_a and S^{\wedge} .

We assume henceforth that a two-phase deformation y_n (n*oc,p) is prescribed. The invertibility (2.4) allows us to consider bulk fields as functions of position x in B, which is the *spatial description*, or as functions of the phase Tt and the material point X in B[^], which is the *referential description*. The spatial description is most convenient, as it allows a direct comparison of the fields at the interface; conversion to the referential description may be accomplished using the *inverse mappings* Y[^].

Precisely, a (spatially described) bulk field is a mapping ip that associates with each xcB, xtZ_t a scalar, vector, or tensor $\langle p(x) \rangle$ with $\langle p(x) \rangle$ a smooth function of x away from Z and up to Z from either side. For such a field, $\langle p^{\wedge} \rangle$ denotes the limit of $\langle p \rangle$ from phase TT at the interface, while kp denotes the jump in q across the interface:

$$\varphi_{\pi}(\mathbf{x}) = \lim_{\mathbf{z} \to \mathbf{x}} \varphi(\mathbf{z}), \quad \mathbf{x} \in \mathcal{S}; \quad [$$

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Analogously, inter/aciaJ fields are functions of $xc \pounds$, examples being q^{n} and [q>]. (Fields subscripted by *n* will generally denote interfacial fields associated with phase IT or bulk fields evaluated at the phase TI interface.)

We define the *deformation gradient* F(x) at points x away from the interface through

$$F(x) * Vy^X,$$
 (27)

with XcB^{\wedge} the point that deforms to x, where the gradient V in (27) is the *material gradient* (with respect to X).

We will consistently write, for **x** & **&**,

n (x)	for the unit normal to Z of	directed outward from
	x€∂B _a ;	
n _a (x)	for the unit normal to S_a (directed outward from
	$XcSB_a$, $X=Y_a(x)$;	
n _p (x)	for the unit normal to S [^] o	directed inward from
	$X \in \partial B_{\beta}, X = Y_{\beta}(x).$	

Then

$$\bar{\mathbf{n}} = \lambda_{\pi} \mathbf{F}_{\pi}^{-\tau} \mathbf{n}_{\pi}, \qquad \lambda_{\pi} = |\mathbf{F}_{\pi}^{-\tau} \mathbf{n}_{\pi}|^{-1}.$$
(2.8)

Further,

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$$P_{\pi}(\mathbf{x}) = 1 - n^{(x)} \mathbb{R} n^{(x)}$$
(2.9)

is the projection of \mathbb{R}^3 onto the tangent plane $n^x)^1$ for S_{π} at $X=Y_{\pi}(\mathbf{x})$,

We denote by

the Jacobian of the deformation; the interfacial field

$$\hat{\mathbf{y}}_{\pi} = \mathbf{J}_{\pi} / \lambda_{\pi} \tag{2.11}$$

is then the surface Jacobian of the mapping that carries S_{π} into Z.

3. INCOHERENCY TENSOR. BURGERS VECTORS

a. The incoherency tensor

Material points $X_a c S_a$ and $X^c S^A$ will be referred to as *compatible* if they deform to the same point **x** ϵ **8**:

$$y \ll x_a$$
) - yW. <3.D

Such points are related by the mapping

$$\mathbf{h}(\mathbf{X}) \ll \mathbf{Y}_{\mathbf{y}}(\mathbf{y}_{\mathbf{a}}(\mathbf{X})) \tag{3.2}$$

from S_a to S^{\wedge} The tangential gradient $V_ah \ll V_s h$ of h maps tangent vectors T to S_a at X into tangent vectors $(V_ah(X))T$ to S^{\wedge} at h(X).

We will refer to

$$\mathbf{H} - \mathbf{F}^{\mathbf{F}} \mathbf{F}, \qquad (3.3)$$

as the *incoherency tensor*. H and V_ah coincide on tangents vectors: for all vectors T tangent to S_a at X,

$$(V_{a}h(X))T * H(x)t, \qquad x \ll y_{a}(X),$$
 (3.4)

or equivalently, using (2.9),

ł

$$\mathbf{V}_{\mathbf{a}}\mathbf{h}(\mathbf{X}) = \mathbf{H}(\mathbf{x})\mathbf{P}_{\mathbf{a}}(\mathbf{x}). \tag{3.5}$$

The incoherency tensor also relates the orientations of the undeformed interfaces, since, by (2.8) and (3.3),

$$\mathbf{n}_a \ll \mathbf{coH}^T \mathbf{n}^{\wedge}, \qquad \mathbf{w} \ll (\mathbf{X}^{\wedge} / \mathbf{X}_a) \ast \mathbf{IH}^T \mathbf{n}^{\wedge} \mathbf{r}^1.$$
 (3.6)

Choose compatible material points X_a and X^A , and let $x^y^X^A$). Further, let dX_n be an "infinitesimal line segment" on S^A at X_n , and let $dx_{tt} \ll F_{ir}(x) dX_{1t}$. If $dx_a \ll dx^A$, then dX_a and dX^A are compatible (coincide when deformed). In this case $dX^A \ll H(x) dX_a$; thus H(x) relates compatible infinitesimal line segments on the undeformed interfaces S_a and S_r . If $dX_p \ll dX_a$ for all compatible infinitesimal line segments, then the deformed lattices are — in some sense — coherent at x; and the same can be said if, for some symmetry transformation Q, $dX^A \ll QdX_a$ for all compatible infinitesimal line segments (Figure 2). This should motivate the following definition: the interface is *infinitesimally coherent* at xc-& if there is a $Q \in Q$ such that $H(X)T^*QT$ for all vectors T tangent to S_a at $X^*Y_a(x)$,

or, more succintly,

$$\mathbf{H}(\mathbf{x})\mathbf{P}_{\mathfrak{H}}(\mathbf{x}) - \mathbf{Q}\mathbf{P}_{\mathbf{J}}\mathbf{x}). \tag{3.7}$$

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Thus infinitesimal coherence at a point x on the deformed interface is the requirement that infinitesimal pieces of the two lattices "fit together" at x. The next proposition is a direct consequence of (3.7).

Proposition 3.1. Given a point X & the following are equivalent:

- (a) The interface is infinitesimally coherent at x.
- (b) There is a Qc9 and a vector a such that

$$\mathbf{H}(\mathbf{x}) = \mathbf{Q} + \mathbf{a} \otimes \mathbf{n}_{\mathbf{a}}(\mathbf{x}). \tag{3.8}$$

(c) There is a Qcg and a vector c such that

$$F_{p}(x)Q - F_{a}(x) * c@n_{a}(x).$$
 (3.9)

Fix the point x and suppress it in what follows. Assume that the interface is infinitesimally coherent at x. Then the vectors a and c are given by

$$\mathbf{a} * \mathbf{H} \mathbf{n}_{\mathbf{a}} - \mathbf{Q} \mathbf{n}_{\mathbf{a}}, \qquad \mathbf{c} = -\mathbf{F}_{\mathbf{p}} \mathbf{a}. \tag{3.10}$$

Further,

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$$K - V$$
 n, • Qn«. (3.11)

To establish (3.11), note first that, by (3.8),

$$detH \ll det(\mathbf{l} + \mathbf{Q}^{\mathrm{T}}\mathbf{a} \otimes \mathbf{n}_{a}) \ll \mathbf{1} + (\mathbf{Q}^{\mathrm{T}}\mathbf{a}) \cdot \mathbf{n}_{a}.$$
(3.12)

On the other hand, (3.6) and (3.8) imply

$$co^{n_a} * Q^{T}n_p + (a < n_p)n_a,$$
 (3.13)

so that $n_a \ll Q^T n_p$; but by (3.12) the minus sign yields $co^{-1}n_{ot} \ll (detH)n_a$, a contradiction, since w and detH are strictly positive. Thus $n_p \ll Qn_a$. Further, this and (3.13) yield

$$(\mathbf{Q}^{\mathrm{T}}\mathbf{a}) \cdot \mathbf{n}_{\mathrm{a}} \ll (\mathbf{X}_{\mathrm{a}}/\mathbf{X}_{\mathrm{p}}) - 1;$$
 (3.14)

since detH- J_a/J_B , (2.11). (3.12), and (3.14) imply J_a-J_B .

b- Burgers vector.³ Burgers set

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Given a curve W in R³, we write

Let Iff be a closed curve in the *deformed body* with Iff a *two-phase loop* in the sense that Iff intersects the interface exactly twice with corresponding undeformed curves

$$W_n \ll Y_n(1ff) \tag{3.16}$$

nontrivial. Here W[^] has orientation induced by Iff (Figure 3). The standard definition of the Burgers vector of Iff, in this setting, yields an expression

$$\int \mathbf{F}^{-1}(\mathbf{x}) d\mathbf{x} * \operatorname{vector} (W_a) \cdot \operatorname{vector} (W_b)$$
(3.17)
Of

that is meaningless, since transformation of the references for phases oc and p by material isometries transforms (3.17) to a vector of the form

$$Qvector(W_a) + \overline{Q}vector(W_s)$$
(3.18)

with Q, $\overline{Q}c9$ » and hence changes (3.17).⁴ Thus rather than a single Burgers vector for Iff there is a *set* b(1ff) consisting of all vectors of the form (3.18). We will refer to bttff) as the *Burgers set* for Iff. What is most important to us is the notion of a "vanishing Burgers vector", which, within our framework, is the assertion that (3.18) vanish for some Q, $\overline{Q}c9$, or equivalently, that OcbClff). Letting X and Z denote the initial and terminal points of W_a, and V[^] the portion of Iff in phase tt, we may use the group structure of 9 ^{to} express the condition OebClff) in the following equivalent forms (for some Qcfc):

³ The concept of a turf act Burger^{*} vector is apparently due to Frank 17 J, who restricts attention to small rotations between phases. The more general situation involving finite deformations is due to Bilby (101, who essentially derives the left side of (3.23) with $Q \gg l$ as an expression for the Burgers vector. See also Brooks 18], Nye 19], Bilby, Buliough. and De Grinberg (111. Christian [12,131, Boliman (14]. Christian and Crocker 115], and Pond [16,171.

⁴Bilby. Buliough, and De Grinberg (111 were apparently the first to notice this indeterminacy of the Burgers vector.

Qvector
$$(W_a) \cdot vector (W_p) \ll 0,$$
 (3.19)

$$h(Z)-h(X) - QIZ-X],$$
 (3.20)

$$JF_{p}^{-1}(x)dx \cdot jQF_{a}^{-1}(x)dx \ll 0.$$
(3.21)

Further, for rc^*a,p , if we let \overline{W}^{\wedge} denote any curve on S_n from the initial point of W_n to its terminal point, then additional conditions equivalent to OcbHff) are (for son Qc9):

$$Qvector(\bar{W}_a) + vector(\bar{W}^{\wedge}) * 0_{\#}$$
(3.22)

$$\frac{J(H(x) - Q)dX \cdot 0.}{W_{\alpha}}$$
(3.23)

4. COHERENT SUBSURFACES

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Let C be a subsurface of Z, and write

$$\mathbf{C}_{\mathbf{n}} = \mathbf{Y}_{\mathbf{.}}(\mathbf{C}) \tag{4.1}$$

for the subsurface of S^{\wedge} that transforms to C. Then C is *infinitesimally coherent* if the interface is anhnitesim^y coherent at each X \in C. A much stronger restriction is the content of the next definition. We say that C is coherent if there is a material isometry f such that

$$X^{\wedge} \ll f(X_a)$$
 whenever $X_a \in C_a$ and $X^{\wedge}eC^{\wedge}$ are compatible (4.2)

(Figure 4). Thus infinitesimal coherence at x is the requirement that infinitesimal segments of the lattices for the two phases fit together at x, while coherency for C is the requirement that the lattices fit together over all of C. Note that (4.2) is equivalent to the assertion that h restricted to C_a is the restriction of a material isometry, so that, for some Qc9»

$$h(Z) - h(X) - QIZ-X$$
 for all X,ZcC_a. (4.3)

In comparing (3.20) and (4.3) it should be remembered that Q in (3.20) depends on X and Z, but Q in (4.3) is *constant*. Note that, for C coherent, not only is the set C_0 obtained by rigidly transporting the set C_a by an isometry f, but, in addition, compatible points of C_a and C[^] are related through I. Note that, for C coherent.

T.

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$$\mathbf{n}_{\mathbf{s}}(\mathbf{x}) = \mathbf{Q}\mathbf{n}_{\mathbf{a}}(\mathbf{x}) \tag{4.4}$$

for all xcC, where Qcfc corresponds to f.

By a two-phase loop for C we mean a two-phase loop that passes twice through C.

Theorem 4.1. Let C be a subsurface of Z.

- (i) C is coherent «+ C is infinitesimally coherent;
- (ii) C is connected and infinitesimally coherent -* C is coherent;
- (iii) C is coherent ** Ocbttff) for any two-phase loop **If** for C;
- (iv) C is connected and Ocbttff) for any two-phase loop Iff for C •• C is coherent.

We now prove this theorem.

(i) Let C be coherent. Differentiating (4.3) with respect to X on C_{a} yields

$$\mathbf{V}_{\mathbf{a}}\mathbf{h}(\mathbf{X}) * \mathbf{Q}\mathbf{P}_{\mathbf{a}}(\mathbf{x}), \tag{4.5}$$

and, by (3.5), the required condition (3.7) for infinitesimal coherence is satisfied. (ii) Let C be connected and infinitesimally coherent. Then, for each XtC_{ω}

$$\mathbf{V}_{\mathbf{a}}\mathbf{h}(\mathbf{X}) \ll \mathbf{Q}(\mathbf{X})\mathbf{P}_{\mathbf{a}}(\mathbf{X}) \tag{4.6}$$

for some Q(X)c9, where, for convenience, we consider P_a as a function of X rather than x. Choose arbitrary points $Z,\overline{Z}cC_a$. Since C_a is connected we can find a smooth curve W in C_a from Z to \overline{Z} . Let X denote the set of all points XcW with Q(X)*Q(Z). Assume, for the purpose of contradiction, that X*W. Then, since X is closed, there is a point $\overline{X}c3X$, $\overline{X}tfdW$, such that Q(\overline{X})*Q(Z). Further, since \overline{X} *dW, there is a sequence X_n -> \overline{X} , X_ncW , such that, for each value of n, Q(X_n)*Q(Z). By (4.6), Q(X)P_a(X) is continuous along W. Thus Q(X_n)P_a(X_n)-*Q(\overline{X})P_a(\overline{X}). But, since 9 is a *finite* group with *orthogonal* elements, and since P_a(X) is continuous, this can happen only if Q(X_n)«Q(\overline{X})«Q(Z) for all sufficiently large n, a contradiction. Therefore X«W and Q(Z)«Q(\overline{Z}); hence Q is constant on C_a. Finally, choosing X,ZcC_a and integrating (d/da)h($\overline{Z}(cx)$) along a smooth path $\overline{Z}(a)cC_a$ with $\overline{Z}(0)*Z$ and $\overline{Z}(1)*X$ yields

$$h(X) - h(Z) \ll [(V_ah(\hat{Z}(a))\hat{Z}'(a)da * QIX-Z], \qquad (4.7)$$

which, by (4.3), yields the coherency of C.

(iii) If C is coherent, then there is a Qcfc such that (4.3) and (hence) (3.20) is satisfied.

(iv) Assume that C is connected and that OcbHff) for any twophase loop Iff for C. Choose X,ZcC_{al} and let $x^*y_a(X)$ and $z^*y_a(Z)$ be the corresponding points on C. Since Z is smooth, it is possible to construct a two-phase loop Iff for C that passes through x and y; hence, by (3.20), there is a symmetry transformation Q(X,Z) such that

 $h(Z) - h(X) \ll Q(X,ZHZ-X).$ (4.8)

This relation must hold for all X,ZcC_a ; thus, since C is connected, an argument similar to that following (4.6) leads to the conclusion that Q(X,Z) is constant. Thus C is coherent.

5. TWO-PHASE MOTIONS

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We now turn our attention to time-dependent situations. A *two-phase motion* is a smooth one-parameter family $y_n(t)$ (ir«oc,p) of two-phase deformations, the time t being the parameter; thus, writing $y^{(X_ft)} = y_{11}(t)(X)$, y_n associates with each time t and each material point X in a closed region $B_n(t)$ a point x^y^tX/t). As before, $Y^{(x_ft)}$ is the (fixed-time) inverse of y_n ,

$$X - Y_n(x,t) * + x - y^X . t),$$
 (5.1)

 $\mathbb{R}n^{*}(B_{lt}(t),t)$ is the region of space occupied by phase TI,

Y,

$$B(t) * S_a(t)uS^{(t)}$$
 (5.2)

is the *deformed body*,

Zit) * 3_a(t)nB,(t) (5.3)

is the *deformed interface*, and

$$\mathbf{S}_{\pi}(\mathbf{t}) = \mathbf{Y}_{\pi}(\mathbf{\hat{s}}(\mathbf{t}), \mathbf{t}) \tag{5.4}$$

is the undeformed phase n interface. We assume that Z(t) evolves

smoothly with t.

We define the *material velocity* at points \mathbf{x} away from the interface through

$$y_{x,t} \ll dy_{x}X/O/dt$$
 (5.5)

with $X \bigoplus_n(t)$ the point that deforms to x, where the derivative is the *material time derivative* (with respect to t holding X fixed). The remaining fields associated with the motion, such as the deformation gradient F(x,t), are defined as before, but now depend on t.

6. INTERFACE VELOCITIES. SLIP

We write V^{\wedge} for the normal velocity of S_n in the direction n^{\wedge} and \overline{V} for the normal velocity of Z in the direction \overline{n} , with V_n and \overline{V} both described spatially.

A vector function z of time that satisfies $z(t)c\pounds(t)$ for all t is called a *trajectory for* Z the normal component of $z^{\#}$ is then the normal velocity ∇ , so that

$$z-(t) * \nabla(z(t),t)\bar{n}(z(t),t) \cdot (z-)_{tan}(t), \qquad (z-)_{tan}(t)-\bar{n}(z(t),t) \ll 0,$$
(6.1)

or more succintly,

z- *
$$\overline{Vn} \cdot (z0_{\tan}, (z^{\#})\tan n * \circ;$$
 (6#2)

if $(z^*)_{tan} \ll 0$, then z is a normal trajectory for %. Normal trajectories satisfy the ordinary differential equation

$$z-(t) \ll \nabla(z(t),t)\overline{n}(z(t)_{f}t); \qquad (6.3)$$

thus (granted sufficient regularity for Z), given an arbitrary time t_0 and an arbitrary point $x_0 \in \&(t_0)$, there is exactly one trajectory z through x_0 at time t_0 , with z(t) defined for all t.

A similar definition applies to the *trajectories* \mathbb{Z}^{\wedge} for S_n . In this case,

$$Z_n^{*}(t) \ll V_{1t}(z_n(t),t)n_{1T}(z_{tl}(t),t) \wedge (Z/)_{Un}(t), \quad (Z_{tt}-)_{tan}(t)-n_n(z_{1t}(t),t) \ll 0,$$

(6.4)

where

$$(t) - y_n(Z_n(t),t)$$
 (6.5)

is the *corresponding trajectory* for Z. As before, we rewrite (6.4) in the abbreviated form

$$Z_{\pi}^{*} = V_{\pi}n_{\pi} + (Z_{\pi}^{*})_{\tan}, \quad (Z_{\pi}^{*})_{u}^{*} \cdot n = 0.$$
 (6.6)

and refer to Z_n as normal if $(Z_{11}^*)_{tan} \ll 0$.

Given an arbitrary time t_0 and an arbitrary point $x_0 \in A(t_0)$, there is exactly one *normal trajectory* Z_n through $XQ^Y CXQ^Q$ at time t_0 . Letting $z_n(t)$ denote the corresponding trajectory (6.5) for Z, we define

$$\langle \mathbf{y}_{\mathbf{w}} \rangle^{\#} (\mathbf{x}_{0} \cdot \mathbf{to} \rangle - \mathbf{V} \wedge \mathbf{o}^{*} \cdot \mathbf{v}^{*}$$

so that the interfacial field $(y^{*})^{*}$ represents the *time derivative of* y^{*} *following the normal trajectories of the undeformed interface* S_{n} . The trajectory z^{*} will generally not be normal, but $\mathbf{\tilde{n}}^{*}(\mathbf{y}_{Tr})^{\circ c} \mathbf{\tilde{V}}$. By the chain rule,

$$(y_w)- \ll (y)_n * V^F^n^;$$
 (6.8)

we therefore have the compatibility relation

$$\mathbf{\bar{n}} \cdot (\mathbf{y}\% + \mathbf{V}_{a}\mathbf{\bar{n}} \cdot \mathbf{F}_{a}\mathbf{n}_{a} \ll \mathbf{\bar{n}} \cdot (\mathbf{y})^{\wedge} \cdot \mathbf{V}^{\wedge}\mathbf{\bar{n}} \cdot \mathbf{F}^{\wedge}, \qquad (6.9)$$

or equivalently, appealing to (2.8),

$$< y V^{fi + x} a^{v} \ll (y^{\#})^{-n} x_{p} v_{p} \ll v.$$
 (6.10)

We write

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$$\mathbf{U}_{\pi} = \mathbf{\overline{V}} - (\mathbf{y}^{*})_{\pi} \cdot \mathbf{\overline{n}} = \lambda_{\pi} \mathbf{V}_{\pi}$$
 (6.11)

for the normal velocity of the deformed interface measured relative to the material of phase tt.

(Possibly nonnormal) trajectories Z_n for S^{\wedge} that satisfy

$$y^{*}(Z_{a}(t).t) \ll y/ZpW.t)$$
 (6.12)

for all t are called *compatible trajectories*, as they correspond to the same trajectory for the deformed interface Z. Differentiating (6.12) we see that, for such trajectories,

$$(y^*)_{\alpha} + F_{\alpha}Z_{\alpha}^* = (y^*)_{\beta} + F_{\beta}Z_{\beta}^*.$$
 (6.13)

Conversely, if (6.13) is satisfied for all time, and if (6.12) is satisfied at some time t_0 , then the trajectories Z_n are compatible.

The interfacial field

* -
$$(y_{a})^{\circ}$$
 - $(y_{a})^{\circ}$ (6.14)

represents the *interfacial slip*; by (6.8),

* - $(y\% \bullet V >_p - \langle y \rangle_a - v_a F_a n_a - ly) + rvmi.$ (6.15)

Further, (6.6), (6.13), and (6.15) yield the alternative expression

» - - W > t a n + F
$$(Z_a)_{tan}$$
 - lF(2')_{tan}l (6.16)

for compatible trajectories Z_a and Z^A . If there is no slip, then, by (3.3),

$$(Z,')_{tan} - H(Z_a^*)_{tan}$$
 (6.17)

and we have the following result.

Proposition 6.1. Assume there is no slip. Then, given any choice of compatible trajectories Z_a and Z_p , if Z_a is normal, then so also is Z_p .

7. PRODUCTION OF REFERENTIAL VOLUME

The field

$$\mathbf{W}^{\mathbf{A}} - \mathbf{V}^{\mathbf{A}} - \mathbf{I} \mathbf{V} \mathbf{J} . \tag{7.1}$$

represents the flow of referential volume across the phase TT interface in the direction $-\bar{n}$, per unit deformed area, and characterizes the production of lattice points at the interface.

Given a control volume (fixed region) 3£ in the deformed body, if m denotes the unit outward normal to 36¢, then

$$L(\mathfrak{R}) = (d/dt) \{ JJ(x,t) - {}^{1}dv(x) \} * JJ(x,t) - V(x,t) - m(x,t) da(x)$$
(7.2)
$$\mathfrak{R} \qquad \mathfrak{R}$$

represents the rate at which referential volume is produced in !fc. A production of referential volume indicates a (positive or negative) production of lattice points (Figure 5) and, since atoms are conserved, this, in turn, signals a production of defects.

Proposition 7.1.

(a) L(tfc)*O if 3£ lies solely in one phase.
(b) Let & shrink to an arbitrary subset Q of Z. Then

$$L(\mathfrak{R}) - J[U/J]da \ll -JIWlda, \qquad (7.3)$$

$$Q \qquad Q$$

12

so that

$$IW] \ll -[U/J]$$
 (7.4)

measures the *interfacial volume-production rate*, *per unit deformed area*.

To establish (a) assume that **3**R, lies in one phase. Let d_t denote partial differentiation with respect to t holding x fixed, and let grad and div denote the gradient and divergence with respect to x holding t fixed. Then differentiating the first term in (7.2) under the integral, applying the divergence theorem to the second, and combining the two integrals leads to an integral over R with integrand

$$-J^{2}_{t}J \cdot J^{divy} - J^{2}_{y} \cdot grad J;$$
 (7.5)

but⁵ vT*Jdivy'*c)_tJ+ $y^{\#}$ «grad J; hence (7.5) vanishes.

On the other hand, letting & contain and shrink to an arbitrary subset Q of i, we find that

which, by (7.1) and (6.11), yields (7.3).

8. WHEN IS AN INTERFACE COHERENT?

We will refer to the interface Z as coherent for all time if $\pounds(t)$ is coherent at each t_f and if the corresponding material isometry f for $\%\{t\}$ is independent of t. Granted this, we may change reference configuration for phase a so that the material isometry f is the identity. Therefore, without loss in generality, we may take f to be the identity in the definition above, and this we shall do. Also, for consistency, the assertion $^{-8}(0)$ is coherent'' will have associated with it the requirement the material $^{5}Cf.$ t.g. 1221. p. 62. «qt. (4); p. 72. «qt. (2). isometry corresponding to Z(0) be the identity. A direct consequence of this definition is

Proposition 8.1. Let Z be coherent for all time. Then: (i) The undeformed interfaces coincide

$$\mathbf{S}_{\mathbf{a}}(\mathbf{t}) \ll \mathbf{S}^{\mathbf{h}}\mathbf{t}) \ll S\mathbf{i}\mathbf{t}. \tag{8.1}$$

(ii) The motion is continuous across the interface in the sense that

 $y_{(X,t)} * y_{(X,t)}$ for all XcS(t). (8.2)

(iii) The normals and normal velocities coincide: for all $xc \mathfrak{t}(t)$,

 $n_a(x,t) \ll n_a(x,t) \ll n(x,t), \quad V_a(x,t) \ll V^{(x,t)} \ll V(x,t).$ (8.3)

A more important result is

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Theorem 8.1. Suppose that the initial interface Z(0) is coherent. Then the interface Z is coherent for all time if and only if, at each time:

(a) the interface is infinitesimally coherent;

(b) the interfacial volume-production rate vanishes identically;

(c) the interfacial slip vanishes identically.

To establish this result assume first that the interface is coherent. Theorem 4.1(i) then implies (a). Next, differentiating (8.2) following an arbitrary normal trajectory of S(t) yields, by (6.14), conclusion (c). Finally, (3.11)! and (8.3) imply that $W_a \ll W_{*}$, which is (b).

Conversely, consider an initially coherent interface consistent with (a)-(c) for all time. By (a), (3.11)! is satisfied. Thus (b), (7.1), and (7.4) imply that, for all $x \in \mathcal{S}(t)$,

$$V_{a}(x,t) * V_{a}(x,t).$$
 (8.4)

Assume first that Zit) is connected. By (a) and Theorem 4.1(ii), Zit) is coherent at each t; thus the function h defined by (3.2) at each t is the restriction to $Z\{t\}$ of a material isometry

$$\mathbf{h}(\mathbf{X},\mathbf{t}) \ll \mathbf{Q}\mathbf{X} \ast \mathbf{q}(\mathbf{t}), \tag{8.5}$$

where Q is independent of t, since 9 is discrete and h(X,t) continuous

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in t; in fact, the initial coherence of the interface and our agreement in the first paragraph of the section yields

$$Q * 1. q(0) * 0,$$
 (8.6)

so that, by (4.4),

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$$n^{(x,t)} * n_{a}(x,t) *:n(x,t).$$
 (87)

Next, let Z_a and 2^h be compatible trajectories; then, by definition, $Z_a(t)$ and Zp(t) coincide in the deformed configuration and

$$Z^{(t)} \ll Z_{a}(t) \cdot q(t).$$
 (8.8)

Assume further, that Z_a is normal (such trajectories always exist), so that, by (a), (c), and Proposition 6.1, 2[^] is also normal. We may therefore differentiate (8.8) and use (8.4) and (8.7) to conclude that $q^{\#}(t) \ll 0$ for all t. But the initial coherence of the interface yields $q(0) \ll 0$; hence $q(t) \approx 0$ for all t, and h(X,t) is the identity on $S_a(t)$ at each t. Thus Z is coherent.

If Z is not connected, then the foregoing argument applied to each connected component of Z again renders h(X,t) the identity on $S_a(t)$, which completes the proof.

One can ask whether Theorem 8.1 remains valid if the no-slip condition (c) is omitted. To answer this let $^{(0)}$ be coherent, and assume that the interface is infinitesimally coherent and that the interfacial volumeproduction rate vanishes identically. Then the results (8.4)-(8.8) remain valid, so that, by (8.4), (8.7), and (8.8),

$$q-(t)-n(x,t) * 0.$$
 (8.9)

Let us agree to call the interface cylindrical at t if there is a unit vector m(t), its axis, such that $xn(t) \ll n(x,t) \approx 0$ for all x. Then (8.9) is satisfied at a planar interface provided $q^{\ast}(t)$ is tangent to the interface, and at a cylindrical interface if $q^{\ast}(t)$ is parallel to the axis of the cylinder. In either case, we may use (6.16), (8.5), and (8.6) to conclude that the slip V is given by

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$$\mathbf{F}^{\mathbf{q}}$$
 - $\mathbf{F}_{\mathbf{a}}\mathbf{q}$ (8.10)

On the other hand, if, at each t, Zit) is neither planar nor cylindrical, then Z is coherent for all time.

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APPENDIX ON LATTICES

a. Lattices. Invariant transformations

We use the term lattice to mean Bravais lattice. To describe these we write

 V^3 * the set of all linearly independent triples (g_1,g_2,B_3) with $Bj^{cR3}>$

and given $(g_1,g_2 \gg g3) \in V^3$, we say that xclR³ is an *integer combination of* the g's if x-Mjgj with $|i_{1f}|_{i_2}$, $anc_* \wedge 3$ integers (summation convention, from 1 to 3, is implied for the subscripts j and k).

A set \pounds of points of \mathbb{R}^3 is a *lattice* if \pounds is *generated by* a triple $(gi^*g2'83) \in \mathbb{R}^3 \mathbb{R}^n$ he sense that \pounds is the set of all integer combinations of the g's. The gj are then called *lattice vectors* for \pounds . Let

7 t * the set of all 3*3 matices M whose determinant is ± 1 and whose entries Mj_k are integers;

if

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 $\overline{g}j - M_{jk}g_k$, Mctni,

then $(\bar{g}_{\nu}62,63)$ also generates £, and conversely (cf., e.g., Ericksen 118]).

Let \pounds be a lattice generated by $(g_1,g_2 \gg g3)$ - Given an invertible tensor F, we write

F£ * the lattice generated by (Fg^Fg^Fgj).

a definition that is independent of the choice of lattice vectors $(g_1,g_2 \gg g3^{\wedge})$ Note that

 $\pounds \bullet \ll F \pounds \quad ++ \quad T \text{-i} f \ll \pounds. \tag{Al}$

By an *invariant transformation of* \pounds we mean an invertible tensor G such that $G\pounds \ll \pounds$, or equivalently,

$$Ggj * M_{ik}g_k \quad \text{for some } MctJIL \tag{A2}$$

The *point group* $P(\pounds)$ of \pounds is then the set of all *orthogonal* invariant transformations of \pounds • Let F and G be invertible tensors. Then

G is an invariant transformation of \pounds «+ FGF¹¹ is an invariant transformation of F \pounds . (A3)

a result which follows from (Al) and the identity $FGF''^{1}(F\pounds)*F\pounds$, which is valid if either G is an invariant transformation of \pounds or FGF''^{1} is an invariant transformation of $F\pounds$.

Given any set T of tensors, we write T^* for the set of all tensors in T with strictly positive determinant, so that

$$P(\pounds)^+$$
 * the set of all *rotations* (proper orthogonal tensors) in the point group $P(\pounds)$.

A direct consequence of (A3) is that, for any orthogonal tensor Q, $P(Q\pounds)-QP(\pounds)Q^{T}$ and $P(Q\pounds)^{*} \ll QP(\pounds)^{+}Q$ so that if F*RU is the *polar* decomposition of F into an orthogonal tensor Q and a positive definite, symmetric tensor U, then

$$P(F \mathfrak{L}) + \ll QP(U \mathfrak{L}) + Q \setminus (A4)$$

and similarly for the point group.

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b. Relation of lattice theory to continuum theory. Admissibility sets for deformation gradients from a configuration with lattice \pounds

Lattice theory is related to continuum theory through the Cauchy-Born rule (cf. Ericksen 1191) in which a reference configuration of a body is a fixed region B of \mathbb{R}^5 together with a lattice $\pounds(X)$ attached to each point XcB; $\pounds(X)$ defines the microstructure of the body at X. Here we restrict attention to homogeneous bodies, for which there is a choice of reference configuration, called *uniform*, such that the *reference lattice* \pounds is independent of X. A deformation y of B then associates with each point $x^*y(X)$ in the deformed region S the lattice $F(X)\pounds$.

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We here limit our discussion to deformations for which — granted an appropriate choice of uniform reference configuration with lattice \pounds — the deformation gradient F lies in an open srt 7 that excludes excessively large shears, but otherwise allows for finite deformations. In particular, we exclude from 7 those invariant transformations of \pounds that do not lie in the point group P(\pounds)+. What seems to us to be a physically reasonable set of properties for 7 are (71)-(74) stated below; there and in what follows

 Lin^+ « the set of all tensors F with detF > 0,

and we write "F is *admissible*" to signify that Fc7.

(71) 7 is an open subset of Lin*.

(72) 1 is admissible,

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(73) QF is admissible for all admissible F and all rotations Q.

(74) Let F be admissible. Then $GcP(\pounds)^*$ if and only if FG is admissible and FGF''¹ is an invariant transformation of F \pounds .

A set 7 with properties (71)-(74) will be referred to as an *admissibility* set for deformations from a reference configuration with lattice \pounds .

In the reference configuration the deformation gradient F is the identity; hence the restriction (72). (73) is the requirement that if the deformed body is rigidly rotated, the resulting deformation gradient remains in 7. (74) requires more explanation. The reference configuration has \pounds as its lattice. Taking F=l in (74) yields the conclusion:

(75) An admissible G is an invariant transformation of \pounds if and only if $G \in \mathcal{P}(\mathcal{L})^+$.

Thus the only admissible invariant transformations of the reference lattice are rotations in its point group so that, in some sense, the reference configuration is undistorted with cspect to 7. But (74) asserts more. If we deform the body B with (constant) deformation gradient F, then F£ is the lattice in the deformed body S, and (74), a consistency condition, asserts that the invariant transformations of F£ with FG admissible are exactly those induced in the natural manner from rotations in the point group P(f).

Another consequence of (72)-(74) is:

(76) Let F be admissible and let G be an invariant transformation of £. Then G is admissible if and only if FG is admissible.

In fact, granted (73),

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$$(74) <* (75), (76).$$
 (A5)

The implication (74)-+(75) has already been established. The remainder of (A5) follows upon using (A3). (72M74) also imply

(77) If U is admissible, symmetric, and positive definite, then $P(U \mathfrak{L})^+ C P(\mathfrak{L})^+$; in fact,

$$P(U \pounds)^+$$
 * the set of all QcPte)* such that $QUQ^T \ll U$. (A6)

This result with (A4) yields the conclusion that if $F \ll RU$ is the polar decomposition of an admissible F, then $P(F \pounds) \approx CRP(\pounds) R^{T}$.

For any lattice £', let

*y($\mathbf{\mathfrak{k}}^{\$}$) * the group of invariant transformations of $\mathbf{\mathfrak{k}}$

To verify (77), choose $RcP(U\pounds)^*$. Then $Rc^{\#}y(U\pounds)$, so that, by (A3),

U-iRUcVO. Hence RU«UF with F $\in^{(\pounds)}$. By (73), RUc7; hence UFc7 and (76) yields Fc7. Thus Fc7n^fy(£), so that, by (75), F*QcP(£)⁺- Therefore RU=Q(Q^TUQ), and by the uniqueness of the polar decomposition of a tensor, R«Q and U*Q^TUQ. These conclusions yield the validity of (77).

The following result, which we shall prove in Subsection d, is a direct corollary of a theorem of Ericksen and Pitteri.

Existence theorem for admissibility sets. Given any lattice \pounds , there exists an admissibility set 7 for deformations from a reference configuration with lattice \pounds .

c. Two-phase systems

Our discussion in the body of the paper is based on a single reference lattice \pounds in conjunction with symmetry transformations of \pounds that are rotations. We now use the theory developed in this Appendix to justify these suppositions.

Consider a two-phase system with phases a and p. Choose fixed uniform reference configurations for a and p with corresponding lattices \pounds_a and \pounds^{\wedge} . Let 7_a and 7^{\wedge} denote admissibility sets for a and p for deformations from their respective reference configurations. At this point it

is most convenient to view the admissibility sets T_a and Ψ_p as unrelated; that is, as lying in unrelated copies of Lin^{*}.

The phases may be related by choosing a tensor U such that

$$f_{a}$$
, « U f_{a} . (A7)

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What is important, we assume that there is a choice of U such that $U \notin 7_a$; granted this we may, modulo a rigid rotation of the reference configuration for oc, choose U to be symmetric and positive definite. By (77), a consequence of this assumption is that the point groups for \pounds_a and $\pounds p$ satisfy

$$\mathbf{P}(\mathbf{\pounds}^{\wedge})\mathbf{c}\mathbf{P}(\mathbf{\pounds}_{a}); \tag{A8}$$

thus a represents a *parent phase*, p a *product phase*.

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Consider the set S_{ap} of all a-admissible transformations of \mathfrak{L}_a into $\mathfrak{L}_{\mathfrak{L}}$:

 J_a^* the set of all Vc?_a such that $\pounds^* V \pounds_a$. (A9)

Choose $Vc3_{aB}$. Then, by (A9), $V\pounds_a *U\pounds_a$, so that $6*V''^1U$ is an invariant transformation of \pounds_a . Trivially, U«VG with both U and V in 7_a ; we may therefore conclude from (76) that $G \notin 7_a$, so that, by (75), G and hence G'' belongs to $P(\pounds_a)^+$. Thus every $Vc \$_a^{A}$ may be written in the form V*UQ, $QcP(\pounds_a)^+$. Since, trivially, the converse is also true, S_{ap} is the set of all tensors UQ, $QcP(\pounds_a)^+$:

$$^{S} U P (C / .$$
 (A10)

Note that, using the right coset decomposition of $P(\pounds_a)^*$ with respect to $P(\pounds_p)^*$, we can also write J_{ap} as the set of all tensors of the form Q^UQ_a with $Q_a \bigoplus (\pounds_a)^+_f Q^A \bigoplus (\pounds_s)^*$; that is, J_a , $\ll P(t/UP(\pounds_a)^+)$.

The theory developed in the body of the paper is easily formulated within the current framework involving "unrelated" references for the two phases. In particular, the discussion of two-phase deformations would now carry the restrictions $F_a \in 7_a$ and $T_p \in 7_p$ on the deformation gradients but would otherwise remain essentially unchanged. (Here we use the * to differentiate the current theory from that discussed in the body of the paper.) The definition of infinitesimal coherency at x would now be the requirement that the incoherency tensor $\hat{H} \ll \hat{F}^{\wedge "} \hat{F}_{ot}$ satisfy

$$fi(x)P_a(x) = GP_a(x)$$
 for some GcJ_{ap} , (All)

and similar changes apply to the material on Burgers vectors.

To convert this theory to the theory discussed in the body of the paper, we change reference configurations for p so that its reference lattice coincides with that of a. We accomplish this by a change in reference configuration via the tensor U; precisely, we change reference configurations via the map $X \ll U^{-1} \hat{X}_f$ so that the class of admissible deformation gradients is 7_a for phase a and $7_p U$ for phase p. Then in terms of the deformation gradients $F_a \ll \hat{F}_a$ and $F \wedge \hat{T} A J$ relative to the common reference with lattice $C^* \pounds_a$, $H^* F^{-1} F_{ot} \ll U''^{-1} \hat{F}_{oc} \ll U''^{-1} \hat{H}$, and, bearing in mind (A10), (All) becomes

$$H(x)P_a(x) * QP_a(x)$$
 for some $QcP(\mathfrak{t}_a)^+$. (A12)

Thus the definition of coherency used in the body of the text — in which the group 9 °f symmetry transformations is a finite subgroup of the proper orthogonal group — follows naturally within the theory discussed in this appendix, with \$ the point group of the parent phase.

d. Proof of the existence theorem for admissibility sets 7. The Ericksen-Pitteri theorem

We now show that there is always an open set 7 with properties (71)-(74) for any choice of reference lattice \pounds . To accomplish this we use a theorem conjectured by Ericksen [18,19,20] and proved by Pitteri I21].⁶ It is convenient to sometimes write (fj) as shorthand for triples $(f_v i_{2s} i_z) \in V^z$. Let TlcV³, let Q be a tensor, and let NU3H; then QII is

 $(f_{\nu}\iota_{2s}\iota_{z}) \in V^{2}$. Let Trev², let Q be a tensor, and let NU3H; then QII is the set of all triples (Qfj) with (fj)c7l; while MJI is the set of all triples $(M_{jk}f_{k})$ with (fj) \in 3ri.

We assume for the remainder of the section that a lattice \pounds with lattice vectors $(g_1, 8_2 * g_3)$ is prescribed.

Ericksen-Pitteri Theorem. There is an open set $71cV^3$ with the following properties:

($\mathfrak{N}1$) (g_1, g_2, g_3) $\in \mathfrak{N}$;

(712) QTU3II for &U orthogonal tensors Q;

(713) for each McW, MTU31 or MJln3l«0;

^{*}Relattd ideas appear also in the work of Schwarzenberger (23] and Parry (24,25].

(714) if M7W71, then

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$$Qgj * M_{ik}g_k$$
 for some $QcP(C)$. (A13)

A dear, concise proof of this theorem is given by Ball and James 126]. We now convert this result to one appropriate to deformation gradients by defining an open neighborhood 7 of lcLin* as follows:

7 * the set of all FcLin* such that (Fg^Fgj.Fgj) lies in 71. (A14)

Then 7 defined by (A14) satisfies (72), (73), (75), and (76); and hence (72)-(74). (72) and (73) follow from (711) and (712). The following result is helpful in proving (75) and (76):

The implication MTU71 -* FGc7 follows from (A2) multiplied by F and the hypothesis Fc7. Conversely, assume that FGc7. Then, since the triples (FGgj) and (Fgj) lie in 71, we may conclude from (A2) that MTln7l*0. Thus (713) yields MJW31.

To prove (76), let Fc7, let Gc'ytC)*, and choose McTII consistent with (A2). Note that (A15) with $F \ll I$ yields the conclusion Gc7 ++ M7I*7I, and this and (A15) for arbitrary F yield Gc7 **«*** FGc7.

To establish (75), let $Gc^{\{\}|(JI)n7$ and choose MctFR consistent with (A2). Then (A15) yields MTU71, so that (A2) and (A13) yield $G \in P(\pounds)+$. Thus 7 satisfies (72)-(74). ;

The conditions (72)-(75) are, in a certain sense, equivalent to (711)-(714) with (712) and (714) restricted to rotations, but a proof is beyond the scope of this paper.

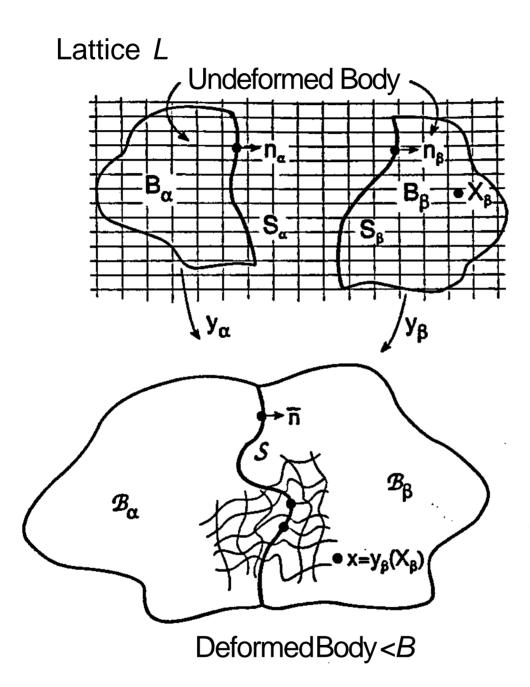
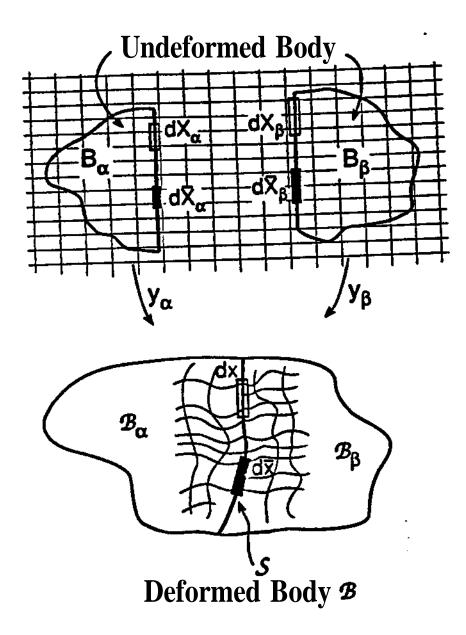


Figure 1. The lattice, the undeformed phase regions, and the deformed body. Note the possibility of dislocations along the interface Z.

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; Figure 2. dX_a and dX^A are compatible infinitesimal line segments at X_a [^ . and X^ that deform to dx, and similarly for dX_a , dX^A_f and $d\bar{x}$. The interface is *not* infinitesimally coherent at x and \bar{x} because of dislocations.

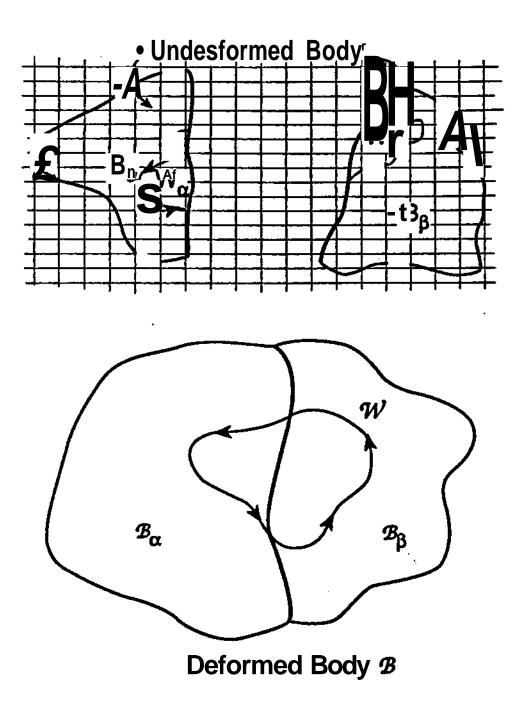


Figure 3. A two-phase loop Iff. W_a and W, are the corresponding undeformed curves.

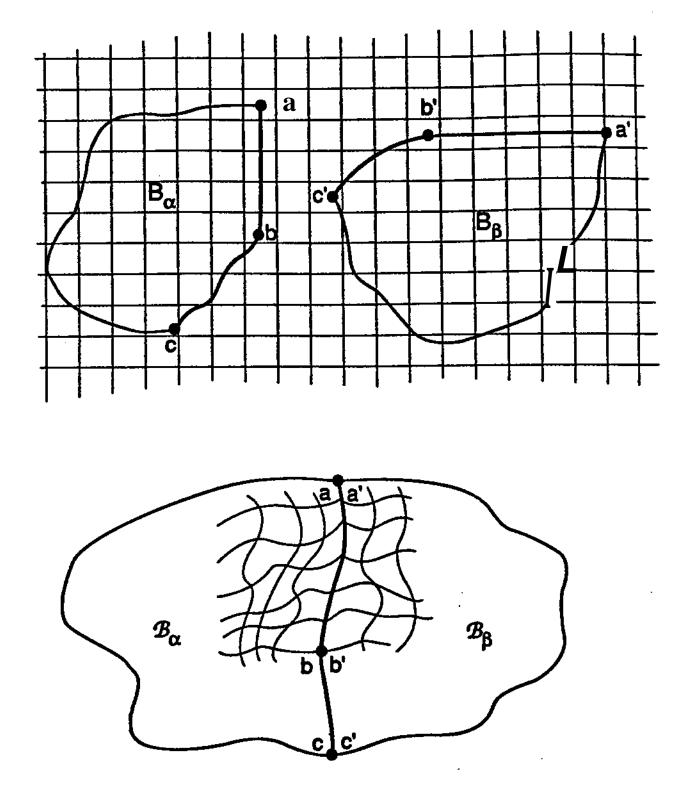


Figure 4. The portion C of the interface from aa* to bb* is coherent. The underlying material isometry is equivalent to a rotation of B clockwise by 90* followed by a suitable translation.

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B_b(t) B_β(t+∆t) Undeformed Body at Time t Undeformed Body at t+At ⊕⊕⊕⊕ ၜၜၜၜ ₲₽₽₽₽₽₽ $B_{\alpha}(t+\Delta t)$ 41 B_c(t)

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