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Phase transitions with interfacial energy: interface null lagrangians, polyconvexity, and existence

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Abstract For interfacial interactions of "separable type" the existence is proved of stable multiphase equilibrium states minimizing the total energy which includes a sharp interface contribution along interfaces separating the phases. The second gradients of deformation do not occur; the theory is based on interfacial null lagrangians as determined in [11–12]. The interfacial interaction is always of separable type if the number of phases does not exceed 3; for the number of phases ≥ 4, the separable nature of the interface interaction is an assumption.

1 The interfacial energies

We consider a body that can exist in states consisting of r inhomogeneous solid phases indexed by $\alpha = 1, \dots, r$. We identify the body with the reference configuration represented by a bounded open set $\Omega \subset \mathbb{R}^3$ with lipschitzian boundary. The states are pairs $(\mathbf{y}, \mathscr{P})$ where $\mathbf{y} : \Omega \to \mathbb{R}^n$ is a deformation function and $\mathscr{P} = (E_1, \dots, E_r)$ is a partition of Ω into subsets E_α of Ω where E_α is the region occupied by phase α. That one or several of the sets E_α is empty is not excluded. The total energy $\mathsf{E}(\mathbf{y}, \mathscr{P})$ of the state $(\mathbf{y}, \mathscr{P})$ is given by

$$\mathsf{E}(\mathbf{y}, \mathscr{P}) = \mathsf{E}_{\mathrm{b}}(\mathbf{y}, \mathscr{P}) + \mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathscr{P}) \tag{1.1}$$

where $\mathsf{E}_{\mathrm{b}}(\mathbf{y}, \mathscr{P})$ and $\mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathscr{P})$ are the bulk and interfacial energies defined as follows. The bulk energy is

$$\mathsf{E}_{\mathrm{b}}(\mathbf{y}, \mathscr{P}) = \sum_{\alpha=1}^{r} \int_{E_\alpha} \hat{f}_\alpha(\nabla \mathbf{y})\, d\mathscr{L}^3 \tag{1.2}$$

where $\hat{f}_\alpha : \mathrm{Lin}_+ \to \mathbb{R}$ is the bulk free energy density of phase α expressed as a function of the deformation gradient

$$\mathbf{F} = \nabla \mathbf{y}.$$

Throughout, Lin denotes the set of all second order tensors in $\mathbb{R}^3$, interpreted as linear transformations from $\mathbb{R}^3$ to $\mathbb{R}^3$, Lin_+ is the set of all second order tensors with positive determinant, and $\mathcal{L}^3$ denotes the Lebesgue measure in $\mathbb{R}^3$. The interfacial energy is given by

$$\mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathcal{P}) = \sum_{1 \le \mathfrak{a} < \mathfrak{b} \le r} \int_{B_{\mathfrak{a},\mathfrak{b}}} \hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}(\mathbb{\nabla}\, \mathbf{y}, \mathbb{m}_{\mathfrak{a},\mathfrak{b}})\, d\mathcal{H}^2. \tag{1.3}$$

Here $\mathcal{H}^2$ is the 2 dimensional Hausdorff measure, $\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}} : \mathrm{G} \to \mathbb{R}$ are the densities of the interfacial energy between the phases $\mathfrak{a}$ and $\mathfrak{b}$, defined on the set G of all pairs $(\mathbb{F}, \mathbb{m}) \in \mathrm{Lin} \times \mathrm{S}^2$ (where S^2 is the unit sphere in $\mathbb{R}^3$) satisfying $\mathbb{F}\mathbb{m} = \mathbf{0}$,

$$B_{\mathfrak{a},\mathfrak{b}} := \mathrm{bd}_* E_{\mathfrak{a}} \cap \mathrm{bd}_* E_{\mathfrak{b}}$$

is the common part of the measure–theoretic boundaries $\mathrm{bd}_* E_{\mathfrak{a}}$ and $\mathrm{bd}_* E_{\mathfrak{b}}$ of phases $\mathfrak{a}$ and $\mathfrak{b}$, $\mathbb{m}_{\mathfrak{a},\mathfrak{b}}$ the measure theoretic normal pointing from $E_{\mathfrak{a}}$ to $E_{\mathfrak{b}}$,

$$\mathbb{F} = \mathbb{\nabla}\, \mathbf{y}$$

is the surface deformation gradient [8, 7, 11–12] with $\mathbb{\nabla}$ the surface gradient [11–12], defined on the union of boundaries

$$\bigcup_{1 \le \mathfrak{a} < \mathfrak{b} \le r} B_{\mathfrak{a},\mathfrak{b}}$$

and satisfying the constraint

$$\mathbb{F}\mathbb{m}_{\mathfrak{a},\mathfrak{b}} = \mathbf{0} \quad \text{on} \quad B_{\mathfrak{a},\mathfrak{b}}$$

as a consequence of the definition of the surface gradient.

The equilibrium states correspond to minimum energy among all states satisfying the boundary conditions. The present paper considers interface interactions of "separable type" as defined below and formulates hypotheses which give the existence of states of minimum energy. For states of at most 3 phases each interface interaction is of separable type and the result extends that of [11–12] where the energy minimizers are proved in the class of 2 phase states. Apart from the separable nature of the interface interaction, the constitutive theory is identical with that of [11–12]; in particular the interfacial stress and Eshelby tensors are derived from the interfacial energy by the same formulas.

Appropriate convexity of the response functions $\hat{f}_{\mathfrak{a}}$ and $\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}$ is needed to prove the minimizers of energy.

The bulk response $\hat{f}_{\mathfrak{a}}$, $\mathfrak{a} = 1, \dots, r$, of the individual phases $\mathfrak{a}$ is assumed to be stable in the sense that $\hat{f}_{\mathfrak{a}}$ is a polyconvex function [2]; hence

$$\hat{f}_{\mathfrak{a}}(\mathbf{F}) = \Phi_{\mathfrak{a}}(\mathbf{F}, \mathrm{cof}\, \mathbf{F}, \det \mathbf{F}) \tag{1.4}$$

for all $\mathbf{F} \in \mathrm{Lin}$ where $\Phi_{\mathfrak{a}} : \mathrm{W} \to \mathbb{R} \cup \{\infty\}$ is a convex function on $\mathrm{W} = \mathrm{Lin} \times \mathrm{Lin} \times \mathbb{R}$. We note that the polyconvexity assumption of $\hat{f}_{\mathfrak{a}}$ is consistent with the existence of r wells (one for each phase) of the minimum energy $\hat{f} : \mathrm{Lin}_+ \to \mathbb{R}$ defined by

$$\hat{f}(\mathbf{F}) = \min \{ \hat{f}_{\mathfrak{a}}(\mathbf{F}) : \mathfrak{a} = 1, \dots, r \},$$

$\mathbf{F} \in \mathrm{Lin}_+$.

The interface free energies $\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}$, $1 \le \mathfrak{a} < \mathfrak{b} \le r$, are assumed to satisfy

$$\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}(\mathbb{F}, \mathbb{m}) = \hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}(\mathbb{F}, -\mathbb{m})$$

for each $(\mathbb{F}, \mathbb{m}) \in \mathrm{G}$; the separable nature of the interface interaction is the assumption that

$$\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}} = \hat{\mathbb{g}}_{\mathfrak{a}} + \hat{\mathbb{g}}_{\mathfrak{b}} \tag{1.5}$$

if $1 \le \mathfrak{b} < \mathfrak{a} \le r$ for some functions $\hat{\mathbb{g}}_{\mathfrak{a}} : \mathrm{G} \to \mathrm{R}$, $\mathfrak{a} = 1, \ldots, r$. We note that the functions $\hat{\mathbb{g}}_{\mathfrak{a}}$ automatically exist if $r \le 3$: one can put $\hat{\mathbb{g}}_1 = \hat{\mathbb{f}}_{1,2}$, $\hat{\mathbb{g}}_2 = 0$ if $r = 2$ and if $r = 3$ then $\hat{\mathbb{g}}_{\mathfrak{a}}$ are unique and given by

$$\hat{\mathbb{g}}_{\mathfrak{a}} = \tfrac{1}{2}(\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}} + \hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{c}} - \hat{\mathbb{f}}_{\mathfrak{b},\mathfrak{c}})$$

for each $\mathfrak{a} \in \{1, 2, 3\}$ where $\mathfrak{b}, \mathfrak{c} \in \{1, 2, 3\} \sim \{\mathfrak{a}\}$, $\mathfrak{b} \ne \mathfrak{c}$ and we have set $\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}} = \hat{\mathbb{f}}_{\mathfrak{b},\mathfrak{a}}$ if $1 \le \mathfrak{b} < \mathfrak{a} \le 3$.

Returning to the case of a general r, we make the basic convexity assumption about the interface response by requiring that the functions $\hat{\mathbb{g}}_{\mathfrak{a}}$ are interface polyconvex [11] for $\mathfrak{a} = 1, \ldots, r$ in the sense that

$$\hat{\mathbb{g}}_{\mathfrak{a}}(\mathbb{F}, \mathbb{m}) = \Psi_{\mathfrak{a}}(\mathbb{m}, \mathbb{F} \times \mathbb{m}, \operatorname{cof} \mathbb{F}\mathbb{m}) \tag{1.6}$$

where $\Psi_{\mathfrak{a}}$ is a positively 1 homogeneous convex nonnegative function and $\mathbb{F} \times \mathbb{m}$ is a second order tensor defined by $(\mathbb{F} \times \mathbb{m})\mathbf{a} = \mathbb{F}(\mathbb{m} \times \mathbf{a})$ for each $\mathbf{a} \in \mathrm{R}^3$.

For the existence theory, states are pairs $(\mathbf{y}, \mathcal{P})$ as before where $\mathbf{y}$ satisfies the requirements necessary to apply the existence theorems based on bulk polyconvexity and such that the expressions $\mathbb{F} \times \mathbb{m}$ and $\operatorname{cof} \mathbb{F}\mathbb{m}$ exist in a weak sense. See Definition 3.1 below; note that every pair $(\mathbf{y}, \mathcal{P})$ where $\mathbf{y}$ is lipschitzian and $\mathcal{P}$ a partition into sets of finite perimeter is a state. For this generalized notion of states and under the hypotheses outlined above one can define the total energy which is an extension of (1.1), (1.2) and (1.3). Assuming appropriate coercivity of $\hat{f}_{\mathfrak{a}}$ and $\hat{\mathbb{g}}_{\mathfrak{a}}$ and imposing the Dirichlet boundary conditions, we prove the existence of global minimizers of energy.

The existence of minimizers of energy is in a sharp contrast with the theory in which the interface energy is neglected: in the latter theory the minimizers generally do not exist. As is well known, in the sequence of states approaching the infimum energy the phases form a mixture which is finer and finer [3–4] with more and more complicated interface. In the present approach the interfacial energy penalizes the formation of the interfaces and thus induces limited fineness of the microstructure.

The framework discussed above assumes a separate bulk energy for each of the phases. Moreover, the regions $E_{\mathfrak{a}}$ are treated as unknowns independent of $\mathbf{y}$. This differs from an alternative view in which all the phases are described at once by a single stored energy and the only unknown is the deformation $\mathbf{y}$. In the later theory, one can, in principle, distinguish the phases constitutively and spatially. On the constitutive level, individual phases correspond to various subregions of the space of all deformation gradients. Spatially, phases are regions separated by interfaces defined as sets of material points of the jump of the deformation gradient. The coercivity of the model requires the dependence of the bulk energies on the second deformation gradient

$$\nabla \mathbf{F} = \nabla^2 \mathbf{y}$$

and the solution is to be sought in the space of deformations $\mathbf{y}$ with bounded hessian. The reader is referred to [5] for a consistent model of this type. The interface part of the constitutive theory of the present model and that of [5] are rather disjoint.

2 Interface quasi– and poly–convexity and interface null lagrangians

We start the detailed exposition with a discussion of the convexity properties of the interface energy functions $\hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}$ and $\hat{\mathbb{g}}_{\mathfrak{a}}$ occurring in (1.5). The basic notions are the interface null lagrangians and interface polyconvex functions to be introduced below; these, in turn, are based on interface quasiconvexity. The last appears to be the right convexity notion for the interfacial energies $\hat{\mathbb{f}} := \hat{\mathbb{f}}_{\mathfrak{a},\mathfrak{b}}$.

Definition 2.1. A continuous function $\hat{\mathbb{f}} : \mathrm{G} \to \mathrm{R} \cup \{\infty\}$ is said to be interface quasiconvex if

$$\int_{\mathcal{S}} \hat{\mathbb{f}}(\nabla \mathbb{y}, \mathbb{m})\, d\mathcal{H}^2 \geq \mathcal{H}^2(\mathcal{T}) \hat{\mathbb{f}}(\mathbb{G}, \mathbb{m}) \tag{2.1}$$

for every $(\mathbb{G}, \mathbb{m}) \in \mathrm{G}$, every planar 2 dimensional region $\mathcal{T}$ of normal $\mathbb{m}$, every (curved) surface $\mathcal{S}$ of normal $\mathbb{m}$ and every smooth map $\mathbb{y} : \mathcal{S} \to \mathrm{R}^3$ such that

$$\operatorname{bd} \mathcal{S} = \operatorname{bd} \mathcal{T}, \quad \mathbb{y}(\mathbf{x}) = \mathbb{G}\mathbf{x}, \quad \mathbf{x} \in \operatorname{bd} \mathcal{T}.$$

Here bd $\mathcal{S}$ and bd $\mathcal{T}$ denote the (relative) boundaries of the 2 dimensional surfaces $\mathcal{S}$ and $\mathcal{T}$ in R^3. We emphasize that the surface $\mathcal{S}$ is not the deformed interface $\mathcal{T}$ but instead a *different interface* consisting of material points different from those of $\mathcal{T}$. Thus testing (2.1) involves implicitly a change of the interface. This is mathematically reflected by the variation of the integration domain, from $\mathcal{T}$ to $\mathcal{S}$, with $\mathcal{H}^2(\mathcal{S}) \geq \mathcal{H}^2(\mathcal{T})$, and physically reflected by the transformation of one phase into another. The variation of domain of integration, which has no counterpart in the standard bulk quasiconvexity notion, has strong consequences which we shall mention below. Here we note that while the constant bulk energies are trivially quasiconvex, a constant interfacial energy $\hat{\mathbb{f}}$ is interface quasiconvex if and only if the constant value of $\hat{\mathbb{f}}$ is nonnegative. The interface quasiconvexity rules out surface wrinkling and prefers homogeneous surface deformations over the inhomogeneous ones.

Working in a different format of the interfacial energy than the present one, Parry [10] and Fonseca [6] established two related but weaker quasiconvexity properties of the interfacial energy; we refer to a discussion in [11; Introduction].

Approaching the notion of interface polyconvex functions, we introduce the interface null lagrangians and determine their form.

Definition 2.2. A function $\hat{\mathbb{f}} : \mathrm{G} \to \mathrm{R} \cup \{\infty\}$ is said to be interface null lagrangian if it is finite-valued, continuous and both $\hat{\mathbb{f}}$ and $-\hat{\mathbb{f}}$ are interface quasiconvex.

Theorem 2.3. *A function $\hat{\mathbb{f}} : \mathrm{G} \to \mathrm{R}$ is an interface null lagrangian if and only if*

$$\hat{\mathbb{f}}(\mathbb{F}, \mathbb{m}) = \mathbf{c} \cdot \mathbb{m} + \mathbf{\Omega} \cdot (\mathbb{F} \times \mathbb{m}) + \mathbf{a} \cdot \operatorname{cof} \mathbb{F}\mathbb{m} \tag{2.2}$$

for each $(\mathbb{F}, \mathbb{m}) \in \mathrm{G}$ *where* $\mathbf{c}$ *and* $\mathbf{a}$ *are constant vectors and* $\boldsymbol{\Omega}$ *a constant second order tensor.*

Recall that we work in the space of dimension 3; see [12; Proposition 3.5.2] for a general dimension and proof. (2.2) shows that the triple

$$\mathbb{m}, \quad \mathbb{F} \times \mathbb{m}, \quad \operatorname{cof} \mathbb{F} \mathbb{m} \tag{2.3}$$

is the basic list of 15 scalar interface null lagrangians.

Definition 2.4. A continuous function $\hat{\mathbb{f}} : \mathrm{G} \to \mathrm{R} \cup \{\infty\}$ is said to be interface polyconvex if it is the supremum of some family of interface null lagrangians.

Clearly, any interface polyconvex function is interface quasiconvex.

Theorem 2.5. *A function* $\hat{\mathbb{f}} : \mathrm{G} \to \mathrm{R}$ *is an interface polyconvex if and only if and only if*

$$\hat{\mathbb{f}}(\mathbb{F}, \mathbb{m}) = \Phi(\mathbb{m}, \mathbb{F} \times \mathbb{m}, \operatorname{cof} \mathbb{F} \mathbb{m})$$

for any $(\mathbb{F}, \mathbb{m}) \in \mathrm{G}$ *where* $\Phi : \mathrm{X} \to \mathrm{R}$ *is a positively* 1 *homogenous convex function on* $\mathrm{X} = \mathrm{R}^3 \times \mathrm{Lin} \times \mathrm{R}^3$, *where the positive* 1 *homogeneity of* Φ *means*

$$\Phi(t\mathrm{A}) = t\,\Phi(\mathrm{A})$$

for each $t \geq 0$ *and each argument* $\mathrm{A} \in \mathrm{X}$.

3 The main result

We introduce the state space for the existence theory, i.e., the competitors in the minimum energy principle.

Definition 3.1. Let $\Omega \subset \mathrm{R}^3$ be a bounded open set with Lipschitz boundary, and let $2 \leq p < \infty$, $3/2 \leq q < \infty$ and let r be an integer $1 \leq r < \infty$. We denote by $\mathcal{G}_r^{p,q}(\Omega)$ the set of all pairs $(\mathbf{y}, \mathcal{P})$ where

(i) $\mathbf{y} \in W^{1,p}(\Omega, \mathrm{R}^3)$, $\operatorname{cof} \nabla \mathbf{y} \in L^q(\Omega, \mathrm{Lin})$,

(ii) $\mathcal{P} = (E_1, \ldots, E_r)$ is a partition of Ω into sets of finite perimeter E_α, $\alpha = 1, \ldots, r$, i.e., the sets E_α, $\alpha = 1, \ldots, r$, are pairwise disjoint and

$$\bigcup_{\alpha=1}^{r} E_\alpha$$

differs from Ω by a set of Lebesgue measure 0;

(iii) for each $\alpha \in \{1, \ldots, r\}$ there exist measures $\mathbb{H}_\alpha$ and $\mathbb{p}_\alpha$ on Ω with values in Lin, and R^3, respectively, such that

$$-\int_{E_\alpha} \nabla \mathbf{y} \operatorname{curl} \mathbf{v}\, d\mathcal{L}^3 = \int_\Omega d\mathbb{H}_\alpha \mathbf{v}, \quad \int_{E_\alpha} \operatorname{cof} \nabla \mathbf{y} \cdot \nabla \mathbf{v}\, d\mathcal{L}^3 = \int_\Omega \mathbf{v} \cdot d\mathbb{p}_\alpha$$

for every $\mathbf{v} \in C_0^\infty(\Omega, \mathrm{R}^3)$.

We call the elements $(\mathbf{y}, \mathcal{P})$ of $\mathcal{G}_r^{p,q}(\Omega)$ states. The measure $\mathbb{H}_\alpha$ and $\mathbb{p}_\alpha$ are uniquely determined by $(\mathbf{y}, \mathcal{P})$ and we write $\mathbb{H}_\alpha(\mathbf{y}, \mathcal{P})$ and $\mathbb{p}_\alpha(\mathbf{y}, \mathcal{P})$ to indicate the dependence on $(\mathbf{y}, \mathcal{P})$.

If $(\mathbf{y}, \mathscr{P})$ is a state with $\mathbf{y}$ is smooth then the integration by parts and the identities

$$\operatorname{curl} \nabla \mathbf{y} = \mathbf{0}, \quad \operatorname{div}(\operatorname{cof} \nabla \mathbf{y}) = \mathbf{0}$$

show that the measures $\mathbb{H}_\alpha$ and $\mathbb{p}_\alpha$ as in Definition 3.1(iii) automatically exist and are given by

$$\mathbb{H}_\alpha = \mathbb{F} \times \mathbb{m}_\alpha \mathscr{H}^2 \llcorner \mathscr{S}_\alpha, \quad \mathbb{p}_\alpha = \operatorname{cof} \mathbb{F} \mathbb{m}_\alpha \mathscr{H}^2 \llcorner \mathscr{S}_\alpha \tag{3.1}$$

where $\mathscr{H}^2 \llcorner \mathscr{S}_\alpha$ is the area measure restricted to the interface $\mathscr{S}_\alpha := \Omega \cap \operatorname{bd}_* E_\alpha$ with $\operatorname{bd}_* E_\alpha$ the measure theoretic boundary of E_α. Hence in the general case the measures

$$\mathbb{b}_\alpha = \mathbb{m}_\alpha \mathscr{H}^2 \llcorner \mathscr{S}_\alpha, \quad \mathbb{H}_\alpha, \quad \mathbb{p}_\alpha$$

provide measure theoretic generalizations of the basic interface null lagrangians (2.3). The requirement (i) in the above definition comes from the refinement of Ball's existence theory [2] given in [9].

We now introduce the interface energy of separable type for states at the level of generality of Definition 3.1.

Definition 3.2. Let p, q, and r be as in Definition 3.1. Let $\hat{\mathbb{g}}_\alpha : \mathrm{G} \to \mathrm{R}$, $\alpha = 1, \ldots, r$, be functions satisfying

$$\hat{\mathbb{g}}_\alpha(\mathbb{F}, -\mathbb{m}) = \hat{\mathbb{g}}_\alpha(\mathbb{F}, \mathbb{m})$$

for each $(\mathbb{F}, \mathbb{m}) \in \mathrm{G}$ and assume that $\hat{\mathbb{g}}_\alpha$ are interface polyconvex in the sense that there exist even convex functions $\Psi_\alpha : \mathrm{X} \to \mathrm{R}$, $\alpha = 1, \ldots, r$, such that (1.6) holds. We define the interfacial energy $\mathsf{E}_{\mathrm{if}} : \mathscr{G}_r^{p,q}(\Omega) \to \mathrm{R}$ by

$$\mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathscr{P}) = \sum_{\alpha=1}^{r} \int_\Omega \Psi_\alpha(\mathbb{A}_\alpha)\, d|\mathbb{J}_\alpha| \tag{3.2}$$

for each $(\mathbf{y}, \mathscr{P}) \in \mathscr{G}_r^{p,q}(\Omega)$, where $\mathbb{A}_\alpha$ and $|\mathbb{J}_\alpha|$ are as follows. We associate with $(\mathbf{y}, \mathscr{P})$ the measures $\mathbb{H}_\alpha$ and $\mathbb{p}_\alpha$ as in Definition 3.1, define $\mathbb{b}_\alpha := \mathbb{m}_\alpha \mathscr{H}^2 \llcorner \mathscr{S}_\alpha$, where $\mathbb{m}_\alpha$ is the measure theoretic normal to $\mathscr{S}_\alpha = \Omega \cap \operatorname{bd}_* E_\alpha$, interpret the triplet $\mathbb{J}_\alpha := (\mathbb{b}_\alpha, \mathbb{H}_\alpha, \mathbb{p}_\alpha)$ as a measure with values in X, denote by $|\mathbb{J}_\alpha|$ the total variation measure of $\mathbb{J}_\alpha$ and let $\mathbb{A}_\alpha : \Omega \to \mathrm{X}$ be a vectorfield such that we have the polar decomposition identity $\mathbb{J}_\alpha = \mathbb{A}_\alpha |\mathbb{J}_\alpha|$.

We note that the individual terms

$$\int_\Omega \Psi_\alpha(\mathbb{A}_\alpha)\, d|\mathbb{J}_\alpha|$$

in (3.2) are the convex functions Ψ_α of the measure $\mathbb{J}_\alpha$ under the standard definition. We refer to [1; Corollary 1.29] for the discussion of the polar decomposition of a measure in a general context and to [1; Section 2.6] for the function of a measure. If $(\mathbf{y}, \mathscr{P})$ is a state with $\mathbf{y}$ sufficiently smooth then (3.1) show that

$$\mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathscr{P}) = \sum_{\alpha=1}^{r} \int_{E_\alpha} \Psi_\alpha(\mathbb{m}_\alpha, \mathbb{F} \times \mathbb{m}_\alpha, \operatorname{cof} \mathbb{F} \mathbb{m}_\alpha)\, d\mathscr{H}^2 = \sum_{\alpha=1}^{r} \int_{E_\alpha} \hat{\mathbb{g}}_\alpha(\mathbb{F}, \mathbb{m}_\alpha)\, d\mathscr{H}^2$$

where $\mathbb{m}_\alpha$ is the measure theoretic normal to E_α and $\mathbb{F} = \nabla \mathbf{y}$ is the surface deformation gradient defined for $\mathscr{H}^2$ a.e. point of $\bigcup_\alpha^r E_\alpha$. This in turn, using the even nature of $\hat{\mathbb{f}}_\alpha$ and the formulas (3.1) enables one to rewrite $\mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathscr{P})$ in the initial form (1.3).

The following is the main result of the paper. We refer to [11–12] for the case $r = 2$.

Theorem 3.3. *Let* $2 \le p < \infty$, $3/2 \le q < \infty$ *and let* r *be an integer,* $1 \le r < \infty$, *let* $\hat f_\alpha : \mathrm{Lin} \to [0,\infty]$, $\Psi_\alpha : \mathrm{X} \to [0,\infty)$, $\alpha = 1, \dots, r$, *be given functions. Assume that*

(i) $\hat f_\alpha$, $\alpha = 1, \dots, r$, *are polyconvex in the sense of* (1.4) *where* $\Phi_\alpha : W \to [0,\infty]$ *are continuous convex functions;*

(ii) *the functions* Ψ_α *are positively* 1 *homogeneous even convex functions,* $\alpha = 1, \dots, r$;

(iii) *for all* $\alpha = 1, \dots, r$ *all* $\mathbf{F} \in \mathrm{Lin}$, *all* $\mathrm{A} \in \mathrm{X}$, *some* $c > 0$ *and some* $d \in \mathrm{R}$ *we have*

$$\hat f_\alpha(\mathbf{F}) \ge c(|\mathbf{F}|^p + |\operatorname{cof}\mathbf{F}|^q) + d, \quad \Psi_\alpha(\mathrm{A}) \ge c|\mathrm{A}|,$$

(iv) $\hat f_\alpha(\mathbf{F}) = \infty$ *if* $\det \mathbf{F} \le 0$.

Let the energy functional $\mathsf{E} : \mathcal{G}_r^{p,q}(\Omega) \to [0,\infty]$ *be defined by* (1.1) *where* E_{b} *is given by* (1.2) *and* E_{if} *is as in Definition* 3.2. *If* $\mathbf{z}_0 \in W^{1,p}(\Omega, \mathrm{R}^3)$ *and* E *is finite for some element of the set*

$$\mathcal{A}(\mathbf{z}_0) = \{(\mathbf{z}, \mathcal{Q}) \in \mathcal{G}_r^{p,q}(\Omega) : \mathbf{z} = \mathbf{z}_0 \text{ on } \operatorname{bd}\Omega\}$$

then there exists an $(\mathbf{y}, \mathcal{P}) \in \mathcal{A}(\mathbf{z}_0)$ *such that*

$$\mathsf{E}(\mathbf{y}, \mathcal{P}) \le \mathsf{E}(\mathbf{z}, \mathcal{Q})$$

for all $(\mathbf{z}, \mathcal{Q}) \in \mathcal{A}(\mathbf{z}_0)$; *we have*

$$\det \nabla \mathbf{y} > 0 \text{ for } \mathcal{L}^3 \text{ a.e. point of } \Omega. \tag{3.3}$$

We allow $\hat f_\alpha$ to take the value ∞ not only to incorporate Condition (iv), which leads to the orientation preserving property (3.3), but also to allow the effective domains

$$\operatorname{eff\,dom} \hat f_\alpha = \{\mathbf{F} \in \mathrm{Lin} : \hat f_\alpha(\mathbf{F}) < \infty\}$$

be proper subsets of the set Lin_+. Thus one may assume that the effective domains are disjoint, and/or exclude states with deformation gradient in the spinodal region.

Proof Let $\mathcal{M}(\Omega, V)$ denote the space of measures on Ω with values in a finite dimensional vectorspace V and let $\mathbf{M}(\mu)$ denote the mass of the measure $\mu \in \mathcal{M}(\Omega, V)$, i.e., $\mathbf{M}(\mu) = |\mu|(\Omega)$ where $|\mu|$ denotes the total variation of μ. Let $(\mathbf{y}^i, \mathcal{P}^i) \in \mathcal{A}(\mathbf{z}_0)$ be a minimizing sequence where we write $\mathcal{P}^i = (E^i_\alpha, \dots, E^i_r)$. By the coercivity assumptions on $\hat f_\alpha$ and Ψ_α the sequences $|\nabla \mathbf{y}^i|_{L^p}$, $|\operatorname{cof}\nabla \mathbf{y}^i|_{L^q}$, $\mathcal{H}^2(\operatorname{bd}_* E^i_\alpha)$, $\mathbf{M}(\mathbb{H}_\alpha(\mathbf{y}^i, \mathcal{P}^i))$ and $\mathbf{M}(\mathbb{p}_\alpha(\mathbf{y}^i, \mathcal{P}^i))$ are bounded. Combining the boundedness of $|\nabla \mathbf{y}^i|_{L^p}$ with the Dirichlet boundary data, one obtains the boundedness of $|\mathbf{y}^i|_{W^{1,p}}$. Standard compactness theorems for Sobolev space and for the spaces of measures give that for some subsequence of $(\mathbf{y}^i, \mathcal{P}^i)$, denoted again $(\mathbf{y}^i, \mathcal{P}^i)$, we have

$$\mathbf{y}^i \rightharpoonup \mathbf{y} \quad \text{in } W^{1,p}(\Omega, \mathrm{R}^3), \tag{3.4}$$

$$\operatorname{cof}\nabla \mathbf{y}^i \rightharpoonup \mathbf{C} \text{ in } L^q(\Omega, \mathrm{Lin})$$

$$(\mathbb{m}^i_\alpha \mathcal{H}^2 \llcorner \operatorname{bd}_* E^i_\alpha, \mathbb{H}_\alpha(\mathbf{y}^i, \mathcal{P}^i), \mathbb{p}_\alpha(\mathbf{y}^i, \mathcal{P}^i)) \rightharpoonup^* \mathbf{\Delta}_\alpha \quad \text{in } \mathcal{M}(\Omega, \mathrm{X}) \tag{3.5}$$

$\alpha = 1, \dots, r$, for some $\mathbf{y} \in W^{1,p}(\Omega, \mathrm{R}^3)$, $\mathbf{C} \in L^q(\Omega, \mathrm{Lin})$, and $\mathbf{\Delta} \in \mathcal{M}(\Omega, \mathrm{X})$ where $\mathbb{m}^i_\alpha$ is the measure theoretic normal to E^i_α. The boundedness of $\mathbb{m}^i_\alpha \mathcal{H}^2 \llcorner E^i_\alpha$ says that the sequence of the derivatives of the characteristic functions $1_{E^i_\alpha}$ of E^i_α in Ω is bounded in $\mathcal{M}(\Omega, \mathrm{R}^3)$. The imbedding theorem from *BV* functions (e.g., [1; Corollary 3.49, Chapter 3]) implies

$$1_{E^i_\alpha} \to 1_{E_\alpha} \quad \text{in } L^1(\Omega). \tag{3.6}$$

for some set $E_\alpha \subset \Omega$ of finite perimeter, i.e.,

$$\mathcal{L}^n(\Delta(E^i_\alpha, E_\alpha)) \to 0, \tag{3.7}$$

where $\Delta(E^i_\alpha, E_\alpha)$ is the symmetric difference of E^i_α and E_α. Moreover, the limit in $\sum^r_\alpha 1_{E^i_\alpha} = 1$ on Ω gives $\sum^r_\alpha 1_{E_\alpha} = 1$ and thus $\mathcal{P} := (E_1, \dots, E_r)$ is a partition of Ω into sets of finite perimeter. Furthermore, if we write

$$\mathbf{\Delta}_\alpha = (\mathbf{\Delta}^1_\alpha, \mathbf{\Delta}^2_\alpha, \mathbf{\Delta}^3_\alpha) \tag{3.8}$$

for the components of the X valued measure $\mathbf{\Delta}_\alpha$ in the product $\mathrm{X} := \mathrm{R}^3 \times \mathrm{Lin} \times \mathrm{R}^3$, then

$$\mathbb{m}^i_\alpha \mathcal{H}^2 \llcorner \operatorname{bd}_* E^i_\alpha \rightharpoonup^* \mathbf{\Delta}^1_\alpha \quad \text{in } \mathcal{M}(\Omega, \mathrm{R}^3) \tag{3.9}$$

and

$$\mathbf{\Delta}^1_\alpha = \mathbb{m}_\alpha \mathcal{H}^2 \llcorner \operatorname{bd}_* E_\alpha$$

where $\mathbb{m}_\alpha$ is the measure theoretic normal to E_α. The condition $\mathsf{E}(\mathbf{y}^i, \mathcal{P}^i) < \infty$ for each i and Hypothesis (iv) imply that $\det \nabla \mathbf{y}^i > 0$ for every i and $\mathcal{L}^n$ a.e. point of Ω. From (3.4) by [9; Lemma 4.1] then

$$\operatorname{cof} \nabla \mathbf{y}^i \rightharpoonup \operatorname{cof} \nabla \mathbf{y} \quad \text{in } L^q(\Omega, \mathrm{Lin}), \tag{3.10}$$

$$\det \nabla \mathbf{y}^i \rightharpoonup \det \nabla \mathbf{y} \quad \text{in } L^1(K, \mathrm{R}) \tag{3.11}$$

for each compact subset K of Ω; recall also that [see (3.4)]

$$\nabla \mathbf{y}^i \rightharpoonup \nabla \mathbf{y} \quad \text{in } L^p(\Omega, \mathrm{Lin}). \tag{3.12}$$

The equiintegrability of the sequences $\nabla \mathbf{y}^i$ and $\operatorname{cof} \nabla \mathbf{y}^i$ and (3.12) and (3.7) yield

$$1_{E^i_\alpha} \nabla \mathbf{y}^i \rightharpoonup 1_{E_\alpha} \nabla \mathbf{y}, \quad 1_{E^i_\alpha} \operatorname{cof} \nabla \mathbf{y}^i \rightharpoonup 1_{E_\alpha} \operatorname{cof} \nabla \mathbf{y} \quad \text{in } L^1(\Omega, \mathrm{Lin})$$

and in particular,

$$\int_\Omega d\,\mathbb{H}(\mathbf{y}^i, \mathcal{P}^i)\mathbf{v} = \int_{E^i_\alpha} \nabla \mathbf{y}^i \operatorname{curl} \mathbf{v}\, d\mathcal{L}^n \to \int_{E_\alpha} \nabla \mathbf{y} \operatorname{curl} \mathbf{v}\, d\mathcal{L}^n,$$

$$\int_\Omega d\,\mathbb{p}(\mathbf{y}^i, \mathcal{P}^i)\mathbf{v} = \int_{E^i_\alpha} \operatorname{cof} \nabla \mathbf{y}^i \cdot \nabla \mathbf{v}\, d\mathcal{L}^n \to \int_{E_\alpha} \nabla \mathbf{y} \cdot \nabla \mathbf{v}\, d\mathcal{L}^n$$

for each $\mathbf{v} \in C^\infty_0(\Omega, \mathrm{R}^3)$. Hence (3.5) yields

$$\int_{E_\alpha} \nabla \mathbf{y} \operatorname{curl} \mathbf{v}\, d\mathcal{L}^n = \int_\Omega d\mathbf{\Delta}^2_\alpha \mathbf{v}, \quad \int_{E_\alpha} \operatorname{cof} \nabla \mathbf{y} \cdot \nabla \mathbf{v}\, d\mathcal{L}^n = \int_\Omega d\mathbf{\Delta}^3_\alpha \mathbf{v}$$

where we use the notation (3.8). Thus $(\mathbf{y}, \mathcal{P}) \in \mathcal{G}^{p,q}_r(\Omega)$ and $\mathbb{H}_\alpha(\mathbf{y}, \mathcal{P}) = \mathbf{\Delta}^2_\alpha$ and $\mathbb{p}_\alpha(\mathbf{y}, \mathcal{P}) = \mathbf{\Delta}^3_\alpha$. Equations (3.5) and (3.9) give

$$\begin{aligned} &(\mathbb{m}^i_\alpha \mathcal{H}^2 \llcorner \operatorname{bd}_* E^i_\alpha, \mathbb{H}_\alpha(\mathbf{y}^i, \mathcal{P}^i), \mathbb{p}_\alpha(\mathbf{y}^i, \mathcal{P}^i)) \rightharpoonup^* \\ &\qquad (\mathbb{m}_\alpha \mathcal{H}^2 \llcorner \operatorname{bd}_* E_\alpha, \mathbb{H}_\alpha(\mathbf{y}, \mathcal{P}), \mathbb{p}_\alpha(\mathbf{y}, \mathcal{P})) \quad \text{in } \mathcal{M}(\Omega, \mathrm{X}). \end{aligned} \tag{3.13}$$

We now recall that Φ_α is nonnegative and convex and apply the Ioffe lowersemicontinuity theorem [1; Theorem 5.8, Chapter 5]. One then deduces from the weak convergences (3.12), (3.10) and (3.11) and the strong convergence (3.6) that for any compact subset K of Ω we have

$$\begin{aligned}\liminf_{i\to\infty} \int_{E_\alpha^i} \hat{f}_\alpha(\nabla \mathbf{y}^i)\, d\mathcal{L}^n &\geq \liminf_{i\to\infty} \int_{E_\alpha^i \cap K} \Phi_\alpha(\nabla \mathbf{y}^i, \operatorname{cof} \nabla \mathbf{y}^i, \det \nabla \mathbf{y}^i)\, d\mathcal{L}^n \\ &\geq \int_{E_\alpha \cap K} \Phi_\alpha(\nabla \mathbf{y}, \operatorname{cof} \nabla \mathbf{y}, \det \nabla \mathbf{y}) \\ &= \int_{E_\alpha \cap K} \hat{f}_\alpha(\nabla \mathbf{y})\ d\mathcal{L}^n.\end{aligned}$$

The arbitrariness of K then gives

$$\liminf_{i\to\infty} \int_{E_\alpha^i} \hat{f}_\alpha(\nabla \mathbf{y}^i)\, d\mathcal{L}^n \geq \int_{E_\alpha} \hat{f}_\alpha(\nabla \mathbf{y})\, d\mathcal{L}^n,$$

which implies

$$\liminf_{i\to\infty} \mathsf{E}_{\mathrm{b}}(\mathbf{y}^i, \mathcal{P}^i) \geq \mathsf{E}_{\mathrm{b}}(\mathbf{y}, \mathcal{P}). \tag{3.14}$$

Using (3.13) and the Reshetnyak lowersemicontinuity theorem (e.g., [1; Theorem 2.38, Chapter 2]), one obtains

$$\liminf_{i\to\infty} \mathsf{E}_{\mathrm{if}}(\mathbf{y}^i, \mathcal{P}^i) \geq \mathsf{E}_{\mathrm{if}}(\mathbf{y}, \mathcal{P}). \tag{3.15}$$

Thus (3.14) and (3.15) provide

$$\liminf_{i\to\infty} \mathsf{E}(\mathbf{y}^i, \mathcal{P}^i) \geq \mathsf{E}(\mathbf{y}, \mathcal{P}).$$

Clearly, $(\mathbf{y}, \mathcal{P}) \in \mathcal{A}(\mathbf{z}_0)$. □

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