Multi-Phase Equilibrium
of Crystalline Solids

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Abstract

A continuum model of crystalline solid equilibrium is presented in which the underlying periodic lattice structure is taken explicitly into account. This model also allows for both point and line defects in the bulk of the lattice and at interfaces, and the kinematics of such defects is discussed in some detail. A Gibbsian variational argument is used to derive the necessary bulk and interfacial conditions for multi-phase equilibrium (crystal-crystal and crystal-melt) where the allowed lattice variations involve the creation and transport of defects in the bulk and at the phase interface. An interfacial energy, assumed to depend on the interfacial dislocation density and the orientation of the interface with respect to the lattices of both phases, is also included in the analysis. Previous equilibrium results based on nonlinear elastic models for incoherent and coherent interfaces are recovered as special cases for when the lattice distortion is constrained to coincide with the macroscopic deformation gradient, thereby excluding bulk dislocations. The formulation is purely spatial and needs no recourse to a fixed reference configuration or an elastic-plastic decomposition of the strain. Such a decomposition can be introduced however through an incremental elastic deformation superposed onto an already dislocated state, but leads to additional equilibrium conditions. The presentation emphasizes the role of configurational forces as they provide a natural framework for the description and interpretation of singularities and phase transitions.

1 Introduction

Consider two phases of a given material separated by a sharp interface and in equilibrium in a heat bath. Let one phase be a crystalline solid, the other phase
may be either the corresponding fluid melt or another crystalline solid (such as in a twinned crystal). This paper is concerned with the determination of the equilibrium conditions for the bulk regions occupied by the two phases and for the interface separating them—a problem of significant interest in diverse fields. Numerous authors have already studied various aspects of it and have derived equations governing the mechanical, thermal, and chemical equilibrium (Eshelby, 1970; Robin, 1974; Larché & Cahn, 1978, 1985; Cahn, 1980, Cahn & Larché, 1982; Grinfeld’d, 1981; Mullins, 1984; Alexander & Johnson, 1985; Johnson & Alexander, 1986; Kaganova & Roitburd, 1988; Leo & Sekerka, 1989; Gurtin, 1993; Cermelli & Gurtin, 1994; Leo & Hu, 1995). A fundamental characteristic of a crystalline solid is its lattice structure, in which the atoms are periodically spaced. Additionally the lattice contains defects, e.g., point defects (interstitials and vacancies) and line defects (dislocations), both types of which can impact on the equilibrium behavior. Larché & Cahn (1978) included point defects in their original analysis by treating the interstitials and vacancies as additional mobile species subject to a lattice or network constraint. This work was later extended to allow for surface energy associated with the interface (Cahn, 1980, Cahn & Larché, 1982; Mullins, 1984; Alexander & Johnson, 1985; Johnson & Alexander, 1986; Leo & Sekerka, 1989; Gurtin, 1993; Cermelli & Gurtin, 1994; Leo & Hu, 1995). In this approach however the lattice does not appear explicitly, so it is not clear how other properties of the lattice, such as the distortion of the lattice or the occurrence of dislocations, affect the governing equations.

In this paper we present a continuum model of crystalline solid equilibrium that explicitly incorporates the underlying lattice structure and includes the possibility of both point and line defects. Following Larché & Cahn (1978), we then give for this model a Gibbsian variational analysis, in which we obtain the necessary conditions for two-phase crystal-crystal equilibrium. We consider general non-equilibrium variations that allow for creation and transport of defects in the bulk and at the interface. We treat both coherent and incoherent interfaces, two extreme cases that characterize many types of interfaces between crystalline solids. In particular, incoherency is important since it can arise from the presence of defects at the phase interface. Additionally, we consider the case of crystal-melt equilibrium. We also include interfacial energy, assuming that it depends on the interfacial dislocation density and the orientation of the interface with respect to the lattices of both phases.

We model a crystalline solid by a continuum microstructural theory where the microstructural variables represent in an average sense the underlying lattice structure:

- 3 linearly independent vector fields denote the average lattice vectors at a spatial point;
- interstitials and vacancies are treated in the usual way by modelling them as additional mobile species subject to a lattice constraint;
- dislocations are related to the anholonomicity (i.e., non-integrability) of
the microstructural lattice vectors.

In this model we introduce neither a fixed reference configuration nor a macroscopic deformation gradient; rather we describe the state only by the microstructural variables through a spatial description, where quantities are defined on a per unit cell basis at a fixed point in space. A spatial description is uncommon in traditional models of solids, but is more convenient when interfaces are incoherent as they remain together in the current configuration. It also seems to be the most appropriate when relating to standard x-ray observations of lattice points, which do not indicate how the lattice points actually evolve. We also assume that the energy per unit cell of the current configuration depends upon the local current state (i.e., lattice vectors, dislocation density, and occupancy density).

Commonly in microstructural models, lattice vectors are assumed to deform as material line elements—the so-called Born rule (Ericksen, 1984)—so that the lattice vectors in the deformed configuration are related to the lattice vectors in the reference configuration by the macroscopic deformation gradient. This assumption however is not always valid: in particular it fails when there are dislocations; it can also fail in other cases (Zanzotto, 1992). We therefore formulate our model without employing the Born rule, but then we show how more classical models for solids are recovered when the Born rule is imposed as a constraint. Thus our equilibrium results are new in that

(1) bulk and surface dislocations are explicitly taken into account; and

(2) no a priori relation between reference lattice vectors and actual lattice vectors is assumed.

When the Born rule is imposed as a constraint, the lattice vectors then deform as material line elements, the dislocation density vanishes in the bulk, the lattice distortion becomes equivalent to the deformation gradient, and we recover equilibrium results equivalent to those of Larché & Cahn (1978), Leo & Sekerka (1989), and Cermelli & Gurtin (1994).

Our approach, however, does not require any recourse to the concept of macroscopic deformation or fixed reference configuration. On the other hand, for a number of applications or in certain special cases, it may be convenient to introduce the often used elastic-plastic decomposition of the strain (Bilby et al., 1957; Kröner, 1960; Lee, 1969). We do so by identifying the dislocated crystal with the intermediate configuration of such a decomposition and then superposing a classical elastic (i.e., defect-preserving) deformation onto this dislocated state. In this approach our “elastic” part of the elastic-plastic decomposition is truly elastic in the traditional sense. This procedure allows one to construct a simple model of dislocated bodies while keeping track of all the different elastic and plastic components of the theory. Due to the additional structure in the theory arising from the incremental elastic deformation, additional equilibrium conditions arise, so that the resulting equilibrium theory is not equivalent to that
without the elastic-plastic decomposition. In particular, when such an intermediate configuration is introduced, both the dislocated intermediate configuration and the current configuration must be in mechanical equilibrium.

There is some precedence for a microstructural approach to modelling crystalline solids. Motivated by the Cosserat director theories for oriented materials (Ericksen & Truesdell, 1958; Truesdell & Toupin, 1960), both Fox (1966,1970) and Toupin (1968) proposed using a triad of continuous vector fields to represent lattice vectors associated with a material point and demonstrated how dislocations could be related to the non-integrability of the directors. The deformation associated with the lattice directors was assumed distinct from the average, macroscopic deformation. Additionally Fox discussed how a notion of lattice slip could be introduced. Mullins & Sekerka (1985) also used a triad of vector fields to model the lattice vectors, which, however, where taken to deform as material line elements (the Born rule). Consequently any constitutive dependence on them could be replaced by a dependence on the macroscopic deformation gradient, which excluded the possibility of bulk dislocations. In this case their model described anisotropic elastic solids (Ericksen & Rivlin, 1954). Davini (1986) and Davini & Parry (1989,1991) discussed in detail the various defect measures and their relation to the lattice directors. They also introduced the neutral deformations—inelastic deformations that do not change the defect content—and demonstrated a corresponding decomposition of the strain. Naghdi & Srinivasa (1993a,b,1994a,b) formulated a director theory as a model of slip in plastic deformations. Similarly, Besseling and van der Giessen (1994) introduced a triad of vector fields for the lattice vectors in their discussion of inelastic deformations, but did not introduce the notion of defects in this model. More recently, Dhzeweski (1996) discussed the driving forces acting on defects in a director model. And Ericksen (1997) discussed an equilibrium theory of crystals in terms of lattice directors without employing the Born rule and without introducing a macroscopic deformation gradient, but did not consider defects. Our approach follows closely that of Davini, Parry, and Ericksen in that it is based entirely on a description in terms of the underlying lattice structure.

Finally, our presentation emphasizes the role of the configurational forces as they provide a natural framework for studying singularities and phase transitions (Eshelby, 1951,1970; Maugin, 1993; Gurtin, 1995). Configurational forces do work over changes in the reference lattice and arise naturally in our theory as the derivatives of the energy with respect to the reciprocal lattice vectors (Cermelli & Sellers, 1998). In our calculations the configurational forces result as primary quantities and provide an immediate interpretation of the resulting equilibrium conditions.

2 Crystalline Solid Model

1 Also called Eshelby forces or energy-momentum.
2.1 Motivation

By the expression crystalline solid, we mean a model for a solid that explicitly incorporates the underlying lattice structure typical of a crystal. Our model of a defective crystalline solid is based on the notion that the regular lattice structure is, on the average, locally recognizable and measurable (Davini, 1986). For instance, x-ray observations can provide local values for the various lattice parameters. Further, such experimental measurements indicate that the dilatation of the lattice parameters does not always correspond to the average macroscopic strain as measured in, for example, tensile tests. These results intimate that the macroscopic deformation gradient can be in some cases an inappropriate measure of the true deformation of the crystal; finer kinematic details of the lattice may be needed. In the following we introduce microstructural variables to represent such kinematic details of the lattice and its distortion. In this point of view, the state of a crystalline solid with defects is completely determined by the crystalline structure, which we take as the set of lattice vectors and the occupancy density of lattice sites. These quantities are viewed as fields over the region of space occupied by the material in its actual or current configuration.

2.2 Lattice microstructure

Let $\mathcal{B} \subset \mathbb{R}^3$ denote the region of space occupied by the crystalline solid in its actual or current configuration. We will consistently use this spatial region as a reference.

To each spatial point $x \in \mathcal{B}$, we associate a triad of vector fields $e_i(x)$ (where $i$ ranges from 1 to 3) that represent the lattice basis vectors at $x$. They describe in an average sense the local microscopic arrangement of the lattice points and vary continuously from one spatial point to another. It is also useful to introduce the reciprocal lattice vectors $e^i(x)$ defined by the relation

$$e^i \cdot e_j = \delta^i_j, \quad e_i \otimes e^i = e_i \otimes e_i = 1,$$

(1)

where $\delta^i_j$ is the Kronecker delta symbol and repeated Latin indices are summed. Generally x-ray observations provide direct measurements of the reciprocal lattice vectors $e^i$. We shall also denote a fixed, constant and uniform lattice basis by $E_i$, with reciprocal basis $E^i$. It provides a convenient reference lattice from which to measure the change of the lattice vectors.

The lattice distortion is by definition the tensor field

$$F_{\text{lat}} = e_i \otimes E^i,$$

(2)

which takes the reference lattice vectors $E_i$ to the actual lattice vectors $e_i$ at each spatial point. Similarly, the inverse lattice distortion

$$F^{-1}_{\text{lat}} = E_i \otimes e^i$$

(3)

2 Although we do not introduce a fixed reference configuration for the current configuration $\mathcal{B}$, we do use the notion of reference lattice.
takes the actual lattice vectors to the reference lattice vector $s$ at each spatial point. We do not assume that $F_{\text{lat}}$ or $F_{\text{lat}}^{-1}$ are gradients. In particular, $F_{\text{lat}}$ need not correspond to the macroscopic deformation gradient $F$.

Since the reference lattice vectors are constant, the actual or current state of the lattice is equivalently characterized by either the fields $e_i$, here taken as spatial fields on $B$, or by the fields $e^i$, due to the relation (1) between lattice vectors and reciprocal lattice vectors.

Furthermore, we interpret $e_1 \cdot (e_2 \times e_3)$ as the volume of a unit cell, so that

$$n := e_1 \cdot (e_2 \times e_3) = \frac{1}{e_1 \cdot (e_2 \times e_3)}$$

is the number of cells per unit volume. It is also a continuously varying spatial field defined on $B$.

### 2.3 Point defects

In a perfect crystal the atoms occupy lattice points. In a defective crystal some of the lattice points may not be occupied, these being called vacancies. Additionally, some atoms may be at points not located at the lattice points, these being called interstitials. Here, to maintain the presentation simple, we assume that there exists a single mobile species of atoms, either vacancies or interstitials. The extension to an arbitrary number of species is straightforward. We thus introduce the following scalar fields:

$$\varrho(x) \quad \text{atoms per unit cell}$$

$$\varrho_{\text{vac}}(x) \quad \text{vacancies per unit cell}$$

If $\varrho_{\text{vac}} > 0$, we will interpret $\varrho_{\text{vac}}$ as a density of vacancies; if $\varrho_{\text{vac}} < 0$, we will interpret $|\varrho_{\text{vac}}|$ as a density of interstitial atoms. Since we allow for only a single mobile species, only the sign of $\varrho_{\text{vac}}$ distinguishes between vacancies and interstitials. These two fields are not independent but are related by the lattice constraint:

$$\varrho + \varrho_{\text{vac}} = \ell = \text{const.},$$

where $\ell$ is the number of lattice points per unit cell. The lattice points are regarded as a geometric constant of the lattice. Consequently only one of the quantities is independent, and we arbitrarily choose $\varrho$ as the independent density.

If independent mobile point defects are allowed, they must also be specified in addition to the lattice vectors. Thus for our model, the current state of a crystalline solid with a single mobile species is given by $(e_i, \varrho)$, specified as spatial fields on $B$. Alternatively and equivalently, the lattice vectors $e_i$ can be replaced by the reciprocal lattice vectors $e^i$ or the molar density $\varrho$ replaced by the vacancy density $\varrho_{\text{vac}}$. 

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Classically, the Burgers vector \( \mathbf{b} = b^i \mathbf{E}_i \) is taken as a measure of the dislocations in the sense that
\[
\mathbf{b}^i = \int_{\partial C} \mathbf{e}^i \cdot d\mathbf{l} = \int_{C} (\text{curl } \mathbf{e}^i) \cdot \mathbf{n}_c \, da,
\]
represents the atomic lattice displacements in the reference lattice for a circuit \( \partial C \) of a fixed surface \( C \subset B \) with unit normal \( \mathbf{n}_c \) (Bilby & Smith, 1956; Davini, 1986). To see this, notice that the quantity \( \mathbf{b}^i \) defined by (6) is the net number of \( i \)-planes (i.e., planes orthogonal to \( \mathbf{e}^i \)) which are crossed by the curve \( \partial C \), so that any term in the combination \( \mathbf{b} = b^i \mathbf{E}_i \) represents: (the net number of added \( i \)-planes encountered upon traveling along \( \partial C \)) times (the reference \( i \)-lattice vector) = (the net Burger vector of the circuit).

By definition the reference lattice vectors \( \mathbf{E}_i \) are constant and dislocation free. Define the 3 quantities
\[
\mathbf{g}^i(x) := \text{curl } \mathbf{e}^i(x).
\]
Commonly \( \mathbf{E}_i \otimes \mathbf{g}^i \) is used as a tensorial measure of the density of dislocations and corresponds to the dislocation density introduced by Nye (1953). Since the reference lattice vectors \( \mathbf{E}_i \) are constant, we use instead the 3 vectorial dislocation densities \( \mathbf{g}^i \), which are taken as a spatial fields on \( B \).

We will frequently use the equivalent fields
\[
\mathbf{g}^{ij} := \frac{1}{n} \mathbf{g}^i \cdot \mathbf{e}^j,
\]
which can be interpreted as the dislocation density per unit cell (Davini, 1986; Davini & Parry, 1991).

We will model phase boundaries as sharp surfaces. To allow for this possibility, suppose now that the circuit \( \partial C \) is intersected by a sharp surface \( S \) across which there is a jump in lattice vectors. Then (6) must be modified to
\[
\mathbf{b}^i = \int_{\partial C} \mathbf{e}^i \cdot d\mathbf{l} = \int_{C} (\text{curl } \mathbf{e}^i) \cdot \mathbf{n}_c \, da - \int_{\partial C \cap S} [\mathbf{e}^i] \cdot d\mathbf{l},
\]
where \([\phantom{x}]\) denotes the jump of a quantity across the surface \( S \) in which the jump is taken as the limit from the portion of \( B \) into which the normal \( \mathbf{n}_s \) to the surface points. Since the above relation is independent of the surface \( C \) (keeping fixed the boundary curve \( \partial C \)), the tangential jump in the lattice vectors provides a measure of the defectivity of the interface. Thus we introduce
\[
[\mathbf{P} \mathbf{e}^i]
\]
as 3 vectorial measures of the surface dislocation density, where
\[
\mathbf{P} := 1 - \mathbf{n}_s \otimes \mathbf{n}_s
\]
is the projection operator onto the tangent plane of $S$. The quantity $[E_i \otimes (Pe^i)]$ corresponds to the tensorial surface density introduced by Bilby (1955). It is equivalent to $\parallel (10)$ since the reference lattice vectors are continuous and linearly independent. To see that $\parallel (10)$ indeed measures the density of interfacial dislocations, let $u$ be a tangent vector to the interface $S$. Then

$$[E_i \otimes (Pe^i)]u = ([e^i] \cdot u) E_i.$$  \hspace{1cm} (12)

And since $(e^i)^\alpha \cdot u$ and $(e^i)^\beta \cdot u$ are the net number of $i$-planes from side $\alpha$ or $\beta$ which intersect the vector $u$ (recall that $|e^i|$ is the reciprocal of the distance between two consecutive $i$-planes), $\parallel (e^i] \cdot u$ is the net number of $i$-planes intersecting $u$. Thus the sum $\parallel (12)$ consists of the net number of added $i$-planes encountered upon traveling along $u$ times the reference $i$-lattice vectors, which equals the net Burgers vector of the interfacial dislocations along $u$.

In classical elastostatics, a deformation is holonomic (i.e., compatible or integrable) if the strain tensor is the gradient of a global, smooth map. For our model of a crystalline solid, this notion is expressed by a compatibility condition stating that there exists a smooth map $\chi$ such that

$$E_i \otimes e^i = \text{grad} \chi.$$ \hspace{1cm} (13)

In other words, the state of a crystalline solid is holonomic if the inverse lattice distortion $F_{\text{lat}}$ is the gradient of a global, smooth map. In this case, the notion of deformation arises naturally since $\chi$ corresponds to the *macroscopic inverse deformation* to the reference lattice. We will call a lattice a *holonomic lattice* (with respect to $E_i$) if $(13)$ is satisfied for some $\chi$. The reference lattice, by definition, is holonomic; the distorted lattice however is in general not holonomic. And since the reference lattice vectors $E_i$ are constant, $(13)$ shows that the bulk dislocation densities $g^i$ vanish identically for a holonomic lattice (though the surface dislocation densities $(10)$ need not vanish at a singular surface $S$ of a holonomic lattice). In this model of a crystalline solid, dislocations are viewed as the obstruction to patching together local measurements of the reciprocal lattice to a single, global lattice.

### 2.5 Born rule

The *Born rule* states that lattice vectors deform as material line elements under a given deformation (Ericksen, 1984). We are primarily concerned with the case when this does not hold, as the Born rule excludes dislocations in the bulk. We will consider however the consequences of imposing it as a constraint, where it will be shown to imply common models for elastic equilibrium as special cases.

Consider now a holonomic lattice in the actual configuration, so that the dislocation density vanishes inside $B$. There is a natural inverse deformation $\chi$ for the lattice, through which we can associate $\chi(B)$ with the region occupied in the undeformed configuration. In this case, the Born rule yields (cf. $(13)$)

$$e_i = (\text{grad} \chi^{-1}) E_i \quad \text{or} \quad e^i = (\text{grad} \chi)^T E^i.$$ \hspace{1cm} (14)
If we assign on $\chi(B)$ the perfect lattice determined by $E^i$, then (14a) states that the lattice vectors deform as material vectors through $\chi^{-1}$. Alternatively, (14b) states that the reciprocal lattice vectors deform as material vectors through $\chi$.

Using the Born rule at a surface of discontinuity $S$, the 3 surface dislocation densities (10) become

$$[P(\text{grad } \chi)^\top]E^i,$$

with $P$ the projection operator onto the tangent plane of $S$. They correspond to the single tensorial quantity $[P(\text{grad } \chi)^\top]$ used by Cermelli & Gurtin (1994).

3 Lattice Variations

Let $(e_i, \varrho)$ denote as before a state of a body occupying the region $B$. We denote an arbitrary smooth variation of this state by $(\delta e_i, \delta \varrho)$, which does not necessarily correspond to any equilibrium state. The external boundary $\partial B$ is assumed rigid and fixed, so the variations vanish on $\partial B$ (but not necessarily on an internal boundary such as the phase interface). Consider now the additive composition of the two configurations

$$e_{i\lambda} := e_i + \lambda \delta e_i, \quad \varrho_{\lambda} := \varrho + \lambda \delta \varrho$$

where $\lambda$ is a small parameter. This composition induces a corresponding variation in any functional $\Phi$ depending on the composed configuration:

$$\delta \Phi = \frac{\partial}{\partial \lambda} \Phi[e_{i\lambda}, \varrho_{\lambda}] \bigg|_{\lambda=0}. \quad (17)$$

In particular, it induces variations in dislocation density $g^i$ and the reciprocal lattice vectors $e^i$, related by the identity

$$\delta g^i = \text{curl } \delta e^i.$$ \hspace{1cm} (18)

The induced variation of the Burgers vector is $\delta b = \delta b^i E_i$ where

$$\delta b^i = \int_{\partial C} \delta e^i \cdot dl.$$ \hspace{1cm} (19)

Generally the $\delta e^i$ induce a dislocation flux (Kosevich, 1962).

A straightforward calculation yields the relations

$$\delta n = n e_i \cdot \delta e^i,$$

$$n \delta g^{ij} = -(g^i \cdot e^j) e_i \cdot \delta e^i + e^i \cdot \delta g^i + g^i \cdot \delta e^i.$$ \hspace{1cm} (20)

which will be needed later.

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4Since we are using a spatial description, the variations correspond to the Eulerian variations of Leo & Sekerka (1989)
Consider now an internal boundary given by the singular surface $S$. We allow the $e_i$ and the dislocation density $g^{ij}$ to be discontinuous across this surface. A variation of the position of the interface in space is described by

$$\delta r = n_S \delta r,$$

(21)

with $n_S$ a choice of unit normal to $S$. Variations of the position of the surface $S$ and of lattice vectors at the surface will involve in general the creation and transport of defects.

4 Equilibrium Equations without Interfacial Energy

In section 2 we developed the kinematics to describe an equilibrium state of a crystalline solid with point and line defects. In section 3 we extended the kinematic structure in order to discuss variations of states that induce creation and transport of such defects. In this section we employ this kinematic structure to derive the equations governing multi-phase equilibria. The approach is variational and involves rendering stationary an appropriate energy potential. We treat crystal-crystal and crystal-melt equilibria separately. Also we consider first the case without interfacial energy, then in the following section extend the equilibrium results to include interfacial energy.

4.1 Crystal-crystal equilibrium

Let two crystalline solid phases (denoted by $\alpha$ and $\beta$) share a common interface $S$ and be immersed in a heat bath at temperature $\theta_B$. Further, let the external boundaries be impermeable and fixed. Such a situation can be in equilibrium only if an appropriate thermodynamic potential is stationary. We now construct such a potential and determine the necessary conditions for it to be stationary. We continue to use a spatial description and take all extensive quantities describing the crystalline solid as per unit cell in the actual state.

Since there is no external mass supply, the total mass of the system is constant and is given by

$$M = M^\alpha + M^\beta = \int_{B^\alpha \cup B^\beta} n_\theta \, dv.$$

(22)

We assume that the total internal energy of the system is given by

$$E = E^\alpha + E^\beta = \int_{B^\alpha \cup B^\beta} n_\epsilon \, dv,$$

(23)

where $\epsilon$ is the internal energy density per unit cell in the actual state, and any surface energy has been assumed negligible. Furthermore, we assume that the entropy is additive:

$$S = S^\alpha + S^\beta = \int_{B^\alpha \cup B^\beta} n_s \, dv,$$

(24)
where \( s \) is the entropy density per unit cell.

A constitutive relation must specify one of these quantities as a function of the current state of the material. As a local measure of the lattice structure, we choose the quantities \((e^i, g^{ij}, \rho)\), since \(e^i\) specifies the periodic structure of the lattice, \(g^{ij}\) the dislocation density per unit cell, and \(\rho\) the atoms per unit cell. This choice is not unique; it is also equivalent to \((e^i, g^i, \rho_{\text{vac}})\). As a measure of the local thermodynamic state, we choose the entropy \( s \) per unit cell. Our constitutive assumptions are then that the internal energy per unit cell of each phase is given by:

\[
\epsilon = \epsilon^\alpha(e^i, g^{ij}, \rho, s) \quad \text{for phase } \alpha,
\]

\[
\epsilon = \epsilon^\beta(e^i, g^{ij}, \rho, s) \quad \text{for phase } \beta.
\]

(25)

Notice that we assume that the energy depends on the current state as determined by the local lattice structure and entropy. In particular, there is no dependence on a macroscopic deformation gradient since we have not introduced a fixed reference configuration for \(B^\alpha \cup B^\beta\).

Following Gibbs (1878), the grand canonical potential

\[
\Omega := E - \theta B S - \mu M
\]

(26)

(at constant total mass and total entropy) is stationary in equilibrium, where \(\mu\) is a constant Lagrange multiplier ensuring conservation of mass. A necessary condition for its stationarity is that the first variation vanish:

\[
\delta \Omega = \delta E - \theta B \delta S - \mu \delta M = 0.
\]

(27)

Thus using (22)–(27) along with (21) and denoting by

\[
[h] = h^\beta - h^\alpha
\]

the jump of a field \( h \) at the interface from the \( \alpha \) and \( \beta \)-sides we have

\[
\delta \Omega = \delta \int_{B^\alpha \cup B^\beta} n \epsilon dv - \theta B \delta \int_{B^\alpha \cup B^\beta} n s dv - \mu \delta \int_{B^\alpha \cup B^\beta} n \rho dv
\]

\[
= \int_{B^\alpha \cup B^\beta} \left[ n(\epsilon - \theta B s - \mu \rho) e_i \cdot \delta e^i + n \frac{\partial \epsilon}{\partial \rho} \mu \delta \rho + n \frac{\partial \epsilon}{\partial s} \delta s + n \frac{\partial \epsilon}{\partial e_i} \cdot \delta e_i + n \frac{\partial \epsilon}{\partial g^{ij}} \delta g^{ij} \right] dv
\]

\[
- \int_S [n(\epsilon - \theta B s - \mu \rho)] \delta r da = 0
\]

(28)

where the surface integral arises from the variation of the interface and reflects the induced change in phase, i.e., accretion.

The main difficulty is to choose an appropriate set of independent variations in the bulk and at the interface that yields equations in a physically transparent form. To this end, let

\[
\omega := \epsilon - \theta B s - \mu \rho.
\]

(29)

5The choice of \( n_S \) pointing outward from phase \( \alpha \) is consistent with our previous convention on the use of \([\cdot]\).

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denote the grand canonical potential per unit cell. Further we introduce
\[ k_i := \frac{\partial \omega}{\partial g^{ij}} e^j, \quad t^i := n_i \frac{\partial \omega}{\partial e_i}, \quad t_i := (t^j \cdot e_i) e_j, \]
and we identify \( E^i \otimes k_i \) as the dislocation couple tensor and \( e^i \otimes t_i \) as the Cauchy stress tensor (Cermelli & Sellers, 1998). The choice of basis indicates that the Cauchy stress acts on the actual lattice, whereas the dislocation couple acts on the reference lattice. We also introduce the configurational stress tensor \( E^i \otimes c_i \), where
\[ c_i := \frac{\partial (n \omega)}{\partial e_i} = n \omega e_i - t_i - (g_j \times e_i) \times k_j. \]
is a generalized Eshelby relation containing an additional term due to the dislocations. Again the choice of basis indicates that the configurational stress, in contrast to the Cauchy stress, acts on the reference lattice. In terms of the quantities (30) and (31) the variation (28) can be expressed alternatively as
\[
\delta \Omega = \int_{\mathcal{B}^a \cup \mathcal{B}^b} \left[ n \left( \frac{\partial \epsilon^\alpha}{\partial \varrho} - \mu \right) \delta \varrho + n \left( \frac{\partial \epsilon^\beta}{\partial s} - \theta_B \right) \delta s + (c_i + \text{curl } k_i) \cdot \delta e^i \right] dv \\
- \int_S \left[ n \omega \delta r + n_s \cdot \left[ \delta e^i \times k_i \right] \right] da = 0, \tag{32}
\]
where we have used the divergence theorem and (18). The expression (32) of the first variation of the energy functional is now in a convenient form for deriving the appropriate necessary conditions.

The choice of the possible independent variations should reflect the relevant physical situation. We consider two different cases: one corresponding to no constraints on the possible variations, the other corresponding to when holonomicity is imposed as a constraint, thus excluding variations that create dislocations in the bulk.

### 4.1.1 Case I: unconstrained variations

- **Bulk Conditions:** We take
\[
\delta \varrho, \quad \delta s, \quad \delta e^i \tag{33}
\]
as the admissible class of independent variations in the continuous bulk regions. These variations allow defect creation and transport in the bulk. With (32) they yield the following necessary conditions:

- uniform chemical potential
\[
\frac{\partial \epsilon^\alpha}{\partial \varrho} = \frac{\partial \epsilon^\beta}{\partial \varrho} = \mu; \tag{34}
\]
- uniform temperature
\[ \frac{\partial e^\alpha}{\partial s} = \frac{\partial e^\beta}{\partial s} = \theta_B; \]  
(35)

- dislocation couple balance for each phase
\[ c_i + \text{curl} \ k_i = 0. \]  
(36)

The uniformity of the chemical potential (34) and temperature (35) are standard and represent chemical and thermal equilibrium. The dislocation couple balance (36) represents mechanical equilibrium. Additionally, it implies immediately the configurational force balance for each phase
\[ \text{div } c_i = 0, \]  
(37)

which, with the Eshelby relation (31), is itself equivalent to the Cauchy force balance
\[ \text{div } (e_i \otimes t_i) = 0, \]  
(38)

which is the more standard mechanical equilibrium condition. But provided that the lattice variations \( \delta e^i \) are arbitrary, relations (34)–(36) are the independent necessary conditions for equilibrium in the bulk.

*Interfacial Conditions:* We want to allow for defect creation and transport at the interface so that we take the variations of the lattice vectors \( \delta e^i \) on each side of the phase interface as independent, but require that \( \delta r \) be continuous across the interface since the two phases remain in contact. Thus the independent variations at \( \Sigma \) are
\[ \delta r, \ (\delta e^i)^\alpha, \ (\delta e^i)^\beta. \]  
(39)

They correspond to an incoherent interface. With this choice of independent variations at the surface, (32) yields as necessary interfacial conditions:

- continuity of the grand canonical potential
\[ [n_\omega] = 0; \]  
(40)

- vanishing of the individual tangential couples
\[ P(k_i)^\alpha = 0 \quad \text{and} \quad P(k_i)^\beta = 0. \]  
(41)

The continuity of the grand canonical potential (40) is standard and is due to the fact that the phases may not separate at the interface. The vanishing of the individual tangential couples reflects the fact that an incoherent interface must be in mechanical equilibrium with respect to both lattices. Moreover, this latter condition implies in turn the
- vanishing of the individual configurational tractions

\[(c_i)\alpha \cdot n_s = 0 \quad \text{and} \quad (c_i)\beta \cdot n_s = 0.\]  

(42)

As in the corresponding bulk conditions on the configurational stress, (42) are not independent conditions since the identity

\[\int_{S'} (c_i)\alpha \cdot n_s \, da = -\int_{\partial S'} (k_i)\alpha \cdot dl,\]  

(43)

(which holds for any subsurface \(S' \subset S\)) and (11) imply (42). Additionally, the identity

\[n_s \cdot [e^i \otimes t_i] n_s = [n_{\omega}] - n_s \cdot [e^i \otimes c_i] n_s - n_s \cdot [e^i \otimes (g^j \times e_i) \times k_j] n_s,\]  

(44)

which follows from the generalized Eshelby relation (31), shows that the continuity of the grand canonical potential is equivalent with (41) and (42) to the

- continuity of the normal Cauchy traction

\[n_s \cdot [e^i \otimes t_i] n_s = 0.\]  

(45)

Thus the independent equilibrium conditions at the incoherent interface are (41) and either (40) or, equivalently, (45).

### 4.1.2 Case II: holonomic variations (Born rule)

Since dislocations are in general created or transported when the lattice variations \(\delta e_i\) are arbitrary, the configurational force balance (37) and corresponding interface conditions (42) are consequences of the dislocation couple balance (36) and corresponding interface condition (41). We now introduce a restricted class of lattice variations that yield (37) and (42) as independent necessary conditions.

Consider the class of holonomically constrained variations for which the Born rule (14) holds: variations of the lattice basis \(\delta e_i\) are such that \(\text{curl} (\delta e_i) = 0\).

Thus away from the surface \(S\) the variations can be expressed in terms of the inverse deformation \(\chi\) by the relation

\[\delta e^i = (\text{grad} \, \delta \chi)^\top E_i.\]  

(46)

Since the external boundary \(\partial B\) is fixed, \(\delta \chi\) vanishes at \(\partial B\), which excludes any rigid body displacements. Thus the actual and varied states may be realized as deformations of the same perfect-lattice reference configuration \((\chi(B), E_i)\). In the terminology of Davini and Parry (1989), the actual and varied states are elastically related. This is false for arbitrary variations not vanishing at \(\partial B\), since in that case rearrangements such as slip may occur, so that the states \(e^i\) and \(e^i + \delta e^i\) are only neutrally related.

\(^7\)Rearrangements are changes of state which do not modify the local lattice microstructure. A discussion of the equilibrium conditions for a crystalline body when global rearrangements are allowed, is due to Fonseca and Parry (1992).
The Born rule excludes dislocations in the bulk but not necessarily at an incoherent interface. Remember that at a coherent interface, \( \chi \) is continuous, whereas at an incoherent interface, \( \chi \) is discontinuous. Thus with the Born rule \([14]\), the continuity of \( \chi \) implies the vanishing of the surface dislocation density \([10]\) whereas discontinuities in \( \chi \) may lead to nonvanishing surface dislocations.

In order to represent these two possibilities more succinctly, we introduce the quantities

\[
\delta_S \chi^i := (\delta \chi + (\nabla_{n_S} \chi) \delta \tau) \cdot E^i, \quad \nabla_{n_S} \chi := (\nabla \chi) n_s, \quad (47)
\]

which are, respectively, the components of the variation of the inverse deformation \( \chi \) following the variation of the interface \( S \) and the derivative of the deformation normal to the current interface. Note that \( \delta_S \chi^i \) is continuous when \( \chi \) is continuous:

\[
[\chi] = 0 \quad \Rightarrow \quad [\delta_S \chi^i] = 0. \quad (48)
\]

By a procedure analogous as before, we may write the first variation of the energy functional in the form

\[
\delta \Omega = \int_{B_\alpha \cup B_\beta} \left[ n \left( \frac{\partial \epsilon}{\partial \varrho} - \mu \delta \varrho + n \left( \frac{\partial \epsilon}{\partial s} - \theta B \right) \delta s + (\text{div} \ c) \delta \chi \cdot E^i \right] dv \\
- \int_S \left[ [c_i \delta_S \chi^i] \cdot n_s - n_s \cdot [(e^i \otimes t_i) n_s \delta \tau] \right] da = 0, \quad (49)
\]

where now the configurational stress component is defined as

\[
c_i := \frac{\partial(n \omega)}{\partial e^i} = n \omega e_i - t_i, \quad (50)
\]

so that

\[
(\nabla \chi)^T (E^i \otimes c_i) = n \omega 1 - e^i \otimes t_i \quad (51)
\]

corresponds to the usual Eshelby relation as expressed in the spatial description. As there are now no dislocations in the bulk, there is no dislocation contribution to \([51]\) and the configurational stress coincides with the classical Eshelby stress.

- **Bulk Conditions:** Taking as independent variations in the bulk

\[
\delta \varrho, \quad \delta s, \quad \delta \chi_i, \quad (52)
\]

we obtain now the following necessary conditions:

- **uniform chemical potential** \([34]\);
- **uniform temperature** \([35]\);
- **configurational force balance** \([37]\) for each phase.
Because of the Eshelby relation (50), the configurational force balance (37) in the bulk is equivalent to the Cauchy force balance (38). But for this holonomic case, the dislocation couples $k_i$ are constitutively indeterminate and are now defined by the couple balance (36). Thus the independent conditions with the class of holonomic variations are (34), (35), and either (37) or (38).

**Incoherent interfacial conditions:** We want to allow for surface dislocations at an incoherent interface, so that we take as the admissible class of independent variations

$$\delta r, \quad (\delta_S \chi^i)^\alpha, \quad (\delta_S \chi^i)^\beta.$$  

(53)

With this choice of independent variations, (49) yields the conditions:

- **vanishing the individual configurational tractions** (42);
- **continuity of the normal Cauchy traction** (45).

Additionally, the continuity of the grand canonical potential (40) is still equivalent to the continuity of the normal Cauchy traction (45), by relations (42) and (50).

The relations (12), (15) for incoherent interfaces with the class of holonomically constrained variations correspond precisely to the equilibrium results of Cermelli & Gurtin (1994) in the spatial description. The equivalent relations (16), (12) correspond to the expressions derived by Larché & Cahn (1978).

**Coherent interfacial conditions:** There are no surface dislocations associated with a coherent interface. Furthermore, variations that keep the interface coherent should preserve the continuity of $\chi$ at $S$, so that we restrict the class of variations to those such that

$$[\delta_S \chi^i] = 0.$$  

(54)

Thus the independent variations at $S$ are

$$\delta r, \quad \delta_S \chi^i.$$  

(55)

With this choice of independent variations, (49) yields the necessary conditions:

- **continuity of the configurational traction**

  $$[\mathbf{c}_i] \cdot \mathbf{n}_S = 0;$$  

  (56)

- **continuity of the normal Cauchy traction** (15).
These two conditions are equivalent to

- continuity of the Cauchy traction

\[ \mathbb{e}^i \otimes t_i n_s = 0; \quad (57) \]

- continuity of the normal configurational traction

\[ n_s \cdot \mathbb{E}' \otimes c_i n_s = [c_i] \cdot n_s = 0. \quad (58) \]

In this case, the continuity of the grand canonical potential does not generally hold. The independent relations \( (54) \) and \( (15) \) (or, equivalently, \( (57) \) and \( (58) \)) correspond to those derived by Cermelli & Gurtin (1994) in the context of nonlinear elasticity. These results are also equivalent to the more standard expressions based on a fixed reference configuration as originally derived by Eshelby (1970) and later by Robin (1974), Larché & Cahn (1978), and Grinfeld (1981).

4.2 Crystal-melt equilibrium

We now turn to the conditions for crystal-melt phase equilibrium. We identify the \( \alpha \)-phase as the crystalline solid and denote the melt quantities with the superscript \( F \).

The external boundaries are assumed impermeable and held fixed. Thus the total mass of the system is constant:

\[ M = M^\alpha + M^F = \int_{B^\alpha} n \rho dv + \int_{B^F} \rho^F dv, \quad (59) \]

with \( \rho^F \) the density per unit volume of the fluid. We assume that the total internal energy of the system is given by

\[ E = E^\alpha + E^F = \int_{B^\alpha} n \epsilon dv + \int_{B^F} \epsilon^F dv, \quad (60) \]

where \( \epsilon^F \) is the internal energy density per unit volume of fluid, and any surface energy has been assumed negligible. Furthermore, we assume that the entropy is additive:

\[ S = S^\alpha + S^F = \int_{B^\alpha} n s dv + \int_{B^F} s^F dv, \quad (61) \]

where \( s^F \) is the entropy density per unit volume of the fluid. Our constitutive assumptions are that:

\[ \epsilon = \epsilon^\alpha (e_i, g^{ij}, s, \rho), \quad \epsilon^F = \epsilon^F (s^F, \rho^F). \quad (62) \]

As before, our condition for equilibrium is

\[ \delta \Omega = \delta E - \theta_B \delta S - \mu \delta M = 0. \quad (63) \]

\(^8\text{The normal configurational traction is also called the driving traction at the interface.}\)
4.2.1 Unconstrained variations

- **Bulk conditions:** We take
  \[ \delta \rho^F, \delta s^F, \delta \varrho, \delta s, \delta \mathbf{e}_i \]  
  as the independent variations in the corresponding continuous bulk regions. With this choice of independent variations, the analog of (49) yields the following independent conditions:

  - uniform chemical potential
    \[ n \frac{\partial e^\alpha}{\partial \varrho} = \frac{\partial e^F}{\partial \rho} = \mu; \]  
    \[ n \frac{\partial e^\alpha}{\partial \varrho} = \frac{\partial e^F}{\partial \rho} = \mu; \]  
  
  - uniform temperature
    \[ n \frac{\partial c^\alpha}{\partial s} = \frac{\partial e^F}{\partial s} = \theta_B; \]  
  
  - dislocation couple balance in the crystalline solid phase
    \[ \mathbf{c}_i + \text{curl } \mathbf{k}_i = 0. \]  

As before, the couple balance (67) implies immediately the **configurational force balance in the crystalline solid phase** which itself is equivalent to the **Cauchy force balance in the crystalline solid phase**. But if we restrict the admissible lattice variations to the holonomically constrained class, then configurational force balance or Cauchy force balance replaces the couple balance (67) as the mechanical equilibrium condition.

- **Interfacial conditions:** We choose
  \[ \delta r, \delta \mathbf{e}_i \]  
  as the independent variations at the interface \( S \). They allow the creation and transport of defects in the crystalline solid phase. We obtain:

  - continuity of the grand canonical potential
    \[ n \omega = \omega^F; \]  
  
  - vanishing of the tangential couples of the crystalline solid
    \[ \mathbf{P} \mathbf{k}_i = 0. \]
Additionally we obtain as a consequence of (70) the vanishing of the configurational traction of the crystalline solid
\[ c_i \cdot n_S = 0. \]  
(71)

The continuity of the normal Cauchy traction
\[ n_S \cdot (e^i \otimes t_i) n_S = \omega^F = \epsilon^F - \theta^F s^F - \mu^F, \]  
(72)
is equivalent to (69) at \( S \) provided (70) and the Eshelby relation (31) for \( c_i \).

Again, if we restrict the admissible lattice variations to the holonomically constrained class, then (71) replaces (70) as the equilibrium conditions at \( S \). In this case, the relations (69), (71) correspond to those derived by Larché & Cahn (1978).

5 Equilibrium Equations with Interfacial Energy

The presence of dislocations at the interface as well as the crystalline structure of the material may modify the equilibrium conditions at the interface. One way to take this into account is to introduce an interfacial energy density that depends upon the local state of the interface. We now extend the previous results to include such an interfacial energy density. Since the conditions for the bulk region do not change, we consider only the appropriate interfacial conditions.

5.1 The interfacial energy density

One possible choice of variables to describe the local state of the interface is
\[ (e^i)^\alpha, \quad (e^i)^\beta, \quad n_S, \]  
(73)
which reflect the local lattice structure on either side of the interface and the orientation of the interface with respect to the current lattice. When the Born rule holds, this choice becomes
\[ (\text{grad} \, \chi)^\alpha, \quad (\text{grad} \, \chi)^\beta, \quad n_S, \]  
(74)
which corresponds to the variables used by Cermelli & Gurtin (1994). Unfortunately, the dependence on the actual orientation is misleading, since \( n_S \) does not properly account for the crystallographic orientations of the individual lattices relative to the interface. A choice of variables that better captures the relevant physics at the interface is
\[ \Phi[e^i], \quad n^\alpha, \quad n^\beta, \]  
(75)
where
\[ n^\alpha = \frac{n_S \cdot (e_i)^\alpha E^i}{|n_S \cdot (e_i)^\alpha E^i|}, \quad n^\beta = \frac{n_S \cdot (e_i)^\beta E^i}{|n_S \cdot (e_i)^\beta E^i|}. \]  
(76)
The choice of variables (75) is motivated by the observation that
• $P[e^i]$ is the dislocation content of the interface (cf. (10));

• $n^\alpha$ and $n^\beta$ are the unit normals to the interface in the reference lattices of each phase. While it is standard in theories of coherent interfaces to include the contribution of the orientation of the interface normal in the superficial energy, for incoherent interfaces the energy depends on the orientation of the interface normal with respect to both lattices;

• the fields $(P[e^i], n^\alpha, n^\beta)$ on $S$ may be assigned independently from each other.

Again, the Born rule simplifies (75) to

$$ P[\nabla \chi], \quad n^\alpha, \quad n^\beta,$$

(77)

where now

$$n^\alpha = \frac{((\nabla \chi)^-)^\alpha n_s}{|((\nabla \chi)^-)^\alpha n_s|}, \quad n^\beta = \frac{((\nabla \chi)^-)^\beta n_s}{|((\nabla \chi)^-)^\beta n_s|}. \quad (78)$$

The variables (77) correspond to a special case of those used by Leo and Sekerka (1989).

Henceforth, we shall restrict the energy density function to have the special form

$$\varphi = \tilde{\varphi}(P[e^i], n^\alpha, n^\beta). \quad (79)$$

For calculations, however, we will find it more convenient to use the more general energy

$$\varphi = \hat{\varphi}((e^i)^\alpha, (e^i)^\beta, n_s) \quad (80)$$

and then insert (79) at the end of the calculation. For example, we denote by

$$\kappa_i^\alpha = \frac{\partial \hat{\varphi}}{\partial (e^i)^\alpha}, \quad \kappa_i^\beta = \frac{\partial \hat{\varphi}}{\partial (e^i)^\beta}, \quad \xi = \frac{\partial \hat{\varphi}}{\partial n_s} \quad (81)$$

the derivatives of (80) with respect to its arguments, which are essentially surface stresses. They must however satisfy the following relations obtained by the chain rule and (74):

$$\kappa_i^\alpha = -P \frac{\partial \tilde{\varphi}}{\partial (P[e^i])} - \frac{n_s \cdot (e_i)^\alpha}{|n_s \cdot (e_j)^\alpha E_j|} \left( P^\alpha \frac{\partial \tilde{\varphi}}{\partial n^\alpha} \cdot E^k \right) (e_k)^\alpha,$$

$$\kappa_i^\beta = P \frac{\partial \tilde{\varphi}}{\partial (P[e^i])} - \frac{n_s \cdot (e_i)^\beta}{|n_s \cdot (e_j)^\beta E_j|} \left( P^\beta \frac{\partial \tilde{\varphi}}{\partial n^\beta} \cdot E^k \right) (e_k)^\beta,$$

$$\xi = \frac{1}{|n_s \cdot (e_j)^\alpha E_j|} \left( P^\alpha \frac{\partial \tilde{\varphi}}{\partial n^\alpha} \cdot E^k \right) (e_k)^\alpha + \frac{1}{n_s \cdot (e_j)^\beta E_j} \left( P^\beta \frac{\partial \tilde{\varphi}}{\partial n^\beta} \cdot E^k \right) (e_k)^\beta - (n_s \cdot [e^i]) P \frac{\partial \tilde{\varphi}}{\partial (P[e^i])} - \left( \frac{\partial \tilde{\varphi}}{\partial (P[e^i])} \cdot n_s \right) P[e^i], \quad (82)$$

20
with projections

\[ P^\alpha := 1 - n^\alpha \otimes n^\alpha, \quad P^\beta := 1 - n^\beta \otimes n^\beta. \]  \tag{83} 

An immediate consequence of (82) is that the surface stresses \( \kappa_i^{\alpha,\beta} \) are tangential to \( S \):

\[ \kappa_i^\alpha \cdot n_s = \kappa_i^\beta \cdot n_s = 0. \]  \tag{84} 

5.2 The variational calculation

When interfacial structure is taken into account, the grand canonical potential (26) includes a contribution from surface energy:

\[ \Omega := E + I - \theta B S - \mu M \]  \tag{85} 

The variation of the interfacial energy is given by

\[ \delta \int_S \varphi \, da = \int_S \left\{ \kappa_i^\alpha \cdot (\delta_S e^i)^\alpha + \kappa_i^\beta \cdot (\delta_S e^i)^\beta + (\text{div}_S \xi - K \varphi) \delta r \right\} \, da, \]  \tag{86} 

where \( \delta_S \) is the variation following the interface (i.e., \( \delta_S f = \delta f + \text{grad}_n f = \delta f + (\text{grad} f)n_s \) for any bulk function restricted to \( S \), \( K \) is the mean curvature of \( S \), \( \text{grad}_S \) and \( \text{div}_S \) are the superficial gradient and divergence on \( S \), and we have used the identities (cf. Leo and Sekerka, 1989)

\[ \delta \int_S \varphi \, da = \int_S (\delta_S \varphi - K \varphi \delta r) \, da, \quad \delta_S n_s = -\text{grad}_S \delta r. \]  \tag{87} 

Remember that the interfacial stresses \( \kappa_i^\alpha, \kappa_i^\beta \) and \( \xi \) are required to satisfy (82).

With (86) added to the surface integral in (32), the interfacial terms in the variation of the grand canonical potential (85) can be expressed as

\[ \int_S \left\{ (\text{div}_S \xi - K \varphi - [n\omega] - [n_s \times k_i \cdot \text{grad}_n e^i]) \right\} \, dr 
+ \kappa_i^\alpha \cdot (\delta_S e^i)^\alpha + \kappa_i^\beta \cdot (\delta_S e^i)^\beta - [n_s \times k_i \cdot (\delta_S e^i)] \right\} \, da. \]  \tag{88} 

5.2.1 Case I: unconstrained variations

When variations are unconstrained in the sense of Section 4.1.1, dislocations are allowed to be created and to move both in the bulk and at the interface. We choose as the admissible class of independent variations at such an incoherent interface

\[ \delta r, \quad (\delta_S e^i)^\alpha, \quad (\delta_S e^i)^\beta. \]  \tag{89} 

This set is more convenient than (39) due to the additional interfacial structure. The interfacial equilibrium conditions which replace (40) and (41) are thus
interfacial normal force balance
\[ \text{div}_S \mathbf{\xi} - K \varphi - [n_\omega] + \kappa^\alpha_i \cdot (\text{grad}_S e^i)^\alpha + \kappa^\beta_i \cdot (\text{grad}_S e^i)^\beta = 0; \quad (90) \]

interfacial couple balances
\[ \kappa^\alpha_i - n_s \times (k^i)^\alpha = 0 \quad \text{and} \quad \kappa^\beta_i + n_s \times (k^i)^\beta = 0. \quad (91) \]

The interfacial relations (91) state that the couples \( n_s \times (k^i)^\alpha \) acting on interfacial dislocations and due to the short-range interactions with bulk dislocations must balance pointwise the forces \( \kappa^\alpha_i, \beta \) in the interface due to interfacial dislocations.

The surface divergence of (91) along with the symmetry of the curvature tensor imply the

interfacial configurational force balances
\[ \text{div}_S \mathbf{\kappa}^\alpha_i - (c^i)^\alpha \cdot n_S = 0, \quad \text{and} \quad \text{div}_S \mathbf{\kappa}^\beta_i + (c^i)^\beta \cdot n_S = 0, \quad (92) \]

which generalizes (42). However these are not independent conditions, but follow as simple consequences of the interfacial couple balances (91). Relations (92) are force balances that state that the “elastic” configurational traction acting on any portion \( R \) of the interface from each phase must be balanced by the interfacial contact force, which tends to reorganize interfacial dislocations in \( R \) according to their mutual interaction.

5.2.2 Case II: holonomic variations.

In this case the variations \( \delta_S e^i \) may be expressed in terms of the inverse deformation through (46) and, by the identity
\[ P \delta_S e^i = \text{grad}_S (\delta_S \chi^i) - (\text{grad}_S (n_s \delta r))^\top e^i, \]
the surface integral in the variation of the grand canonical potential (85) becomes, granted (84),
\[ -\int_S \left\{ [\text{div}_S \kappa^\alpha_i - (c^i)^\alpha \cdot n_s] (\delta_S \chi^i)^\alpha + [\text{div}_S \kappa^\beta_i + (c^i)^\beta \cdot n_s] (\delta_S \chi^i)^\beta \right. \\
- \left. \left( \text{div}_S \mathbf{\xi} - K \varphi + (e^i)^\alpha \cdot n_s \text{div}_S \kappa^\alpha_i + (e^i)^\beta \cdot n_s \text{div}_S \kappa^\beta_i \right. \\
+ \kappa^\alpha_i \cdot (\text{grad}_S e^i))^\alpha + \kappa^\beta_i \cdot (\text{grad}_S e^i))^\beta - n_s \cdot \left[ e^i \otimes t_i \right] n_s \delta r \right\} d\theta^3 \]
where \( c_i \) is now given by (50).

- Incoherent interfacial conditions: We take
\[ \delta r, \quad (\delta_S \chi^i)^\alpha, \quad (\delta_S \chi^i)^\beta \quad (94) \]
as the admissible class of independent variations. This yields as generalizations of (12) and (43) the interfacial equilibrium conditions:
- interfacial normal force balance

\[
\text{div}_S \xi - K \varphi + (e^i)^\alpha \cdot n_S \text{div}_S \kappa_i^\alpha + (e^i)^\beta \cdot n_S \text{div}_S \kappa_i^\beta + \kappa_i^\alpha \cdot (\text{grad}_{n_S} e^i)^\alpha + (\kappa_i)^\beta \cdot (\text{grad}_{n_S} e^i)^\beta = n_S \cdot \left[ e^i \otimes t_i \right] n_S \quad (95)
\]

- interfacial configurational force balances (92).

Now however (92) are independent conditions. Furthermore, (95) is equivalent, granted (92), to (90). The equilibrium interfacial conditions (90) and (92) are appropriate to a constrained situation in which dislocations cannot be created or move in the bulk and, for this case, are equivalent to the relations derived by Cermelli & Gurtin (1994).

The non-holonomic equilibrium conditions (91) are stricter than their holonomic counterparts (92); interfaces which are in equilibrium governed by (91), i.e., when dislocations are absent in bulk, need not be in equilibrium if dislocations were allowed, since these dislocations could exert forces on the interface. As an example, consider a grain boundary between undeformed grains in a polycrystalline material, and assume that the grains are rotated one relative to another:

\[
(e_i)^\alpha = E_i, \quad (e_i)^\beta = Q E_i, \quad (96)
\]

with \(Q\) a rigid body rotation. Assume that dislocations are not allowed in bulk (holonomy), fix \(\varrho = \varrho_0\) and \(s = s_0\), and take the grand canonical potential such that, by objectivity, \(\omega(E_i, \varrho_0, s_0) = \omega(Q E_i, \varrho_0, s_0) = 0\) is a minimum, so that \((e_i)^\alpha = (e_i)^\beta = 0\) (cf. (50)). Then, according to the holonomic equilibrium condition (92), any interface such that \(\kappa_i^{\alpha,\beta}\) is a constant (for instance planar interfaces with a uniform dislocation density) is in equilibrium. On the other hand, if dislocations are free to move to and from the interface from the bulk, equilibrium is established by the non-holonomic relations (91), and such an interface (planar with a uniform dislocation density) may well not be at equilibrium, as for instance when \(\kappa_i^{\beta,\alpha}\) is non-zero but \(k_i\) is zero.

5.3 The equilibrium conditions projected on a slip system

The transport of defects is commonly interpreted in terms of a crystallographic slip system, where slip typically takes place along lattice vectors. Some insight into the structure of the bulk and interfacial equilibrium conditions may be gained by introducing such a crystallographic slip system and projecting the equations onto this slip system. The resulting relations involve forces acting within the slip plane, which may be interpreted as forces on the dislocations moving by glide on such a plane.

More precisely, let

\[
\sigma \otimes \mu, \quad (97)
\]
be a slip system, with $\sigma$ a slip vector and $\mu$ the slip-plane normal, with the restriction that $\mu \cdot \sigma = 0$. The slip vectors are taken to be lattice vectors, which correspond to the Burgers vectors of the dislocations whose motion generates the slip, while the slip-plane normals are reciprocal lattice vectors.

The slip system is measured in the reference lattice. Its counterpart in the current lattice is represented by the set of vectors

$$\sigma^i m^i, \quad \text{with} \quad \sigma^i := \sigma \cdot E^i, \quad (98)$$

and

$$m^i = \mu_j e^j, \quad \text{with} \quad \mu_j := \mu \cdot E_j. \quad (99)$$

Note that $\sigma^i$ and $\mu_i$ are constants.

Projecting the bulk dislocation couple balance (36) onto the slip system (98), we obtain

$$\sigma^i c_i \cdot m^i + \sigma^i \mu_j (k_i \cdot g^j) + \sigma^i \text{div} (k_i \times m) = 0, \quad (100)$$

with the configurational stress given by (31). Each term in (100) has a suggestive interpretation, namely:

- the term $\sigma^i c_i \cdot m^i$ is the configurational shear across the slip plane (recall in fact that $m^i$ is the current slip-plane normal, while $\sigma^i$ is contained in the referential slip plane), and may be viewed as forcing or inhibiting slip along the corresponding system. It may be identified with the so-called long-range stress on dislocations in a dislocated crystal.

- the term $\sigma^i k_i \times m^i$ is the couple acting in the slip plane on dislocations with Burgers vectors parallel to $\sigma^i$. It may be identified with the short-range contact couple due to the presence of other dislocations.

Projection of the interfacial couple balances (91) onto a phase-$\alpha$ slip system yields

$$({\sigma}^i)^{\alpha} m^i \cdot \kappa_i^{\alpha} - (\sigma^i)^{\alpha} (k_i^{\alpha} \times m) \cdot n_s = 0. \quad (101)$$

The couple $m \times (k_i^{\alpha})$ is tangential to the slip plane, while $\kappa_i^{\alpha}$ is tangential to the interface. Consider now the intersection line (say $L$) of the slip plane with the tangent plane to the interface. A straightforward calculation shows that

- the term $(\sigma^i)^{\alpha} m^i \cdot \kappa_i^{\alpha}$ represents the projection onto the direction $m - (m \cdot n_s) n_s$, the perpendicular to $L$ in the tangent plane to the interface, of the interfacial force on a dislocation with Burgers vector $\sigma$.

- the term $(\sigma^i)^{\alpha} (m \times (k_i^{\alpha})) \cdot n_s$ represents the projection onto the direction $n_s - (m \cdot n_s) m$, the perpendicular to $L$ in the slip plane, of the couple due to bulk dislocations on a defect with Burgers vector $\sigma$. 

24
A dislocation lying along the intersection of the slip plane and the interface is parallel to \( L \); the only relevant component of any force acting on this dislocation is the component orthogonal to \( L \). The couple balance requires that these components of the opposing couples on the dislocation be equal. Therefore \((101)\) represents a balance of couples which tend to redistribute the dislocation density at the interface and couples which tend to move the dislocations away from the interface along their slip planes, due to the presence of bulk dislocations. Two such independent balances are needed, one for each phase, since dislocations may be transferred to and from the interface from each crystal phase, and their slip systems are independent.

6 Incremental Deformations (without Interfacial Energy)

In many models of defective materials, it is common to introduce an elastic-plastic decomposition of the macroscopic deformation. In our formulation there is no need to introduce the notion of deformation from a fixed reference configuration. In order to compare the two approaches, however, we now introduce such an elastic-plastic decomposition. We follow the procedure of Davini (1989) by superposing a conventional elastic deformation onto a dislocated crystalline solid, where the elastic deformation does not change the defectivity of the crystal. We then derive the necessary equilibrium conditions for the resulting incremental theory.

We identify \( B \), which corresponds to the region occupied by the crystalline solid in a dislocated state, to the intermediate configuration in an elastic-plastic decomposition. In contrast to the standard formulations of the elastic-plastic decomposition, we do not assume that \( B \) is stress-free. Now consider a deformation \( f : B \to \mathbb{R}^3 \) from this dislocated state that is continuous but possibly non-smooth across the surface \( S \). Although the incremental deformation is continuous everywhere, the interface can be incoherent due to the presence of surface dislocations in the dislocated intermediate configuration. We assume that the lattice vectors transform according to the Born rule under the deformation \( f \):

\[
\mathbf{e}_i \mapsto \mathbf{e}_i := F \mathbf{e}_i, \quad \mathbf{e}^i \mapsto \mathbf{e}^i := F^{-\top} \mathbf{e}^i,
\]

(102)

where the \( \mathbf{e}_i \) are the current lattice vectors in the deformed region \( f(B) \) and \( \mathbf{F} = \text{grad} f \). The dislocation density associated to the field \( \mathbf{e}^i \) is given by

\[
\mathbf{g}^i = \det (\mathbf{F}^{-1}) \mathbf{F} g^i,
\]

(103)

which yields

\[
\mathbf{g}^{ij} = g^{ij}.
\]

(104)

Thus the dislocation density per unit cell is unaffected by the incremental elastic deformation.
The lattice variations of this resulting state can be expressed as \((\delta \mathbf{e}_i, \delta \varrho)\), which, as before, are assumed to vanish on the external boundary \(\partial \mathcal{B}\). Consider now the additive composition of the two configurations

\[
\mathbf{e}_i \lambda := \mathbf{e}_i + \lambda \delta \mathbf{e}_i, \quad \varrho_\lambda := \varrho + \lambda \delta \varrho
\]

where \(\lambda\) is a small parameter. This composition induces a corresponding variation in any functional \(\Phi\) depending on the composed configuration:

\[
\delta \Phi = \frac{\partial}{\partial \lambda} \Phi[\mathbf{e}_i \lambda, \varrho_\lambda] \bigg|_{\lambda=0}.
\]

Note however that

\[
\delta \mathbf{e}_i = (\delta F) \mathbf{e}_i - (\mathbf{e}_i \cdot \delta \mathbf{e}_j) \mathbf{F}_{ij}.
\]

Because of (102) and (104), we may assume that the energy densities are functions of the form

\[
\epsilon = \epsilon^\alpha(\mathbf{e}_i, \mathbf{F}, g, \varrho, \psi, s) \quad \text{for phase } \alpha,
\]

\[
\epsilon = \epsilon^\beta(\mathbf{e}_i, \mathbf{F}, g, \varrho, \psi, s) \quad \text{for phase } \beta,
\]

where the unbarred quantities refer to the dislocated configuration \(\mathcal{B}\). We introduce the incremental Piola stress

\[
\mathbf{T}_R := n \frac{\partial \epsilon}{\partial \mathbf{e}_i} \otimes \mathbf{e}_i = n \frac{\partial \epsilon}{\partial \mathbf{F}},
\]

so that the Eshelby relation (31) becomes

\[
c_i := \frac{\partial (n \omega)}{\partial \mathbf{e}_i} = n \omega \mathbf{e}_i - \mathbf{T}_R \mathbf{F}_{ii} - (g_{ij} \times \mathbf{e}_i) \times \mathbf{k}_j
\]

due to the superposed deformation.

Thus the expression (28) for the variation of the energy functional becomes

\[
\delta \Omega = \int_{\mathcal{B}^0 \cup \mathcal{B}^\beta} \left[ n \left( \frac{\partial \epsilon}{\partial \varrho} - \mu \right) \delta \varrho + n \left( \frac{\partial \epsilon}{\partial \psi} - \theta_B \right) \delta \psi \right.
\]
\[
+ (c_i + \text{curl } \mathbf{k}_i) \cdot \delta \mathbf{e}_i - (\text{div } \mathbf{T}_R) \cdot \delta \mathbf{f} \bigg] \, dv
\]
\[
- \int_S \left[ (n \omega - \mathbf{n}_s \cdot \mathbf{F}^T \mathbf{T}_R \mathbf{n}_s) \delta r + \mathbf{n}_s \cdot \| \delta \mathbf{e}_i \times \mathbf{k}_i \|ight.
\]
\[
+ \| \mathbf{T}_R \mathbf{n}_s \| \cdot \delta \mathbf{f} \bigg] \, da = 0,
\]

where we have used the identity

\[
-\| \mathbf{T}_R \mathbf{n}_s \cdot \delta \mathbf{f} \| = -\| \mathbf{T}_R \mathbf{n}_s \| \cdot \delta \mathbf{s} + \mathbf{n}_s \cdot \| \mathbf{F}^T \mathbf{T}_R \mathbf{n}_s \| \delta r,
\]

and introduced

\[
\delta \mathbf{s} := \delta \mathbf{f} + (\text{grad}_{\mathbf{n}_s} \mathbf{f}) \delta r = \delta \mathbf{f} + \mathbf{F} \mathbf{n}_s \delta r,
\]
which is the variation of the deformation \( f \) following the variation of the interface. Notice that the continuity of \( f \) implies the continuity of \( \delta_S f \). The difference between (111) and (32) is due to the superposed elastic deformation \( f \).

We take as the admissible class of independent variations in bulk:

\[
\delta \rho, \quad \delta s, \quad \delta f, \quad \delta e. \tag{114}
\]

The introduction of the incremental deformation \( f \) provides an additional admissible variation to (33). This choice in (111) leads to the following necessary conditions:

9 - uniform chemical potential

\[
\frac{\partial \epsilon^\alpha}{\partial \rho} = \frac{\partial \epsilon^\beta}{\partial \rho} = \mu; \tag{115}
\]

- uniform temperature

\[
\frac{\partial \epsilon^\alpha}{\partial s} = \frac{\partial \epsilon^\beta}{\partial s} = \theta_B; \tag{116}
\]

- Piola force balance for each phase

\[
\text{div} \, \mathbf{T}_R = 0; \tag{117}
\]

- dislocation couple balance for each phase

\[
\mathbf{c}_i + \text{curl} \, \mathbf{k}_i = 0. \tag{118}
\]

As in the previous unconstrained cases, the couple balance (118) implies immediately the configurational force balance for each phase

\[
\text{div} \, \mathbf{c}_i = 0, \tag{119}
\]

but, importantly, it is \textit{not equivalent} to the force balance (117). The independent conditions in the bulk are (115)–(118). In particular, there are two distinct mechanical equilibrium conditions: the couple balance (118) enforces mechanical equilibrium of the dislocated intermediate region \( B \); the force balance (117) enforces mechanical equilibrium of the elastically deformed region \( f(B) \). Interestingly, both the intermediate and the current configurations must be in mechanical equilibrium.\(^9\)

\(^9\)The derivatives are, as before, with respect to the position \( x \), which is now in the reference configuration for the incremental elastic deformation.

\(^{10}\) Both (117) and (118) correspond to equations derived variationally by Le & Stumpf (1996) in a continuum theory of dislocations with a postulated elastic-plastic decomposition, though they were not interpreted as the mechanical equilibrium conditions in the actual and intermediate configurations.
If we restrict the admissible lattice variations to the holonomically con-
strained class (i.e., the Born rule) then (119) replaces (118) as the mechanical
equilibrium condition in the intermediate configuration. Then both the config-
urational force balance (119) and the standard force balance (117) are needed
to enforce mechanical equilibrium.

At the interface we take as the admissible independent variations
\[ \delta r, \quad \delta S, \quad (\delta e^i)^\alpha, \quad (\delta e^i)^\beta. \] (120)
They yield the following interface conditions:

- continuity of incremental normal Eshelby traction
  \[ n_s \cdot [n_\omega 1 - F^T T_R] n_s = 0; \] (121)

- continuity of incremental Piola traction
  \[ [T_R] n_s = 0; \] (122)

- vanishing of the individual tangential couples
  \[ P(\mathbf{k}_i)^\alpha = 0 \quad \text{and} \quad P(\mathbf{k}_i)^\beta = 0. \] (123)

Both (121) and (123) are standard equilibrium conditions for coherent interfaces,
whereas (123) is the condition for mechanical equilibrium for an incoherent in-
terface. Both sets of conditions arise because the interface is coherent under the
superposed elastic deformation, but incoherent in the intermediate dislocated
configuration. As in the bulk, we see that the interface must be in equilibrium
in both configurations when an elastic-plastic decomposition is introduced.

If we restrict the lattice variations in the intermediate configuration to the
holonomically constrained class, then the vanishing of the individual configura-
tional tractions in the intermediate configuration replaces the equilibrium con-
dition (123). Note that this configurational stress differs from the incremental
Eshelby stress, which arises from the elastic part of the deformation.

7 Discussion

One way of introducing the notion of a discrete crystalline lattice into a macro-
scopic continuum model is through additional fields that represent, for example,
the lattice basis vectors of the crystalline structure at each point. It is com-
mon however to eliminate these additional degrees of freedom by means of the
Born rule, which states that the lattice vectors at each point deform with the
gradient of the macroscopic deformation. Thus a crystalline body is reduced
to an anisotropic elastic continuum, which remembers its lattice structure only
through the symmetry of the constitutive relations. This approach fails when
defects such as dislocations have to be accounted for in the model, since the
Born-rule no longer holds. In this case the macroscopic deformation gradient
fails to describe the true local ordering of the lattice.

In this work, we use the kinematic ideas of Davini and Parry on defective
crystals to construct a model of crystalline solid equilibrium. The basic assump-
tion is that the defect density is sufficiently small, so that an average ordering
is still recognizable locally. At each spatial point of the solid a lattice basis may
therefore be assigned, but these local descriptions need not match globally to
yield a smooth deformation of a perfect crystal. Dislocations are then viewed as
the obstruction to patching together such local lattice bases to a global lattice
basis.

Using a variational framework, we obtain equilibrium equations for the bulk
and for incoherent interfaces in the presence of vacancies and dislocations with-
out assuming the validity of the Born rule. Although the mechanical equilib-
rium equations involve dislocation couples, indeed they also imply the more
familiar equilibrium conditions ensuing from the Cauchy and configurational
force balances. We discuss how these equations simplify when the Born rule
is imposed as a constraint on the possible lattice variations so that the defect
density vanishes in bulk, and also when coherent boundaries are considered. In
these constrained cases, our results correspond to those previously derived by
Larché & Cahn (1978), Leo & Sekerka (1989), and Cermelli & Gurtin (1994).
Importantly, our unconstrained results provide a generalization to their work,
which only dealt with conventional elastic bodies, or, in our language, holonomic
microstructures.

In order to compare to common models involving an elastic-plastic decom-
position of the strain, we also discuss an extended model, in which we superpose
conventional elastic deformations onto equilibrium states of a dislocated crystal.
The resulting system for the bulk is composed of a force balance that enforces
mechanical equilibrium of the current configuration, together with a couple bal-
ance enforcing the mechanical equilibrium of the dislocated intermediate con-
figuration. Such bulk conditions have also been derived by Le & Stumpf (1996)
in a slightly different context. The interfacial conditions are composed of the
standard coherency relations requiring the continuity of the Piola traction and
the continuity of the usual Eshelby-stress traction, but complemented by an
incoherent relation requiring the vanishing of the individual tangential couples,
which enforces the equilibrium of the interface with respect to the lattices of
each phase in the intermediate dislocated configuration.

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