

Article

An Algebraic Reparametrization of Phase-Specific Strains in Phase-Field Models for Microstructure Evolution

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Abstract

In a recently published continuum thermodynamic approach to the phase-field method, the order parameter is considered an internal state variable, and the phase-field method is interpreted as an approximation of the corresponding sharp-interface theory. The approach involves phase-specific strains and stresses within the diffuse interface region. In the present contribution, the interpolation relation for the effective strain within the diffuse interface is used to obtain an algebraic reparametrization in which the phase-specific strains and their rates are expressed by the effective strain, the effective strain rate, and the corresponding strain jump and its rate. The reparametrization defines a bijective mapping from the two phase-specific strains to the effective strain and the strain jump and therefore preserves the dimension of the mechanical state space. It modifies the thermodynamic forces conjugate to the selected rates and, consequently, the order-parameter and mechanical contributions to the diffuse-interface dissipation, while the total dissipation remains unchanged. At the same time, the heat conduction equation obtained in the original formulation remains unchanged since the corresponding derivation already uses the phase-specific stresses and strain rates in the mechanical power contribution. The algebraic reparametrization is generalized to the multiphase-field method based on internal state variables.

Keywords: phase-field method; diffuse interface; internal state variable; continuum thermodynamics; dissipation inequality; crystalline materials



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1. Introduction

1.1. Motivation and Scope

The phase-field method provides a numerically efficient framework for the treatment of evolving microstructures with complex interface geometries since no explicit tracking of sharp interfaces is required, cf., e.g., [1–3]. It is widely applied to simulations of solidification, crack propagation, and microstructure evolution in crystalline materials, including precipitate evolution, grain growth, and mechanically coupled phase transformations, cf., e.g., [4–9]. Multiphase-field models have also been applied to isothermal and non-isothermal polymer crystallization and the associated evolution of crystal morphologies, cf., e.g., [10,11]. In Prahs et al. [12], the phase-field method is formulated from the viewpoint of continuum thermodynamics by interpreting the order parameter as an internal state

variable. In this approach, a volumetric diffuse-interface region approximates the sharp singular surface. The corresponding dissipation inequality is then exploited to determine the evolution of the order parameter. In this regard, the formulation contains phase-specific strains and stresses in the diffuse interface region. The present contribution shows how the phase-specific strains and their rates can be reparametrized in terms of the effective strain, the strain jump, and the corresponding rates.

1.2. Relation to Previous Work

Different approaches exist for the treatment of mechanical fields in diffuse interfaces, including interpolation-based and homogenization-based schemes as well as approaches motivated by sharp-interface jump conditions, cf., e.g., [8,13–15]. Mosler et al. [16] determine the mechanical coupling between coexisting phases through partial rank-one relaxation of the averaged (incremental) bulk energy in a finite-deformation setting. Svendsen et al. [17] develop a finite-deformation chemomechanical framework in which phase-specific compositions and deformation gradients are expressed in terms of mixture quantities and phase differences. These differences are treated as internal variables of the mixture, with their evolution governed by relaxation equations. In the equilibrium limit, the corresponding phase contrasts are determined by minimization of the mixture bulk free energy. In the method of Schneider et al. [13], the phase-specific deformation gradients are first expressed in terms of the averaged deformation gradient and deformation-gradient jump vectors by volumetric averaging and the Hadamard condition, cf., Schneider et al. [13], Equations (13)–(15). The jump vectors are then determined from traction continuity, cf., [13], Equations (17)–(19), with the corresponding multiphase construction given in [13], Equations (28)–(35). Consequently, the phase-specific deformation gradients enter the strain energy density in [13], Equation (44), as dependent reconstructed quantities. Their induced order-parameter dependence is accounted for by the chain rule in [13], Equation (45), leading to the stress-interaction contributions in [13], Equations (49) and (50). The present contribution does not introduce an additional jump-condition-based homogenization method. Instead, it starts from the phase-specific strains as mechanical state variables while retaining the order parameter as an internal state variable of the continuum thermodynamic approach of Prahs et al. [12]. For each fixed value of the order parameter, the phase-specific strains are replaced by the effective strain and the strain jump through an invertible transformation. The order parameter itself remains unchanged, and the dimension of the mechanical state space is preserved.

1.3. Objectives of the Present Work

The objective of the present work is to determine the thermodynamic consequences of the invertible strain reparametrization within the continuum thermodynamic phase-field and multiphase-field methods based on internal state variables developed by Prahs et al. [12,18]. For this purpose, the material time derivatives of the phase-specific free energies are expressed in terms of the transformed mechanical rates, and the resulting order-parameter and mechanical contributions to the diffuse-interface dissipation are derived. The relation of the resulting stress-interaction contributions to the variational method of Schneider et al. [13] is established, and the implications of the reparametrization for the heat conduction equations are assessed.

1.4. Contribution and Scope

The stress-interaction contribution itself is established in mechanically coupled phase-field formulations, including in the work of Schneider et al. [13], Equations (49) and (50). Its counterpart is already present in sharp-interface equilibrium conditions for coherent solids, cf. Johnson and Alexander [19], Equation (32), and Voorhees and Johnson [20],

Equation (34). The connection between the corresponding phase-field contribution and the Gibbs–Thomson condition is explicitly discussed by Schneider et al. [21], Section 3.4, Equations (75)–(77). The present work shows that the stress-interaction contribution is implicitly contained in the phase-specific free-energy rates of the internal state variable framework developed by Prahs et al. [12] but is revealed explicitly in the order-parameter part of the dissipation inequality through the invertible strain reparametrization introduced here. The analysis also addresses the associated mechanical rates, multiphase constraints, and heat-conduction equations.

1.5. Notation

The notation follows Prahs et al. [12] as far as possible. Quantities associated with the two phases are indicated by the labels $+$ and $-$, used as superscripts or subscripts depending on the quantity. The jump of a quantity $\bullet$ across the diffuse interface is denoted by $\{\bullet\} = \bullet^+ - \bullet^-$. A superposed dot denotes the material time derivative. The spatial position and time are denoted by x and t , respectively. For equations containing multiple relations, a subscript attached to an equation reference identifies the corresponding relation, counted from left to right. The symbols, mathematical operations, and dimensional conventions used below are summarized in the Nomenclature section at the end of the manuscript. Quantities normalized by the surface mass density are distinguished from mass-specific bulk quantities. Units of unspecified internal variables remain constitutive-model dependent.

2. Revisiting the Internal State Variable Approach to the Phase-Field Method

2.1. Diffuse-Interface Setting

2.1.1. Relation to the Sharp-Interface

In the present setting, the order parameter φ is treated as an internal state variable (ISV). Its evolution is determined by exploiting a dissipation inequality motivated by the corresponding sharp-interface theory. For this purpose, the approximation introduced by Prahs et al. [12], Equations (11)–(15), relates the entropy production Γ of the sharp-interface model to the entropy production $\tilde{\Gamma}$ of the diffuse-interface model according to

$$\tilde{\Gamma} \approx \Gamma, \quad \tilde{\Gamma} \geq 0. \quad (1)$$

The diffuse-interface approximation replaces the sharp interface $\mathcal{S}$ by the volumetric region $\delta\mathcal{S}$. As a consequence, the adjacent regions $\mathcal{V}^+$ and $\mathcal{V}^-$ are reduced to $\tilde{\mathcal{V}}^+$ and $\tilde{\mathcal{V}}^-$, respectively. The material domain is denoted by $\mathcal{V} = \tilde{\mathcal{V}}^+ \cup \tilde{\mathcal{V}}^- \cup \delta\mathcal{S}$. The entropy production of the regularized domain is then decomposed as

$$\tilde{\Gamma} = \tilde{\Gamma}_{\tilde{\mathcal{V}}^+} + \tilde{\Gamma}_{\tilde{\mathcal{V}}^-} + \tilde{\Gamma}_{\delta\mathcal{S}} \geq 0, \quad \tilde{\Gamma}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}} -\rho_{\mathcal{S}} \frac{\dot{\theta}}{\theta} \tilde{\eta}_{\mathcal{S}} - \rho_{\mathcal{S}} \frac{\dot{\psi}_{\mathcal{S}}}{\theta} dv. \quad (2)$$

Here, $\tilde{\Gamma}_{\tilde{\mathcal{V}}^+}$ and $\tilde{\Gamma}_{\tilde{\mathcal{V}}^-}$ denote the entropy production associated with the reduced bulk regions $\tilde{\mathcal{V}}^+$ and $\tilde{\mathcal{V}}^-$, respectively, while $\tilde{\Gamma}_{\delta\mathcal{S}}$ denotes the contribution of the diffuse interface region $\delta\mathcal{S}$. The temperature is denoted by θ . Following Prahs et al. [12], Equations (16) and (17), $\tilde{\psi}_{\mathcal{S}}$ and $\tilde{\eta}_{\mathcal{S}}$ denote the free-energy and entropy densities in $\delta\mathcal{S}$, respectively, each divided by the surface mass density $\rho_{\mathcal{S}}$.

2.1.2. Free-Energy Structure

The interpolation functions associated with the two phases are denoted by $h(\varphi)$ and $\bar{h}(\varphi)$. Within the present small-deformation setting, the free energy and entropy are given by

$$\begin{aligned} \tilde{\psi}_S = & \frac{h(\varphi)\rho_+ + \bar{h}(\varphi)\rho_-}{\rho_S} \psi_S (\psi_{\text{grad}} + \psi_{\text{pot}}) \\ & + \frac{1}{\rho_S} (h(\varphi)\rho_+ \psi^+ + \bar{h}(\varphi)\rho_- \psi^-), \quad \tilde{\eta}_S = -\frac{\partial \tilde{\psi}_S}{\partial \theta} \end{aligned} \quad (3)$$

In this regard, ρ_+ and ρ_- denote the phase-specific mass densities, ψ_S the specific surface free energy of the material singular surface, ψ_{grad} and ψ_{pot} the gradient and potential contributions associated with the diffuse interface, and ψ^+ and ψ^- the specific free energy for each phase. No explicit temperature dependence is assigned to $h(\varphi)$, $\bar{h}(\varphi)$, ψ_{pot} , ψ_{grad} , ρ_+ , ρ_- , or ρ_S . The potential relations for the bulk entropy and the surface entropy are assumed to hold pointwise in δS , cf., Prahs et al. [12], Equations (9)₂ and (9)₃. Consequently, the second relation in Equation (3) follows. The bulk part of Equation (3)₁ can be stated as the interpolated free-energy density

$$\bar{f}_V = h(\varphi)f^+ + \bar{h}(\varphi)f^- = h(\varphi)\rho_+ \psi^+ + \bar{h}(\varphi)\rho_- \psi^- = \bar{\rho} \bar{\psi} \quad (4)$$

where $\bar{f}_V$ denotes the interpolated bulk free-energy density within δS , cf., Prahs et al. [12], Equation (18). The phase-specific volumetric free-energy densities are denoted by $f^+ = \rho_+ \psi^+$ and $f^- = \rho_- \psi^-$. The notation $\bar{\rho} \bar{\psi}$ denotes the same phase-weighted bulk free-energy density.

Following Prahs et al. [12], Equation (19), the constitutive arguments retained for the two interfacial contributions are

$$\psi_{\text{grad}} = \psi_{\text{grad}}(\varphi, \nabla \varphi), \quad \psi_{\text{pot}} = \psi_{\text{pot}}(\varphi). \quad (5)$$

The interpolation functions satisfy

$$\bar{h}(\varphi) = 1 - h(\varphi), \quad \frac{\partial \bar{h}(\varphi)}{\partial \varphi} = -\frac{\partial h(\varphi)}{\partial \varphi}, \quad (6)$$

cf., e.g., [13]. Admissible choices for $h(\varphi)$ and $\bar{h}(\varphi)$, together with their limitations, are discussed in [18,22].

2.2. Global Dissipation and Strain Reparametrization

2.2.1. Diffuse-Interface Dissipation

As in Prahs et al. [12], Equation (21), non-negativity is imposed separately on the contributions associated with $\tilde{\mathcal{V}}^+$, $\tilde{\mathcal{V}}^-$, and δS :

$$\tilde{\Gamma}_{\tilde{\mathcal{V}}^+} \geq 0, \quad \tilde{\Gamma}_{\tilde{\mathcal{V}}^-} \geq 0, \quad \tilde{\Gamma}_{\delta S} \geq 0. \quad (7)$$

Only the third inequality in Equation (7) is required for the reparametrization considered below. The first two reduce to the standard Clausius–Duhem inequalities in the bulk regions and are omitted. For this purpose, the reduced entropy contribution

$$\tilde{\eta}_S^* = h(\varphi) \frac{\rho_+}{\rho_S} \eta^+ + \bar{h}(\varphi) \frac{\rho_-}{\rho_S} \eta^- \quad (8)$$

and the derivative of the gradient contribution with respect to the order-parameter gradient,

$$\xi = \frac{\partial \psi_{\text{grad}}}{\partial \nabla \varphi} \quad (9)$$

are introduced. Regarding Equation (8), the specific bulk entropies of the two phases are denoted by η^+ and η^- . The localization and integration steps follow Prahs et al. [12], Equations (24)–(29). After differentiating Equation (3) with respect to time, accounting for Equations (5) and (6), and applying the product rule and the divergence theorem, one obtains the diffuse-interface dissipation functional $\mathcal{D}_{\delta\mathcal{S}}$ in the form

$$\begin{aligned} \mathcal{D}_{\delta\mathcal{S}} := & \int_{\delta\mathcal{S}} -\rho_S \dot{\theta} \tilde{\eta}_S^* - \left\{ (\rho_+ - \rho_-) \frac{\partial h(\varphi)}{\partial \varphi} \dot{\varphi} \psi_S (\psi_{\text{grad}} + \psi_{\text{pot}}) \right. \\ & + (h(\varphi)\rho_+ + (1 - h(\varphi))\rho_-) \psi_S \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi} \dot{\varphi} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi} \dot{\varphi} \right) - \text{div}(\Xi) \dot{\varphi} \\ & + (\rho_+ \psi^+ - \rho_- \psi^-) \frac{\partial h(\varphi)}{\partial \varphi} \dot{\varphi} + \Omega \left. \right\} dv \\ & - \int_{\partial\delta\mathcal{S}} (\Xi \cdot \mathbf{n}_V^{\delta\mathcal{S}}) \dot{\varphi} da \geq 0, \end{aligned} \quad (10)$$

where $\mathbf{n}_V^{\delta\mathcal{S}}$ denotes the outward normal to $\delta\mathcal{S}$ on its boundary $\partial\delta\mathcal{S}$. Here, Ξ denotes the weighted gradient-energy derivative, and Ω collects the specific bulk free-energy rates weighted by the interpolation functions and the corresponding phase densities, reading

$$\Xi = (h(\varphi)\rho_+ + (1 - h(\varphi))\rho_-) \psi_S \xi, \quad \Omega := (h(\varphi)\rho_+ \dot{\psi}^+ + (1 - h(\varphi))\rho_- \dot{\psi}^-). \quad (11)$$

Let $\partial\delta\mathcal{S}_N$ and $\partial\delta\mathcal{S}_D$ denote the Neumann and rate-type Dirichlet parts of $\partial\delta\mathcal{S}$, respectively. The conditions used in Prahs et al. [12], Equation (28), are imposed in the form

$$\Xi \cdot \mathbf{n}_V^{\delta\mathcal{S}} = 0 \quad \rightsquigarrow \quad \xi \cdot \mathbf{n}_V^{\delta\mathcal{S}} = 0, \quad \forall \mathbf{x} \in \partial\delta\mathcal{S}_N, \quad \dot{\varphi} = 0, \quad \forall \mathbf{x} \in \partial\delta\mathcal{S}_D, \quad (12)$$

cf., e.g., [23]. Since $(h(\varphi)\rho_+ + \bar{h}(\varphi)\rho_-) \neq 0$, these conditions eliminate the boundary contribution. They are required on $\partial\delta\mathcal{S}$, not on the external boundary $\partial\mathcal{V}$ of $\mathcal{V} = \tilde{\mathcal{V}}^+ \cup \tilde{\mathcal{V}}^- \cup \delta\mathcal{S}$.

2.2.2. Phase-Specific Free Energy

To isolate the effect of the strain reparametrization, the state space in Prahs et al. [12], Equation (30), is restricted by omitting an explicit dependence of ψ^+ and ψ^- on φ . The retained dependencies are

$$\psi^+ = \psi^+(\varepsilon^+, \varepsilon^{*+}, \alpha^+, \theta), \quad \psi^- = \psi^-(\varepsilon^-, \varepsilon^{*-}, \alpha^-, \theta). \quad (13)$$

Here, ε^+ and ε^- denote the phase-specific strains, ε^{*+} and ε^{*-} the phase-specific inelastic strains, and α^+ and α^- the phase-specific sets of internal variables. Equation (13) specifies the constitutive arguments of the phase-specific free energies. The particular material behavior remains to be defined. No additive separation into thermal and non-thermal free-energy contributions, as discussed in [24], is imposed. Consequently, the constitutive setting permits thermomechanically coupled material behavior, cf., e.g., [25].

3. Algebraic Reparametrization of the Phase-Specific Strains

3.1. Kinematic Coupling and Reformulation of Interpolated Free Energy Density Rates

3.1.1. Kinematic Coupling

For the subsequent considerations, the effective displacement gradient $\bar{H}$ within the diffuse interface is introduced as an interpolation of the phase-specific displacement gradients H^+ and H^- . Moreover, the corresponding displacement-gradient jump is defined, reading

$$\bar{H} = h(\varphi)H^+ + (1 - h(\varphi))H^-, \quad \{H\} = H^+ - H^-. \quad (14)$$

Rearranging Equation (14) yields the formulation for the phase-specific displacement gradients as

$$H^+ = \bar{H} + \{H\}, \quad H^- = \bar{H} - \{H\}. \quad (15)$$

Substituting Equation (15)₁ and Equation (15)₂ into Equation (14) yields

$$H^+ = \bar{H} + (1 - h(\varphi))\{H\}, \quad H^- = \bar{H} - h(\varphi)\{H\}. \quad (16)$$

Symmetrization of H^+ and H^- according to Equation (16) yields the phase-specific strain tensors as

$$\varepsilon^+ = \bar{\varepsilon} + \{\varepsilon\} - h(\varphi)\{\varepsilon\}, \quad \varepsilon^- = \bar{\varepsilon} - h(\varphi)\{\varepsilon\} \quad (17)$$

Here, $\bar{\varepsilon}$ denotes the effective infinitesimal strain, and $\{\varepsilon\}$ the corresponding strain jump. Thus, based on Equation (17), the material time derivatives of ε^+ and ε^- read

$$\dot{\varepsilon}^+ = \dot{\bar{\varepsilon}} + \{\dot{\varepsilon}\} - \frac{\partial h(\varphi)}{\partial \varphi} \dot{\varphi} \{\varepsilon\} - h(\varphi) \{\dot{\varepsilon}\}, \quad \dot{\varepsilon}^- = \dot{\bar{\varepsilon}} - \frac{\partial h(\varphi)}{\partial \varphi} \dot{\varphi} \{\varepsilon\} - h(\varphi) \{\dot{\varepsilon}\}, \quad (18)$$

respectively.

The relations in Equation (17) define, for each fixed value of φ , an invertible change of the mechanical variables from $(\varepsilon^+, \varepsilon^-)$ to $(\bar{\varepsilon}, \{\varepsilon\})$. Consequently, the effective strain and the strain jump retain the mechanical information contained in the two phase-specific strains, and the dimension of the mechanical state space is preserved. The order parameter remains an internal state variable of the diffuse-interface theory, although it is not included as an explicit constitutive argument of the restricted phase-specific free energies in Equation (13). Its appearance in the inverse relations through the interpolation function is induced by the change of mechanical variables. Because the strain jump is retained as an independent mechanical state-space coordinate, the inverse relations constitute a change of variables rather than a constitutive closure. A related change of mechanical state variables occurs in classical infinitesimal elastoplasticity, where the additive strain decomposition permits equivalent representations in terms of total and plastic strains or elastic and plastic strains, cf., Lemaitre and Chaboche [26], Sections 2.4.1, 2.4.2 and 5.3.2. Application of the chain rule therefore changes the representation of the thermodynamic forces conjugate to the selected rates without introducing an additional constitutive assumption.

3.1.2. Reformulating Ω

The phase-specific free energies retain the constitutive arguments specified in Equation (13). Their material time derivatives in the contribution Ω introduced in Equation (11) are first expanded with respect to these arguments by application of the chain rule, leading to

$$\begin{aligned}\Omega &= (h(\varphi)\rho_+\dot{\psi}^+ + (1-h(\varphi))\rho_-\dot{\psi}^-) \\ &= h(\varphi)\left(\rho_+\frac{\partial\psi^+}{\partial\varepsilon^+}\cdot\dot{\varepsilon}^+ + \rho_+\frac{\partial\psi^+}{\partial\varepsilon^{*+}}\cdot\dot{\varepsilon}^{*+} + \rho_+\frac{\partial\psi^+}{\partial\alpha^+}\cdot\dot{\alpha}^+ + \rho_+\frac{\partial\psi^+}{\partial\theta}\dot{\theta}\right) \\ &\quad + (1-h(\varphi))\left(\rho_-\frac{\partial\psi^-}{\partial\varepsilon^-}\cdot\dot{\varepsilon}^- + \rho_-\frac{\partial\psi^-}{\partial\varepsilon^{*-}}\cdot\dot{\varepsilon}^{*-} + \rho_-\frac{\partial\psi^-}{\partial\alpha^-}\cdot\dot{\alpha}^- + \rho_-\frac{\partial\psi^-}{\partial\theta}\dot{\theta}\right)\end{aligned}\quad (19)$$

The phase-specific strain rates in Equation (19) are then replaced using Equation (18). Together with the potential relations for the Cauchy stresses σ^+ and σ^- , adapted for $\tilde{\mathcal{V}}^+$ and $\tilde{\mathcal{V}}^-$, respectively, $\rho_+\partial\psi^+/\partial\varepsilon^+ = \sigma^+$ and $\rho_-\partial\psi^-/\partial\varepsilon^- = \sigma^-$, cf., Prahs et al. [12], Equation (9)₁, this gives

$$\begin{aligned}\Omega &= h(\varphi)\sigma^+ \cdot \left(\dot{\varepsilon} + \{\varepsilon\} - \frac{\partial h(\varphi)}{\partial\varphi}\dot{\varphi}\{\varepsilon\} - h(\varphi)\{\dot{\varepsilon}\}\right) \\ &\quad + h(\varphi)\left(\rho_+\frac{\partial\psi^+}{\partial\varepsilon^{*+}}\cdot\dot{\varepsilon}^{*+} + \rho_+\frac{\partial\psi^+}{\partial\alpha^+}\cdot\dot{\alpha}^+ + \rho_+\frac{\partial\psi^+}{\partial\theta}\dot{\theta}\right) \\ &\quad + (1-h(\varphi))\sigma^- \cdot \left(\dot{\varepsilon} - \frac{\partial h(\varphi)}{\partial\varphi}\dot{\varphi}\{\varepsilon\} - h(\varphi)\{\dot{\varepsilon}\}\right) \\ &\quad + (1-h(\varphi))\left(\rho_-\frac{\partial\psi^-}{\partial\varepsilon^{*-}}\cdot\dot{\varepsilon}^{*-} + \rho_-\frac{\partial\psi^-}{\partial\alpha^-}\cdot\dot{\alpha}^- + \rho_-\frac{\partial\psi^-}{\partial\theta}\dot{\theta}\right)\end{aligned}\quad (20)$$

Rearrangement of Equation (20) leads to

$$\begin{aligned}\Omega &= \{\dot{\varepsilon}\} \cdot \left(h(\varphi)\sigma^+ - h(\varphi)^2\sigma^+ - h(\varphi)(1-h(\varphi))\sigma^-\right) \\ &\quad + \dot{\varepsilon} \cdot (h(\varphi)\sigma^+ + (1-h(\varphi))\sigma^-) \\ &\quad - \frac{\partial h(\varphi)}{\partial\varphi}\dot{\varphi}\{\varepsilon\} \cdot (h(\varphi)\sigma^+ + (1-h(\varphi))\sigma^-) \\ &\quad + h(\varphi)\left(\rho_+\frac{\partial\psi^+}{\partial\varepsilon^{*+}}\cdot\dot{\varepsilon}^{*+} + \rho_+\frac{\partial\psi^+}{\partial\alpha^+}\cdot\dot{\alpha}^+ + \rho_+\frac{\partial\psi^+}{\partial\theta}\dot{\theta}\right) \\ &\quad + (1-h(\varphi))\left(\rho_-\frac{\partial\psi^-}{\partial\varepsilon^{*-}}\cdot\dot{\varepsilon}^{*-} + \rho_-\frac{\partial\psi^-}{\partial\alpha^-}\cdot\dot{\alpha}^- + \rho_-\frac{\partial\psi^-}{\partial\theta}\dot{\theta}\right)\end{aligned}\quad (21)$$

Accounting for

$$h(\varphi)\sigma^+ - h(\varphi)^2\sigma^+ - h(\varphi)(1-h(\varphi))\sigma^- = h(\varphi)(1-h(\varphi))(\sigma^+ - \sigma^-) \quad (22)$$

as well as the stress jump and the interpolated Cauchy stress $\bar{\sigma}$, defined by

$$\{\sigma\} = \sigma^+ - \sigma^-, \quad \text{and} \quad \bar{\sigma} = h(\varphi)\sigma^+ + (1-h(\varphi))\sigma^- \quad (23)$$

Equation (21) reads

$$\begin{aligned}\Omega &= h(\varphi)(1-h(\varphi))\{\dot{\varepsilon}\} \cdot \{\sigma\} + \dot{\varepsilon} \cdot \bar{\sigma} - \frac{\partial h(\varphi)}{\partial\varphi}\dot{\varphi}\{\varepsilon\} \cdot \bar{\sigma} \\ &\quad + h(\varphi)\left(\rho_+\frac{\partial\psi^+}{\partial\varepsilon^{*+}}\cdot\dot{\varepsilon}^{*+} + \rho_+\frac{\partial\psi^+}{\partial\alpha^+}\cdot\dot{\alpha}^+ + \rho_+\frac{\partial\psi^+}{\partial\theta}\dot{\theta}\right) \\ &\quad + (1-h(\varphi))\left(\rho_-\frac{\partial\psi^-}{\partial\varepsilon^{*-}}\cdot\dot{\varepsilon}^{*-} + \rho_-\frac{\partial\psi^-}{\partial\alpha^-}\cdot\dot{\alpha}^- + \rho_-\frac{\partial\psi^-}{\partial\theta}\dot{\theta}\right)\end{aligned}\quad (24)$$

For brevity, the stress-interaction contribution

$$\Delta l := \frac{\partial h(\varphi)}{\partial \varphi} [\varepsilon] \cdot \bar{\sigma} \quad (25)$$

is introduced.

3.2. Evolution Equation of the Order Parameter and Reduced Mechanical Dissipation Inequality

3.2.1. Rewriting the Dissipation Inequality

Taking into account Equation (24) and (12), Equation (10) can be written as

$$\mathcal{D}_{\delta S} = \mathcal{D}_{\delta S}^{\varphi} + \mathcal{D}_{\delta S}^{\theta} + \mathcal{D}_{\delta S}^{\text{mech}} \geq 0, \quad (26)$$

where $\mathcal{D}_{\delta S}^{\varphi}$ denotes the part conjugate to the order-parameter rate

$$\begin{aligned} \mathcal{D}_{\delta S}^{\varphi} := \int_{\delta S} & - \left\{ [\rho] \frac{\partial h(\varphi)}{\partial \varphi} \psi_S (\psi_{\text{grad}} + \psi_{\text{pot}}) + [\rho \psi] \frac{\partial h(\varphi)}{\partial \varphi} - \Delta l \right. \\ & \left. + (h(\varphi)\rho_+ + (1 - h(\varphi))\rho_-) \psi_S \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi} \right) - \text{div}(\Xi) \right\} \dot{\varphi} \, dv, \end{aligned} \quad (27)$$

$\mathcal{D}_{\delta S}^{\theta}$ denotes the part conjugate to the temperature rate

$$\mathcal{D}_{\delta S}^{\theta} = \int_{\delta S} - \left\{ \rho_S \tilde{\eta}_S^* + h(\varphi)\rho_+ \frac{\partial \psi^+}{\partial \theta} + (1 - h(\varphi))\rho_- \frac{\partial \psi^-}{\partial \theta} \right\} \dot{\theta} \, dv, \quad (28)$$

and $\mathcal{D}_{\delta S}^{\text{mech}}$ denotes the part conjugate to the remaining mechanical rates

$$\begin{aligned} \mathcal{D}_{\delta S}^{\text{mech}} := \int_{\delta S} & - \left\{ h(\varphi)(1 - h(\varphi)) [\dot{\varepsilon}] \cdot [\sigma] + \dot{\varepsilon} \cdot \bar{\sigma} + h(\varphi)\rho_+ \left(\frac{\partial \psi^+}{\partial \varepsilon^{*+}} \cdot \dot{\varepsilon}^{*+} + \frac{\partial \psi^+}{\partial \alpha^+} \cdot \dot{\alpha}^+ \right) \right. \\ & \left. + (1 - h(\varphi))\rho_- \left(\frac{\partial \psi^-}{\partial \varepsilon^{*-}} \cdot \dot{\varepsilon}^{*-} + \frac{\partial \psi^-}{\partial \alpha^-} \cdot \dot{\alpha}^- \right) \right\} \, dv. \end{aligned} \quad (29)$$

3.2.2. Decoupled Dissipative Contributions

The terms in Equation (26) are grouped by their conjugate rates. Using the notation of [12], $\mathcal{D}_{\delta S}^{\varphi}$ and $\mathcal{D}_{\delta S}^{\theta}$ contain the terms multiplied by $\dot{\varphi}$ and $\dot{\theta}$, respectively. The remaining mechanical part $\mathcal{D}_{\delta S}^{\text{mech}}$ contains the rates $\dot{\varepsilon}$, $[\dot{\varepsilon}]$, $\dot{\varepsilon}^{*+}$, $\dot{\alpha}^+$, $\dot{\varepsilon}^{*-}$, and $\dot{\alpha}^-$. These rate groups are distinct. Hence, the following separate inequalities provide a sufficient condition for Equation (26)

$$\mathcal{D}_{\delta S}^{\varphi} \geq 0, \quad \mathcal{D}_{\delta S}^{\theta} \geq 0, \quad \mathcal{D}_{\delta S}^{\text{mech}} \geq 0. \quad (30)$$

Since $\mathcal{D}_{\delta S}^{\theta}$ according to Equation (28) coincides with Prahs et al. [12], Equation (33), the fulfillment of $\mathcal{D}_{\delta S}^{\theta} \geq 0$ is not discussed further. The present contribution focuses on $\mathcal{D}_{\delta S}^{\varphi} \geq 0$ and $\mathcal{D}_{\delta S}^{\text{mech}} \geq 0$, since these contributions differ from Prahs et al. [12], Equations (32) and (34), due to the algebraic reparametrization of the phase-specific strains.

3.2.3. Fulfillment of $\mathcal{D}_{\delta S}^{\varphi} \geq 0$

Several kinetic relations can satisfy Equation (30)₁. Here, the linear relation used in Prahs et al. [12], Equation (36), is extended by the stress-interaction contribution, giving

$$\begin{aligned} \dot{\varphi} = \dot{\varphi}_0 \left\{ -[\rho] \frac{\partial h(\varphi)}{\partial \varphi} \psi_S (\psi_{\text{grad}} + \psi_{\text{pot}}) - [\rho \psi] \frac{\partial h(\varphi)}{\partial \varphi} + \Delta l \right. \\ \left. + \operatorname{div}(\Xi) - (h(\varphi)\rho_+ + (1 - h(\varphi))\rho_-) \psi_S \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi} \right) \right\}, \quad \dot{\varphi}_0 \geq 0 \quad (31) \end{aligned}$$

where $\dot{\varphi}_0$ is a non-negative kinetic coefficient with units $\text{m}^3 \text{J}^{-1} \text{s}^{-1}$, so that the right-hand side has units s^{-1} . The algebraic reparametrization of the dissipation and the choice of the kinetic relation in Equation (31) represent distinct steps. The former provides an equivalent representation of the total diffuse-interface dissipation, whereas the latter constitutes a kinetic choice based on the transformed force conjugate to $\dot{\varphi}$. Equation (31) therefore contains the stress-interaction contribution Δl , in contrast to Prahs et al. [12], Equation (36). If the Hadamard condition and traction continuity are additionally imposed, Δl is the small-deformation counterpart of the stress-interaction contribution obtained variationally by Schneider et al. [13], Equation (49). In the method of Schneider et al. [13], the deformation-gradient jump vector introduced through the Hadamard condition is treated as a dependent quantity obtained from the traction-continuity problem. Consequently, the phase-specific deformation gradients enter the variational derivative of the strain energy as dependent reconstructed quantities, while the jump vector is not retained as an independent kinematic coordinate.

Mosler et al. [16] likewise express the phase-specific deformation gradients in terms of their average and jump. In their partial rank-one relaxation, Hadamard compatibility is imposed with the interface normal determined by the order-parameter gradient. Local minimization of the averaged (incremental) bulk energy with respect to the jump vector then yields the traction-continuity condition used directly by Schneider et al. The local stress-interaction contribution follows from the chain rule, while stationarity eliminates the term involving the implicit order-parameter derivative of the jump vector. In the present derivation, Δl is identified by applying the chain rule to the phase-specific free-energy rates in the dissipation inequality. The strain jump is retained as an independent mechanical state-space coordinate, keeping its mechanical closure separate from the invertible reparametrization. Related stress-interaction contributions occur in further mechanically coupled phase-field and multiphase-field approaches, cf., e.g., [27], Equation (53), [8], Equation (A.30), [28], Equation (35), and [9], Equation (11).

3.2.4. Remark on Sharp Interface Pendant and Applications

The corresponding mechanical contribution is already present in sharp-interface equilibrium conditions for coherent solids, cf. Johnson and Alexander [19], Equation (32), and Voorhees and Johnson [20], Equation (34). Schneider et al. [21], Section 3.4, Equations (75)–(77), Figure 5, relate the phase-field contribution to the Gibbs–Thomson condition and assess inclusion growth and shrinkage against the predicted equilibrium. Related applications include precipitate shape evolution under applied stress, cf. Johnson [29], and martensitic transformation, cf. Schneider et al. [14], Section 7.3, Figures 7 and 8. The present work demonstrates that the stress interaction contribution is already present in the ISV framework of Prahs et al. [12] but becomes apparent within that framework only through the reparametrization presented here.

3.2.5. Fulfillment of $\mathcal{D}_{\delta S}^{\text{mech}} \geq 0$

Taking into account $\{\dot{\epsilon}\} \cdot \{\sigma\} = 0$, cf. Prahs et al. [12], Equation (A.29), Equation (29) reads

$$\mathcal{D}_{\delta S}^{\text{mech}} := \int_{\delta S} - \left\{ \dot{\bar{\epsilon}} \cdot \bar{\sigma} + h(\varphi) \rho_+ \left(\frac{\partial \psi^+}{\partial \epsilon^{*+}} \cdot \dot{\epsilon}^{*+} + \frac{\partial \psi^+}{\partial \alpha^+} \cdot \dot{\alpha}^+ \right) + (1 - h(\varphi)) \rho_- \left(\frac{\partial \psi^-}{\partial \epsilon^{*-}} \cdot \dot{\epsilon}^{*-} + \frac{\partial \psi^-}{\partial \alpha^-} \cdot \dot{\alpha}^- \right) \right\} dv. \quad (32)$$

The rate of the effective strain is assumed to satisfy $\dot{\bar{\epsilon}} = \text{sym}(\text{grad}(\dot{\bar{u}}))$, where $\bar{u}$ denotes the effective displacement field. The kinematic continuity of a material singular surface implies $\{v\} = 0$, cf., Truesdell and Toupin [30], p. 519, with v denoting the velocity field of the body. With $\dot{u}_+$ and $\dot{u}_-$ denoting the phase-specific displacement rates, the corresponding jump therefore vanishes, $\{\dot{u}\} = 0$. A common displacement rate $\dot{u}_+ = \dot{u}_- = \dot{u}$ is used. Using the symmetry of $\bar{\sigma}$, application of the divergence theorem to Equation (32) yields

$$\begin{aligned} \mathcal{D}_{\delta S}^{\text{mech}} := & \int_{\delta S} \left\{ \text{div}(\bar{\sigma}) \cdot \dot{u} - h(\varphi) \rho_+ \left(\frac{\partial \psi^+}{\partial \epsilon^{*+}} \cdot \dot{\epsilon}^{*+} + \frac{\partial \psi^+}{\partial \alpha^+} \cdot \dot{\alpha}^+ \right) \right. \\ & \left. - (1 - h(\varphi)) \rho_- \left(\frac{\partial \psi^-}{\partial \epsilon^{*-}} \cdot \dot{\epsilon}^{*-} + \frac{\partial \psi^-}{\partial \alpha^-} \cdot \dot{\alpha}^- \right) \right\} dv \\ & - \int_{\partial \delta S} \bar{t} \cdot \dot{u} da \geq 0. \end{aligned} \quad (33)$$

Regarding Equation (33), the interpolated stress vector $\bar{t}$ is used as

$$\bar{t} := h(\varphi) t^+ + (1 - h(\varphi)) t^-, \quad \text{with } t^+ = \sigma^+ n_{\mathcal{V}}^{\delta S} \text{ and } t^- = \sigma^- n_{\mathcal{V}}^{\delta S}, \quad (34)$$

cf., Prahs et al. [12], Equation (4). Here, t^+ and t^- are the phase-specific traction vectors on $\partial \delta S$. The inequality stated in Equation (33), and therefore also Equation (30)₃, can be further reduced by imposing

$$\text{div}(\bar{\sigma}) = 0, \forall x \in \delta S, \quad \bar{t} = 0, \forall x \in \partial \delta S_N, \quad \dot{u} = 0, \forall x \in \partial \delta S_D. \quad (35)$$

Here, $\partial \delta S_N$ and $\partial \delta S_D$ denote the Neumann and Dirichlet parts of the boundary, respectively. The reduced form of Equation (33) then reads

$$\begin{aligned} & \int_{\delta S} - h(\varphi) \rho_+ \left(\frac{\partial \psi^+}{\partial \epsilon^{*+}} \cdot \dot{\epsilon}^{*+} + \frac{\partial \psi^+}{\partial \alpha^+} \cdot \dot{\alpha}^+ \right) \\ & - (1 - h(\varphi)) \rho_- \left(\frac{\partial \psi^-}{\partial \epsilon^{*-}} \cdot \dot{\epsilon}^{*-} + \frac{\partial \psi^-}{\partial \alpha^-} \cdot \dot{\alpha}^- \right) dv \geq 0. \end{aligned} \quad (36)$$

Further evaluation of Equation (36) requires specific forms of the free energies ψ^+ and ψ^- , together with evolution equations for the inelastic strains and internal variables.

3.2.6. Remark on the Heat Conduction Equation

The reparametrization of the phase-specific strain rates $\dot{\epsilon}^+$ and $\dot{\epsilon}^-$ derived in the present contribution does not modify the heat conduction equation obtained in [12]. In that derivation, the stress power $\bar{\sigma} \cdot \dot{\bar{\epsilon}}$ in the diffuse interface is already expressed in terms of the phase-specific stresses and strain rates, cf. Prahs et al. [12], Equation (A.26). The corresponding mechanical interaction contribution is then collected in $\Delta L = \Delta l \dot{\varphi}$, cf. Prahs et al. [12], Equation (A.31). Accordingly, the reparametrization affects the contri-

butions $\mathcal{D}_{\delta S}^{\phi}$ and $\mathcal{D}_{\delta S}^{\text{mech}}$, but does not introduce an additional contribution into the heat conduction equation.

4. Transition to Multiple Phases

4.1. Multiphase-Field Setting

4.1.1. Multiple Phases

The transition to multiple phases uses the domain decomposition introduced by Prahs et al. [18], Equations (1)–(3). In addition to diffuse two-phase interfaces, this decomposition includes diffuse junction regions in which more than two phases meet. The corresponding unions are given by

$$\delta S^{II} = \bigcup_{\substack{A \subseteq \mathcal{I} \\ |A|=2}} \delta S^A, \quad \delta S^{III} = \bigcup_{\substack{A \subseteq \mathcal{I} \\ |A| \geq 3}} \delta S^A. \quad (37)$$

In Equation (37), the set $\mathcal{I}$ contains the indices of all phases. A subset $A \subseteq \mathcal{I}$ identifies the phases involved in a particular interface or junction. For $|A| = 2$, δS^A denotes the diffuse interface region between the phases in A . For $|A| \geq 3$, δS^A denotes their diffuse junction region. Here, $|A|$ denotes the number of elements in A . The corresponding set is empty if that interface or junction is absent. The region occupied by phase α in the corresponding sharp-interface description is denoted by $\mathcal{V}^\alpha$. Upon replacing the sharp interfaces by diffuse-interface regions of finite width, the remaining bulk region of phase α is denoted by $\tilde{\mathcal{V}}^\alpha \subset \mathcal{V}^\alpha$. Hence, the material domain is decomposed as

$$\mathcal{V} = \bigcup_{\alpha=1}^N \mathcal{V}^\alpha = \left(\bigcup_{\alpha=1}^N \tilde{\mathcal{V}}^\alpha \right) \cup \delta S^{II} \cup \delta S^{III}. \quad (38)$$

The cardinality $N = |\mathcal{I}|$ gives the total number of material phases occurring in $\mathcal{V}$ at the considered instant. The order parameter associated with phase α is denoted by φ_α . Within the bulk region $\tilde{\mathcal{V}}^\alpha$, $\varphi_\alpha = 1$, while $\varphi_\beta = 0$ holds for every $\beta \neq \alpha$. In contrast, more than two order parameters may be nonzero simultaneously within a diffuse junction region.

4.1.2. Locally Active Phases

The multiphase-field formulation of Prahs et al. [18] provides the basis for the present analysis. Only the notation and relations required for the algebraic reparametrization are recalled below. At a material point within a diffuse-interface or junction region, only a subset of the N phases may be active. A phase is referred to as locally active if its corresponding order parameter is nonzero. The number of locally active phases is denoted by $\tilde{N} \leq N$. For the local relations, these phases are indexed by $\alpha = 1, \dots, \tilde{N}$. Their order parameters are collected in

$$\boldsymbol{\phi} = \{\varphi_1, \dots, \varphi_{\tilde{N}}\}, \quad (39)$$

cf., Prahs et al. [18], Equation (7). They satisfy the local summation constraint of Prahs et al. [18], Equation (13)

$$\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha(\mathbf{x}, t) = 1 \quad \rightsquigarrow \quad \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha(\mathbf{x}, t) = 0. \quad (40)$$

In accordance with the restriction derived by Prahs et al. [18], Equation (64) and Equations (A.14)–(A.39), the interpolation functions $h_\alpha(\boldsymbol{\phi})$ are identified with the corresponding order parameters according to

$$h_\alpha(\boldsymbol{\phi}) = \varphi_\alpha, \quad \alpha = 1, \dots, \tilde{N}. \quad (41)$$

Consequently,

$$\dot{h}_\alpha(\boldsymbol{\phi}) = \dot{\varphi}_\alpha, \quad \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\kappa} = \delta_{\alpha\kappa}. \quad (42)$$

Here, $\delta_{\alpha\kappa}$ denotes the Kronecker delta, and $\kappa = 1, \dots, \tilde{N}$ is a locally active phase index.

4.1.3. Free-Energy Structure

With Equation (41), the free-energy ansatz of Prahs et al. [18], Equation (6), specializes to

$$\tilde{\psi}_S = \frac{1}{\rho_S} \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \right) \psi_S(\psi_{\text{grad}} + \psi_{\text{pot}}) + \frac{1}{\rho_S} \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \psi^\alpha \right). \quad (43)$$

Here, ρ^α and ψ^α denote the mass density and specific bulk free energy of phase α , respectively. The constitutive arguments of ψ_{grad} and ψ_{pot} are adopted from Prahs et al. [18], Equations (11) and (12), reading

$$\psi_{\text{grad}} = \psi_{\text{grad}}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}), \quad \psi_{\text{pot}} = \psi_{\text{pot}}(\boldsymbol{\phi}), \quad \nabla \boldsymbol{\phi} = \{\nabla \varphi_1, \dots, \nabla \varphi_{\tilde{N}}\}. \quad (44)$$

Here, $\nabla \boldsymbol{\phi}$ denotes the collection of the gradients of the locally active order parameters. The quantities ψ_{grad} , ψ_{pot} , ρ^α , and ρ_S are assumed not to depend explicitly on the temperature. Moreover, the order parameters are treated as independent state variables. Thus, $\boldsymbol{\phi}$ and $\nabla \boldsymbol{\phi}$ are held fixed when the partial derivative of $\tilde{\psi}_S$ with respect to θ is evaluated. This does not exclude a thermal coupling of the order-parameter evolution through the corresponding driving forces. The specific surface entropy associated with ψ_S is denoted by η_S . Under the assumptions stated above and using the surface-entropy potential relation in Prahs et al. [18], Equation (A.13), the entropy takes the form given in their Equation (8), reading

$$\tilde{\eta}_S = -\frac{\partial \tilde{\psi}_S}{\partial \theta} = \frac{\bar{\rho}}{\rho_S} \eta_S(\psi_{\text{grad}} + \psi_{\text{pot}}) + \tilde{\eta}_S^*. \quad (45)$$

The interpolated density $\bar{\rho}$ and the interpolated bulk entropy $\tilde{\eta}_S^*$ are defined by

$$\bar{\rho} := \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha, \quad \tilde{\eta}_S^* := \frac{1}{\rho_S} \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \eta^\alpha, \quad (46)$$

cf., Prahs et al. [18], Equation (9). Here, η^α denotes the specific bulk entropy of phase α .

4.1.4. Diffuse-Interface Dissipation

Following Prahs et al. [18], Equation (23), the dissipation regarding δS^{III} is given by

$$\begin{aligned} \mathcal{D}_{\delta S}^{III} = & \int_{\delta S^{III}} -\rho_S \dot{\theta} \dot{\eta}_S^* \\ & - \left(\sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \left(-\operatorname{div}(\Xi^\alpha) + \bar{\rho} \psi_S \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_\alpha} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\alpha} \right) \right. \right. \\ & \left. \left. + \rho^\alpha \psi^\alpha + \rho^\alpha \psi_S (\psi_{\text{grad}} + \psi_{\text{pot}}) \right) \right) - \Omega \, dv + \mathcal{B} \geq 0 \end{aligned} \quad (47)$$

Here, Ξ^α denotes the weighted gradient-energy derivative associated with φ_α , and $\mathcal{B}$ is the boundary contribution to the dissipation. The corresponding unweighted derivative is denoted by ξ^α . The contribution Ω now collects the specific bulk free-energy rates of all locally active phases weighted by their order parameters and mass densities. Regarding Equation (47),

$$\Omega := \left(\sum_{\alpha=1}^{\tilde{N}} \rho^\alpha \varphi_\alpha \dot{\psi}^\alpha \right), \quad \Xi^\alpha := \bar{\rho} \psi_S \xi^\alpha, \quad \xi^\alpha = \partial \psi_{\text{grad}} / \partial \nabla \varphi_\alpha \quad (48)$$

and

$$\mathcal{B} := - \int_{\partial \delta S^{III}} \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \Xi^\alpha \cdot \mathbf{n}_V^{\delta S} \, da \quad (49)$$

are introduced. In Equation (49), $\mathbf{n}_V^{\delta S}$ denotes the outward unit normal to the junction region δS^{III} on $\partial \delta S^{III}$. The boundary contribution $\mathcal{B}$ vanishes under the phase-field boundary conditions

$$\xi^\alpha \cdot \mathbf{n}_V^{\delta S} = 0, \quad \forall \mathbf{x} \in \partial \delta S_N^{III}, \quad \dot{\varphi}_\alpha = 0, \quad \forall \mathbf{x} \in \partial \delta S_D^{III}, \quad (50)$$

for each $\alpha = 1, \dots, \tilde{N}$. In this regard, $\partial \delta S_N^{III}$ and $\partial \delta S_D^{III}$ denote the Neumann and rate-type Dirichlet parts of $\partial \delta S^{III}$, respectively.

4.1.5. Phase-Specific Free Energy

Relative to the state space in Prahs et al. [18], Equation (24), an explicit dependence of the phase-specific free energies on the corresponding order parameter is omitted. The restricted dependencies are

$$\psi^\alpha = \psi^\alpha(\boldsymbol{\varepsilon}^\alpha, \boldsymbol{\varepsilon}^{*\alpha}, \boldsymbol{\alpha}^\alpha, \theta). \quad (51)$$

Here, $\boldsymbol{\varepsilon}^\alpha$ denotes the infinitesimal strain, $\boldsymbol{\varepsilon}^{*\alpha}$ the inelastic strain, and $\boldsymbol{\alpha}^\alpha$ the set of internal variables of phase α . Accounting for the constitutive dependencies, application of the chain rule gives

$$\Omega = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \left(\frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^\alpha} \cdot \dot{\boldsymbol{\varepsilon}}^\alpha + \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha}} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha + \frac{\partial \psi^\alpha}{\partial \theta} \dot{\theta} \right). \quad (52)$$

4.2. Algebraic Reparametrization of Phase-Specific Strains

4.2.1. Kinematic Coupling

In the following, the effective displacement gradient $\bar{\mathbf{H}}$ is introduced as the interpolation of the phase-specific displacement gradients,

$$\bar{\mathbf{H}} = \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \mathbf{H}^{\alpha}, \quad (53)$$

For two arbitrary locally active phases α and β , the corresponding pairwise displacement-gradient jump is defined as

$$\{\mathbf{H}\}^{\alpha\beta} := \mathbf{H}^{\alpha} - \mathbf{H}^{\beta}, \quad \{\mathbf{H}\}^{\alpha\beta} = -\{\mathbf{H}\}^{\beta\alpha}. \quad (54)$$

Accounting for Equation (40)₁, the difference between the phase-specific and effective displacement gradients is obtained as

$$\begin{aligned} \mathbf{H}^{\alpha} - \bar{\mathbf{H}} &= \mathbf{H}^{\alpha} \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} - \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} \mathbf{H}^{\beta} = \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} (\mathbf{H}^{\alpha} - \mathbf{H}^{\beta}) \\ &= \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} \{\mathbf{H}\}^{\alpha\beta}. \end{aligned} \quad (55)$$

Thus, the displacement gradient of phase α is expressed as

$$\mathbf{H}^{\alpha} = \bar{\mathbf{H}} + \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} \{\mathbf{H}\}^{\alpha\beta}. \quad (56)$$

Within the small-strain framework, symmetrization of Equation (56) gives the phase-specific strain tensor

$$\boldsymbol{\varepsilon}^{\alpha} = \bar{\boldsymbol{\varepsilon}} + \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} \{\boldsymbol{\varepsilon}\}^{\alpha\beta}, \quad (57)$$

with the effective strain $\bar{\boldsymbol{\varepsilon}}$ and the pairwise strain jump $\{\boldsymbol{\varepsilon}\}^{\alpha\beta}$ defined by

$$\bar{\boldsymbol{\varepsilon}} = \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \boldsymbol{\varepsilon}^{\alpha}, \quad \{\boldsymbol{\varepsilon}\}^{\alpha\beta} := \boldsymbol{\varepsilon}^{\alpha} - \boldsymbol{\varepsilon}^{\beta}. \quad (58)$$

Taking the material time derivative of Equation (57) yields

$$\dot{\boldsymbol{\varepsilon}}^{\alpha} = \dot{\bar{\boldsymbol{\varepsilon}}} + \sum_{\beta=1}^{\tilde{N}} \varphi_{\beta} \{\dot{\boldsymbol{\varepsilon}}\}^{\alpha\beta} + \sum_{\beta=1}^{\tilde{N}} \dot{\varphi}_{\beta} \{\boldsymbol{\varepsilon}\}^{\alpha\beta}. \quad (59)$$

Accordingly, the phase-specific strain rates are represented by the effective strain rate, the pairwise strain-jump rates, and a contribution that is linear in the rates of the order parameter. For $\tilde{N} > 2$, the pairwise strain jumps do not constitute an independent set since their definitions imply

$$\{\boldsymbol{\varepsilon}\}^{\alpha\beta} + \{\boldsymbol{\varepsilon}\}^{\beta\gamma} + \{\boldsymbol{\varepsilon}\}^{\gamma\alpha} = 0 \quad (60)$$

for any three distinct phases α , β , and γ . The corresponding relation for the strain-jump rates follows by taking the material time derivative. Consequently, only $\tilde{N} - 1$ pairwise strain jumps, and correspondingly their rates, can be chosen independently. Together with

the effective strain, any independent set of $\tilde{N} - 1$ strain jumps contains the same number of mechanical degrees of freedom as the $\tilde{N}$ phase-specific strains. The reparametrization therefore preserves the dimension of the local mechanical state space. Nevertheless, all pairwise jumps are retained below to preserve the pairwise symmetric structure of the algebraic relations. The algebraic reparametrization does not provide a closure relation for these jumps. They have to be determined by additional mechanical assumptions or a suitable closure approach, such as partial rank-one relaxation or a method based on mechanical jump conditions, cf., e.g., [13,16,17,31]. Consequently, the pairwise interaction contribution in Equation (75) and the evolution equation stated in Equation (78) remain closure dependent. Before such a closure is specified, Equation (78) defines a thermodynamically admissible structure but not a closed phase-field model. No specific constitutive law is required for the reparametrization. The mechanical closure for the pairwise strain jumps is therefore kept separate from the thermodynamic derivation and may be selected according to the material behavior and interface conditions under consideration.

4.2.2. Reformulation of Ω

Introducing the phase-specific Cauchy stresses by the potential relations $\sigma^\alpha = \rho^\alpha \partial \psi^\alpha / \partial \epsilon^\alpha$ and the interpolated stress $\bar{\sigma} := \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \sigma^\alpha$, the stress-power contribution in Equation (52) reads

$$\Omega_\epsilon := \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \sigma^\alpha \cdot \dot{\epsilon}^\alpha. \quad (61)$$

Insertion of Equation (59) gives

$$\Omega_\epsilon = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \sigma^\alpha \cdot \dot{\bar{\epsilon}} + \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_\alpha \varphi_\beta \sigma^\alpha \cdot \{\dot{\epsilon}\}^{\alpha\beta} + \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_\alpha \dot{\varphi}_\beta \sigma^\alpha \cdot \{\epsilon\}^{\alpha\beta}. \quad (62)$$

The first term in Equation (62) directly becomes

$$\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \sigma^\alpha \cdot \dot{\bar{\epsilon}} = \bar{\sigma} \cdot \dot{\bar{\epsilon}}. \quad (63)$$

The second term in Equation (62) contains a double sum over all ordered pairs of locally active phases, subsequently denoted as χ and defined as

$$\chi := \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_\alpha \varphi_\beta \sigma^\alpha \cdot \{\dot{\epsilon}\}^{\alpha\beta}. \quad (64)$$

The terms with identical indices vanish because

$$\{\dot{\epsilon}\}^{\alpha\alpha} = \dot{\epsilon}^\alpha - \dot{\epsilon}^\alpha = \mathbf{0}. \quad (65)$$

Consequently, only terms with $\alpha \neq \beta$ contribute to χ stated in Equation (64). By restricting the summation indices and limits, Equation (64) becomes

$$\chi = \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_\alpha \varphi_\beta \sigma^\alpha \cdot \{\dot{\epsilon}\}^{\alpha\beta} = \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1}^{\tilde{N}} \varphi_\alpha \varphi_\beta [\sigma]^\alpha \cdot \{\dot{\epsilon}\}^{\alpha\beta}, \quad (66)$$

A detailed derivation of the second equality is provided in the Appendix A. In this regard, $[\sigma]^\alpha = \sigma^\alpha - \sigma^\beta$ denotes the pairwise jump of the Cauchy stress tensor. The third

term in Equation (62) contains the rates of the order parameters. Expanding the strain jump gives

$$\sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_{\alpha} \dot{\varphi}_{\beta} \sigma^{\alpha} \cdot [\varepsilon]^{\alpha\beta} = \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_{\alpha} \dot{\varphi}_{\beta} \sigma^{\alpha} \cdot \varepsilon^{\alpha} - \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_{\alpha} \dot{\varphi}_{\beta} \sigma^{\alpha} \cdot \varepsilon^{\beta}. \quad (67)$$

Since $\sum_{\beta=1}^{\tilde{N}} \dot{\varphi}_{\beta} = 0$, the first term on the right-hand side of Equation (67) vanishes. The remaining contribution is rearranged as

$$- \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_{\alpha} \dot{\varphi}_{\beta} \sigma^{\alpha} \cdot \varepsilon^{\beta} = - \sum_{\beta=1}^{\tilde{N}} \dot{\varphi}_{\beta} \varepsilon^{\beta} \cdot \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \sigma^{\alpha} \right) = - \sum_{\beta=1}^{\tilde{N}} \dot{\varphi}_{\beta} \varepsilon^{\beta} \cdot \bar{\sigma}. \quad (68)$$

Combining Equations (63), (66), and (68), the stress-power contribution becomes

$$\Omega_{\varepsilon} = \dot{\varepsilon} \cdot \bar{\sigma} + \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1}^{\tilde{N}} \varphi_{\alpha} \varphi_{\beta} [\dot{\varepsilon}]^{\alpha\beta} \cdot [\sigma]^{\alpha\beta} - \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_{\alpha} \varepsilon^{\alpha} \cdot \bar{\sigma}. \quad (69)$$

For subsequent use, the mechanical interaction contribution associated with phase α is denoted by l_{α} and defined as

$$l_{\alpha} := \varepsilon^{\alpha} \cdot \bar{\sigma}. \quad (70)$$

4.2.3. Decomposition of Diffuse-Interface Dissipation

Insertion of the reparametrized free-energy rates into the diffuse-interface dissipation inequality modifies the contributions conjugate to the order-parameter rates and to the remaining mechanical rates. The thermal contribution and the boundary contribution retain their previous forms. Accordingly, the diffuse-interface dissipation is decomposed as

$$\mathcal{D}_{\delta S}^{\text{III}} = \mathcal{D}_{\delta S}^{\varphi} + \mathcal{D}_{\delta S}^{\theta} + \mathcal{D}_{\delta S}^{\text{mech}} + \mathcal{B} \geq 0. \quad (71)$$

Using the notation of Prahs et al. [18], Equations (26)–(32), $\mathcal{D}_{\delta S}^{\varphi}$ and $\mathcal{D}_{\delta S}^{\theta}$ collect the terms conjugate to $\dot{\varphi}_{\alpha}$ and $\dot{\theta}$, respectively. The remaining rate-dependent terms enter $\mathcal{D}_{\delta S}^{\text{mech}}$, while $\mathcal{B}$ is defined on the boundary. Since the three volume contributions involve distinct rate groups, the following conditions are sufficient for Equation (71):

$$\mathcal{D}_{\delta S}^{\varphi} \geq 0, \quad \mathcal{D}_{\delta S}^{\theta} \geq 0, \quad \mathcal{D}_{\delta S}^{\text{mech}} \geq 0, \quad \mathcal{B} \geq 0. \quad (72)$$

Accounting for Equations (49) and (50), $\mathcal{B} = 0$ holds. Thus, the condition $\mathcal{B} \geq 0$ is already fulfilled.

4.2.4. Reparametrized Multiphase-Field Evolution Equations

Let F_{α} denote the phase-field driving-force contribution obtained prior to the kinematic reparametrization. In the present work, this contribution is specialized by identifying the interpolation function $h_{\alpha}(\boldsymbol{\phi})$ with the order parameter φ_{α} , cf., Equation (41), and by considering the restricted thermodynamic state space introduced in Equation (51). In contrast to the state space considered by Prahs et al. [18], the phase-specific free energy does not depend explicitly on the corresponding order parameter. Thus, $\partial \psi^{\alpha} / \partial \varphi_{\alpha} = 0$, and the corresponding term in Prahs et al. [18, Equation (25)] vanishes. Consequently, the driving-force contribution considered here reads

$$F_{\alpha} := -\text{div}(\Xi^{\alpha}) + \bar{\rho} \psi_S \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_{\alpha}} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_{\alpha}} \right) + \rho^{\alpha} \psi^{\alpha} + \rho^{\alpha} \psi_S (\psi_{\text{grad}} + \psi_{\text{pot}}). \quad (73)$$

Since the final term in Equation (69) contributes with the opposite sign after Ω is inserted into the dissipation inequality, the order-parameter contribution becomes

$$\mathcal{D}_{\delta S}^{\varphi} = \int_{\delta S^{III}} - \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_{\alpha} (F_{\alpha} - l_{\alpha}) \, dv. \quad (74)$$

The pairwise mechanical interaction contribution is defined as

$$\Delta l^{\alpha\beta} := l_{\alpha} - l_{\beta} = (\boldsymbol{\varepsilon}^{\alpha} - \boldsymbol{\varepsilon}^{\beta}) \cdot \bar{\boldsymbol{\sigma}} = [\boldsymbol{\varepsilon}]^{\alpha\beta} \cdot \bar{\boldsymbol{\sigma}}. \quad (75)$$

For brevity, the modified driving force $\hat{F}_{\alpha} := F_{\alpha} - l_{\alpha}$ is introduced. The order-parameter dissipation then reads

$$\mathcal{D}_{\delta S}^{\varphi} = \int_{\delta S^{III}} - \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_{\alpha} \hat{F}_{\alpha} \, dv. \quad (76)$$

The dual-interaction structure of Prahs et al. [18], Equation (33), is applied to the modified driving forces, giving

$$\dot{\varphi}_{\alpha} = -\frac{1}{\tilde{N}} \sum_{\beta=1, \beta \neq \alpha}^{\tilde{N}} M_{\alpha\beta} (\hat{F}_{\alpha} - \hat{F}_{\beta}), \quad M_{\alpha\beta} = M_{\beta\alpha} \geq 0. \quad (77)$$

Here, $M_{\alpha\beta}$ denotes the non-negative mobility assigned to the pair of phases α and β . Equivalently,

$$\dot{\varphi}_{\alpha} = -\frac{1}{\tilde{N}} \sum_{\beta=1, \beta \neq \alpha}^{\tilde{N}} M_{\alpha\beta} (F_{\alpha} - F_{\beta} - \Delta l^{\alpha\beta}). \quad (78)$$

The diffuse-interface dissipation is first reformulated algebraically, while its total value remains unchanged. The dual-interaction ansatz then specifies a particular kinetic relation in terms of the modified driving forces. Insertion of Equation (77) into Equation (76) gives

$$\begin{aligned} \mathcal{D}_{\delta S}^{\varphi} &= \int_{\delta S^{III}} \frac{1}{\tilde{N}} \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1, \beta \neq \alpha}^{\tilde{N}} M_{\alpha\beta} (\hat{F}_{\alpha} - \hat{F}_{\beta}) \hat{F}_{\alpha} \, dv \\ &= \int_{\delta S^{III}} \frac{1}{\tilde{N}} \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1}^{\tilde{N}} M_{\alpha\beta} (\hat{F}_{\alpha} - \hat{F}_{\beta})^2 \, dv \geq 0, \end{aligned} \quad (79)$$

cf., Prahs et al. [18], Equations (34) and (35). Thus, the dual-interaction evolution equation based on the modified driving forces satisfies the order-parameter dissipation inequality. Under pairwise Hadamard compatibility and traction continuity, the pairwise stress-interaction contribution in Equation (78) agrees with the small-deformation limit of the stress-dependent part of Schneider et al. [13], Equation (50), when expressed as pairwise driving-force differences. In the variational approach of Schneider et al. [13], the deformation-gradient jump vectors required by the multiphase construction are treated as dependent quantities determined by solving the system of traction-continuity equations, cf., Schneider et al. [13], Equations (31)–(35). Consequently, the phase-specific deformation gradients enter the variation as dependent reconstructed quantities rather than independent kinematic coordinates. The present reparametrization instead retains the effective strain and $\tilde{N} - 1$ independent strain jumps as mechanical state-space coordinates. Agreement with the stress-dependent variational contribution is therefore conditional on a mechanical closure enforcing pairwise Hadamard compatibility and traction continuity.

4.2.5. Mechanical Part of the Reduced Dissipation Inequality

The mechanical contribution after the algebraic reparametrization is

$$\mathcal{D}_{\delta S}^{\text{mech}} = \int_{\delta S^{III}} \left[\dot{\bar{\epsilon}} \cdot \bar{\sigma} + \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1}^{\tilde{N}} \varphi_{\alpha} \varphi_{\beta} [\dot{\epsilon}]^{\alpha\beta} \cdot [\sigma]^{\alpha\beta} + \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \rho^{\alpha} \left(\frac{\partial \psi^{\alpha}}{\partial \epsilon^{*\alpha}} \cdot \dot{\epsilon}^{*\alpha} + \frac{\partial \psi^{\alpha}}{\partial \alpha^{\alpha}} \cdot \dot{\alpha}^{\alpha} \right) \right] dv. \quad (80)$$

Equation (80) is the general mechanical contribution obtained from the algebraic reparametrization. Its subsequent reduction is restricted to the additional assumptions stated below. As in the two-phase case, the rate of the effective strain is assumed to be kinematically compatible, $\dot{\bar{\epsilon}} = \text{sym}(\text{grad}(\dot{\bar{u}}))$. Moreover, pairwise orthogonality of the strain-rate and stress jumps is imposed for every pair of locally active phases in the junction region, leading to

$$[\dot{\epsilon}]^{\alpha\beta} \cdot [\sigma]^{\alpha\beta} = 0, \quad \forall x \in \delta S^{III}, \quad 1 \leq \alpha < \beta \leq \tilde{N}. \quad (81)$$

For an individual pair of phases α and β , Equation (81) follows if a pairwise unit normal $\mathbf{n}^{\alpha\beta}$ and a jump vector $\mathbf{d}^{\alpha\beta}$ exist such that $[\dot{\epsilon}]^{\alpha\beta} = \text{sym}(\mathbf{d}^{\alpha\beta} \otimes \mathbf{n}^{\alpha\beta})$ and $[\sigma]^{\alpha\beta} \mathbf{n}^{\alpha\beta} = \mathbf{0}$. This is the pairwise extension of the two-phase result obtained by Prahs et al. [12], Equation (A.29). At a general junction, however, the sharp-interface conditions are formulated on the individual pairwise interfaces and do not by themselves establish that Equation (81) holds simultaneously for every locally active phase pair throughout the diffuse junction region. The subsequent reduction is therefore restricted to configurations for which Equation (81) holds for every locally active phase pair. Otherwise, Equation (80) remains applicable. For the junction region, the effective stress vector is defined analogously to Equation (34) as $\bar{\mathbf{t}} := \bar{\sigma} \mathbf{n}_{\delta S}^{\delta S}$. Using Equation (81), the kinematic compatibility relation, the symmetry of the Cauchy stress, the divergence theorem, and the equilibrium and boundary conditions given in Equation (35), applied to δS^{III} , Equation (80) reduces to

$$\mathcal{D}_{\delta S}^{\text{mech}} = \int_{\delta S^{III}} - \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \rho^{\alpha} \left(\frac{\partial \psi^{\alpha}}{\partial \epsilon^{*\alpha}} \cdot \dot{\epsilon}^{*\alpha} + \frac{\partial \psi^{\alpha}}{\partial \alpha^{\alpha}} \cdot \dot{\alpha}^{\alpha} \right) dv \geq 0. \quad (82)$$

For the restricted state space considered here, Equation (82) has the same structure as Prahs et al. [18], Equation (58).

4.2.6. Implication for the Heat Conduction Equation

Compared with the heat conduction equation derived by Prahs et al. [18], Equation (70), the equation considered here differs only through the restriction of the thermodynamic state space introduced in Equation (51). However, the algebraic reparametrization of the phase-specific strain rates does not introduce an additional contribution into this equation. The mechanical power in Prahs et al. [18], Equation (70), already contains the effective and phase-specific stress-power contributions. Accounting for Equations (69) and (81), the reparametrization only provides an equivalent representation of this existing mechanical contribution.

5. Summary and Conclusions

5.1. Thermodynamic Consequences

The thermodynamic consequences of an algebraic reparametrization of phase-specific strains have been established within the phase-field and multiphase-field formulations based on internal state variables. The principal findings are as follows:

- The effective strain and an independent set of strain jumps provide an invertible representation of the phase-specific strains. For $\tilde{N}$ locally active phases, $\tilde{N} - 1$ independent jump tensors preserve the dimension of the local mechanical state space.
- The reparametrization preserves the total diffuse-interface dissipation but changes the representation of the forces conjugate to the selected rates. The kinetic relations used for order-parameter evolution constitute separate constitutive assumptions.
- The reparametrization makes the stress-interaction contribution already contained in the underlying internal-state-variable formulations explicit in the order-parameter dissipation. This contribution has a counterpart in the sharp-interface equilibrium conditions of Johnson and Alexander [19], Equation (32), and Voorhees and Johnson [20], Equation (34). Under the stated compatibility and traction-continuity conditions, the two-phase and multiphase expressions recover the corresponding small-deformation stress-dependent contributions of Schneider et al. [13], Equations (49) and (50).
- The reparametrization introduces no additional contribution into the heat-conduction equations of the underlying formulations.

These results clarify the representation of mechanical coupling within the internal-state-variable framework and its relation to established sharp-interface and phase-field formulations.

5.2. Practical Applicability

The applications cited in Section 3.2 provide relevant contexts for the use of the reparametrized representation. For a particular application, the phase-specific strains must be computed by means of a mechanical closure. A procedure based on mechanical jump conditions is given by Schneider et al. [13], Sections 3.1 and 3.2. The resulting phase-specific strains and stresses provide the strain jumps and interpolated stress needed to evaluate Δl or $\Delta l^{\alpha\beta}$ in the selected order-parameter kinetics.

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Nomenclature

Symbols and dimensional conventions. Units refer to the dimensional formulation in SI units.

Symbol	Meaning	SI Unit/Type
Geometry and phase labels		
x, t	Spatial position and time	m, s
$\mathcal{V}, \mathcal{V}^\alpha, \mathcal{V}^\pm$	Material domain and sharp-description phase regions	Sets
$\tilde{\mathcal{V}}^\alpha, \tilde{\mathcal{V}}^\pm$	Reduced bulk regions after diffuse regularization	Sets
$\mathcal{S}, \delta\mathcal{S}$	Sharp interface and its volumetric diffuse region	Sets
$\delta\mathcal{S}^{II}, \delta\mathcal{S}^{III}$	Unions of diffuse two-phase interfaces and junction regions	Sets
$\delta\mathcal{S}^A, \delta\mathcal{C}^A$	Interface or junction associated with the phase subset A	Sets
$\partial(\cdot), \partial\delta\mathcal{S}_N, \partial\delta\mathcal{S}_D$	Boundary, Neumann part, and Dirichlet part. Superscript III has the analogous meaning	Sets
$\mathcal{I}, A, A $	Global phase-index set, subset, and its cardinality	Set/count
$N, \tilde{N}, \alpha, \beta, \gamma, \kappa$	Global and local phase counts and phase indices	Counts/indices
$n_{\mathcal{V}}^{\delta\mathcal{S}}, n^{\alpha\beta}$	Outer boundary normal and pairwise interface normal	1
dv, da	Volume and area elements	m ³ , m ²
Order parameters and mechanical variables		
$\varphi, \varphi_\alpha, \boldsymbol{\phi}$	Two-phase order parameter, phase-specific order parameters, and their collection	1
$h(\varphi), \bar{h}(\varphi), h_\alpha$	Interpolation functions. $\bar{h}(\varphi) = 1 - h(\varphi)$ in the two-phase setting	1
$\nabla\varphi, \nabla\boldsymbol{\phi}$	Order-parameter gradient and collection of gradients	m ^{−1}
$\bar{\mathbf{u}}, \dot{\mathbf{u}}_\pm, \mathbf{v}$	Effective displacement, phase-specific displacement rates, and velocity	m, m s ^{−1}
$\bar{\mathbf{H}}, \mathbf{H}^\pm, \mathbf{H}^\alpha$	Effective and phase-specific displacement gradients	1
$\bar{\boldsymbol{\varepsilon}}, \boldsymbol{\varepsilon}^\pm, \boldsymbol{\varepsilon}^\alpha$	Effective and phase-specific infinitesimal strains	1
$\boldsymbol{\varepsilon}^{*\pm}, \boldsymbol{\varepsilon}^{*\alpha}$	Phase-specific inelastic strains	1
$\boldsymbol{\alpha}^\pm, \boldsymbol{\alpha}^\alpha$	Collections of phase-specific internal variables	Model dependent
$\bar{\boldsymbol{\sigma}}, \boldsymbol{\sigma}^\pm, \boldsymbol{\sigma}^\alpha$	Interpolated and phase-specific Cauchy stresses	Pa
$\bar{\mathbf{t}}, \mathbf{t}^\pm$	Interpolated and phase-specific traction vectors on the diffuse-region boundary	Pa

Symbol	Meaning	SI Unit/Type
$\mathbf{d}^{\alpha\beta}$	Pairwise jump vector in the strain-rate compatibility condition following Equation (81)	s^{-1}
Thermodynamic fields and interface contributions		
$\theta, \dot{\theta}$	Absolute temperature and material temperature rate	K, K s^{-1}
$\rho_{\pm}, \rho^{\alpha}, \bar{\rho}$	Phase-specific and interpolated bulk mass densities	kg m^{-3}
ρ_S	Surface mass density	kg m^{-2}
$\psi^{\pm}, \psi^{\alpha}, \psi_S$	Mass-specific bulk free energies and mass-specific surface free energy	J kg^{-1}
$f^{\pm}, \bar{f}_V, \bar{\rho}\bar{\psi}$	Phase-specific volumetric free energies and their interpolated bulk density	J m^{-3}
$\eta^{\pm}, \eta^{\alpha}, \eta_S$	Mass-specific bulk and surface entropies	$\text{J kg}^{-1} \text{K}^{-1}$
$\tilde{\psi}_S$	Diffuse free-energy density divided by ρ_S	$\text{J kg}^{-1} \text{m}^{-1}$
$\tilde{\eta}_S, \tilde{\eta}_S^*$	Diffuse entropy density and interpolated bulk-entropy contribution, each divided by ρ_S	$\text{J kg}^{-1} \text{m}^{-1} \text{K}^{-1}$
$\psi_{\text{grad}}, \psi_{\text{pot}}$	Normalized gradient and potential contributions in the adopted free-energy ansatz	1
ξ, ξ^{α}	Derivatives of ψ_{grad} with respect to the corresponding order-parameter gradients	m
Ξ, Ξ^{α}	Density- and surface-energy-weighted gradient derivatives	J m^{-2}
Rates, dissipation, and conjugate forces		
$\Gamma, \tilde{\Gamma}$	Total entropy-production rates of sharp and diffuse descriptions	$\text{J K}^{-1} \text{s}^{-1}$
$\tilde{\Gamma}_{\tilde{V}^{\pm}}, \tilde{\Gamma}_{\delta S}$	Bulk and diffuse-region entropy-production rates	$\text{J K}^{-1} \text{s}^{-1}$
$\mathcal{D}_{\delta S}, \mathcal{D}_{\delta S}^{\text{III}}$	Integrated dissipation in the diffuse interface and junction regions	J s^{-1}
$\mathcal{D}_{\delta S}^{\varphi}, \mathcal{D}_{\delta S}^{\theta}, \mathcal{D}_{\delta S}^{\text{mech}}$	Order-parameter, thermal, and mechanical contributions to the integrated dissipation	J s^{-1}
$\mathcal{B}$	Boundary contribution to the integrated dissipation	J s^{-1}
$\Omega, \Omega_{\varepsilon}$	Weighted bulk free-energy rates and their strain-rate contribution	$\text{J m}^{-3} \text{s}^{-1}$
$\chi, A_{\alpha\beta\alpha}, A_{\beta\alpha\beta}$	Pairwise stress-power sum and auxiliary ordered-pair contractions	$\text{J m}^{-3} \text{s}^{-1}$
$\Delta l, l_{\alpha}, \Delta l^{\alpha\beta}$	Two-phase, phase-specific, and pairwise mechanical interaction contributions	J m^{-3}
$F_{\alpha}, \hat{F}_{\alpha}$	Original and modified order-parameter force densities	J m^{-3}
$\dot{\phi}_0, M_{\alpha\beta}$	Kinetic coefficient in Equation (31) and pairwise mobilities in Equation (77)	$\text{m}^3 \text{J}^{-1} \text{s}^{-1}$
$\Delta L = \Delta l \dot{\phi}$	Mechanical interaction power density in the heat-equation discussion	$\text{J m}^{-3} \text{s}^{-1}$
Mathematical notation		
$\{\bullet\}, \{\bullet\}^{\alpha\beta}$	Two-phase jump and ordered pairwise jump, with phase order + minus – and α minus β , respectively	As $\bullet$
$\dot{\bullet}$	Material time derivative	Unit of $\bullet$ per s
$\cdot, \otimes$	Euclidean scalar product (full contraction for second-order tensors) and tensor product	By operands

Symbol	Meaning	SI Unit/Type
sym, ∇ , div	Symmetric part, spatial gradient, and divergence	Operators
$\delta_{\alpha\kappa}$, $\mathbf{0}$	Kronecker delta and zero tensor	1 / by context

Appendix A

Auxiliary Calculation for the Pairwise Stress-Power Contribution

The diagonal contributions to χ vanish since $\{\dot{\epsilon}\}^{\alpha\alpha} = 0$. Consequently, the double sum can first be restricted to ordered phase pairs with $\alpha \neq \beta$, i.e.,

$$\begin{aligned}\chi &:= \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \varphi_{\alpha} \varphi_{\beta} \sigma^{\alpha} \cdot \{\dot{\epsilon}\}^{\alpha\beta} \\ &= \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1, \beta \neq \alpha}^{\tilde{N}} \varphi_{\alpha} \varphi_{\beta} \sigma^{\alpha} \cdot \{\dot{\epsilon}\}^{\alpha\beta}.\end{aligned}\quad (\text{A1})$$

For an arbitrary phase pair $\alpha \neq \beta$, the two ordered contributions are denoted by

$$\begin{aligned}A_{\alpha\beta\alpha} &:= \{\dot{\epsilon}\}^{\alpha\beta} \cdot \sigma^{\alpha} \\ &= (\dot{\epsilon}^{\alpha} - \dot{\epsilon}^{\beta}) \cdot \sigma^{\alpha}\end{aligned}\quad (\text{A2})$$

and

$$\begin{aligned}A_{\beta\alpha\beta} &:= \{\dot{\epsilon}\}^{\beta\alpha} \cdot \sigma^{\beta} \\ &= (\dot{\epsilon}^{\beta} - \dot{\epsilon}^{\alpha}) \cdot \sigma^{\beta}.\end{aligned}\quad (\text{A3})$$

Since $\varphi_{\alpha} \varphi_{\beta} = \varphi_{\beta} \varphi_{\alpha}$, the two ordered contributions associated with the same unordered phase pair can be collected. Applying the rearrangement of the ordered double sum given by Prahs et al. [18], Equations (47)–(50), to the stress-power contributions considered here, Equation (A1) becomes

$$\chi = \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1}^{\tilde{N}} \varphi_{\alpha} \varphi_{\beta} (A_{\alpha\beta\alpha} + A_{\beta\alpha\beta}). \quad (\text{A4})$$

Insertion of Equations (A2) and (A3) gives

$$\begin{aligned}A_{\alpha\beta\alpha} + A_{\beta\alpha\beta} &= \sigma^{\alpha} \cdot (\dot{\epsilon}^{\alpha} - \dot{\epsilon}^{\beta}) + \sigma^{\beta} \cdot (\dot{\epsilon}^{\beta} - \dot{\epsilon}^{\alpha}) \\ &= \sigma^{\alpha} \cdot \dot{\epsilon}^{\alpha} - \sigma^{\alpha} \cdot \dot{\epsilon}^{\beta} + \sigma^{\beta} \cdot \dot{\epsilon}^{\beta} - \sigma^{\beta} \cdot \dot{\epsilon}^{\alpha} \\ &= \sigma^{\alpha} \cdot \dot{\epsilon}^{\alpha} - \sigma^{\alpha} \cdot \dot{\epsilon}^{\beta} - \sigma^{\beta} \cdot \dot{\epsilon}^{\alpha} + \sigma^{\beta} \cdot \dot{\epsilon}^{\beta}.\end{aligned}\quad (\text{A5})$$

On the other hand, expansion of the scalar product of the corresponding stress and strain-rate jumps yields

$$\begin{aligned}\{\sigma\}^{\alpha\beta} \cdot \{\dot{\epsilon}\}^{\alpha\beta} &= (\sigma^{\alpha} - \sigma^{\beta}) \cdot (\dot{\epsilon}^{\alpha} - \dot{\epsilon}^{\beta}) \\ &= \sigma^{\alpha} \cdot \dot{\epsilon}^{\alpha} - \sigma^{\alpha} \cdot \dot{\epsilon}^{\beta} - \sigma^{\beta} \cdot \dot{\epsilon}^{\alpha} + \sigma^{\beta} \cdot \dot{\epsilon}^{\beta}.\end{aligned}\quad (\text{A6})$$

Comparison of Equations (A5) and (A6) shows that

$$A_{\alpha\beta\alpha} + A_{\beta\alpha\beta} = \{\sigma\}^{\alpha\beta} \cdot \{\dot{\epsilon}\}^{\alpha\beta}. \quad (\text{A7})$$

Finally, insertion of Equation (A7) into Equation (A4) gives

$$\chi = \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1}^{\tilde{N}} \varphi_{\alpha} \varphi_{\beta} [\sigma]^{\alpha\beta} \cdot [\dot{\epsilon}]^{\alpha\beta}. \quad (\text{A8})$$

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