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ORIGINAL ARTICLE

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The multiphase-field method based on internal state variables

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Abstract The multiphase-field method is widely used to simulate the evolution of complex microstructures in computational materials science and is commonly derived via a variational approach. When coupled with heat conduction, it is desirable to derive both the multiphase-field method and the heat conduction equation from a unified, consistent framework. In the present work, this is accomplished by introducing order parameters as internal state variables and exploiting the entropy production inequality of the diffuse interface region for multiple intersecting phases. The approach represents a generalization of the method of Prahs *et al.* (Prahs *et al. Continuum Mech. Thermodyn.* **37**, 55 (2025). https://doi.org/10.1007/s00161-025-01383-y) via a dual-interaction ansatz and its Lagrange multiplier simplification, while maintaining thermodynamical consistency. This requirement, in turn, restricts the choice of the interpolation functions. Moreover, the coupling effects in the heat conduction equation as well as connections to established evolution equations from the literature are demonstrated through an illustrative derivation.

Keywords Multiphase-field method · Continuum thermodynamics · Internal state variable · Heat conduction · Dual-interaction ansatz · Lagrange multiplier

1 Introduction

From two to multiple phases The phase-field method (PFM) was initially developed to describe nanoscale and microscale phenomena (see the seminal works [1–6]). Today, it is widely used for modeling phase transitions and, more generally, the evolution of singular surfaces [7–10]. The PFM employs order parameters, which are continuous indicator functions that satisfy a nonlocal (kinetic) evolution equation [6,11]. This equation is

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usually derived using a variational approach: the variational derivative of a functional depending on the order parameters is balanced by their rate and a positive mobility factor. Notably, the strong form of the evolution equation remains a postulate. An alternative formulation by Penrose and Fife uses an entropy functional rather than a free-energy functional, which allows for spatiotemporal variations in the temperature field [11]. While the PFM was originally formulated for two phases, e.g., [4,6,11], it was extended to multiple phases by [7,12–14], referred to as the multiphase-field method (MPFM). Since the order parameters are formulated as scalar fields, the numerical tracking of diffuse interfaces can be performed efficiently, cf., e.g., [15–17]. Hence, the MPFM is a well-established approach for simulating the evolution of complex microstructures and is applied in contexts such as solidification, solid–solid phase transitions, precipitation growth and coarsening, and grain growth, cf. [8–10]. Moreover, the MPFM was further extended to account for mechanical contributions [18–21], with non-linear constitutive behavior, e.g., [22–24], crack propagation [25,26], and many more.

Approaches to derive the (M)PFM The evolution equation of the order parameter is typically derived via a variational approach. However, in the case of coupling with heat conduction, it is imperative to adopt a consistent framework in which the derivation of the MPFM and the derivation of the modified heat conduction equation are obtained in a unified manner. A generalization of the PFM was proposed by Gurtin [27] via an extended principle of virtual power (POVP), rooted in continuum thermodynamics. Unlike variational approaches, this framework separates balance equations, reflecting universal physical laws, from constitutive relations, describing material behavior. In continuum mechanics, the evolution of the order parameter is commonly derived either from the extended POVP [27,28] or from the invariance of an extended energy balance under Euclidean transformations [29]. In both cases, the order parameter is introduced as an additional generic degree of freedom (DOF), implying that the PFM is formulated within an extended continuum. Another approach is given by [30], [31], considering the order parameter as an internal state variable (ISV) instead of as an additional DOF, since it represents an observable rather than a controllable quantity, e.g., [32,33]. In this regard, the order parameter is considered to be of dissipative nature [33] and its evolution equation, consequently, follows from the exploitation of the dissipation inequality. In deriving the evolution equation of the order parameter, [31] employs the dissipation inequality associated with the singular surface, in contrast to [30], which bases the derivation on the bulk dissipation inequality. The distinction originates from the modeling framework: [30] assumes a Cauchy continuum with a diffuse interfacial region, from the outset, while [31] employs a Cauchy continuum with a material singular surface for the derivation of the evolution equation. The latter approach interprets the PFM as an approximation of the sharp interface theory for the quasi-static special case of a slowly evolving non-material singular surface without body forces, within the framework of continuum thermodynamics, [34]. For this special case, the balances of mass, linear momentum, and internal energy of a non-material singular surface are identical to those of a material singular surface.

Objectives of the current work This work derives the MPFM by introducing the order parameters as ISVs and systematically exploiting the entropy production inequality of the diffuse interface region for multiple intersecting phases within the framework of continuum thermodynamics. Thermodynamically consistent evolution equations for the order parameters are presented, and the corresponding heat conduction equation is derived. A comparison with the classical variational approach is also provided.

Originality This work represents a direct generalization of Prahs et al. [31] to multiple intersecting phases. Following this approach, this work:

- demonstrates the thermodynamic consistency of the dual-interaction ansatz in the multiphase setting, as well as the Lagrange multiplier formulation as a simplified version of this,
- demonstrates that $h_\alpha(\varphi_\alpha) = \varphi_\alpha$ is not only one but the only admissible interpolation function under consistent with continuum thermomechanics[1]
- derives a fully consistent heat-conduction equation including coupling contributions due to microstructure evolution.

Finally, the relationships between the dual-interaction approach and the evolution equation of Steinbach and Pezzolla [7], as well as between the simplified approach and the evolution equation of Nestler et al. [14], are demonstrated through a derivation of the MPFM using the classical variational approach for an illustrative special case.

Outline The derivation of the multiphase-field method based on introducing the order parameters as ISVs and exploiting the entropy production inequality of the diffuse interface domain is presented in Sect. (2).

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[1] While Steinbach [35, p.12] mentions that $h_\alpha(\varphi_\alpha) = \varphi_\alpha$ represents a thermodynamically consistent interpolation function, it is shown that this is the only thermodynamically consistent choice within the presented framework.

Moreover, the thermodynamical consistency of the proposed evolution equations is demonstrated, and the associated equation of heat conduction is derived. Special cases of the MPFM obtained by restrictions of the considered free energy are discussed in Sect. (3). The comparison of the proposed evolution equations with well-established evolution equations from literature is carried out by deriving the MPFM via the variational approach in Sect. (4). Section (5) presents the conclusion of the work at hand.

Notation Tensors are represented using a direct notation: first-order tensors by lowercase bold letters and second-order tensors by uppercase bold letters, e.g., $\boldsymbol{a}$ and $\boldsymbol{A}$. Scalar products are written as $\boldsymbol{a} \cdot \boldsymbol{b}$ and $\boldsymbol{A} \cdot \boldsymbol{B}$, the dyadic product as $\boldsymbol{a} \otimes \boldsymbol{b}$, and the composition of second-order tensors as $\boldsymbol{A}\boldsymbol{B}$. The material time derivative of a quantity $\boldsymbol{\alpha}$ of arbitrary tensorial order is $\dot{\boldsymbol{\alpha}}$.

2 Diffuse interface theory

2.1 Approximation of entropy production in the diffuse interface

Brief sketch of the idea In this work, the order parameter is considered as an internal state variable but not as an additional degree of freedom. Consequently, the evolution equation of the order parameter is obtained by exploitation of the dissipation inequality. The balances of mass, linear momentum, and internal energy of a i) slowly evolving, ii) quasi-static, non-material singular surface with iii) no body forces acting on it resemble those of a material singular surface, cf. the discussion in [31]. In this particular case, the phase-field method is regarded as an approximation of the sharp interface theory, employed within the framework of evolving microstructure. Thus, the balance equations (mass, linear momentum, internal energy, cf. Eq. (A.8)), derived for a material singular surface, are assumed to hold true at each point of the diffuse interface domain. Moreover, the constitutive restriction regarding the dependency of the specific free energy, cf. Eq. (A.12), as well as the potential relation for the specific entropy, cf. Eq. (A.13), derived for a material singular surface, are also assumed to hold true in the diffuse interface. Consequently, the free energy contribution related to the sharp interface is assumed to depend only on the absolute temperature, also in the diffuse interface context. For brevity, considerations are limited to a small-strain framework. Summarizing, the present phase-field formulation is interpreted as a thermodynamically consistent diffuse approximation of a sharp-interface theory for quasi-static, slowly evolving non-material singular surfaces governed by balances of mass, linear momentum, and internal energy.

Diffuse interfaces in the multiphase context This section extends the approach of Prahs et al. [31] to multiple phases, as illustrated by Fig. 1.

In addition to [31], surfaces that intersect at a common line are considered.[2] Regarding Fig. 1, the material singular surfaces $\mathcal{S}^{\alpha\beta}$, $\mathcal{S}^{\beta\gamma}$, and $\mathcal{S}^{\gamma\alpha}$ are replaced by the diffuse interface regions of finite width, referred to as $\delta\mathcal{S}^{\alpha\beta}$, $\delta\mathcal{S}^{\beta\gamma}$, and $\delta\mathcal{S}^{\gamma\alpha}$, respectively, except for the region around the common line. In general, the union of interfaces between two phases is referred to as $\delta\mathcal{S}^{II}$ and given by

$$\delta\mathcal{S}^{II} = \bigcup_{\substack{A \subseteq \mathcal{I} \\ |A|=2}} \delta\mathcal{S}^{A}, \qquad \text{with } \delta\mathcal{S}^{A} = \varnothing \text{ if no } A\text{-interface occurs.} \tag{1}$$

Regarding Eq. (1), $\mathcal{I}$ denotes the index set of all phases and $A \subseteq \mathcal{I}$ with $|A| = 2$ denotes a subset of indices corresponding to two intersecting phases. A brief remark on the notation used in Eq. (2) is provided in the appendix, cf. Eqs. (A.1) - (A.5). Regarding again Fig. 1, the diffuse interface $\delta\mathcal{C}^{\alpha\beta\gamma}$ is introduced around the common line of $\mathcal{S}^{\alpha\beta}$, $\mathcal{S}^{\beta\gamma}$, and $\mathcal{S}^{\gamma\alpha}$. In general, the union of the diffuse interfaces between three or more intersecting phases, i.e. around common lines, is denoted as $\delta\mathcal{S}^{III}$ and given by

$$\delta\mathcal{S}^{III} = \bigcup_{\substack{A \subseteq \mathcal{I} \\ |A|\geq 3}} \delta\mathcal{C}^{A}, \qquad \text{with } \delta\mathcal{C}^{A} = \varnothing \text{ if no } A\text{-junction occurs.} \tag{2}$$

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[2] In the two-dimensional sketch of the continuum shown in Fig. 1, singular surfaces are depicted as lines, and their common line corresponds to the point of intersection of these lines.

Regarding Eq. (2), $\mathcal{I}$ denotes the index set of all phases and $A \subseteq \mathcal{I}$ with $|A| \geq 3$ denotes a subset of indices corresponding to intersecting phases. A brief remark on the notation used in Eq. (2) is provided in the appendix, cf. Eqs. (A.1) - (A.5). In addition, the volumetric regions $\mathcal{V}^\alpha$ are replaced by smaller volumes $\tilde{\mathcal{V}}^\alpha$, such that

$$\mathcal{V} = \bigcup_{\alpha=1}^{N} \mathcal{V}^\alpha = \left(\bigcup_{\alpha=1}^{N} \tilde{\mathcal{V}}^\alpha \right) \cup \delta\mathcal{S}^{II} \cup \delta\mathcal{S}^{III} \tag{3}$$

holds true. Here, N denotes the number of all material phases at a given instant of time. The spatial distribution of different phases is described by order parameters, which act as continuous indicator functions governed by a nonlocal evolution equation. Within the bulk domain $\tilde{\mathcal{V}}^\alpha$, the corresponding order parameter satisfies $\varphi_\alpha = 1$, while in $\tilde{\mathcal{V}}^\beta$, $\varphi_\alpha = 0$ holds true. In contrast, inside diffuse interfacial regions separating multiple phases, several order parameters attain nonzero values simultaneously. For instance, along two-phase interfaces both associated order parameters are nonzero, while in multiphase regions the product of all involved order parameters differs from zero.

Entropy production in the diffuse interface The entropy production of a Cauchy continuum with several material singular surfaces (considered sharp interfaces) is approximated by that of a Cauchy continuum with diffuse interfaces. Accordingly, the entropy production $\tilde{\Gamma}$ of the latter is required to be non-negative. It consists of a surface contribution $\tilde{\Gamma}_{\delta\mathcal{S}}$, associated with the diffuse interface domain $\delta\mathcal{S}$, and bulk contributions $\tilde{\Gamma}_{\tilde{\mathcal{V}}^\alpha}$ for each phase α, associated with its respective domain $\tilde{\mathcal{V}}^\alpha$, reading

$$\tilde{\Gamma} = \tilde{\Gamma}_{\delta\mathcal{S}} + \sum_{\alpha=1}^{N} \tilde{\Gamma}_{\tilde{\mathcal{V}}^\alpha} \geq 0, \quad \tilde{\Gamma}_{\delta\mathcal{S}} = \tilde{\Gamma}^{II}_{\delta\mathcal{S}} + \tilde{\Gamma}^{III}_{\delta\mathcal{S}}. \tag{4}$$

In this regard, $\tilde{\Gamma}^{II}_{\delta\mathcal{S}}$ denotes the entropy production within the diffuse interface between two phases, while $\tilde{\Gamma}^{III}_{\delta\mathcal{S}}$ denotes the entropy production within a diffuse interface between at least three phases. The exploitation of $\tilde{\Gamma}_{\tilde{\mathcal{V}}^\alpha}$ and $\tilde{\Gamma}^{II}_{\delta\mathcal{S}}$ is carried out in detail in [31]. Therefore, the exploitation of $\tilde{\Gamma}^{III}_{\delta\mathcal{S}}$, given by

$$\tilde{\Gamma}^{III}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}^{III}} -\rho_{\mathcal{S}} \frac{\dot{\theta}}{\theta} \tilde{\eta}_{\mathcal{S}} - \rho_{\mathcal{S}} \frac{\dot{\tilde{\psi}}_{\mathcal{S}}}{\theta} \, \mathrm{d}v, \tag{5}$$

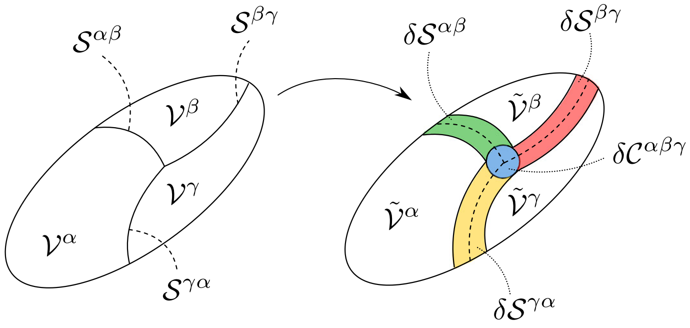

Fig. 1 Representation of the transition between sharp and diffuse interface descriptions exemplified by a material volume divided by three intersecting material surfaces. The sharp material surfaces $\mathcal{S}^{\alpha\beta}$, $\mathcal{S}^{\beta\gamma}$, and$\mathcal{S}^{\gamma\alpha}$ are substituted by the diffuse interface regions $\delta\mathcal{S}^{\alpha\beta}$, $\delta\mathcal{S}^{\beta\gamma}$, and $\delta\mathcal{S}^{\gamma\alpha}$ of finite width. To represent the neighborhood of their common line, the diffuse region $\delta\mathcal{C}^{\alpha\beta\gamma}$ is introduced. Furthermore, the bulk regions $\mathcal{V}^\alpha$ are replaced by smaller domains $\tilde{\mathcal{V}}^\alpha$. Within the bulk domain $\tilde{\mathcal{V}}^\alpha$, the corresponding order parameter satisfies $\varphi_\alpha = 1$, while in $\tilde{\mathcal{V}}^\beta$, $\varphi_\alpha = 0$ holds. In contrast, diffuse interfacial regions are characterized by products of order parameters: along a two-phase interface $\delta\mathcal{S}^{\alpha\beta}$, separating phases α and β, one has $\varphi_\alpha\varphi_\beta \neq 0$. Similarly, in the multiphase region $\delta\mathcal{C}^{\alpha\beta\gamma}$, where phases α, β, and γ intersect, the product $\varphi_\alpha\varphi_\beta\varphi_\gamma \neq 0$ holds, indicating the simultaneous presence of all involved phases. The depicted sketch is closely inspired by and adapted from Slattery et al. [36, Fig. 1.3.8-1] and Steinbach and Pezzolla [7, Fig.2].

is discussed, in the work at hand. The temperature θ is assumed to be a continuous field across the phases. The mass density of the material singular surface from the approximated sharp interface theory is referred to as $\rho_{\mathcal{S}}$. Regarding the diffuse interface $\delta\mathcal{S}^{III}$, the contributions $\tilde{\psi}_{\mathcal{S}}$ and $\tilde{\eta}_{\mathcal{S}}$ represent the approximations of $\psi_{\mathcal{S}}$ and $\eta_{\mathcal{S}}$ which denote the specific free energy and the specific entropy of the material singular surface in the sharp interface context. Here, a Cauchy continuum with intersecting material singular surfaces provides the starting point for deriving the evolution equations of the order parameters. The velocity fields of the material singular surfaces coincide with that of the common line, cf. Slattery et al. [36, Eq.(1.3.7-13)]. Thus, no energy contribution is present on the common line.

Ansatz for surface free energy and surface entropy The ansatz for the contribution $\tilde{\psi}_{\mathcal{S}}$ represents a direct generalization of Prahs et al. [31, Eq. 16] towards multiple phases, reading

$$\tilde{\psi}_{\mathcal{S}} = \frac{1}{\rho_{\mathcal{S}}}\left(\sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi})\rho^\alpha\right)\psi_{\mathcal{S}}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) + \frac{1}{\rho_{\mathcal{S}}}\left(\sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi})\rho^\alpha\psi^\alpha\right), \tag{6}$$

with the set of the order parameter defined as

$$\boldsymbol{\phi} = \{\varphi_1, \dots, \varphi_{\tilde{N}}\}. \tag{7}$$

Here, $\tilde{N}$ denotes the number of locally active phases. Interfaces and junctions are not counted explicitly and may form or vanish naturally through the evolution of the order parameters. Moreover, ψ_{grad} and ψ_{pot} denote, the gradient and potential contribution of the specific free energy, and ψ^α the specific free energy of phase α. The potential relation for the surface entropy, cf. Eq. (A.13) is considered to hold true in the diffuse interface context. Moreover, it is assumed that the interpolation functions $h_\alpha(\boldsymbol{\phi})$, the gradient and potential contributions ψ_{grad} and ψ_{pot}, as well as the mass densities ρ^α and $\rho_{\mathcal{S}}$ do not depend on the temperature. Consequently, the entropy is given by

$$\tilde{\eta}_{\mathcal{S}} = -\frac{\partial\tilde{\psi}_{\mathcal{S}}}{\partial\theta} = \frac{\overline{\rho}}{\rho_{\mathcal{S}}}\eta_{\mathcal{S}}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) + \tilde{\eta}^*_{\mathcal{S}}. \tag{8}$$

Here, the interpolated density $\overline{\rho}$ is introduced along with the interpolated bulk entropy $\tilde{\eta}^*_{\mathcal{S}}$, reading

$$\overline{\rho} := \sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi})\rho^\alpha, \quad \tilde{\eta}^*_{\mathcal{S}} := \frac{1}{\rho_{\mathcal{S}}}\sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi})\rho^\alpha\eta^\alpha. \tag{9}$$

The second term of Eq. (6) illustrates that the considered ansatz for $\tilde{\psi}_{\mathcal{S}}$ accounts for the interpolation of the free energy density $\overline{f_{\mathcal{V}}}$ in the sense that

$$\overline{f_{\mathcal{V}}} = \sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi}) f^\alpha = \sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi})\rho^\alpha\psi^\alpha = \overline{\rho\psi} \tag{10}$$

holds true.

Gradient and potential contribution to the free energy It is assumed that the potential contribution ψ_{pot} depends on the set of order parameters $\boldsymbol{\phi}$, while the gradient contribution ψ_{grad} depends on both the set of order parameters $\boldsymbol{\phi}$ and the set of the gradients of the order parameters $\nabla\boldsymbol{\phi}$, i.e.,

$$\psi_{\text{grad}} = \psi_{\text{grad}}(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}), \quad \psi_{\text{pot}} = \psi_{\text{pot}}(\boldsymbol{\phi}) \tag{11}$$

holds true, e.g., [14], with the set of the gradients of the order parameters defined as

$$\nabla\boldsymbol{\phi} = \{\nabla\varphi_1, \dots, \nabla\varphi_{\tilde{N}}\}. \tag{12}$$

The focus of this work is on the derivation of the MPFM based on the interpretation of the order parameters as ISVs. Thus, a discussion of specific choices for ψ_{grad} and ψ_{pot} is omitted in this manuscript. For a detailed discussion of these contributions and their implications regarding the phase evolution, the reader is referred to [37]. As a consequence, no asymptotic analysis, cf., e.g., Bender and Orszag [38], Hinch [39] is carried out as done, e.g., by the seminal works of Caginalp [40], Karma and Rappel [41], Elder et al. [42]. The order parameters may be interpreted as the volume fractions associated with the respective phase α and must consequently satisfy the summation constraint

$$\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha(\boldsymbol{x}, t) = 1 \quad \rightsquigarrow \quad \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha(\boldsymbol{x}, t) = 0, \quad \forall \boldsymbol{x} \in \mathcal{V}, \quad t \geq 0, \tag{13}$$

cf. Garcke et al. [13, Eq.(4)], Stinner et al [43, Eq.(2)$_2$], Nestler et al. [14, p.2]. Moreover, the summation constraint is also applied to the interpolation functions $h_\alpha(\boldsymbol{\phi})$, reading

$$\sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi}) = 1, \quad \forall \boldsymbol{x} \in \mathcal{V}, \quad t \geq 0, \tag{14}$$

cf. Moelans [44, p.1078]. The time derivative of Eq. (14) yields

$$\sum_{\alpha=1}^{\tilde{N}} \dot{h}_\alpha(\boldsymbol{\phi}) = 0 \quad \rightsquigarrow \quad \sum_{\alpha=1}^{\tilde{N}} \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha} \dot{\varphi}_\alpha = 0, \quad \forall \boldsymbol{x} \in \mathcal{V}, \quad t \geq 0. \tag{15}$$

Dissipation in the diffuse interface The non-negativity of the entropy of the diffuse interface, cf. Eq. (4), is fulfilled if each contribution is non-negative. Thus, it is required that

$$\tilde{\Gamma}_{\tilde{\mathcal{V}}^\alpha} \geq 0, \quad \tilde{\Gamma}^{II}_{\delta\mathcal{S}} \geq 0, \quad \tilde{\Gamma}^{III}_{\delta\mathcal{S}} \geq 0 \tag{16}$$

hold true. The fulfillment of Eqs. (16)$_1$ and (16)$_2$ has already been examined in detail in [31]; a brief recapitulation is given in the appendix of the present work. Accordingly, the present work provides an in-depth discussion of Eq. (16)$_3$. Accounting for Eqs. (6) and (8), the integrand of Eq. (5) is referred to as $\mathcal{L}_\mathcal{S}$, in the following. It is given by

$$\mathcal{L}^{III}_\mathcal{S} = -\rho_\mathcal{S}\frac{\dot{\theta}}{\theta}\tilde{\eta}_\mathcal{S} - \frac{\rho_\mathcal{S}}{\theta}\left(\frac{\overline{\rho}}{\rho_\mathcal{S}}\psi_\mathcal{S}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) + \frac{1}{\rho_\mathcal{S}}\left(\sum_{\alpha=1}^{\tilde{N}} h_\alpha(\boldsymbol{\phi})\rho^\alpha\psi^\alpha\right)\right)^{\boldsymbol{\cdot}}, \quad \mathcal{L}^{III}_\mathcal{S} \geq 0. \tag{17}$$

Here, Eq. (17)$_2$ represents the Clausius–Duhem inequality for points in $\delta\mathcal{S}^{III}$. Considering small deformations, $\dot{\rho}_+ = 0, \quad \dot{\rho}_- = 0, \quad \dot{\rho}_\mathcal{S} = 0$ hold true. Consequently, the application of the product rule transforms Eq. (17) into

$$\begin{aligned} \mathcal{L}^{III}_\mathcal{S} = -\rho_\mathcal{S}\frac{\dot{\theta}}{\theta}\tilde{\eta}_\mathcal{S} - \frac{1}{\theta}\Bigg(&\left(\sum_{\alpha=1}^{\tilde{N}} \dot{h}_\alpha(\boldsymbol{\phi})\rho^\alpha\right)\psi_\mathcal{S}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) + \overline{\rho}\dot{\psi}_\mathcal{S}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) \\ &+ \overline{\rho}\psi_\mathcal{S}\left(\dot{\psi}_{\text{grad}} + \dot{\psi}_{\text{pot}}\right) + \left(\sum_{\alpha=1}^{\tilde{N}} \rho^\alpha\dot{h}_\alpha(\boldsymbol{\phi})\psi^\alpha + \rho^\alpha h_\alpha(\boldsymbol{\phi})\dot{\psi}^\alpha\right)\Bigg). \end{aligned} \tag{18}$$

This work assumes that the balance equations and potential relations derived for a material singular surface within a Cauchy continuum hold. For this case it is possible to show $\psi_\mathcal{S} = \psi_\mathcal{S}(\theta)$, cf., e.g., Prahs et al. [31, Eq.(A.15)], and $\eta_\mathcal{S} = -\partial\psi_\mathcal{S}/\partial\theta$. Accounting for this and inserting Eq. (8) into Eq. (18) yields

$$\begin{aligned} \mathcal{L}^{III}_\mathcal{S} =& -\rho_\mathcal{S}\frac{\dot{\theta}}{\theta}\frac{\overline{\rho}}{\rho_\mathcal{S}}\eta_\mathcal{S}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) - \rho_\mathcal{S}\frac{\dot{\theta}}{\theta}\tilde{\eta}^*_\mathcal{S} \\ &- \frac{1}{\theta}\left(\sum_{\alpha=1}^{\tilde{N}} \dot{h}_\alpha(\boldsymbol{\phi})\rho^\alpha\right)\psi_\mathcal{S}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) + \frac{1}{\theta}\overline{\rho}\eta_\mathcal{S}\dot{\theta}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) \\ &- \frac{1}{\theta}\overline{\rho}\psi_\mathcal{S}\left(\dot{\psi}_{\text{grad}} + \dot{\psi}_{\text{pot}}\right) - \frac{1}{\theta}\left(\sum_{\alpha=1}^{\tilde{N}} \rho^\alpha\dot{h}_\alpha(\boldsymbol{\phi})\psi^\alpha + \rho^\alpha h_\alpha(\boldsymbol{\phi})\dot{\psi}^\alpha\right). \end{aligned} \tag{19}$$

With $\boldsymbol{\xi}^\alpha = \partial\psi_{\text{grad}}/\partial\nabla\varphi_\alpha$, Eq. (19) simplifies upon multiplication by θ, resulting in

$$\begin{aligned}\theta\mathcal{L}_{\mathcal{S}}^{III} =& -\rho_{\mathcal{S}}\dot{\theta}\tilde{\eta}_{\mathcal{S}}^{*} - \left(\sum_{\alpha=1}^{\tilde{N}} \dot{h}_\alpha(\boldsymbol{\phi})\rho^\alpha\right)\psi_{\mathcal{S}}\left(\psi_{\text{grad}}+\psi_{\text{pot}}\right)\\ & -\overline{\rho}\psi_{\mathcal{S}}\left(\sum_{\alpha=1}^{\tilde{N}} \frac{\partial\psi_{\text{grad}}}{\partial\varphi_\alpha}\dot{\varphi}_\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla\dot{\varphi}_\alpha + \frac{\partial\psi_{\text{pot}}}{\partial\varphi_\alpha}\dot{\varphi}_\alpha\right) - \left(\sum_{\alpha=1}^{\tilde{N}} \rho^\alpha\dot{h}_\alpha(\boldsymbol{\phi})\psi^\alpha + \rho^\alpha h_\alpha(\boldsymbol{\phi})\dot{\psi}^\alpha\right). \end{aligned} \tag{20}$$

Defining $\boldsymbol{\Xi}^\alpha := \overline{\rho}\psi_{\mathcal{S}}\boldsymbol{\xi}^\alpha$, integration of Eq. (20) over $\delta\mathcal{S}^{III}$ yields

$$\begin{aligned}\int_{\delta\mathcal{S}^{III}} \theta\mathcal{L}_{\mathcal{S}}^{III}\,\mathrm{d}v = \int_{\delta\mathcal{S}^{III}} & -\rho_{\mathcal{S}}\dot{\theta}\tilde{\eta}_{\mathcal{S}}^{*} - \left(\sum_{\alpha=1}^{\tilde{N}} \dot{h}_\alpha(\boldsymbol{\phi})\rho^\alpha\right)\psi_{\mathcal{S}}\left(\psi_{\text{grad}}+\psi_{\text{pot}}\right)\\ & -\overline{\rho}\psi_{\mathcal{S}}\left(\sum_{\alpha=1}^{\tilde{N}} \frac{\partial\psi_{\text{grad}}}{\partial\varphi_\alpha}\dot{\varphi}_\alpha + \frac{\partial\psi_{\text{pot}}}{\partial\varphi_\alpha}\dot{\varphi}_\alpha\right) - \left(\sum_{\alpha=1}^{\tilde{N}} \boldsymbol{\Xi}^\alpha\cdot\nabla\dot{\varphi}_\alpha\right)\\ & -\left(\sum_{\alpha=1}^{\tilde{N}} \rho^\alpha\dot{h}_\alpha(\boldsymbol{\phi})\psi^\alpha + \rho^\alpha h_\alpha(\boldsymbol{\phi})\dot{\psi}^\alpha\right)\mathrm{d}v. \end{aligned} \tag{21}$$

Rewriting $\dot{h}_\alpha(\boldsymbol{\phi})$ as

$$\dot{h}_\alpha(\boldsymbol{\phi}) = \sum_{\alpha=1}^{\tilde{N}} \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial\varphi_\gamma}\dot{\varphi}_\gamma = \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial\varphi_\alpha}\dot{\varphi}_\alpha + \sum_{\gamma=1,\gamma\neq\alpha}^{\tilde{N}} \frac{\partial h_\gamma(\boldsymbol{\phi})}{\partial\varphi_\gamma}\dot{\varphi}_\gamma, \tag{22}$$

Eq. (21) yields

$$\begin{aligned}\int_{\delta\mathcal{S}^{III}} \theta\mathcal{L}_{\mathcal{S}}^{III}\,\mathrm{d}v = \int_{\delta\mathcal{S}^{III}} & -\rho_{\mathcal{S}}\dot{\theta}\tilde{\eta}_{\mathcal{S}}^{*}\\ & -\left(\sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha\left(-\operatorname{div}\left(\boldsymbol{\Xi}^\alpha\right) + \overline{\rho}\psi_{\mathcal{S}}\left(\frac{\partial\psi_{\text{grad}}}{\partial\varphi_\alpha} + \frac{\partial\psi_{\text{pot}}}{\partial\varphi_\alpha}\right)\right.\right.\\ & \left.\left. + \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial\varphi_\alpha}\left(\rho^\alpha\psi^\alpha + \rho^\alpha\psi_{\mathcal{S}}\left(\psi_{\text{grad}}+\psi_{\text{pot}}\right)\right)\right)\right)\\ & -\left(\sum_{\alpha=1}^{\tilde{N}} \left(\rho^\alpha\psi^\alpha + \rho^\alpha\psi_{\mathcal{S}}\left(\psi_{\text{grad}}+\psi_{\text{pot}}\right)\right)\left(\sum_{\gamma=1,\gamma\neq\alpha}^{\tilde{N}} \frac{\partial h_\gamma(\boldsymbol{\phi})}{\partial\varphi_\gamma}\dot{\varphi}_\gamma\right)\right)\\ & -\left(\sum_{\alpha=1}^{\tilde{N}} \rho^\alpha h_\alpha(\boldsymbol{\phi})\dot{\psi}^\alpha\right)\mathrm{d}v - \int_{\partial\delta\mathcal{S}^{III}} \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha\boldsymbol{\Xi}^\alpha\cdot\boldsymbol{n}_{\mathcal{V}}^{\delta\mathcal{S}}\,\mathrm{d}a. \end{aligned} \tag{23}$$

Constitutive assumptions and further exploitation For the further exploitation of Eq. $(16)_3$, it is assumed that the specific free energy of phase α depends on the phase-specific strain $\boldsymbol{\varepsilon}^\alpha$, the phase-specific inelastic strain $\boldsymbol{\varepsilon}^{*\alpha}$, the order parameter φ_α, a set of additional phase-specific internal state variables $\boldsymbol{\alpha}^\alpha$, and the temperature θ, i.e.

$$\psi^\alpha = \psi^\alpha(\boldsymbol{\varepsilon}^\alpha, \boldsymbol{\varepsilon}^{*\alpha}, \varphi_\alpha, \boldsymbol{\alpha}^\alpha, \theta) \tag{24}$$

holds true. Based on Eq. (6) and Eq. (24), the phase-specific strains and, consequently, phase-specific stresses are accounted for, in the following. A closure, providing a relation between the phase-specific strains is not discussed, deliberately. Different closure approaches such as homogenization schemes, e.g., Voigt/Reuss or the jump condition approach, cf., e.g., Durga et al. [45], Mosler et al. [46], Schneider et al. [21,47], Svendsen et al. [48] can be applied straightforward. However, the subsequently carried out calculations differ slightly, depending on the considered closure ansatz. Application of the chain rule, accounting for the divergence theorem and introducing the driving force contribution F_α as

$$\begin{aligned} F_\alpha :=& -\operatorname{div}\left(\boldsymbol{\Xi}^\alpha\right) + \overline{\rho}\psi_{\mathcal{S}}\left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_\alpha} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\alpha}\right) \\ &+ \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha}\left(\rho^\alpha \psi^\alpha + \rho^\alpha \psi_{\mathcal{S}}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) + \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \varphi_\alpha}\right) \end{aligned} \tag{25}$$

Eq. (21) can be expressed as

$$\int_{\delta\mathcal{S}^{III}} \theta \mathcal{L}_{\mathcal{S}}^{III}\, \mathrm{d}v = \mathcal{D}_{\delta\mathcal{S}}^{\varphi} + \mathcal{D}_{\delta\mathcal{S}}^{\theta} + \mathcal{D}_{\delta\mathcal{S}}^{\text{mech}} + \mathcal{D}_{\delta\mathcal{S}}^{\text{h}} + \mathcal{B} \geq 0 \tag{26}$$

with the contribution linear in the rate of the order parameters denoted by

$$\mathcal{D}_{\delta\mathcal{S}}^{\varphi} := \int_{\delta\mathcal{S}^{III}} -\left(\sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha F_\alpha\right) \mathrm{d}v, \tag{27}$$

the contribution linear in the temperature rate denoted by

$$\mathcal{D}_{\delta\mathcal{S}}^{\theta} := \int_{\delta\mathcal{S}^{III}} -\left(\rho_{\mathcal{S}} \tilde{\eta}_{\mathcal{S}}^{*} + \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \theta}\right) \dot{\theta}\, \mathrm{d}v, \tag{28}$$

the contribution related to the interpolation functions denoted by

$$\mathcal{D}_{\delta\mathcal{S}}^{\text{h}} := \int_{\delta\mathcal{S}^{III}} -\left(\sum_{\alpha=1}^{\tilde{N}} \left(\rho^\alpha \psi^\alpha + \rho^\alpha \psi_{\mathcal{S}}\left(\psi_{\text{grad}} + \psi_{\text{pot}}\right)\right)\left(\sum_{\gamma=1,\gamma\neq\alpha}^{\tilde{N}} \frac{\partial h_\gamma(\boldsymbol{\phi})}{\partial \varphi_\gamma} \dot{\varphi}_\gamma\right)\right) \mathrm{d}v, \tag{29}$$

the contribution linear in the remaining rates denoted by

$$\mathcal{D}_{\delta\mathcal{S}}^{\text{mech}} := \int_{\delta\mathcal{S}^{III}} -\left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \left(\frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^\alpha} \cdot \dot{\boldsymbol{\varepsilon}}^\alpha + \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha}} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha\right)\right) \mathrm{d}v, \tag{30}$$

and the boundary contribution denoted by

$$\mathcal{B} := -\int_{\partial\delta\mathcal{S}^{III}} \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \boldsymbol{\Xi}^\alpha \cdot \boldsymbol{n}_{\mathcal{V}}^{\delta\mathcal{S}}\, \mathrm{d}a. \tag{31}$$

The contributions $\mathcal{D}_{\delta\mathcal{S}}^{\varphi}$, $\mathcal{D}_{\delta\mathcal{S}}^{\theta}$, $\mathcal{D}_{\delta\mathcal{S}}^{\text{mech}}$ are decoupled regarding the rates and defined in $\delta\mathcal{S}^{III}$. Moreover, $\mathcal{B}$ is defined on the boundary. Thus, Eq. (26) is fulfilled by demanding

$$\mathcal{D}_{\delta\mathcal{S}}^{\varphi} \geq 0, \quad \mathcal{D}_{\delta\mathcal{S}}^{\theta} \geq 0, \quad \mathcal{D}_{\delta\mathcal{S}}^{\text{h}} \geq 0, \quad \mathcal{D}_{\delta\mathcal{S}}^{\text{mech}} \geq 0, \quad \mathcal{B} \geq 0. \tag{32}$$

independently of each other.

2.2 Exploitation of the dissipation inequality

Thermodynamical consistency of dual interaction evolution equation To fulfill Eq. (32)$_1$, the following ansatz is considered for $\dot{\varphi}_\alpha$

$$\dot{\varphi}_\alpha = -\frac{1}{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \left(F_\alpha - F_\beta\right), \tag{33}$$

with $M_{\alpha\beta}$ denoting the so-called mobility of the diffuse interface between phase α and β. The ansatz for the evolution equation according to Eq. (33) is closely related to that proposed by Steinbach and Pezzolla [7], as will be discussed in Sect. (4.2). It represents the pair-wise interactions between phase β and phase α. Inserting Eq. (33) in Eq. (27) yields

$$\mathcal{D}^{\varphi}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}^{III}} \frac{1}{\tilde{N}} \sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \left(F_\alpha - F_\beta\right) F_\alpha \,\mathrm{d}v, \quad M_{\alpha\beta} \geq 0, \quad \forall \alpha, \beta \tag{34}$$

$$= \int_{\delta\mathcal{S}^{III}} \frac{1}{\tilde{N}} \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \left(F_\alpha - F_\beta\right)^2 \,\mathrm{d}v \geq 0 \tag{35}$$

The transformation from Eq. (34) to Eq. (35) is carried out in Proof 1, cf. Eqs. (47)-(52). In this context, explicit use is made of the symmetry of the mobilities, i.e. $M_{\alpha\beta} = M_{\beta\alpha}$, for symmetrizing the double sum. Since the simplification of Eq. (34) results in the third binomial formula, the non-negativity of $\mathcal{D}^{\varphi}_{\delta\mathcal{S}}$ is ensured. The evolution equation according to Eq. (33) can also be written as

$$\begin{aligned} \dot{\varphi}_\alpha = -\frac{1}{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \Bigg(& -\operatorname{div}\left(\boldsymbol{\Xi}^\alpha - \boldsymbol{\Xi}^\beta\right) \\ & + \bar{\rho}\psi_{\mathcal{S}} \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_\alpha} - \frac{\partial \psi_{\text{grad}}}{\partial \varphi_\beta} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\alpha} - \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\beta} \right) \\ & + \Delta^{\alpha\beta}_{\psi} + \Delta^{\alpha\beta}_{\rho} + \Delta^{\alpha\beta}_{\text{bulk}} \Bigg), \end{aligned} \tag{36}$$

with the corresponding driving forces defined as,

$$\Delta^{\alpha\beta}_{\psi} := \rho^\alpha \psi^\alpha \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha} - \rho^\beta \psi^\beta \frac{\partial h_\beta(\boldsymbol{\phi})}{\partial \varphi_\beta} = \left\llbracket \rho\psi \frac{\partial h}{\partial \varphi} \right\rrbracket^{\alpha\beta}, \tag{37}$$

$$\Delta^{\alpha\beta}_{\rho} := \left(\rho^\alpha \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha} - \rho^\beta \frac{\partial h_\beta(\boldsymbol{\phi})}{\partial \varphi_\beta} \right) \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}}\right) = \left\llbracket \rho \frac{\partial h}{\partial \varphi} \right\rrbracket^{\alpha\beta} \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}}\right), \tag{38}$$

$$\Delta^{\alpha\beta}_{\text{bulk}} := \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \varphi_\alpha} \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha} - \varphi_\beta \rho^\beta \frac{\partial \psi^\beta}{\partial \varphi_\beta} \frac{\partial h_\beta(\boldsymbol{\phi})}{\partial \varphi_\beta} = \left\llbracket \varphi\rho \frac{\partial \psi}{\partial \varphi} \frac{\partial h}{\partial \varphi} \right\rrbracket^{\alpha\beta}. \tag{39}$$

Here, the notation $\llbracket \zeta \rrbracket^{\alpha\beta} = \zeta^\alpha - \zeta^\beta$ is introduced and employed for an arbitrary quantity ζ.

Remark regarding identical mobilities The evolution equation stated in Eq. (33) can be rewritten for the special case of identical mobilities, i.e., assuming $M_{\alpha\beta} = M_0$, reading

$$\dot{\varphi}_\alpha = -M_0 \frac{1}{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} \left(F_\alpha - F_\beta\right). \tag{40}$$

Subsequently, the following identity is used

$$\frac{1}{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} \left(F_\alpha - F_\beta\right) = \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \left(F_\alpha - F_\beta\right), \tag{41}$$

since $F_\alpha - F_\beta = 0$ holds true for $\beta = \alpha$ regarding the right-hand side of Eq. (41). Expansion of the right-hand side of Eq. (41) yields

$$\frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \left(F_\alpha - F_\beta\right) = \frac{1}{\tilde{N}} \left(\sum_{\beta=1}^{\tilde{N}} F_\alpha\right) - \frac{1}{\tilde{N}} \left(\sum_{\beta=1}^{\tilde{N}} F_\beta\right) \tag{42}$$

$$= \frac{1}{\tilde{N}} \tilde{N} F_\alpha - \frac{1}{\tilde{N}} \left(\sum_{\beta=1}^{\tilde{N}} F_\beta\right) \tag{43}$$

Consequently, Eq. (40) can be written as

$$\dot{\varphi}_\alpha = -M_0 \left(F_\alpha - \Lambda\right), \quad \Lambda := \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} F_\beta. \tag{44}$$

with Λ denoting the Lagrange multiplier. Here, the Lagrange multiplier follows from enforcing the summation constraint within the dissipation inequality framework and does not stem from a variational stationarity condition. The ansatz for the evolution equation according to Eq. (44) is closely related to that proposed by Nestler et al. [14, Eq.(6)], as will be discussed in Sect. (4.2). The Lagrange multiplier enforces the summation constraint given in Eq. (14). By substituting Eqs. (44) into Eq. (15), one obtains

$$-M_0 \sum_{\alpha=1}^{\tilde{N}} \left(F_\alpha - \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} F_\beta\right) = 0. \tag{45}$$

Since Λ is independent of α, Eq. (45) simplifies to

$$\left(\sum_{\alpha=1}^{\tilde{N}} F_\alpha\right) - \tilde{N} \left(\frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} F_\beta\right) = 0, \tag{46}$$

which vanishes identically. This confirms that Eq. (15) is satisfied.

$$\sum_{\alpha=1}^{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} A_{\alpha\beta\alpha}, \quad A_{\alpha\beta\alpha} := \left(F_\alpha - F_\beta\right) F_\alpha \tag{47}$$

$$\begin{aligned}
&= M_{12} A_{121} + M_{13} A_{131} + M_{14} A_{141} + \ldots + M_{1\tilde{N}} A_{1\tilde{N}1} \\
&+ M_{21} A_{212} + M_{23} A_{232} + M_{24} A_{242} + \ldots + M_{2\tilde{N}} A_{2\tilde{N}2} \\
&+ M_{31} A_{313} + M_{32} A_{323} + M_{34} A_{343} + \ldots + M_{3\tilde{N}} A_{3\tilde{N}3} \\
&+ M_{41} A_{414} + M_{42} A_{424} + M_{43} A_{434} + \ldots + M_{4\tilde{N}} A_{4\tilde{N}4} \\
&+ \ldots \\
&+ M_{\tilde{N}1} A_{\tilde{N}1\tilde{N}} + M_{\tilde{N}2} A_{\tilde{N}2\tilde{N}} + M_{\tilde{N}3} A_{\tilde{N}3\tilde{N}} + \ldots + M_{\tilde{N}(\tilde{N}-1)} A_{\tilde{N}(\tilde{N}-1)\tilde{N}}
\end{aligned} \tag{48}$$

$$\begin{aligned}
&= M_{12} \left(A_{121} + A_{212}\right) + M_{13} \left(A_{131} + A_{313}\right) + \ldots + M_{1\tilde{N}} \left(A_{1\tilde{N}1} + A_{\tilde{N}1\tilde{N}}\right) \\
&+ M_{23} \left(A_{232} + A_{323}\right) + \ldots + M_{2\tilde{N}} \left(A_{2\tilde{N}2} + A_{\tilde{N}2\tilde{N}}\right) \\
&+ M_{34} \left(A_{343} + A_{434}\right) + \ldots + M_{3\tilde{N}} \left(A_{3\tilde{N}3} + A_{\tilde{N}3\tilde{N}}\right) \\
&+ \ldots \\
&+ M_{(\tilde{N}-1)\tilde{N}} \left(A_{(\tilde{N}-1)\tilde{N}(\tilde{N}-1)} + A_{\tilde{N}(\tilde{N}-1)\tilde{N}}\right)
\end{aligned} \tag{49}$$

$$= \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \left(A_{\alpha\beta\alpha} + A_{\beta\alpha\beta}\right) \tag{50}$$

$$= \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \left(\left(F_\alpha - F_\beta\right) F_\alpha + \left(F_\beta - F_\alpha\right) F_\beta\right) \tag{51}$$

$$= \sum_{\alpha=1}^{\tilde{N}-1} \sum_{\beta=\alpha+1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta} \left(F_\alpha - F_\beta\right)^2 \tag{52}$$

Proof 1: The double sum occurring in $\mathcal{D}^{\varphi}_{\delta\mathcal{S}}$, cf. Eqs. (34) and (35), can be transformed by using $M_{\alpha\beta} = M_{\beta\alpha}$, for symmetrization.

Fulfillment of $\mathcal{D}^{\theta}_{\delta\mathcal{S}} \geq 0$ To fulfill Eq. $(32)_2$, $\tilde{\eta}^{*}_{\mathcal{S}}$ is inserted, cf. Eq. (9), leading to

$$\mathcal{D}^{\theta}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}^{III}} - \left(\rho_{\mathcal{S}} \left(\frac{1}{\rho_{\mathcal{S}}} \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \eta^\alpha\right) - \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \eta^\alpha\right)\right) \dot{\theta} \, \mathrm{d}v = 0. \tag{53}$$

It is evident that the terms eliminate each other, and the vanishing of $\mathcal{D}^{\theta}_{\delta\mathcal{S}}$ ensures its non-negativity.

Fulfillment of $\mathcal{D}^{\mathrm{mech}}_{\delta\mathcal{S}} \geq 0$ Taking into account $\boldsymbol{\sigma}^\alpha = \rho^\alpha \partial \psi^\alpha / \partial \boldsymbol{\varepsilon}^\alpha$ Eq. $(32)_4$ can be rewritten as

$$\mathcal{D}^{\mathrm{mech}}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}^{III}} - \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^\alpha\right) - \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha}} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha\right) \mathrm{d}v \tag{54}$$

Considering the symmetry of $\boldsymbol{\sigma}^\alpha$ and the equality $\dot{\boldsymbol{u}}_\alpha = \dot{\boldsymbol{u}}$, which follows from the derivation being based on a material singular surface, and introducing the interpolated stress $\overline{\boldsymbol{\sigma}}$ as well as the interpolated stress vector $\overline{\boldsymbol{t}}$ by

$$\overline{\boldsymbol{\sigma}} := \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \boldsymbol{\sigma}^\alpha, \quad \overline{\boldsymbol{t}} := \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \boldsymbol{t}^\alpha \tag{55}$$

the application of the divergence theorem to Eq. (54) yields

$$\mathcal{D}^{\text{mech}}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}^{III}} \dot{\boldsymbol{u}} \cdot \operatorname{div}\left(\overline{\boldsymbol{\sigma}}\right) - \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha}} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha\right) \mathrm{d}v \\ - \int_{\partial\delta\mathcal{S}^{III}} \dot{\boldsymbol{u}} \cdot \bar{\boldsymbol{t}}\, \mathrm{d}a. \tag{56}$$

A reduction of the inequality Eq. $(32)_4$ is achieved by

$$\operatorname{div}\left(\overline{\boldsymbol{\sigma}}\right) = \boldsymbol{0},\ \forall \boldsymbol{x} \in \delta\mathcal{S}, \quad \bar{\boldsymbol{t}} = \boldsymbol{0},\ \forall \boldsymbol{x} \in \partial\delta\mathcal{S}^{III}_N, \quad \dot{\boldsymbol{u}} = \boldsymbol{0},\ \forall \boldsymbol{x} \in \partial\delta\mathcal{S}^{III}_D. \tag{57}$$

Here, $\partial\delta\mathcal{S}^{III}_N$ and $\partial\delta\mathcal{S}^{III}_D$ designate the Neumann and Dirichlet portions of the boundary $\partial\delta\mathcal{S}^{III}$, respectively. Finally, the reduced form of Eq. $(32)_4$ reads

$$\mathcal{D}^{\text{mech}}_{\delta\mathcal{S}} = \int_{\delta\mathcal{S}^{III}} - \left(\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha}} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha\right) \mathrm{d}v \geq 0. \tag{58}$$

The free-energy dependencies in Eq. (24) define a general framework, without prescribing a specific constitutive behavior. As no decoupling between thermal and non-thermal contributions is assumed, contrary to [49], the results remain valid for a thermomechanically coupled theory, as discussed by [50]. To further evaluate Eq. (58), the specific forms of the specific free energies ψ^α must be defined, as well as the relations between $\dot{\boldsymbol{\varepsilon}}^{*\alpha}$ and $\dot{\boldsymbol{\alpha}}^\alpha$. Selected special cases based on restrictions of the specific free energy are addressed in Sect. (3).

Fulfillment of $\mathcal{B} \geq 0$ Inserting the definition of Ξ^α in Eq. $(32)_5$ yields

$$\mathcal{B} = -\int_{\partial\delta\mathcal{S}^{III}} \left(\sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \bar{\rho} \psi_{\mathcal{S}} \boldsymbol{\xi}^\alpha \cdot \boldsymbol{n}^{\delta\mathcal{S}}_{\mathcal{V}}\right) \mathrm{d}a \geq 0, \quad \bar{\rho} \geq 0, \quad \psi_{\mathcal{S}} \neq 0 \tag{59}$$

Accounting for the non-negativity of $\bar{\rho}$ and $\psi_{\mathcal{S}}$, the non-negativity of $\mathcal{B}$ is fulfilled by the two boundary conditions

$$\boldsymbol{\xi}^\alpha \cdot \boldsymbol{n}^{\delta\mathcal{S}}_{\mathcal{V}} = 0,\ \forall \boldsymbol{x} \in \partial\delta\mathcal{S}^{III}_N, \quad \dot{\varphi}_\alpha = 0,\ \forall \boldsymbol{x} \in \partial\delta\mathcal{S}^{III}_D, \tag{60}$$

representing a generalization of the boundary conditions given by Prahs et al. [31, Eq.(28)].

Fulfillment of $\mathcal{D}^{\text{h}}_{\delta\mathcal{S}} \geq 0$ Without restricting the contributions $\rho^\alpha \psi^\alpha + \rho^\alpha \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}}\right)$ of Eq. (29), Eq. $(32)_3$ is fulfilled by demanding

$$\sum_{\gamma=1,\gamma\neq\alpha}^{\tilde{N}} \frac{\partial h_\gamma(\boldsymbol{\phi})}{\partial \varphi_\gamma} \dot{\varphi}_\gamma = 0. \tag{61}$$

since $(D^h_{\delta\mathcal{S}})$ is the 3rd item in Eq. (32).

By means of Eq. (22), Eq. (61) can be written as

$$\dot{h}_\alpha(\boldsymbol{\phi}) - \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha} \dot{\varphi}_\alpha = 0 \quad \rightsquigarrow \quad \dot{h}_\alpha(\boldsymbol{\phi}) = \frac{\partial h_\alpha(\boldsymbol{\phi})}{\partial \varphi_\alpha} \dot{\varphi}_\alpha. \tag{62}$$

This constitutes a restriction of the interpolation function,

$$h_\alpha(\boldsymbol{\phi}) = h_\alpha(\varphi_\alpha). \tag{63}$$

Accounting for Eq. (63) as well as for Eqs. (13) and (14), it follows that

$$h_\alpha(\varphi_\alpha) = \varphi_\alpha \tag{64}$$

is the only admissible choice. A proof is provided in the appendix, cf. Eqs. (A.14) - (A.39). It is emphasized that the restriction according to Eq. (64) does not control interface width or strength. These properties are governed by the gradient and potential contributions ψ_{pot} and ψ_{grad}. The subsequent sections take Eq. (64) and, thus, $\partial h_\alpha(\varphi_\alpha)/\partial \varphi_\alpha = 1$ directly into account.

2.3 Implications for the heat conduction equation

Balance of internal energy in the multiphase-domain The balance of internal energy, cf. Eq. (A.6), for the diffuse interface domain is given by

$$(\overline{\rho e})^{\cdot} = \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}(\overline{\boldsymbol{q}})\,. \tag{65}$$

In this context, the interpolated internal energy $\overline{\rho e}$, the heat source $\overline{\rho r}$ and heat flux $\overline{\boldsymbol{q}}$ are defined as

$$\overline{\rho e} = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha e^\alpha, \quad \overline{\rho r} = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha r_\alpha, \quad \overline{\boldsymbol{q}} = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \boldsymbol{q}^\alpha. \tag{66}$$

In the following, $\overline{\rho r}$ and $\overline{\boldsymbol{q}}$ are not replaced by the relations according to Eq. (66), for brevity. While $\overline{\boldsymbol{\sigma}}$ is considered according to Eq. $(55)_1$, the interpolated strain $\overline{\boldsymbol{\varepsilon}}$ is given by

$$\overline{\boldsymbol{\varepsilon}} = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \boldsymbol{\varepsilon}^\alpha. \tag{67}$$

Heat conduction in the multiphase-domain Application of the Legendre transformation, i.e. $e^\alpha = \theta\eta^\alpha + \psi^\alpha$, cf., e.g., [51], yields

$$\left(\overline{\rho\psi}\right)^{\cdot} + \dot{\theta}\overline{\rho\eta} + \theta\,(\overline{\rho\eta})^{\cdot} = \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}(\overline{\boldsymbol{q}})\,. \tag{68}$$

In this context, $\overline{\rho\psi}$ is considered according to Eq. (10) and the interpolated entropy is introduced as

$$\overline{\rho\eta} = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \eta^\alpha. \tag{69}$$

Reformulation of Eq. (68) yields

$$\begin{aligned}
\bar{c}_\varepsilon\dot{\theta} &= \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}(\overline{\boldsymbol{q}}) - \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^\alpha \\
&\quad + \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \left(\frac{\partial \boldsymbol{\sigma}^\alpha}{\partial\theta} \cdot \left(\dot{\boldsymbol{\varepsilon}}^\alpha - \dot{\boldsymbol{\varepsilon}}^{*\alpha}\right) + \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha \partial\theta} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right) \\
&\quad + \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \left(\boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} - \rho^\alpha \frac{\partial\psi^\alpha}{\partial\boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right) \\
&\quad + \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \left(\varphi_\alpha \theta \rho^\alpha \frac{\partial^2\psi^\alpha}{\partial\varphi_\alpha \partial\theta} - \varphi_\alpha \rho^\alpha \frac{\partial\psi^\alpha}{\partial\varphi_\alpha} - \rho^\alpha e^\alpha \right),
\end{aligned} \tag{70}$$

with the interpolated specific heat

$$\bar{c}_\varepsilon = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha c_\varepsilon^\alpha, \quad c_\varepsilon^\alpha = -\theta \frac{\partial^2\psi^\alpha}{\partial\theta^2}. \tag{71}$$

A detailed derivation of Eq. (70) is provided in the appendix. It is stressed that Eq. (70) remains general with respect to the underlying mechanical and thermal behavior, as the contributions $\boldsymbol{\sigma}^\alpha$, $\boldsymbol{\varepsilon}^{*\alpha}$, and $\boldsymbol{q}^\alpha$ have not been specified at this stage. It is convenient to apply the Legendre transformation $e^\alpha = \theta\eta^\alpha + \psi^\alpha$, cf., e.g., [51], together with the entropy relation, cf. Eq. (A.10), to substitute e^α by

$$e^\alpha = \psi^\alpha + \theta \frac{\partial\psi^\alpha}{\partial\theta}. \tag{72}$$

Eq. (70) is a generalization of the heat conduction equation used in [52] in the context of non-isothermal polymer crystallization.

3 Selected special cases

3.1 Special case S_1

Constitutive assumption In the remainder of this section, it is assumed that the mass densities ρ^α are identical, i.e., $\rho^\alpha = \rho$. Taking into account Eq. (9),

$$\overline{\rho} = \rho \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha = \rho \tag{73}$$

holds true.

Effect on the driving force contribution If S_1 is considered from the outset,

$$\frac{\overline{\rho}}{\rho_{\mathcal{S}}} \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}} \right) \equiv \frac{\rho}{\rho_{\mathcal{S}}} \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}} \right) \tag{74}$$

holds true regarding Eq. (17). Consequently,

$$\left(\sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \rho^\alpha \right) \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}} \right) \equiv 0 \tag{75}$$

holds true with respect to Eq. (18) and the contribution $\rho^\alpha \psi_{\mathcal{S}} \left(\psi_{\text{grad}} + \psi_{\text{pot}} \right)$ is not present in F_α. Thus, Eq. (76) reduces to

$$F_\alpha := -\operatorname{div}\left(\boldsymbol{\Xi}^\alpha \right) + \rho \psi_{\mathcal{S}} \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_\alpha} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\alpha} \right) + \rho \psi^\alpha + \varphi_\alpha \rho \frac{\partial \psi^\alpha}{\partial \varphi_\alpha} \tag{76}$$

with $\boldsymbol{\Xi}^\alpha = \rho \psi_{\mathcal{S}} \boldsymbol{\xi}^\alpha$.

Effect on the evolution equation Based on Eq. (73) and Eq. $(38)_2$, $\Delta_\rho^{\alpha\beta} = 0$ holds true. Consequently, Eq. (36) reads

$$\begin{aligned} \dot{\varphi}_\alpha = -\frac{1}{\tilde{N}} \sum_{\beta=1, \beta \neq \alpha}^{\tilde{N}} M_{\alpha\beta} \Big(& -\operatorname{div}\left(\boldsymbol{\Xi}^\alpha - \boldsymbol{\Xi}^\beta \right) \\ & + \rho \psi_{\mathcal{S}} \left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_\alpha} - \frac{\partial \psi_{\text{grad}}}{\partial \varphi_\beta} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\alpha} - \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\beta} \right) \\ & + \Delta_\psi^{\alpha\beta} + \Delta_{\text{bulk}}^{\alpha\beta} \Big), \end{aligned} \tag{77}$$

with the modified driving forces

$$\Delta_\psi^{\alpha\beta} = \rho \,{-}\!\!\left[\psi \right]\!\!{-}^{\alpha\beta}, \quad \Delta_{\text{bulk}}^{\alpha\beta} = \rho \,{-}\!\!\left[\varphi \frac{\partial \psi}{\partial \varphi} \right]\!\!{-}^{\alpha\beta}. \tag{78}$$

3.2 Special case S_2

Constitutive assumptions Following the special case S_1 it is assumed that the specific free energies admit an additive decomposition as

$$\psi^\alpha = \psi_{\text{e}}^\alpha (\boldsymbol{\varepsilon}^\alpha, \boldsymbol{\varepsilon}^{*\alpha}, \varphi_\alpha) + \psi_{\text{p}}^\alpha (\boldsymbol{\alpha}^\alpha, \varphi_\alpha) + \psi_\theta^\alpha (\theta, \varphi_\alpha) + \psi_{\text{ch}}^\alpha, \tag{79}$$

with the elastic contribution ψ_{e}^α, the inelastic contribution ψ_{p}^α, the thermal contribution ψ_θ^α, and the constant chemical contribution ψ_{ch}^α. This corresponds to a thermomechanical decoupling of the specific free energy, cf. [50].

Effect on the driving force contribution Based on the assumption S_2, the driving force contribution F_α as stated in Eq. (76) is further specified, reading

$$\begin{aligned} F_\alpha := &- \operatorname{div}\left(\boldsymbol{\Xi}^\alpha\right) + \rho\psi_{\mathcal{S}}\left(\frac{\partial\psi_{\mathrm{grad}}}{\partial\varphi_\alpha} + \frac{\partial\psi_{\mathrm{pot}}}{\partial\varphi_\alpha}\right) + \rho\psi_{\mathrm{e}}^\alpha + \rho\psi_{\mathrm{p}}^\alpha + \rho\psi_\theta^\alpha \\ &+ \varphi_\alpha\rho\frac{\partial\psi_{\mathrm{e}}^\alpha}{\partial\varphi_\alpha} + \varphi_\alpha\rho\frac{\partial\psi_{\mathrm{p}}^\alpha}{\partial\varphi_\alpha} + \varphi_\alpha\rho\frac{\partial\psi_\theta^\alpha}{\partial\varphi_\alpha}. \end{aligned} \tag{80}$$

Effect on the evolution equation Both the evolution equation according to Eq. (77) as well as $\Delta_\psi^{\alpha\beta}$ remain in their current form. However, the bulk driving force $\Delta_{\mathrm{bulk}}^{\alpha\beta}$ is expressed as the sum of the following contributions

$$\Delta_{\mathrm{bulk}}^{\alpha\beta} = \Delta_{\mathrm{e}}^{\alpha\beta} + \Delta_{\mathrm{p}}^{\alpha\beta} + \Delta_\theta^{\alpha\beta}, \tag{81}$$

with the following definitions

$$\Delta_{\mathrm{e}}^{\alpha\beta} = \rho\left[\!\!\left[\varphi\frac{\partial\psi_{\mathrm{e}}}{\partial\varphi}\right]\!\!\right]^{\alpha\beta}, \quad \Delta_{\mathrm{p}}^{\alpha\beta} = \rho\left[\!\!\left[\varphi\frac{\partial\psi_{\mathrm{p}}}{\partial\varphi}\right]\!\!\right]^{\alpha\beta}, \quad \Delta_\theta^{\alpha\beta} = \rho\left[\!\!\left[\varphi\frac{\partial\psi_\theta}{\partial\varphi}\right]\!\!\right]^{\alpha\beta}. \tag{82}$$

3.3 Special case S_3

Constitutive assumptions Following the special cases S_1 and S_2, it is assumed that the inelastic and the thermal contributions do not depend on the order parameter, i.e.,

$$\psi_{\mathrm{p}}^\alpha = \psi_{\mathrm{p}}^\alpha(\boldsymbol{\alpha}^\alpha), \quad \psi_\theta^\alpha = \psi_\theta^\alpha(\theta) \tag{83}$$

hold true.

Effect on the driving force contribution Based on the assumption S_3, the driving force contribution F_α as stated in Eq. (80) is further specified, reading

$$F_\alpha := - \operatorname{div}\left(\boldsymbol{\Xi}^\alpha\right) + \rho\psi_{\mathcal{S}}\left(\frac{\partial\psi_{\mathrm{grad}}}{\partial\varphi_\alpha} + \frac{\partial\psi_{\mathrm{pot}}}{\partial\varphi_\alpha}\right) + \rho\psi_{\mathrm{e}}^\alpha + \rho\psi_{\mathrm{p}}^\alpha + \rho\psi_\theta^\alpha + \varphi_\alpha\rho\frac{\partial\psi_{\mathrm{e}}^\alpha}{\partial\varphi_\alpha}. \tag{84}$$

Effect on the evolution equation Accounting for Eq. (83), $\Delta_{\mathrm{p}}^{\alpha\beta} = 0$ and $\Delta_\theta^{\alpha\beta} = 0$ are obtained. Thus, the evolution equation for φ_α reads

$$\begin{aligned} \dot{\varphi}_\alpha = -\frac{1}{\tilde{N}}\sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta}\Bigg(&-\operatorname{div}\left(\boldsymbol{\Xi}^\alpha - \boldsymbol{\Xi}^\beta\right) \\ &+ \rho\psi_{\mathcal{S}}\left(\frac{\partial\psi_{\mathrm{grad}}}{\partial\varphi_\alpha} - \frac{\partial\psi_{\mathrm{grad}}}{\partial\varphi_\beta} + \frac{\partial\psi_{\mathrm{pot}}}{\partial\varphi_\alpha} - \frac{\partial\psi_{\mathrm{pot}}}{\partial\varphi_\beta}\right) \\ &+ \rho\left[\!\!\left[\psi_{\mathrm{e}}\right]\!\!\right]^{\alpha\beta} + \rho\left[\!\!\left[\psi_{\mathrm{p}}\right]\!\!\right]^{\alpha\beta} + \rho\left[\!\!\left[\psi_\theta\right]\!\!\right]^{\alpha\beta} + \Delta_{\mathrm{e}}^{\alpha\beta}\Bigg). \end{aligned} \tag{85}$$

4 Comparison with classical approach

4.1 Energy functional and variational derivative

Energy functional The classical derivation of the multiphase-field method is commonly based on an energy functional $\mathcal{F}$ defined on $\mathcal{V}$, consisting of the interface contribution $f_{\mathcal{S}}$ and the bulk contribution $\overline{f}_{\mathcal{V}}$, reading

$$\mathcal{F} = \int_{\mathcal{V}} f\,\mathrm{d}v, \quad f = f_{\mathcal{S}} + \overline{f}_{\mathcal{V}}, \quad f_{\mathcal{S}} = \rho\psi_{\mathcal{S}}\left(\psi_{\mathrm{grad}} + \psi_{\mathrm{pot}}\right) = f_{\mathrm{grad}} + f_{\mathrm{pot}}, \tag{86}$$

The surface contribution $f_{\mathcal{S}}$ is additively decomposed into a gradient part f_{grad} and a potential part f_{pot}, which are related to ψ_{grad} and ψ_{pot}, respectively, as shown in Eq. (86)$_3$. Thus, the dependencies of f_{grad} and f_{pot} on $\boldsymbol{\phi}$ and $\nabla\boldsymbol{\phi}$ correspond to those of ψ_{grad} and ψ_{pot}. The contribution $\overline{f}_{\mathcal{V}}$ is defined according to Eq. (10). For the comparison in this section, the special case S_3 is considered, allowing the contribution $\overline{f}_{\mathcal{V}}$ to be simplified to

$$\overline{f}_{\mathcal{V}} = \rho \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \psi^\alpha = \rho \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \left(\psi_{\text{e}}^\alpha + \psi_{\text{p}}^\alpha + \psi_\theta^\alpha\right). \tag{87}$$

Variational derivative For the classical derivation of the evolution equation, the variational derivative is introduced, defined as

$$\frac{\delta f}{\delta \varphi_\alpha} = \left(\frac{\partial f}{\partial \varphi_\alpha} - \operatorname{div}\left(\frac{\partial f}{\partial \nabla \varphi_\alpha}\right)\right). \tag{88}$$

Considering the definition of f according to Eq. (86) and accounting for special case S_3, the variational derivative of f is given by

$$\frac{\delta f}{\delta \varphi_\alpha} = -\operatorname{div}\left(\boldsymbol{\Xi}^\alpha\right) + \rho\psi_{\mathcal{S}}\left(\frac{\partial \psi_{\text{grad}}}{\partial \varphi_\alpha} + \frac{\partial \psi_{\text{pot}}}{\partial \varphi_\alpha}\right) + \varphi_\alpha \rho \frac{\partial \psi_{\text{e}}^\alpha}{\partial \varphi_\alpha} + \rho\psi_{\text{e}}^\alpha + \rho\psi_{\text{p}}^\alpha + \rho\psi_\theta^\alpha \tag{89}$$

with $\boldsymbol{\Xi}^\alpha = \rho\psi_{\mathcal{S}}\partial\psi_{\text{grad}}/\partial\nabla\varphi_\alpha$. Comparison of Eq. (89) and Eq. (84) yields

$$\frac{\delta f}{\delta \varphi_\alpha} = F_\alpha. \tag{90}$$

4.2 Variational approach to the multiphase-field method

Evolution equation The ansatz for the evolution equation of the order parameter is given by

$$\dot{\varphi}_\alpha = -\frac{1}{\tilde{N}} \sum_{\beta=1,\beta\neq\alpha}^{\tilde{N}} M_{\alpha\beta}\left(\frac{\delta f}{\delta \varphi_\alpha} - \frac{\delta f}{\delta \varphi_\beta}\right), \tag{91}$$

cf. Steinbach and Pezzolla [7]. With $\delta f/\delta\varphi_\alpha = F_\alpha$, cf. Eq. (90), the ansatz for the evolution equation of the order parameter given in Eq. (91) corresponds to the formulation stated in Eq. (33). Consequently, the evolution equation obtained from Eq. (91) coincides with Eq. (85) for the special case S_3.

Remark regarding identical mobilities Accounting for Eq. (90), Eq. (44) can be written as

$$\dot{\varphi}_\alpha = -M_0\left(\frac{\delta f}{\delta \varphi_\alpha} - \Lambda\right), \quad \Lambda := \frac{1}{\tilde{N}} \sum_{\beta=1}^{\tilde{N}} \frac{\delta f}{\delta \varphi_\beta} \tag{92}$$

with Λ denoting the Lagrange Multiplier. The Lagrange multiplier enforces the summation constraint given in Eq. (14) as already illustrated by Eqs. (45) and (46). The formulation according to Eq. (92) was similarly introduced in Nestler et al. [14, Eq.(6)].

5 Concluding remarks

In this work, the multiphase-field method was systematically derived for multiple intersecting phases by introducing the order parameters as internal state variables and exploiting the entropy production inequality of the diffuse interface region within the framework of continuum thermodynamics. Thus, it represents a direct generalization of [31] to multiple intersecting phases. The key results are summarized as follows:

- The thermodynamical consistency of the dual-interaction ansatz for the evolution equation of the order parameters, as well as its simplification via the Lagrange-multiplier ansatz, was demonstrated.

- To ensure thermodynamical consistency within the framework of continuum thermomechanics, the restriction $h_\alpha(\boldsymbol{\phi}) = h_\alpha(\varphi_\alpha)$ has to be fulfilled, i.e., the interpolation function h_α must only depend on the order parameter φ_α, but not on the remaining order parameters. Moreover, it was shown that $h_\alpha(\varphi_\alpha) = \varphi_\alpha$ is the only admissible choice for the interpolation function in the multiphase-field context. All further considerations apply for this case.
- The corresponding heat conduction equation was consistently derived, with special emphasis on coupling contributions arising from microstructure evolution.
- Special cases of the multiphase-field method were discussed by restricting the considered phase-specific free energy contributions.
- The relation of the dual-interaction and Lagrange-multiplier ansatz to the well-established approaches by Steinbach and Pezzolla [7] and Nestler et al. [14] is illustrated for an introduced special case.

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Data Availability No datasets were generated or analysed during the current study.

Declarations

Conflicts of Interest The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix

Remark on used notation

Set notation In Fig. 1 the considered sharp interfaces are referred to as $\mathcal{S}^{\alpha\beta}$, $\mathcal{S}^{\beta\gamma}$, and $\mathcal{S}^{\gamma\alpha}$ while the corresponding diffuse interfaces are denoted by $\delta\mathcal{S}^{\alpha\beta}$, $\delta\mathcal{S}^{\beta\gamma}$, and $\delta\mathcal{S}^{\gamma\alpha}$, respectively. Moreover, the multiphase region $\delta\mathcal{C}^{\alpha\beta\gamma}$ is introduced. Regarding δS and δC, juxtaposed superscripts (e.g., $S^{\alpha\beta}$) denote unordered index sets. In formulas the equivalent notation $\delta S^{\{\alpha,\beta\}}$ is used, i.e.

$$\delta S^{\alpha\beta} := \delta S^{\{\alpha,\beta\}}, \qquad \alpha \neq \beta, \tag{A.1}$$

is used. This affects only the remarks in this section of the appendix.

Notation used for two-phase unions in Eq. (1) Let $\mathcal{I} = \{1, 2, 3, 4, 5\}$. Then

$$\delta S^{\mathrm{II}} = \bigcup_{\substack{A \subseteq \mathcal{I} \\ |A|=2}} \delta S^{A} \tag{A.2}$$

expands to

$$
\begin{aligned}
\delta S^{\mathrm{II}} = {} & \delta S^{\{1,2\}} \cup \delta S^{\{1,3\}} \cup \delta S^{\{1,4\}} \cup \delta S^{\{1,5\}} \\
& \cup\ \delta S^{\{2,3\}} \cup \delta S^{\{2,4\}} \cup \delta S^{\{2,5\}} \\
& \cup\ \delta S^{\{3,4\}} \cup \delta S^{\{3,5\}} \cup \delta S^{\{4,5\}}.
\end{aligned}
\tag{A.3}
$$

Notation used for multiple phase unions in Eq. (2) Let $\mathcal{I} = \{1, 2, 3, 4, 5\}$. Then

$$
\delta S^{\mathrm{III}} = \bigcup_{\substack{A \subseteq \mathcal{I} \\ |A| \geq 3}} \delta C^{A}
\tag{A.4}
$$

expands to

$$
\begin{aligned}
\delta S^{\mathrm{III}} = {} & \delta C^{\{1,2,3\}} \cup \delta C^{\{1,2,4\}} \cup \delta C^{\{1,2,5\}} \cup \delta C^{\{1,3,4\}} \\
& \cup\ \delta C^{\{1,3,5\}} \cup \delta C^{\{1,4,5\}} \cup \delta C^{\{2,3,4\}} \\
& \cup\ \delta C^{\{2,3,5\}} \cup \delta C^{\{2,4,5\}} \cup \delta C^{\{3,4,5\}} \\
& \cup \delta C^{\{1,2,3,4\}} \cup \delta C^{\{1,2,3,5\}} \cup \delta C^{\{1,2,4,5\}} \cup \delta C^{\{1,3,4,5\}} \cup \delta C^{\{2,3,4,5\}} \\
& \cup \delta C^{\{1,2,3,4,5\}}.
\end{aligned}
\tag{A.5}
$$

Balance equations for a Cauchy continuum with a material singular surface

Remark For enhancing readability, the superscript α is omitted in this and the subsequent section. However, the considerations regarding regular points are applicable to points in $\mathcal{V}^{\alpha}$ as well as $\tilde{\mathcal{V}}^{\alpha}$.

Balance equations for points in $\mathcal{V}^{\alpha} \backslash \tilde{\mathcal{V}}^{\alpha}$ In the work at hand, the derivation of the MPFM is based on a Cauchy continuum containing several intersecting material singular surfaces. In this context, no additional degrees of freedom are considered. The balance equations for a Cauchy continuum can be derived, e.g., by requiring invariance of the total energy balance, cf. Prahs et al. [31, Eq.(1)] under a change of observer, cf., e.g., [53]. In this appendix, the balance equations are only provided but not derived, for brevity. A detailed derivation of the balance including additional degrees of freedom is provided in [54]; neglecting these yields the standard balance equations adopted here. The balance of mass, linear and angular momentum along with the balance of internal energy are given by

$$
\dot{\rho} + \rho \operatorname{div}(\boldsymbol{v}) = 0, \quad \rho\,(\boldsymbol{a} - \boldsymbol{b}) = \operatorname{div}(\boldsymbol{\sigma}), \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathsf{T}}, \quad \rho \dot{e} = \boldsymbol{\sigma} \cdot \boldsymbol{D} + \rho r - \operatorname{div}(\boldsymbol{q}).
\tag{A.6}
$$

Moreover, the existence of the Cauchy stress tensor and the heat flux vector, i.e.,

$$
\boldsymbol{\sigma} \boldsymbol{n}_{\mathcal{V}} = \boldsymbol{t}, \quad \boldsymbol{q} \cdot \boldsymbol{n}_{\mathcal{V}} = -h
\tag{A.7}
$$

also follows from requiring the invariance of the total energy balance under a change of observer.

Remark The results presented are obtained for the volumes $\mathcal{V}^{\alpha}$, representing a single phase in the context of a sharp interface theory. They are also valid for the volumes $\tilde{\mathcal{V}}^{\alpha}$ of the diffuse interface theory.

Balance equations for points on $\mathcal{S}$ The balance equations for points on the singular surface $\mathcal{S}$ are also obtained by requiring the invariance of the balance of total energy with respect to a change of observer. This yields the balance of mass, linear momentum, and internal energy on $\mathcal{S}$, reading

$$
\dot{\rho}_{\mathcal{S}} + \rho_{\mathcal{S}} \operatorname{div}_{\mathrm{S}}(\boldsymbol{v}) = 0, \quad \rho_{\mathcal{S}} \boldsymbol{a} - \rho_{\mathcal{S}} \boldsymbol{b}^{\mathcal{S}} = [\![\boldsymbol{t}]\!], \quad \rho_{\mathcal{S}} \dot{e}_{\mathcal{S}} = \rho_{\mathcal{S}} r_{\mathcal{S}} - [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n}_{\mathcal{S}}.
\tag{A.8}
$$

Remark In the present context, only the quasi-static case is considered, neglecting body forces and assuming small deformations, such that $\boldsymbol{a} = \boldsymbol{0}$, $\boldsymbol{b} = \boldsymbol{0}$, $\boldsymbol{b}^{\mathcal{S}} = \boldsymbol{0}$, and $\boldsymbol{D} = \dot{\boldsymbol{\varepsilon}}$.

Constitutive behavior

Constitutive behavior for points in $\mathcal{V}^\alpha \backslash \tilde{\mathcal{V}}^\alpha$ The specific free energy is assumed to depend on the total strain $\boldsymbol{\varepsilon}$, the inelastic strain $\boldsymbol{\varepsilon}^*$, additional internal state variables $\boldsymbol{\alpha}$ and the temperature θ i.e.,

$$\psi = \psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^* \boldsymbol{\alpha}, \theta) \tag{A.9}$$

holds true. Accounting for Eq. (A.9), the exploitation of the Clausius–Duhem inequality, cf., e.g., Prahs et al. [31, Eq.(A.3)] yields the potential relations for the Cauchy stress and the entropy, reading

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \quad \eta = -\frac{\partial \psi}{\partial \theta}. \tag{A.10}$$

The rate of the entropy is given by

$$\dot{\eta} = \left(-\frac{\partial \psi}{\partial \theta}\right)^{\bullet} = -\frac{\partial \dot{\psi}}{\partial \theta}. \tag{A.11}$$

Constitutive behavior for points on $\mathcal{S}$ The application of the Coleman–Noll procedure for the Clausius–Duhem inequaltiy on a material singular surface, cf. Prahs et al. [31, Eq.(A.6)] yields that $\psi_{\mathcal{S}}$ can only depend on the temperature, i.e.

$$\psi_{\mathcal{S}} = \psi_{\mathcal{S}}(\theta), \tag{A.12}$$

as well as the potential relation for $\psi_{\mathcal{S}}$, reading

$$\eta_{\mathcal{S}} = -\frac{\partial \psi_{\mathcal{S}}}{\partial \theta}. \tag{A.13}$$

Admissible interpolation functions

Remark on the idea The constraints according to Eqs. (13) and (14) must be satisfied on the $\tilde{N}$-simplex. Since Eq. (13) holds on the $\tilde{N}$-simplex, it must also hold on every subsimplex obtained by setting some of the order parameters to zero. The minimal non-trivial case is the three-phase subsystem, represented by a triangular face of the simplex. Restricting the proof to a three-phase region simplifies the discussion. The arbitrariness of the chosen triple ensures that the conclusions apply to every sub-simplex, and therefore to the general case for arbitrary $\tilde{N}$. The proof strategy then proceeds by showing that the vanishing Hessian on such a three-phase slice implies that each interpolation function is affine. Imposing the summation constraints according to Eqs. (13) and (14) and the pure-phase conditions finally reduces these affine functions uniquely to the identity mapping, i.e., $h_\alpha(\varphi_\alpha) = \varphi_\alpha$.

Interpolation functions as affine functions

Assume the functions $h_\alpha(\varphi_\alpha)$ are twice differentiable. Subsequently, considerations are restricted to a three-phase region of phases ξ, η, and ζ, where

$$\varphi_\xi \varphi_\eta \varphi_\zeta \neq 0 \tag{A.14}$$

holds true and all other order parameters vanish. According to Eq. (13)

$$\varphi_\xi + \varphi_\eta + \varphi_\zeta = 1 \tag{A.15}$$

holds true in this three-phase region. Accounting for Eq. (63), the constraint according to Eq. (14) reads

$$H := h_\xi(\varphi_\xi) + h_\eta(\varphi_\eta) + h_\zeta(\varphi_\zeta) \equiv 1. \tag{A.16}$$

Taking into account Eq. (A.15), Eq. (A.16) can be written as

$$H := h_\xi(\varphi_\xi) + h_\eta(\varphi_\eta) + h_\zeta(1 - \varphi_\xi - \varphi_\eta) \equiv 1. \tag{A.17}$$

Differentiating gives

$$\begin{aligned}\frac{\partial H}{\partial \varphi_\xi} &= \frac{\partial h_\xi(\varphi_\xi)}{\partial \varphi_\xi} - \frac{\partial h_\zeta(1-\varphi_\xi-\varphi_\eta)}{\partial \varphi_\xi}\\ \frac{\partial H}{\partial \varphi_\eta} &= \frac{\partial h_\eta(\varphi_\eta)}{\partial \varphi_\xi} - \frac{\partial h_\zeta(1-\varphi_\xi-\varphi_\eta)}{\partial \varphi_\eta}.\end{aligned} \tag{A.18}$$

The mixed second derivative is given by

$$\frac{\partial^2 H}{\partial \varphi_\xi \partial \varphi_\eta} = \frac{\partial}{\partial \varphi_\eta}\left(\frac{\partial H}{\partial \varphi_\xi}\right) = \frac{\partial^2 h_\zeta(1-\varphi_\xi-\varphi_\eta)}{\partial \varphi_\xi \partial \varphi_\eta}. \tag{A.19}$$

Taking into account the summation constraint, i.e. $H = 1$, $\partial^2 H/\left(\partial \varphi_\xi \partial \varphi_\eta\right) = 0$ holds true. To fulfill

$$\frac{\partial^2 h_\zeta(1-\varphi_\xi-\varphi_\eta)}{\partial \varphi_\xi \partial \varphi_\eta} = 0 \tag{A.20}$$

the function $h_\zeta(\varphi_\zeta)$ has to be an affine function, reading

$$h_\zeta(\varphi_\zeta) = a_\zeta \varphi_\zeta + b_\zeta. \tag{A.21}$$

Since the choice of the triple of indices is arbitrary,

$$h_\alpha(\varphi_\alpha) = a_\alpha \varphi_\alpha + b_\alpha, \quad \forall \alpha \tag{A.22}$$

must hold.

Identical slopes Inserting Eq. (A.22) in Eq. (14) yields

$$L(\boldsymbol{\phi}) + B = 1, \quad L(\boldsymbol{\phi}) := \sum_{\alpha=1}^{\tilde{N}} a_\alpha + \varphi_\alpha, \quad B := \sum_{\alpha=1}^{\tilde{N}} b_\alpha. \tag{A.23}$$

Consequently,

$$L(\boldsymbol{\phi}) = B - 1 = \text{constant} \tag{A.24}$$

must hold for every tuple $\boldsymbol{\phi}$ with $\left\{\boldsymbol{\phi} \in \mathbb{R}^{\tilde{N}} : \varphi_\alpha \geq 0,\ \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha = 1\right\}$. Subsequently, define a new tuple $\boldsymbol{\phi}^{\text{new}}$ with

$$\varphi_\mu^{\text{new}} = \varphi_\mu + \tau, \quad \varphi_\nu^{\text{new}} = \varphi_\nu - \tau, \quad \varphi_\beta^{\text{new}} = \varphi_\beta, \quad \beta \notin \mu, \nu, \quad \tau \in R. \tag{A.25}$$

The parameter τ is chosen small and feasible such that

$$\sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha^{\text{new}} = \left(\varphi_\mu + \tau\right) + \left(\varphi_\nu - \tau\right) + \left(\sum_{\beta=1, \beta \notin \{\tau,\nu\}}^{\tilde{N}} \varphi_\beta\right) = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha = 1. \tag{A.26}$$

Regarding $\boldsymbol{\phi}^{\text{new}}$, Eq. $(\text{A.23})_2$ reads

$$\begin{aligned}L(\boldsymbol{\phi}^{\text{new}}) = \sum_{\alpha=1}^{\tilde{N}} a_\alpha \varphi_\alpha^{\text{new}} &= a_\mu \varphi_\mu^{\text{new}} + a_\nu \varphi_\nu^{\text{new}} + \left(\sum_{\beta=1, \beta \notin \{\tau,\nu\}}^{\tilde{N}} a_\beta \varphi_\beta\right)\\ &= a_\mu\left(\varphi_\mu + \tau\right) + a_\nu\left(\varphi_\nu - \tau\right) + \left(\sum_{\beta=1, \beta \notin \{\tau,\nu\}}^{\tilde{N}} a_\beta \varphi_\beta\right),\end{aligned} \tag{A.27}$$

while regarding $\boldsymbol{\phi}$ it is given by

$$L(\boldsymbol{\phi}) = a_\mu \varphi_\mu + a_\nu \varphi_\nu + \left(\sum_{\beta=1, \beta \notin \{\tau, \nu\}}^{\tilde{N}} a_\beta \varphi_\beta \right). \tag{A.28}$$

Since Eq. (A.24) must hold for every tuple $\boldsymbol{\phi}$, it is required that

$$L(\boldsymbol{\phi}) = L(\boldsymbol{\phi}^{\text{new}}) \quad \rightsquigarrow \quad L(\boldsymbol{\phi}) - L(\boldsymbol{\phi}^{\text{new}}) = 0. \tag{A.29}$$

Exploiting Eq. (A.28) yields

$$\left(a_\mu - a_\nu\right) \tau = 0, \tag{A.30}$$

which can be fulfilled for admissible τ only by choosing $a_\mu = a_\nu$. Since the choice of the indices μ and ν was arbitrary

$$a_1 = a_2 = \ldots = a \tag{A.31}$$

must hold, i.e., the slopes of all affine functions need to coincide and Eq. (A.22) reads

$$h_\alpha(\varphi_\alpha) = a\varphi_\alpha + b_\alpha \quad \forall \alpha. \tag{A.32}$$

Reduction to linear functions Considering a *single phase* γ

$$\varphi_\gamma = 1, \quad \text{and} \quad \varphi_\beta = 0 \quad \forall \beta \neq \gamma \tag{A.33}$$

holds true. Consequently, the interpolation functions according to Eq. (A.32) must satisfy

$$h_\gamma(\varphi_\gamma = 1) = a + b_\gamma = 1, \quad h_\gamma(\varphi_\beta = 0) = b_\beta = 0 \quad \forall \beta \neq \gamma. \tag{A.34}$$

Again, the choice of the index γ was arbitrary. However, since Eq. (A.34) must hold for every single phase, leading to

$$\gamma = 1 \quad \rightsquigarrow \quad b_1 = 1 - a, \quad b_\beta = 0 \quad \forall \beta \neq 1 \tag{A.35}$$

$$\gamma = 2 \quad \rightsquigarrow \quad b_2 = 1 - a, \quad b_\beta = 0 \quad \forall \beta \neq 2 \tag{A.36}$$

$$\gamma = \ldots \tag{A.37}$$

Fulfilling Eq. (A.35), $b_2 = b_3 = \ldots = 0$ has to hold true, while fulfilling Eq. (A.36), $b_1 = b_3 = \ldots = 0$ must hold. Consequently, to satisfy Eqs. (A.35), (A.36), and Eq. (A.37) for all choices of γ, the only possibility is

$$b_\beta = 0 \quad \forall \beta, \quad 0 = 1 - a \quad \rightsquigarrow \quad a = 1 \tag{A.38}$$

Accounting for Eq. (A.38), Eq. (A.32) finally reads

$$h_\alpha(\varphi_\alpha) = \varphi_\alpha. \tag{A.39}$$

Heat conduction equation

Derivation of equation of heat conduction Application of the chain rule to Eq. (68) yields

$$
\begin{aligned}
&\sum_{\alpha=1}^{\tilde{N}} \left(\dot{\varphi}_\alpha \rho^\alpha \psi^\alpha + \varphi_\alpha \rho^\alpha \dot{\psi}^\alpha\right) + \dot{\theta} \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \eta^\alpha + \theta \sum_{\alpha=1}^{\tilde{N}} \left(\dot{\varphi}_\alpha \rho^\alpha \eta^\alpha + \varphi_\alpha \rho^\alpha \dot{\eta}^\alpha\right) \\
&\quad = \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}\left(\overline{\boldsymbol{q}}\right) .
\end{aligned}
\tag{A.40}
$$

Taking into account the dependencies of the specific free energy as stated in Eq. (24), the potential relation for the entropy,cf. Eq. (A.10)$_2$, and the relation for the entropy rate according to Eq. (A.11), yields

$$
\begin{aligned}
&\sum_{\alpha=1}^{\tilde{N}} \left(\dot{\varphi}_\alpha \rho^\alpha \psi^\alpha + \varphi_\alpha \left(\rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^\alpha} \cdot \dot{\boldsymbol{\varepsilon}}^\alpha + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha}} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \varphi_\alpha} \dot{\varphi}_\alpha + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right.\right. \\
&\quad \left.\left. + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \theta} \dot{\theta}\right)\right) - \dot{\theta} \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial \psi^\alpha}{\partial \theta} + \theta \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \rho^\alpha \eta^\alpha - \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial \dot{\psi}^\alpha}{\partial \theta} \\
&\quad = \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}\left(\overline{\boldsymbol{q}}\right) ,
\end{aligned}
\tag{A.41}
$$

Using the potential relation for the Cauchy stress according to Eq. (A.10) and accounting for Eq. (24) with respect to $\partial \dot{\psi}^\alpha / \partial \theta$ yields

$$
\begin{aligned}
&\sum_{\alpha=1}^{\tilde{N}} \left(\dot{\varphi}_\alpha \rho^\alpha \psi^\alpha + \varphi_\alpha \left(\boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^\alpha - \boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \varphi_\alpha} \dot{\varphi}_\alpha + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right)\right) \\
&\quad + \theta \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \rho^\alpha \eta^\alpha - \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \left(\rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \boldsymbol{\varepsilon}^\alpha \partial \theta} \cdot \dot{\boldsymbol{\varepsilon}}^\alpha + \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \boldsymbol{\varepsilon}^{*\alpha} \partial \theta} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \varphi_\alpha \partial \theta} \dot{\varphi}_\alpha \right. \\
&\quad \left. + \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha \partial \theta} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right) - \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \theta^2} \dot{\theta} = \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}\left(\overline{\boldsymbol{q}}\right) ,
\end{aligned}
\tag{A.42}
$$

Introducing the specific heat c_ε^α as well as the interpolated specific heat $\overline{c}_\varepsilon$ as

$$
-\theta \frac{\partial^2 \psi^\alpha}{\partial \theta^2} = c_\varepsilon^\alpha , \quad \overline{c}_\varepsilon = \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \rho^\alpha c_\varepsilon^\alpha
\tag{A.43}
$$

and using again the potential relation for the Cauchy stress according to Eq. (A.10) leads to

$$
\begin{aligned}
&\sum_{\alpha=1}^{\tilde{N}} \left(\dot{\varphi}_\alpha \rho^\alpha \psi^\alpha + \varphi_\alpha \left(\boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^\alpha - \boldsymbol{\sigma}^\alpha \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \varphi_\alpha} \dot{\varphi}_\alpha + \rho^\alpha \frac{\partial \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right)\right) \\
&\quad + \theta \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_\alpha \rho^\alpha \eta^\alpha - \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_\alpha \left(\frac{\partial \boldsymbol{\sigma}^\alpha}{\partial \theta} \cdot \left(\dot{\boldsymbol{\varepsilon}}^\alpha - \dot{\boldsymbol{\varepsilon}}^{*\alpha}\right) + \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \varphi_\alpha \partial \theta} \dot{\varphi}_\alpha \right. \\
&\quad \left. + \rho^\alpha \frac{\partial^2 \psi^\alpha}{\partial \boldsymbol{\alpha}^\alpha \partial \theta} \cdot \dot{\boldsymbol{\alpha}}^\alpha \right) + \overline{c}_\varepsilon \dot{\theta} = \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}\left(\overline{\boldsymbol{q}}\right) .
\end{aligned}
\tag{A.44}
$$

Rearranging the terms gives

$$
\begin{aligned}
\overline{c}_{\varepsilon}\dot{\theta} &= \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}\left(\overline{\boldsymbol{q}}\right) - \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_{\alpha} \rho^{\alpha} \theta \eta^{\alpha} - \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_{\alpha} \rho^{\alpha} \psi^{\alpha} \\
&\quad + \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \left(\frac{\partial \boldsymbol{\sigma}^{\alpha}}{\partial \theta} \cdot \left(\dot{\boldsymbol{\varepsilon}}^{\alpha} - \dot{\boldsymbol{\varepsilon}}^{*\alpha} \right) + \rho^{\alpha} \frac{\partial^{2} \psi^{\alpha}}{\partial \varphi_{\alpha} \partial \theta} \dot{\varphi}_{\alpha} + \rho^{\alpha} \frac{\partial^{2} \psi^{\alpha}}{\partial \boldsymbol{\alpha}^{\alpha} \partial \theta} \cdot \dot{\boldsymbol{\alpha}}^{\alpha} \right) \\
&\quad - \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \boldsymbol{\sigma}^{\alpha} \cdot \left(\dot{\boldsymbol{\varepsilon}}^{\alpha} - \dot{\boldsymbol{\varepsilon}}^{*\alpha} \right) - \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \left(\rho^{\alpha} \frac{\partial \psi^{\alpha}}{\partial \varphi_{\alpha}} \dot{\varphi}_{\alpha} + \rho^{\alpha} \frac{\partial \psi^{\alpha}}{\partial \boldsymbol{\alpha}^{\alpha}} \cdot \dot{\boldsymbol{\alpha}}^{\alpha} \right).
\end{aligned}
\tag{A.45}
$$

Considered form of the equation heat conduction Application of the Legendre transformation, i.e., $e^{\alpha} = \theta \eta^{\alpha} + \psi^{\alpha}$, cf., e.g., [51] yields the equation of heat conduction

$$
\begin{aligned}
\overline{c}_{\varepsilon}\dot{\theta} &= \overline{\boldsymbol{\sigma}} \cdot \dot{\overline{\boldsymbol{\varepsilon}}} + \overline{\rho r} - \operatorname{div}\left(\overline{\boldsymbol{q}}\right) - \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \boldsymbol{\sigma}^{\alpha} \cdot \dot{\boldsymbol{\varepsilon}}^{\alpha} \\
&\quad + \theta \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \left(\frac{\partial \boldsymbol{\sigma}^{\alpha}}{\partial \theta} \cdot \left(\dot{\boldsymbol{\varepsilon}}^{\alpha} - \dot{\boldsymbol{\varepsilon}}^{*\alpha} \right) + \rho^{\alpha} \frac{\partial^{2} \psi^{\alpha}}{\partial \boldsymbol{\alpha}^{\alpha} \partial \theta} \cdot \dot{\boldsymbol{\alpha}}^{\alpha} \right) \\
&\quad + \sum_{\alpha=1}^{\tilde{N}} \varphi_{\alpha} \left(\boldsymbol{\sigma}^{\alpha} \cdot \dot{\boldsymbol{\varepsilon}}^{*\alpha} - \rho^{\alpha} \frac{\partial \psi^{\alpha}}{\partial \boldsymbol{\alpha}^{\alpha}} \cdot \dot{\boldsymbol{\alpha}}^{\alpha} \right) \\
&\quad + \sum_{\alpha=1}^{\tilde{N}} \dot{\varphi}_{\alpha} \left(\varphi_{\alpha} \theta \rho^{\alpha} \frac{\partial^{2} \psi^{\alpha}}{\partial \varphi_{\alpha} \partial \theta} - \varphi_{\alpha} \rho^{\alpha} \frac{\partial \psi^{\alpha}}{\partial \varphi_{\alpha}} - \rho^{\alpha} e^{\alpha} \right),
\end{aligned}
\tag{A.46}
$$

which is also stated in Eq. (70).

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