MODELLING PHASE TRANSITIONS VIA YOUNG MEASURES

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Abstract. We consider the elastic theory of single crystals at constant temperature where the free energy density depends on the local concentration of one or more species of particles in such a way that for a given local concentration vector certain lattice geometries (phases) are preferred. Furthermore we consider possible large deformations of the crystal lattice. After deriving the physical model, we indicate by means of a suitable implicite time discretization an existence result for measure-valued solutions that relies on a new existence theorem for Young measures in infinite settings. This article is an overview of [2].

1. Introduction. We consider the general elastic theory of single crystals at constant temperature where the free energy density depends on the local concentration of one or more species of particles in such a way that for a given local concentration vector certain lattice geometries (phases) are preferred. Large deformations of the crystal lattice are explicitly allowed.

The local concentration of the molecules may change due to diffusion. The time scales typical for diffusion and for elastic deformation are usually significantly different. In good approximation it is admissible to assume that the deformation adjusts infinitely fast to the local situation. In the developed model there is surface energy contributing to the free energy of the crystal. The model allows for different coexisting macroscopic phases. We assume that the crystal does not possess interstitials and that the time-evolution of the boundary of the domain is known.

After deriving the physical model with the above properties we discuss the existence of solutions to this model by means of an implicit time discretization which results from a $Q - Q^*$ formulation, see section 3. In the Langrangian picture we will show for a special class of volumetric free energy densities that in the limit of vanishing time step the time-discrete solutions converge in the sense of Young measures on suitable separable and reflexive Banach spaces. Finally we state an energy inequality for the limit solution.

In this overview of [2] we focus on presenting a general strategy to solve the model equations. We omit all proofs of the stated theorems which can be found in german in [2].

For symbols not defined in the text see the List of Symbols at the end of this paper.

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2. Derivation of the model. In this section we derive a model of the physical phenomenon outlined in the introduction. We make use of non-equilibrium thermodynamics, see [15], [20], in the context of continuum mechanics, see [16], [9]. In particular we neglect the atomistic structure of the crystal and disregard possible effects of the microstructure. The model is based on the following fundamental considerations: Diffusion is caused by gradients of chemical potentials. The diffusive flux causes a local change of crystal’s free energy. The free energy shall depend on particle density, elasticity of the crystal and phase parameter only with a term representing the surface energy of the boundary layers.

In good approximation the system is in mechanical equilibrium. For the analytical treatment, we assume that deformation and phase parameters are global minimisers of the free energy.

Furthermore we assume a constant temperature, no interstials and that the boundary of the crystal is fixed.

A crucial point of the model is that it allows possible large deformations of the crystal lattice that can especially occur at the phase boundaries and for which the assumptions of linear elasticity theory does not hold. Because of these deformations we also consider surface energies between different phases. Our approach generalizes existing models of solid-solid phase transitions which assume linear elasticity laws, see [18], [29], [30], [23], [8], [28], [14], and it is applicable to materials with non-linear elastic behaviour, see [17], [24].

Remark 1. All theorems presented here hold also for a given boundary evolution if this evolution allows an energy releasing process, see (1.1.38) in [2], p.23.

We describe the crystal by a non-empty, bounded Lipschitz domain \( \Omega \subset \mathbb{R}^3 \). The mechanical deformation is given by a family of mappings \( \{ \Phi_t : \Omega \to \Omega : t \geq 0 \} \) that satisfy for all \( t \geq 0 \)

\[
\Phi_0 = \text{Id}_\Omega, \quad (1)
\]

\[
\Phi_t \in W^{1,a}(\Omega, \mathbb{R}^3) \quad \text{and} \quad \Theta_t := \Phi_t^{-1} \in W^{1,a}(\Omega, \mathbb{R}^3) \quad \text{exists}, \quad (2)
\]

\[
\det \nabla \Phi_t > 0 \quad \text{a.e. in } \Omega. \quad (3)
\]

Here, \( a > 3 \) can be arbitrary. The conditions (2) and (3) ensure that \( \Phi_t \) are deformations. The condition \( a > 3 \) guarantees the integrability of the functional determinant and therefore that positive volumes will be transformed into positive ones. Condition (1) reflects the fact that the initial state is undeformed.

The space- and time-dependent particle densities of the \( n \in \mathbb{N} \) different species of molecules are described by \( \rho(t) : \Omega \to \mathbb{R}^n, t \geq 0 \), with the natural conditions are postulated for \( t \geq 0 \):

\[
\rho(t) \in L^1(\Omega, \mathbb{R}^n), \quad \rho(t) \geq 0 \quad \text{a.e. in } \Omega, \quad \int_{\Omega} \rho(t,x) \, dx = \int_{\Omega} \rho_0(x) \, dx, \quad (4)
\]

\[
\rho(0) = \rho_0, \quad |\rho(t)|_1 \circ \Phi_t \det \nabla \Phi_t \leq 1 \quad \text{a.e. in } \Omega. \quad (5)
\]

\( \rho_0 \) is a given initial density-vector with

\[
\rho_0 \in L^1(\Omega, \mathbb{R}^n), \quad \rho_0 \geq 0 \quad \text{a.e. in } \Omega, \quad \int_{\Omega} \rho_0(x) \, dx > 0, \quad (6)
\]

\[
|\rho_0|_1 \leq 1 \quad \text{a.e. in } \Omega \quad \text{and} \quad \|\rho_0\| < |\Omega| \quad (7)
\]
Equation (4) ensures the conservation of particles, (5) is due to the fact that the crystal does not possess interstitials and that the number of lattice positions in a volume element is a uniform constant. We assume (7) with strict inequality: This means that we always allow for vacancies in our system in order to permit diffusion.

Let \( m \in \mathbb{N} \) denote the number of different possible phases. At each time \( t \geq 0 \) every \( x \in \Omega \) belongs to exactly one phase. The evolution of the phases is described by a family of phase-vectors \( \{ \chi_t : \Omega \to \mathbb{R}^m : t \geq 0 \} \) with given \( \chi_0 \) which have to fulfil

\[
\chi_t \in \{0,1\}^m, \quad |\chi_t|_1 = 1, \quad \chi_t \in \text{BV}(\Omega, \mathbb{R}^m) \quad \text{for all } t \geq 0.
\]

Therefore at each time \( t \geq 0 \) there is a well-defined surface area between phase \( i \) and phase \( j \) given by \( S(\chi_i, \chi_j) \), where

\[
S(\alpha, \beta) := \begin{cases} \frac{1}{2} \int_\Omega |\nabla \alpha + \nabla \beta| - |\nabla (\alpha + \beta)|, & \text{if } \int_\Omega |\nabla \alpha| + |\nabla \beta| < \infty, \\ \infty, & \text{else,} \end{cases} \quad \alpha, \beta \in L^1(\Omega).
\]

Assuming further that the densities of the surface energy \( \varsigma_{ij} \) on the interface between phase \( i \) and phase \( j \) are positive constants with \( \varsigma_{ij} = \varsigma_{ji} \), the surface energy \( F^s(\chi_t) \) at time \( t \geq 0 \) can be introduced by

\[
F^s(\chi) := \sum_{i=1}^m \sum_{j=1}^m \sigma_{ij} S(\chi_i, \chi_j), \quad \chi \in L^1(\Omega, \mathbb{R}^m),
\]

where \( \sigma_{ij} := \frac{\varsigma_{ij}}{2} \). Additionally we postulate for all \( i, j, k \in \{1, \ldots, m\} \)

\[
0 < \sigma_{ij} = \sigma_{ji},
\]

\[
\sigma_{ij} \leq \sigma_{ik} + \sigma_{kj}, \quad \text{if } i \neq j \text{ and } k \notin \{i, j\}.
\]

Therefore energetically it is not favourable to add a third phase between two other existing phases.

We assume that the volumetric free energy density \( f \) depends on the phase-vector, the gradient of the deformation and the particle densities and that there is a representation

\[
f(\chi, A, \rho) = \sum_{j=1}^m \chi_j f_j(A, \rho), \quad \chi \in \mathbb{R}_+^m, A \in \mathbb{R}^{3 \times 3}, \rho \in \mathbb{R}^n,
\]

where \( f_j : \mathbb{R}^{3 \times 3} \times \mathbb{R}^n \to [0, \infty] \) are measurable functions.

At each time \( t \geq 0 \) holds

\[
f(\chi_t, \nabla \Phi_t \circ \Theta_t, \rho(t)) = f \left( \chi_t, (\nabla \Theta_t)^{-1}, \rho(t) \right) = f \left( \chi_t, \frac{\text{cof} \nabla \Theta_t}{\det \nabla \Theta_t}, \rho(t) \right),
\]

where \( \text{cof} A \) denotes the matrix of co-factors of the quadratic matrix \( A \). By introducing

\[
F^v(\chi, A, \rho) := \int_\Omega f \left( \chi(y), \frac{\text{cof} A(y)}{\det A(y)}, \rho(y) \right) \, dy \in [0, \infty],
\]

for \( (\chi, A, \rho) \in L^1(\Omega, \mathbb{R}^m) \times L^1(\Omega, \mathbb{R}^{3 \times 3}) \times L^1(\Omega, \mathbb{R}^n) \) the free volumetric energy at time \( t \geq 0 \) can be computed by \( F^v(\chi_t, \nabla \Theta_t, \rho(t)) \). Consequently the free
energy of the system at $t \geq 0$ is given by $F(\chi_t, \nabla \Theta_t, \rho(t))$, where

$$F(\chi, A, \rho) := F^v(\chi, A, \rho) + F^s(\chi), \quad (\chi, A, \rho) \in L^1. \quad (11)$$

To model the dynamics of the system we use the following notation.

**Notation.** We define (formally) for quantities $J : \Omega \rightarrow \mathbb{R}^3$ and $\mu : \Omega \rightarrow \mathbb{R}^n$:

$$\text{div} J := (\text{div} J_i)_{i=1}^n \quad \text{and} \quad \nabla \mu := (\nabla \mu_i)_{i=1}^n.$$ 

The evolution of the particle densities can be described by a continuity equation

$$\partial_t \rho(t) = -\text{div} J^m_t \quad \text{in} \quad \Omega, \quad t > 0, \quad (12)$$

or equivalently

$$\partial_t (\rho(t) \circ \Phi_t \det \nabla \Phi_t) = (\text{div} J_t) \circ \Phi_t \det \nabla \Phi_t \quad \text{in} \quad \Omega, \quad t > 0. \quad (13)$$

At a fixed constant temperature the diffusive fluxes are caused by the negative gradients of the chemical potentials which are the thermodynamical forces, [15]. According to Onsager’s postulate, [25], [26]), every thermodynamical flux is a linear combination of the thermodynamical forces. Therefore we set for $t > 0$

$$J_t = L \nabla \mu_t := \left( \sum_{k=1}^n L_{ik} \nabla \mu_k \right)_{i=1}^n \quad \text{in} \quad \Omega \quad (14)$$

with a symmetric and positive definite matrix $L := (L_{ik})_{i,k=1}^n$ and the chemical potential $\mu_k$ of species $k$, where the symmetry and positive definiteness of $L$ comes from Onsager’s reciprocity relation, [25], [26], [15]. Due to the definition of the chemical potential one has in $\Omega$ at each time $t > 0$

$$\mu_t = \nabla \rho f(\chi_t, \nabla \Theta_t \circ \Theta_t, \rho(t)) = \nabla \rho f \left( \chi_t, \frac{\text{cof} \nabla \Theta_t}{\det \nabla \Theta_t}, \rho(t) \right). \quad (15)$$

Let us formulate now the aforementioned minimality condition on the free energy. Considering the time-evolution of the deformation of a representative volume element and keeping in mind that the number of particles only changes due to diffusion, we find for two possible deformations $\Phi^1_t$, $\Phi^2_t$ the relation

$$\rho^1(t) \circ \Phi^1_t \det \nabla \Phi^1_t = \rho^2(t) \circ \Phi^2_t \det \nabla \Phi^2_t \quad \text{in} \quad \Omega \quad (16)$$

where $\rho^1(t), \rho^2(t)$ are the densities corresponding to $\Phi^1_t, \Phi^2_t$. The minimality condition for any $t > 0$ reads

$$F(\chi_t, \nabla \Theta_t, \rho(t)) = \min_{\chi \in \mathcal{P}, \Theta \in \mathcal{D}} F(\chi, \nabla \Theta, \rho(t) \circ \Theta \det \nabla \Theta), \quad (17)$$
where
\[ P := \{ \chi \in BV(\Omega, \mathbb{R}^m) : \chi \in \{0,1\}^m, |\chi|_1 = 1 \text{ a.e. in } \Omega \}, \] (18)
\[ D := \{ \Theta \in W^{1,\alpha}(\Omega, \mathbb{R}^3) : \Theta(\Omega) = \Omega, \Theta^{-1} \in W^{1,\alpha}(\Omega, \mathbb{R}^3), \det \nabla \Theta > 0 \text{ a.e. in } \Omega \}, \] (19)
\[ \hat{\rho}(t) := \rho(t) \circ \Phi_t \det \nabla \Phi_t, \quad t \geq 0. \] (20)

Finally our model consists of the equations (1) - (5), (8), (13) - (15) and (17). We refer to this as the Eulerian description or picture.

3. Solution strategy and implicit time discretization. A suitable strategy to solve our equations was developed by Luckhaus and named Q – Q*-ansatz or principle. It has its roots in a special treatment of the heat equation, see section 1.2 in [2]. Up to now this principle is not published. We exemplify it by our equations. To this end we compute formally the time derivative of the free energy by exploiting the minimality condition (17). The following argument is only heuristic.

If we formally consider the free energy \( F \) due to the relation \( \Theta = \Phi^{-1} \) as a function of the phase-vector \( \chi \), the deformation \( \Phi \) and the particle-density-vector \( \rho \) then for \( t > 0 \) we find
\[ d_t F(t) = \partial_\chi F(t) \partial_t \chi_t + \partial_\rho F(t) \partial_t \Phi_t + \partial_\rho F(t) \partial_t \rho(t). \]
From (17) it follows \( \partial_\chi F(t) \partial_t \chi_t = 0, \partial_\rho F(t) \partial_t \rho(t) + \partial_\rho F(t) = 0 \) Consequently
\[ d_t F(t) = \partial_\rho F(t)(\partial_t \rho(t) - \partial_\Phi \rho(t) \partial_t \Phi_t). \] (21)

Now we compute \( \partial_\Phi \rho(t) \partial_t \Phi_t \) from (16) by using
\[ G(\Phi) := \rho(\Phi) \circ \Phi \det \nabla \Phi, \]
\[ d_\Phi G(\Phi_t) = 0, \]
\[ \det'(A)(\cdot) = \text{Tr}(A^{-1}) \det A \text{ for invertible matrices } A \]
to obtain:
\[ \partial_\Phi \rho(t) \partial_t \Phi_t = -\rho(t) \text{Tr}(\nabla \Phi_t^{-1} \nabla \partial_t \Phi_t \circ \Theta_t) - \sum_{i=1}^n \langle \nabla \rho_i(t), \partial_t \Phi_t \circ \Theta_t \rangle \]
\[ = -\text{div}(\rho(t) \partial_t \Phi_t \circ \Theta_t) \] (22)

If we plug (12) and (22) into (21) we find
\[ d_t F(t) = \partial_\rho F(t)(\text{div}(J_t) - \text{div}(\rho(t) \partial_t \Phi_t \circ \Theta_t) + \text{div}(\rho(t) \partial_t \Phi_t \circ \Theta_t)) \]
\[ = \partial_\rho F(t) \text{div}(J_t). \]

Assuming that the surface terms do not depend on \( \rho \) and the normal component of \( J_t \) vanishes on \( \partial \Omega \), cf. (13) and (4)_3, it follows, see [5] p.58,
\[ d_t F(t) = \int_\Omega \langle \nabla \rho(t)(\chi_t(y), \nabla \Phi_t \circ \Theta_t(y), \rho(t, y)), \text{div}(J_t(y)) \rangle \, dy \] (23)
\[ = \int_\Omega \langle \nabla \mu_t(y), J_t(y) \rangle \, dy \] (24)
\[ = Q(J_t) - Q^*(\nabla \mu_t), \quad t > 0, \] (25)
where
\[
Q(G) = \frac{1}{2} ||L^{-\frac{1}{2}}G||^2_2, \ G \in L^2(\Omega, \mathbb{R}^{3 \times n}),
\]
\[
Q^*(G) = \frac{1}{2} ||L^{\frac{1}{2}}G||^2_2, \ G \in L^2(\Omega, \mathbb{R}^{3 \times n}).
\]

$Q^*$ is the Fenchel conjugate of $Q$, see [7], p.49. We call the continuity equation (13) together with (15), (25) and the minimality condition (17) the $Q - Q^*$ formulation of our system. A solution to the $Q - Q^*$ formulation can be regarded as a weak solution to our original system. This is due to the fact that such a weak solution also fulfills Onsager’s Law (14) if we assume (23) to be true. (14) is then an immediate consequence of (25) and of the Fenchel-Young equality, see proposition 3.3.4 in [7], p.51.

An advantage of the $Q - Q^*$-formulation is that it provides a natural implicit time discretization of our original system. For similar discretizations see also [29], [21], [22].

Replacing (13), (23), (25) in use of (20) by their time-discrete versions for time-step $h > 0$ and $t \geq 0$:
\[
\rho(t + h) = \hat{\rho}(t) \circ \Theta_{t+h} \det \nabla \Omega_{t+h} + \operatorname{div} J_{t+h},
\]
\[
F(t + h) - F(t) = h \int_\Omega \left\langle \nabla \mu \left( \Theta_{t+h} J_{t+h} \rho(t + h) \right), \mu(t + h) \right\rangle,
\]
\[
F(t + h) - F(t) = -h \left[ Q(J_{t+h}) + Q^*(\nabla \mu_{t+h}) \right],
\]

yields
\[
\frac{d}{dt} Q(J_{t+h})[J_{t+h}] = -h \left[ Q(J(t + h)) + Q^*(\nabla \mu(t + h)) \right]
\]
\[
\frac{d}{dt} E^h_{\hat{\rho}(t)}(\chi_{t+h}, \Theta_{t+h}, J_{t+h}) = dJ E^h_{\hat{\rho}(t)}(\chi_{t+h}, \Theta_{t+h}, J_{t+h}) \big[ \chi_{t+h}, \Omega_{t+h}, J_{t+h} \big],
\]

where $E^h_{\hat{\rho}(t)}(\chi, \Theta, J)$ for $\chi \in L^1(\Omega, \mathbb{R}^{m}), \Theta \in W^{1,\alpha}(\Omega, \mathbb{R}^3), J \in L^2(\Omega, \mathbb{R}^{3 \times n})$ is formally defined by
\[
E^h_{\hat{\rho}(t)}(\chi, \Theta, J) := F(\chi, \Theta, \hat{\rho}(t) \circ \Theta) \det \nabla \Theta + h \operatorname{div} J.
\]

If $(\chi_{t+h}, \Theta_{t+h}, J_{t+h})$ is a minimizer of the functional $F^h_{\hat{\rho}(t)} := E^h_{\hat{\rho}(t)} + hQ$ so (31) is automatically satisfied and there holds for all $\eta \in C^1(\Omega, \mathbb{R}^{3 \times n})$
\[
0 = \lim_{\epsilon \to 0} \int_\Omega \frac{F^h_{\hat{\rho}(t)}(\chi_{t+h}, \Theta_{t+h}, J_{t+h} + \epsilon \eta) - F^h_{\hat{\rho}(t)}(\chi_{t+h}, \Theta_{t+h}, J_{t+h})}{\epsilon}
\]
\[
= \int_\Omega \left\langle L^{-1} J_{t+h} - \nabla \rho \left( \Theta_{t+h} \frac{\det \nabla \Omega_{t+h}}{\det \nabla \Theta_{t+h}} \rho(t + h) \right), \eta \right\rangle
\]

where $\rho(t + h)$ is defined by (28). Hence
\[
J_{t+h} = L \nabla \mu_{t+h}, \text{ where } \\
\mu_{t+h} := \nabla \rho \left( \Theta_{t+h} \frac{\det \nabla \Omega_{t+h}}{\det \nabla \Theta_{t+h}} \hat{\rho}(t + h) \right).
\]

Therefore for given time step $h > 0$ we suggest the following algorithm to compute a time-discrete solution:
The time-discrete model.

its analysis.

of the model equations.

system and then to show that the time-discrete solutions converge for vanishing
time step \( h \) to an object that can be interpreted as a physically meaningful solution
of the model equations.

The next step is to give the precise definition of the time-discrete solution and
its analysis.

4. The time-discrete model. To define the notion of a time-discrete solution we
have to clarify first what we will understand by the divergence of a \( L^2 \)-mapping.
This is done in a way adapted to the equations such that the conservation of particles (4)
and the implication (23) ⇒ (24) holds. The deeper reasons why we need a definition
for all \( L^2 \)-mappings are that \( Q \) is defined on \( L^2(\Omega, \mathbb{R}^{3n}) \) and that we want to
apply the direct method of variational analysis to show existence of a time-discrete
solution (see below).

Definition 4.1. The divergence for \( j \in L^2(\Omega, \mathbb{R}^3) \) resp. \( J \in L^2(\Omega, \mathbb{R}^{3n}) \) is defined by

\[
\text{div} j(\xi) := -\int_\Omega (j(y), \nabla \xi(y)) \, dy, \quad \xi \in W^{1,2}(\Omega),
\]

\[
\text{div} J := (\text{div} J_l)_{l=1}^n.
\]

Remark 2. Take notice of the following properties of the divergence, see Bemerkung 2.1.3, p.41 in [2].

• If \( \text{div} j \in L^1(\Omega) \) then \( \int_\Omega \text{div} j(y) \, dy = 0 \).

• Let \( C > 0, 1 < p < \infty \) and \( (\text{div} j_l) \in L^p(\Omega) \) with \( \lim_{l \to \infty} \text{div} j_l(\xi) = \text{div} j(\xi) \)
for all \( \xi \in W^{1,2}(\Omega) \) and \( \|\text{div} j_l\|_p \leq C \) for all \( l \in \mathbb{N} \) then \( \text{div} j \in L^p(\Omega) \).

• Let \( g : \mathbb{R} \to [0, \infty] \) be measurable with \( C_1 g(x) + C_2 \geq |x|^p \) for all \( x \in \mathbb{R} \)
for some constants \( C_1, C_2 > 0 \) and \( p > 1 \). Furthermore let \( j \in L^2(\Omega, \mathbb{R}^3) \),
\( (j_l) \in C_0^1(\Omega, \mathbb{R}^3) \) such that \( \lim_{l \to \infty} \text{div} j_l(\xi) = \text{div} j(\xi) \) for all \( \xi \in W^{1,2}(\Omega) \) and
\( \text{div} j \notin L^p(\Omega) \) then \( \lim_{l \to \infty} \int_\Omega g(\text{div} j_l(z)) \, dz = \infty \).

We define a time-discrete solution as follows.

Definition 4.2. (time-discrete solution) Let \( F, Q, P, D \) be defined as in (11), (26),
(18), (19) and

\[
\Pi_d := L^1(\Omega, \mathbb{R}^m) \times W^{1,\infty}(\Omega, \mathbb{R}^3) \times L^2(\Omega, \mathbb{R}^{3n}),
\]

\[
\Pi_e := \Pi_d \times W^{1,2}(\Omega, \mathbb{R}^n) \times L^1(\Omega, \mathbb{n}),
\]

\[
M := P \times D \times L^2(\Omega, \mathbb{R}^{3n}).
\]

Furthermore let for \( \hat{\rho} \in L^\infty(\Omega, \mathbb{R}^n) \), \( h > 0 \) and \( (\chi, \Theta, J) \in \Pi_d \)

\[
E^h_\hat{\rho}(\chi, \Theta, J) := \begin{cases} F(\chi, \nabla \Theta, \hat{\rho} \circ \Theta \det \nabla \Theta + h \text{div} J), & \text{if div} J \in L^1(\Omega, \mathbb{R}^n), \\ \infty, & \text{if div} J \notin L^1(\Omega, \mathbb{R}^n), \end{cases}
\]

\[
F^h_\hat{\rho}(\chi, \Theta, J) := E^h_\hat{\rho}(\chi, \Theta, J) + h Q(J).
\]
For fixed time step $h > 0$ we call every mapping
\[
\gamma : [0, \infty[ \rightarrow \Pi, \ t \mapsto (\chi_t, \Theta_t, J_t, \mu_t, \rho(t))
\]
a time-discrete solution if it satisfies
\[
\chi_0 \in P, \ 
\Theta_0 = \text{Id}_\Omega, \ 
\rho(0) = \rho_0
\]
and for $k \in \mathbb{N}_0$, $0 \leq \tau < h$, $t \geq h$
\[
\gamma(\tau + \tau) = \gamma(\tau), \quad (\chi_t, \Theta_t) \in P \times D,
\]
\[
\mu_t = \nabla \rho f (\chi_t, \Theta_t, \partial \nabla \Theta_t, \rho(t)),
\]
\[
J_t = L \nabla \mu_t,
\]
\[
\rho(t) \geq 0 \text{ a.e. in } \Omega,
\]
\[
\int_\Omega \rho(t, y) \, dy = \int_\Omega \rho_0(x) \, dx,
\]
\[
|\hat{\rho}(t)|_1 \leq 1 \text{ a.e. in } \Omega
\]
and for $t \geq 0$
\[
\rho(t + h) = \hat{\rho}(t) \circ \Theta_{t+h} \det \nabla \Theta_{t+h} + h \text{ div } J_{t+h},
\]
\[
F^h_{\hat{\rho}(t)} (\chi_{t+h}, \Theta_{t+h}, J_{t+h}) = \inf_{(\chi, \Theta, J) \in \mathcal{M}} F^h_{\hat{\rho}(t)} (\chi, \Theta, J),
\]
where for $t \geq 0$
\[
\Phi_t := \Theta_t^{-1},
\]
\[
\hat{\rho}(t) \equiv \rho(t) \circ \Phi_t \det \nabla \Phi_t.
\]

Crucial to prove existence of a time-discrete solution is to show that the minimization problem $F^h_{\hat{\rho}} \rightarrow \min$, $(\chi, \Theta, J) \in \mathcal{M}$ has a solution. We try to apply the direct method. To this end we need additional mathematical conditions on the volumetric free energies $f_j$, especially convexity, lower semicontinuity and growth conditions. They are specified in the following theorem. Using the abbreviations
\[
A := (A, \text{cof } A, \det A), \ A \in \mathbb{R}^{3 \times 3},
\]
\[
Z := \{(A, \rho) \in \mathbb{R}^{3 \times 3} \times \mathbb{R}^n : \rho \geq 0, \det A > 0, |\rho|_1 \leq \det A \}.
\]

we state, see Theorem 2.2.1, p.44 in [2]:

**Theorem 4.3.** Let $h > 0$ and let $\hat{\rho} \in L^\infty(\Omega, \mathbb{R}^n)$ be satisfying (6), (7). Furthermore let there be convex, lsc functions $f_j : \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \times \mathbb{R} \times \mathbb{R}^n \rightarrow [0, \infty[$, $j = 1, ..., m$, such that there holds for all $j \in \{1, ..., m\}$

i. $f_j (\text{cof } A, \rho) = f_j (A, \rho)$ for all $A \in \mathbb{R}^{3 \times 3}$ with $\det A > 0$ and all $\rho \in \mathbb{R}^n$.

ii. There are $c_1, c_2 > 0$ such that $c_1 f_j (A, \rho) + c_2 \geq \max \left[ |A|_1, \frac{|\text{cof } A|_1}{|\det A|^{1 - \gamma}} \right]$ for all $A \in \mathbb{R}^{3 \times 3}$ with $\det A > 0$ and all $\rho \in \mathbb{R}^n$.

iii. For $A \in \mathbb{R}^{3 \times 3}$, $\rho \in \mathbb{R}^n$ there holds $f_j (A, \rho) < \infty$ iff $(A, \rho) \in Z$.

iv. $\sup_{(E, \rho) \in Z} f_j (E, \rho) < \infty$, where $E$ denotes the unity in $\mathbb{R}^{3 \times 3}$.
Then there is \((\chi^*, \Theta^*, J^*) \in M\) such that \(F^h_\rho(\chi^*, \Theta^*, J^*) = \inf_{(\chi, \Theta, J) \in M} F^h_\rho(\chi, \Theta, J)\), \(\rho^* := \tilde{\rho} \circ \Theta^* \text{det} \nabla \Theta^* + \text{hdiv} J^*\) fulfills (4), (5) where \(\rho_0\) is replaced by \(\tilde{\rho}\).

The first assumption i., this is polyconvexity and lower semicontinuity of the volumetric free energy densities, is mainly needed to apply the direct method. ii. assures that there is a sequence \((\Theta_i)_{i \in \mathbb{N}}\) such that \(\Theta_i \overset{W^{1,n}}{\rightharpoonup} \Theta, \text{cof} \nabla \Theta_i \overset{L^p}{\rightharpoonup} H, \text{det} \nabla \Theta_i \overset{L^q}{\rightharpoonup} \Delta, i \to \infty\) which implies \(H = \text{cof} \nabla \Theta, \Delta = \text{det} \nabla \Theta\), see theorem 7.6-1, p.365 in [9]. It also guarantees the same for the deformations \(\Phi_i\) due to

\[
\int_\Omega |\nabla \Phi(x)|^p \, dx = \int_\Omega |\nabla \Phi(\Theta(y))|^p \text{det} \nabla \Theta(y) \, dy = \int_\Omega \left| \text{cof} \nabla \Theta(y) \right|^p \frac{1}{(\text{det} \nabla \Theta(y))^{\alpha - 1}} \, dy
\]

for \(\Theta \in D\) with \(\Phi = \Theta^{-1}\). To satisfy (4), (5) we need iii. while iv. yields \(\inf_M F^h_\rho < \infty\). Beside of this the proof relies on the following statements

- Sobolev embeddings, Mazur’s lemma and Fatou’s lemma.
- For a minimizing sequence there holds \(\|J_i\|_2^2 \leq \frac{2\|L - \frac{d}{h}\|}{h} Q(J_i)\) and \(\|\text{div} J_i\|_2 \leq \frac{\|\text{det} \nabla \Theta_i\|_2}{h}\).
- \(Q\) is weakly sequentially lower semicontinuous.

- The unit ball in \(B^1(\Omega)\) is strongly compact in \(L^1(\Omega)\).
- \(F^x\) is strongly lower semicontinuous on \(P\) and it holds \(\sum_{j=1}^m \int_{\Omega} |\nabla \chi_j| \leq CF^x(\chi)\) for some fixed constant \(C > 0\) and all \(\chi \in P\).

By means of this theorem we can construct to every \(h > 0\) a mapping \(\gamma_h : [0, \infty[ \to \Pi_e\) which fulfills all restrictions of definition 4.2 but (45) and (46). Beside the existence of vacancies (7) we need some extra informations about the behavior of the \(f_j\) at their effective domains to assure this relations. The reason for this is that the argument (32) doesn’t work in general, because we cannot exclude concentrations of \((\nabla \Theta_i, \rho(t))\) near or at

\[
\partial Z_u := \{(A, \rho) \in Z : \text{there is } i \in \{1, \ldots, n\} \text{ with } \rho_i = 0\}, \quad (55)
\]

\[
\partial Z_o := \{(A, r) \in Z : \rho > 0, |\rho|_1 = \text{det}A\}. \quad (56)
\]

If the \(f_j\) satisfy the following conditions 1.-4. then Onsager’s relations does hold, see Korollar 2.2.2, p.45 in [2]:

**Corollary 1.** Let \(\partial Z_u, \partial Z_o\) be defined as in (55), (56) and let

\[
Z_0 := \{(A, \rho) \in Z : 0 < \rho, |\rho|_1 < \text{det}A\} ,
\]

\[
R := \mathbb{R}^m_+ \times \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \times \mathbb{R} \times \mathbb{R}^n ,
\]

\[
f(\chi, A, B, d, \rho) := \sum_{j=1}^m \chi_j f_j(A, B, d, \rho), \quad (\chi, A, B, d, \rho) \in R ,
\]

\[
C_m := \{e \in \{0,1\}^m : |e|_1 = 1\} \quad (57)
\]
and for $A \in \mathbb{R}^{3 \times 3}$ with $\det A > 0$

$$u(A) := \max \left\{ \frac{|A|^a}{\det a^{-1} A}, \sqrt{\frac{|A|^a}{\det a^{-1} A}}, \det \frac{a^2}{2} \right\}.$$ 

If $f$ satisfies

1. To every $(A, \rho) \in \partial Z_o$ and every $\chi \in C_n$ there exists $\nabla \rho f(\chi, A, \rho)$,
2. To every $(A, \rho) \in \partial Z_u$ there is $z \in \mathbb{R}^n$ such that for all $\chi \in C_n$ there holds
   $$\lim_{r \downarrow 0} \frac{f(\chi, A, \rho + r \epsilon)}{r} = -\infty,$$
3. To every $(A, \rho) \in \partial Z_o$ there is $z \in \mathbb{R}^n$ such that for all $\chi \in C_n$ there holds
   $$\lim_{r \downarrow 0} \frac{f(\chi, A, \rho - r \epsilon)}{r} = \infty,$$
4. There are $0 < \epsilon < 1$, $b, v_1, v_2 > 0$, such that for all $(A, \rho) \in \mathbb{Z}$, $\chi, e \in C_n$, $0 \leq r_1 \leq \min \left\{ \epsilon (\det A - |\rho|_1), b \right\}$, $0 \leq r_2 \leq \min \left\{ \epsilon (\rho, e), b \right\}$ there holds
   $$|f(\chi, A, \rho + r_1 e) - f(\chi, A, \rho)| \leq v_1 u(A) + v_2,$$
   $$|f(\chi, A, \rho - r_2 e) - f(\chi, A, \rho)| \leq v_1 u(A) + v_2$$

then under the assumptions of theorem 4.3 there holds

$$\mu^* := \nabla \rho f(\chi^*, \nabla \Theta^*, \rho^*) \in W^{1,2}(\Omega, \mathbb{R}^n),$$

$$J^* = L\nabla \mu^*$$

where we used the abbreviation $(54)$. 

The idea of proof is to approximate the $f_j$ by suitable smooth and convex functions from below and to show by using $(32)$ that the solution of the corresponding variational problem fulfils $(45), (46)$. Then one shows that this solutions converge to the solution of the original problem where in the limit Onsager’s relation remains valid. This is done by a subgradient argument where 1.-4. enters.

Theorem 4.3 and corollary 1 imply together with their assumptions and together with the inequality

$$F_h^b(\chi_{t+h}, \Theta_{t+h}, J_{t+h}) \leq F(\chi_t, \nabla \Theta_t, \rho(t))$$

the main theorem for the time-discrete system, see Korollar 2.2.3, p.56 and Korollar 2.2.4, p.63 in [2]. It deals mainly with estimates on the time-discrete solutions.

**Theorem 4.4.** Let $h > 0$ and the assumptions of theorem 4.3 and corollary 1 be satisfied. Then there is a time-discrete solution and for every $T > 0$. Furthermore there is $C > 0$ independent of $h$ such that there holds for all $t \in [0, T]$

$$\int_0^\infty \|J_r\|^2 \, dr, \|\Theta_t\|_{1, a}, \|\Phi_t\|_{1, a}, \|\chi_a\|_{\text{BV}} \leq C$$

(60)

If there are $0 < \epsilon < 1$, $0 < \gamma_1, \gamma_2$ such that for all $(A, \tau) \in Z_0$, $\chi, e \in C_n$ and all $0 \leq s_1 \leq \epsilon (\det A - |\rho|_1)$, $0 \leq s_2 \leq \epsilon (\rho, e)$ there holds

$$\frac{|f(\chi, A, \rho + s_1 e) - f(\chi, A, \rho)|}{\det A} \leq \gamma_1 u(A) + \gamma_2,$$

$$\frac{|f(\chi, A, \rho - s_2 e) - f(\chi, A, \rho)|}{\det A} \leq \gamma_1 u(A) + \gamma_2$$

(61)
then there is also
\[ \int_0^T \| \mu_\tau \|_{1,2}^2 \, d\tau \leq C \]  
(63)

fulfilled. In addition there holds an energy inequality.

\[ F (\chi_{t+h}, \nabla \Theta_{t+h}, \rho(t+h)) - F (\chi_t, \nabla \Theta_t, \rho(t)) \leq -h \left[ Q (J_{t+h}) + Q^* (\nabla \mu_{\inf t}) \right] \]  
(64)

where for \( t \geq 0 \)

\[ J_{\inf t} := \arg \min_{J \in L^2(\Omega, \mathbb{R}^3 \cdot n)} F_h (\hat{\rho}(t)) (\chi_t, \Theta_t, J), \]
\[ \rho_{\inf t}(t) := \rho(t) + h \text{div} J_{\inf t}, \]
\[ \mu_{\inf t} := \nabla \rho^f (\chi_t, \nabla \Theta_t, \rho_{\inf t}). \]

Furthermore (58), (59) is fulfilled for \( \mu_{\inf t}, J_{\inf t}, t \geq 0 \) and (60), (63) remains true for the mappings \( \tau \mapsto \| J_{\inf \tau} \|_{2,2}, \tau \mapsto \| \mu_{\inf \tau} \|_{1,2}, \tau \geq 0 \).

The reason for the conditions (61), (62) is that they allow to estimate
\[ \left| \int_0^T \right| \mu_\tau \left. \right|_{1,2}^2 \, d\tau \right|^2. \]
(63) is then a consequence of the second Poincaré-inequality. The time-discrete energy inequality (64) results easily by Fenchel-Young’s inequality.

**Remark 3.** (61), (62) can be relaxed if \( a \geq 6 \).

(64) in combination with Jensen’s inequality and Kolmogorov’s criterion allows to prove a statement about the convergence of the Lagrangian particle densities \( \hat{\rho} \) as \( h \to 0 \), see Korollar 2.2.5, p.65 in [2].

**Corollary 2.** Let \((h_k > 0)_{k \in \mathbb{N}}\) with \( \lim_{k \to \infty} h_k = 0 \) and let \( \gamma_k \) be a time-discrete solution to time step \( h_k \) for \( k \in \mathbb{N} \). Then to every \( \phi \in C^1_0(\mathbb{R}^3) \) and \( T > 0 \) there is a subsequence of \((\gamma_k)_{k \in \mathbb{N}}\) also labeled by \( k \) and \( \hat{\rho} \in L^2 ([0, T] \times \Omega, \mathbb{R}^n) \) such that there holds
\[ \lim_{k \to \infty} \int_0^T \| \hat{\rho}_k(t) * \phi - \hat{\rho}(t) \|_2^2 \, dt = \lim_{k \to \infty} \int_0^T \| \hat{\rho}_{\inf_k}(t) * \phi - \hat{\rho}(t) \|_2^2 \, dt = 0. \]

Note that the folding is in space and understood to be componentwise.

5. **The time-continuous model.** The next step according to our strategy is to give an answer to the question: Can we find a sequence of time steps \((h_k)_{k \in \mathbb{N}}\) with \( h_k \downarrow 0, k \to \infty \) and a corresponding sequence \((\gamma_k)_{k \in \mathbb{N}}\) of time-discrete solutions which converges (in some sense) to a physically meaningful solution of the time-continuous problem as \( k \to \infty \)?

We restrict ourselves to finite time intervals \([0, T], T > 0\). At first one would try to show convergence to a weak solution in the sense of Sobolev. Due to the nonlinearities of the model and the fact that the equations do not provide estimates on \( \chi_t, \Theta_t \) in time there is no hope to find a weak solution like that.

An inspiration to get a useful notation of solution gives the original Young measure theorem, see [31]:
Theorem 5.1. Let $I \subset \mathbb{R}$ be an interval, $p \in \mathbb{N}$ and let $(u_k : I \to \mathbb{R}^p)_{k \in \mathbb{N}}$ be a sequence of measurable mappings with $\sup_{k \in \mathbb{N}} \sup_{\tau \in I} |u_k(\tau)| < \infty$. Then there is a subsequence $(u_{k_l} : I \to \mathbb{R}^p)_{l \in \mathbb{N}}$ and for almost all $\tau \in I$ there is a probability measure $P_\tau$ on $\mathbb{R}^p$ such that for all $f \in C(\mathbb{R}^p)$ and $\psi \in L^1(I)$ there holds
\[
\lim_{l \to \infty} \int_I \psi(\tau) f(u_{k_l}(\tau)) \, d\tau = \int_I \psi(\tau) \bar{f}(\tau) \, d\tau,
\]
(65)
where
\[
\bar{f}(\tau) := \int_{\mathbb{R}^p} f(x) \, dP_\tau(x),
\]
(66)
holds for $\tau \in \{t \in I : P_t \text{ exists}\}$.

If we consider the time-discrete solutions as mappings $\gamma_h : [0,T] \to \Pi_c$, see definition 4.2, having in mind the estimates of theorem 4.4 and suppose that there is a generalisation of theorem 5.1 to a function space $\mathcal{X}$ with $\Pi_c \subset \mathcal{X}$ then by (65) it would be natural to look for a formulation of our time-continuous model in terms of functionals according to the right-hand side of (65) where in (66) $\mathbb{R}^p$ has to be replaced by $\mathcal{X}$. This is the underlying idea of the following notion of a measure-valued solution, see Definition 3.1.1, p.71 in [2].

A weak formulation of our problem belongs to the following class of weak diffusion problems.

Definition 5.2. Let $T > 0$, $X, I, J$ be sets, $(N_t)_{t \in [0,T]}$ be a family of subsets of $X$ and $(D_i)_{i \in I}, (F_i)_{i \in I}, (C_j)_{j \in J}$ be families of functionals on $[0,T] \times X$ with values in $[-\infty, \infty]$. By a weak diffusion problem with respect to $T$, $X$, $(N_t)_{t \in [0,T]}$, $(D_i)_{i \in I}, (F_i)_{i \in I}, (C_j)_{j \in J}$ we understand the following task.

Find a mapping $\gamma : [0,T] \to X$ such that for all $\vartheta \in C_0^\infty(\mathbb{R})$ and all $t \in [0,T]$ there holds
\[
\int_0^T \dot{\vartheta}(\tau) D_i(\tau, \gamma(\tau)) + \vartheta(\tau) F_i(\tau, \gamma(\tau)) \, d\tau = 0 \text{ for all } i \in I, \quad (67)
\]
\[
\int_0^T \dot{\vartheta}(\tau) C_j(\tau, \gamma(\tau)) \, d\tau = 0 \text{ for all } j \in J, \quad (68)
\]
\[
\gamma(t) \in N_t. \quad (69)
\]

(67) is an abstract diffusion equation, (68) can be regarded as a coupling of the different (physical) quantities represented by $\gamma$ and (69) is an abstract formulation of the side conditions.

“Averaging over the values of $\gamma(t)$” leads to the notion of a measure-valued solution for weak diffusion problems.

Definition 5.3. We say there is a measure-valued solution to (67) - (69), if there is an $\sigma$–Algebra $\Sigma$ on $X$ and to almost every $t \in [0,T]$ a probability measure $P_t$
on $\Sigma$ such that for all $\vartheta \in C^\infty_c([0,T])$ and almost all $t \in [0,T]$ there holds
\[
\int_0^T \left( \vartheta(\tau) \int_X D^i(\tau,x) \, dP_\tau(x) + \vartheta(\tau) \int_X F^j(\tau,x) \, dP_\tau(x) \right) \, d\tau = 0 \quad \text{for all } i \in I,
\]
\[
\int_0^T \vartheta(\tau) \int_X C^j(\tau,x) \, dP_\tau(x) \, d\tau = 0 \quad \text{for all } j \in J,
\]
\[
P_t(X \setminus N_t) = 0.
\]
We will denote a measure-valued solution by $(X, \Sigma, P_t)_{t \in [0,T]}$.

**Remark 4.** Every solution $\gamma$ of (67) - (69) in the sense of definition 5.2 corresponds to the measure-valued solution $(X, 2^X, \delta_{\gamma(t)})_{t \in [0,T]}$. For the notion of measure-valued solutions see also [28].

As mentioned below theorem 5.1 our hope to find a measure-valued solution to our problem is based on a generalisation of Young’s theorem to function spaces $X$ with $\Pi \subset X$. Fortunately this is possible as the following theorem and its corollary shows, see Theorem 3.2.8, p.105 and Theorem 3.2.11 p.106 in [2].

**Theorem 5.4.** (Analogon to Young measures in the infinite setting.) Let $T > 0$ and $\lambda_T$ be the Lebesgue measure on $[0, T]$, $(\nu_k)_{k \in \mathbb{N}}$ be a sequence of positive Radon measures on $[0,T]$ with $\nu_k \rightharpoonup \lambda_T$ for $k \to \infty$, let $X_1, X_2$ be Banach spaces with separable $X_1^*, X_2^*$, define $(X, \tau) := (X_1 \times X_2, \|\cdot\|_{X_1} \times w_{X_2})$, and $(\gamma_k : [0,T] \to X)_{k \in \mathbb{N}}$ be a sequence of mappings. If there are monoton increasing sequences of compact sets $(K_{1\lambda} \subset (X_1, \|\cdot\|_{X_1}))_{\lambda \in \mathbb{N}}$, $(K_{2\lambda} \subset (X_2, w_{X_2}))_{\lambda \in \mathbb{N}}$ such that holds
\[
\nu_k (M_{k\lambda} := \{t \in [0,T] : \gamma_k(t) \notin K_{1\lambda} \times K_{2\lambda}\}) < \frac{1}{\lambda} \quad \text{for all } k, \lambda \in \mathbb{N},
\]
then there exists a subsequence $(\gamma_{k_j})_{j \in \mathbb{N}}$ and a mapping $P : [0,T] \to R(X)$ with $P_t \geq 0, P_t(X) = 1$ for almost all $t \in [0,T]$ and
\[
\lim_{l \to \infty} \int_0^T f(t, \gamma_{k_l}(t)) \, d\nu_{k_l}(t) = \int_0^T \int_X f(t,x) \, dP_t(x) \, dt
\]
for all $f \in C_b([0,T] \times X)$.

**Corollary 3.** Let $\|x\|_X := \|x_1\|_{X_1} + \|x_2\|_{X_2}, x \in X$. Additional to the assumptions stated above let there exist a $q \geq 0$ such that for all $k, \lambda \in \mathbb{N}$
\[
\|\gamma_{k_i}\|_X \leq L^1([0,T]),
\]
\[
\int_{M_{\lambda k}} \|\gamma_{k_i}\|_X^q \, d\nu_{k_i}(t) < \frac{1}{\lambda}.
\]
Let $f : ([0,T] \times X, |\cdot| \times \tau) \to \mathbb{R}$ fulfil for a constant $C > 0$
\[
f(t,x) \leq C (1 + \|x\|^q) \quad \text{for all } (t,x) \in [0,T] \times X.
\]
Let $f$ be bounded from below and let $f$ be either lower sequentially semicontinuous or lower sequentially semicontinuous with respect to the second argument and satisfy a
uniform continuity in time, i.e. for any \( \lambda \in \mathbb{N} \) and given \( \epsilon > 0 \) there exists a \( \delta(\lambda, \epsilon) \) with \( |f(t,x) - f(t',x)| < \epsilon \) for \( |t-t'| < \delta(\lambda, \epsilon) \), \( t, t' \in [0,T] \) and all \( x \in K_{1\lambda} \times K_{2\lambda} \). If one of these two conditions is met, it follows

\[
\begin{align*}
  f(t, \cdot) & \in L^1(X, B(X, \tau), P_t) \text{ f.a.a. } t \in [0,T], \\
  \left( \int_{[0,T]} f(t,x) \, dP_t(x) \, dt \right) & \in L^1([0,T]), \\
  \lim\inf_{t \to t} \int_{[0,T]} f(t, \gamma_{k_i}(t)) \, d\nu_{k_i}(t) & \geq \int_{[0,T]} f(t,x) \, dP_t(x) \, dt. \quad (75)
\end{align*}
\]

A sequentially continuous function \( f \) that is not necessarily bounded from below and satisfies (74) fulfills

\[
\lim_{t \to \infty} \int_{[0,T]} f(t, \gamma_{k_i}(t)) \, d\nu_{k_i}(t) = \int_{[0,T]} f(t,x) \, dP_t(x) \, dt. \quad (76)
\]

Remark 5. 1. \((X, \tau)\) can be replaced by \( \left( K := \bigcup_{\lambda=1}^{\infty} K_{1\lambda} \times K_{2\lambda}, \tau|_K \right) \). 2. For our model we need only the case where \( \nu_k = \lambda T \), \( k \in \mathbb{N} \). 3. A semi-constructive method to compute the measures \( P_t \) by means of cylindric functions is given in section 3.2 in [2].

Theorem 5.4, corollary 3 and the estimates stated in theorem 4.4 restrict the choice of the function space \( X \). On one hand one has to guarantee the existence of a sequence of compact subsets such that (70) holds and on the other hand the functionals that corresponds to \( D_1, F_1, C_1 \) in definition 5.2 have to be (lower semi-)continuous and to fulfill growth conditions like (74). Obviously these are contrarily requirements and so it turns out that 5.4 and corollary 3 are not directly applicable to our system. The reason lies in the fact that we cannot prove the weak sequential continuity of the functional which corresponds to the continuity resp. diffusion equation (13), because there enters a term \( \text{cof} \nabla \Phi(f \circ \Phi) \), see p.119 in [2]. This is due to the fact that we can find only sequences of weakly compact sets in \( W^{1,n}(\Omega, \mathbb{R}^3) \) resp. in \( L^2(\Omega, \mathbb{R}^{3-n}) \) for the mappings \( \Theta_k \) resp. \( J_k, k \in \mathbb{N} \), which correspond to \((K_{2\lambda})_{\lambda \in \mathbb{N}}\) in theorem 5.4. Now one can try to use the Lagrangian picture instead of the Eulerian one, i.e. one uses for \( t \geq 0 \) the quantities \( \Phi_t \) and

\[
\begin{align*}
  \hat{\chi}_t & := \chi_t \circ \Phi_t, \\
  \hat{J}_t & := \text{cof} \nabla \Phi_t J_t \circ \Phi_t := (\text{cof} \nabla \Phi_t J_t \circ \Phi_t)^n, \\
  \hat{\mu}_t & := \mu_t \circ \Phi_t, \\
  \hat{\rho}(t) & := \rho(t) \circ \Phi_t \text{det} \nabla \Phi_t,
\end{align*}
\]

where the Langrangian volume energy density is given by

\[
\hat{f}(\hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) = \begin{cases} f \left( \hat{\chi}, \hat{B} \cdot \frac{\hat{A}}{\hat{d}}, \frac{\hat{B}}{\hat{d}} \right) \hat{d} & \text{if } \hat{d} > 0, \\
+\infty & \text{if } \hat{d} \leq 0,
\end{cases} \quad (X, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) \in \mathbb{R}.
\]

Note that the transformation \( f \mapsto \hat{f} \) preserves all presumed properties of \( f \).

In this picture the continuity equation reads as \( \partial_t \hat{\rho}(t) = \text{div} \hat{J}_t \) but because of the integrability and differentiability properties of the \( \Phi_t \) we cannot prove existence of the corresponding compact sets with (70). For instance there is no integral estimate for \( t \mapsto \hat{J}_{k_i} \) like (60) and \( \hat{\chi}_t \) loses the BV-property.
A way to overcome these problems is to use a mixture of the Langrangian and the Eulerian description and splitting up the model equations by introducing extra variables. In addition to the Langrangian variables we use the following Eulerian variables for $t \geq 0$: $\chi_t, \Theta_t, J_t, \mu_t, J_{inf}, \mu_{inf}$, and

\[
\begin{align*}
\hat{A}_t := \nabla \Phi_t, & \quad \hat{B}_t := \text{cof} \nabla \Phi_t, \\
\hat{d}_t := \det \nabla \Phi_t, & \quad A_t := \nabla \Theta_t, \\
G_t := \nabla \mu_t, & \quad \mu_{inf} := \mu_{inf} \circ \Phi_t, \\
G_{inf} := \nabla \mu_{inf}, & \quad \rho_{inf}(t) := \rho_{inf}(t) \circ \Phi_t \text{det} \nabla \Phi_t.
\end{align*}
\]

Remark 6. We need the quantities indicated by $\inf$ to prove an energy inequality, see (64).

Now we model the time-continuous problem by this quantities and define functionals according to definition (5.2) to give a weak formulation.

Let for $\chi, \hat{\chi} \in L^1(\Omega, \mathbb{R}^n), A, B \in L^1(\Omega, \mathbb{R}^{3 \times 3}), d \in L^1(\Omega), \hat{\rho} \in L^1(\Omega, \mathbb{R}^n)$

\[
\begin{align*}
\hat{F}^v(\hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) & := \int_{\Omega} \hat{F}(\hat{\chi}(x), \hat{A}(x), \hat{B}(x), \hat{d}(x), \hat{\rho}(x)) \, dx, \\
\hat{F}(\chi, \hat{\chi}, A, B, d, \hat{\rho}) & := F^s(\chi) + \hat{F}^v(\hat{\chi}, A, B, d, \hat{\rho}).
\end{align*}
\]

Let furthermore

\[
\begin{align*}
\hat{P} & := \{ \hat{\chi} \in L^1(\Omega, \mathbb{R}^n): \hat{\chi} \in \{0, 1\}^m, |\hat{\chi}|_1 = 1 \text{ a.e. in } \Omega \}, \\
\hat{M} & := \{ (\chi, \hat{\chi}, \Phi) \in P \times \hat{P} \times D: \hat{\chi} = \chi \circ \Phi \}, \\
\hat{S} & := \{ \hat{s} \in \mathbb{R}^n_+: |\hat{s}|_1 = 1 \}, \\
\hat{E} & := \{ (A, B, d) \in \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \times \mathbb{R}: \text{cof} B = \det A \}, \\
\hat{X}_p & := L^{p_1}(\Omega, \mathbb{R}^n) \times L^{p_2}(\Omega, \mathbb{R}^n) \times L^{p_3}(\Omega, \mathbb{R}^3) \times L^{p_4}(\Omega, \mathbb{R}^{3 \times 3}) \\
& \times L^{p_5}(\Omega, \mathbb{R}^{3 \times 3}) \times L^{p_6}(\Omega, \mathbb{R}) \times L^{p_7}(\Omega, \mathbb{R}^3) \times L^{p_8}(\Omega, \mathbb{R}^{3 \times 3}) \\
& \times L^{p_9}(\Omega, \mathbb{R}^{3 \times 3}) \times L^{p_{10}}(\Omega, \mathbb{R}^3) \times L^{p_{11}}(\Omega, \mathbb{R}^n) \times L^{p_{12}}(\Omega, \mathbb{R}^n) \\
& \times L^{p_{13}}(\Omega, \mathbb{R}^n) \times L^{p_{14}}(\Omega, \mathbb{R}^n) \times L^{p_{15}}(\Omega, \mathbb{R}^{3 \times n}) \times L^{p_{16}}(\Omega, \mathbb{R}^n) \\
& \times L^{p_{17}}(\Omega, \mathbb{R}^n) \times L^{p_{18}}(\Omega, \mathbb{R}^{3 \times n}) \times L^{p_{19}}(\Omega, \mathbb{R}^n) \text{ for } p \in \mathbb{R}^{19}, \\
1 & := (1)^{19}_{i=1}, \\
\hat{N} & := \{ \hat{x} \in \hat{X}_1: (\chi, \hat{\chi}, \Phi) \in \hat{M}, \Theta = \Phi^{-1}, (\hat{A}, \hat{B}, \hat{d}, \hat{\rho}) \in \hat{E} \times \hat{S} \text{ a.e. in } \Omega, \\
& \hat{\mu}_t = \mu \circ \Phi, \hat{\mu}_{inf} = \mu_{inf} \circ \Phi, \|\hat{\rho}\|_1 = \|\rho_0\|_1 \}
\end{align*}
\]

where we used for the components of $\hat{x} = (\hat{x}_i)_{i=1}^{19} \in \hat{X}_1$ the notation

\[
(\hat{x}_i)_{i=1}^{19} := (\chi, \hat{\chi}, \Phi, \hat{A}, \hat{B}, \hat{d}, \Theta, A, \hat{J}, J, J_{inf}, \hat{\mu}, \mu, \hat{\mu}_{inf}, \mu_{inf}, G, G_{inf}, \hat{\rho}, \hat{\rho}_{inf}).
\]
The time-continuous system modeled by the above mentioned quantities reads then for \( t > 0 \)

\[
\begin{align*}
\partial_t \hat{\rho}(t) &= \text{div}\hat{J}_t, \\
\hat{J}_t &= \hat{d}_t \hat{A}_t^{-1} \circ \Phi_t, \\
J_t &= LG_t, \\
G_t &= \nabla \mu_t, \\
\hat{\mu}_t &= \nabla_\rho \hat{F}(\hat{x}_t, \hat{\chi}_t, \hat{A}_t, \hat{B}_t, \hat{d}_t, \hat{\rho}(t)), \\
\hat{F}(\chi_t, \hat{\chi}_t, \hat{A}_t, \hat{B}_t, \hat{d}_t, \hat{\rho}(t)) &= \min_{(x, \hat{x}, \Phi) \in M} \hat{F}(x, \hat{\chi}, \nabla \Phi, \hat{\rho}(t)),
\end{align*}
\]

where we used in \((89)\) an abbreviation as \((77)\).

To give a formulation in the sense of definition 5.2 of the above stated model we use

\[
\begin{align*}
D_\xi(\textbf{\hat{x}}) &:= \int_\Omega \langle \hat{\rho}(x), \xi(x) \rangle \, dx, \\
F_\xi(\textbf{\hat{x}}) &:= \int_\Omega \left\langle -\hat{J}(x), \nabla \xi(x) \right\rangle \, dx, \\
C_{1n\xi}(\textbf{\hat{x}}) &:= \int_\Omega \langle \hat{J}(x), \eta(x) \rangle - \langle A(x)J(x), \eta \circ \Theta(x) \rangle \, dx, \\
C_{2n\xi}(\textbf{\hat{x}}) &:= \int_\Omega \langle J(x) - LG(x), \eta(x) \rangle \, dx, \\
C_{3n\xi}(\textbf{\hat{x}}) &:= \int_\Omega \mu(x) \text{div} \eta(x) + \langle G(x), \eta(x) \rangle \, dx, \\
C_{4n\xi}(\textbf{\hat{x}}) &:= \int_\Omega \hat{F}(\textbf{\hat{x}}, \hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) \, dx, \\
C_{5n\xi}(\textbf{\hat{x}}) &:= \begin{cases} \\
\hat{F}(\textbf{\hat{x}}, \hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) - \min_{(x, \hat{x}, \Phi) \in M} \hat{F}(x, \hat{\chi}, \nabla \Phi, \hat{\rho}) & \text{if } \hat{\rho} \in \hat{\mathcal{S}} \text{ a.e. in } \Omega, \\
0 & \text{else,} \end{cases} \\
C_{6n\xi}(\textbf{\hat{x}}) &:= \int_\Omega \Phi(x) \text{div} \zeta(x) + \hat{A}(x)\zeta(x) \, dx, \\
C_{7n\xi}(\textbf{\hat{x}}) &:= \int_\Omega \Theta(x) \text{div} \zeta(x) + A(x)\zeta(x) \, dx.
\end{align*}
\]
Define the topology \( \hat{\tau} \) to be understood componentwise and \( \hat{\tau} \) the corresponding right-hand sides in (90) - (101) are well-defined with values in \( \xi \) for \( \hat{\xi} \in \hat{X}_1 \) whenever the corresponding right-hand side is not well-defined.

**Remark 7.** We set the values of the functionals defined by (90) - (101) to \( \infty \) whenever the corresponding right-hand side is not well-defined.

**Definition 5.5.** Let \( T > 0 \) be fixed and define
\[
I := C^\infty(\Omega, \mathbb{R}^n), \quad J := \{1, \ldots, 10\} \times C^\infty_0(\Omega, \mathbb{R}^{3-n}) \times C^\infty_0(\Omega, \mathbb{R}^{3-3})
\]
then a weak formulation of (78) - (89) is given by the weak diffusion problem with respect to \( T, \hat{X}_1, \left( N_t := \hat{N} \right)_{t \in [0, T]}, (D_\xi)_{\xi \in \hat{\Xi}}, (F_\xi)_{\xi \in \hat{\Xi}} \) and (C \( \lambda \eta \xi \)) \( (\lambda, \eta, \xi) \in \hat{\Xi} \), see definition 5.2.

If \( \hat{X}_1 \) is replaced by a suitable subspace \( \hat{X}_p, p > 1 \), equipped with a suitable topology \( \hat{\tau} \), then theorems 4.4, 5.4 and corollaries 2, 3 yield the existence of a measure-valued solution in the sense of definition 5.3 to the weak diffusion problem stated in definition 5.5, see Theorem 3.3.1, p.147 and Theorem 3.3.2, p.150 in [2].

**Main Theorem.** Let \( \sigma_{jk}, j, k \in \{1, \ldots, m\} \), fulfill (9), (10) and let (61), (62) and the assumptions of theorem 4.3 and corollary 1 be satisfied.

Let \( a > \frac{12}{13} \) and \( 1 < p < \infty \) such that there holds \( p_1 = p_8 = p_{18} = p_{19} = 2 \), \( p_{10} = p_{11} = p_{16} = p_{17}, p_{12} = p_{14}, p_{13} = p_{15} \) and
\[
\begin{align*}
p_5 &= \min\left(\frac{3}{2}, 2\right), \quad p_6 = \min\left(\frac{3}{2}, 2\right), \quad p_9 < 1 + \frac{(a-3)(a-2)}{(a-3)^2 + 11(a-3) + 18} \\
p_{10} &< 2, \quad p_{12} < \min\left(\frac{6(a-3)}{a}, 3\right), \quad p_{13} = p_{12} \left\{ \begin{array}{ll} \frac{a}{a-3} & \text{if } a < 6, \\ 2 & \text{if } 6 \leq a. \end{array} \right. \\
p_{15} &= \min\left(\frac{6(a-3)}{a}, 3\right)
\end{align*}
\]

**Define the topology \( \hat{\tau}_p \) on \( \hat{X}_p \) by**
\[
\hat{\tau}_p := \| \cdot \|_{p_1} \times \| \cdot \|_{p_2} \times \| \cdot \|_{p_3} \times \| \cdot \|_{p_4} \times \| \cdot \|_{p_5} \times \| \cdot \|_{p_6} \times \| \cdot \|_{p_7} \times \| \cdot \|_{p_8} \times \| \cdot \|_{p_9} \\
\times \| \cdot \|_{p_{10}} \times \| \cdot \|_{p_{11}} \times \| \cdot \|_{p_{12}} \times \| \cdot \|_{p_{13}} \times \| \cdot \|_{p_{14}} \times \| \cdot \|_{p_{15}} \times \| \cdot \|_{p_{16}} \times \| \cdot \|_{p_{17}} \\
\times \| \cdot \|_{p_{18}} \times \| \cdot \|_{p_{19}}.
\]

Furthermore we assume that following conditions are fulfilled.

I. \( \hat{f}(e, \cdot) \in C(\hat{E} \times \hat{R}) \) for all \( e \in C_m \), see (57).
II. There is an open set \( O \subset \mathbb{R}^{3x3} \times \mathbb{R}^{3x3} \times \mathbb{R} \times \mathbb{R}^n \) such that there holds
\[
\hat{E} \times \text{re}(\hat{R}) \subset O, \ f(e, \cdot) \in C^2(O) \text{ for all } e \in C_m \text{ and }
\min_{e \in C_m} \inf_{u \in O} \left( \inf_{v \in \mathbb{R}^{12+n}} \frac{\langle v, D^2 f(e, u) v \rangle}{\langle v, v \rangle} \right) > 0.
\]

Hereby we identified \( \mathbb{R}^{3x3} \times \mathbb{R}^{3x3} \times \mathbb{R} \times \mathbb{R}^n \) with \( \mathbb{R}^{19+n} \) and the \( \hat{f}(e, \cdot) \) with the corresponding functions defined on \( \mathbb{R}^{19+n} \).

III. There are \( \hat{\varphi}_1 : \mathbb{R}^m_+ \times \mathbb{R}^{3x3} \times \mathbb{R}^{3x3} \times \mathbb{R} \to \mathbb{R}_+ \) und \( \hat{\varphi}_2 : \mathbb{R}^m_+ \times \mathbb{R}^n \to \mathbb{R}_+ \) such that there holds
\[
\hat{f}(\hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) = \hat{\varphi}_1(\hat{\chi}, \hat{A}, \hat{B}, \hat{d}) + \hat{\varphi}_2(\hat{\chi}, \hat{\rho}) \text{ for all } (\hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) \in \mathbb{R}.
\]

If in definition 5.5 \( \hat{X}_1 \) is replaced by \( (\hat{X}_p, \hat{\tau}_p) \) then under the above stated assumptions there is a measure-valued solution \( (\hat{X}_p, B(\hat{X}_p, \hat{\tau}_p), \hat{P}_t)_{t \in [0,T]} \) to the weak diffusion problem stated in definition 5.5 such that f.a.a. \( t \in [0,T] \) there is a product representation
\[
\hat{P}_t = \bar{\hat{P}}_t \times \delta_{\hat{\rho}(t)} \times \delta_{\hat{\rho}(t)}
\]
where \( \delta_{\hat{\rho}(t)} \) fulfills \( 0 \leq \hat{\rho}(t), |\hat{\rho}(t)|_1 \leq 1 \text{ a.e. in } \Omega \) and \( \|\hat{\rho}(t)\|_1 = \|\rho_0\|_1 \).

Additionally there holds a weak energy inequality
\[
\int_0^T \hat{\theta}(t) \int_{\hat{X}_p} F(\hat{\chi}, \hat{\chi}, \hat{A}, \hat{B}, \hat{d}, \hat{\rho}) \, d\hat{P}_t(\hat{\chi}) \, dt \geq \int_0^T \hat{\theta}(t) \left( \int_{\hat{X}_p} Q(J) + Q^*(G_{\text{inf}}(x)) \, d\hat{P}_t(\hat{\chi}) \right) \, dt
\]
for all \( \hat{\theta} \in C_0^\infty([0,T]) \) with \( \hat{\theta} \geq 0 \) and the relation
\[
\int_0^T \hat{\theta}(t) \int_{\hat{X}_p} \langle G(x) - G_{\text{inf}}(x), \eta(x) \rangle \, dx \, d\hat{P}_t(\hat{\chi}) \, dt = 0
\]
is fulfilled for all \( \theta \in C_0^\infty([0,T]) \) and all \( \eta \in C_0^\infty(\Omega, \mathbb{R}^{3-n}) \).

Remark 8. 1. The condition \( a > \frac{18}{\gamma} \) is needed to assure that there is \( q > 1 \) such that \( \hat{\mu} \in L^q(\Omega, \mathbb{R}^n) \).

2. The most restricting condition on \( \hat{f} \) is III. But because of the fact that for the discrete system doesn’t hold a minimality condition we were not able to prove the existence of a measure-valued solution without this assumption.

III. is equivalent to
\[
f(\chi, A, B, d, \rho) = \varphi_1(\chi, A, B, d) + d \varphi_2 \left( \chi, \frac{\rho}{d} \right)
\]
for \( (\chi, A, B, d, \rho) \in \mathbb{R}, d > 0 \).

3. Note that we proved for almost all \( t \in [0,T] \) that there is a well-defined Langrangian particle density.

Comment. This survey preludes articles with emphasis on technical aspects of the model stated in section 2 together with S. Luckhaus and T. Blesgen which is work in progress.
List of symbols. Let $p, q \in \mathbb{N}$ and $r \in \mathbb{N} \cup \{\infty\}$.

| Symbol | Description |
|--------|-------------|
| $\mathbb{N}$ | $\mathbb{N} \cup \{0\}$ |
| $\mathbb{R}^+_q$ | $[0, \infty[q$ |
| $\mathbb{R}^{q \times q}$ | $(\mathbb{R}^q)^q$ |
| $\langle \cdot, \cdot \rangle$ | euclidean scalar product |
| $\text{Id}_\Omega$ | Identity on $\Omega$ |
| $r \leq s$ | means $s - r \in \mathbb{R}^+_q$ for $r, s \in \mathbb{R}^q$ |
| $r < s$ | means $s - r \in \mathbb{R}^+_q \setminus \{0\}$ for $r, s \in \mathbb{R}^q$ |
| $|r|_1$ | $\sum_{k=1}^q |r_i|$ for $r \in \mathbb{R}^q$ |
| $|A|$ | spectral norm of $A \in \mathbb{R}^{q \times q}$ |
| $	ext{Tr}A$ | $\sum_{k=1}^q A_{kk}$ for $A \in \mathbb{R}^{q \times q}$ |
| $\parallel \cdot \parallel_q$ | $q$-norm on some given $L^q$ space |
| $\parallel \cdot \parallel_{p,q}$ | Sobolev-norm on some given $W^{p,q}$ space |
| $\parallel \cdot \parallel_{BV}$ | natural norm on $BV(\Omega, \mathbb{R}^m)$ |
| $C^\omega_0(U)$ | set of all $C^\omega$-functions with compact support in the open set $U \subset \mathbb{R}^q$ |
| $\rightharpoonup$ | denotes weak convergence in the Banach space $X$ |
| $\rightharpoonup^*$ | denotes convergence in the sense of Radon measures |
| $X^*$ | norm-dual of the Banach space $X$ |
| $w_X$ | weak topology on the Banach space $X$ |
| $w_q$ | weak topology on some given $L^q$ space |
| $\mathbb{R}(X)$ | space of Radon measures on the topological space $X$ |
| $C_b(Y)$ | space of continuous and bounded functions on the topological space $Y$ |
| $\mathcal{B}(Y,\omega)$ | Borel $\sigma$-algebra on the topological space $(Y,\omega)$ |
| $\text{ri}(V)$ | relative interior of $V \subset \mathbb{R}^q$ |

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