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ORIGINAL ARTICLE

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A viscoelastic damage model for polycrystalline ice, inspired by Weibull-distributed fiber bundle models. Part II: Thermodynamics of a rank-4 damage model

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Abstract We consider a viscoelastic–viscoplastic continuum damage model for polycrystalline ice. The focus lies on the thermodynamics particularities of such a constitutive model and restrictions on the constitutive theory which are implied by the entropy principle. We use Müller's formulation of the entropy principle, together with Liu's method of exploiting it with the aid of Lagrange multipliers.

Keywords Damage mechanics · Delayed elastic response · Nonlinear viscous heat conducting fluid · Polycrystalline ice

1 Introduction

Continuum damage mechanics has been introduced into the mechanics of polycrystalline ice, e.g., by [2,4,9, 11,13,15–17]. Efforts on the consistency of the proposed constitutive relations with the second law of thermodynamics are by [6,7,12]. The latter work demonstrates that in anisotropic damage formulations, rank-4 damage tensors are required to reach consistent formulations of damage with the second law of thermodynamics. All the above models treat the damage variable as internal variable, for which an evolution equation is postulated. Its production term is expressed as a constitutive relation of the material class of the theory in question.

This is not the approach dealt with in part I of this paper [5]. Instead of writing a suitable damage evolution law, i.e., treating damage as one or several degrees of freedom, we treat it as a function of the delayed-elastic deformation (i.e., the component of deformation which is recoverable but not instantaneous). The likely earliest proposal of this approach in ice mechanics was given in [14]. Part I of this paper [5] formulates a nonlinear theory of such a model in three dimensional space; in this second part, we examine its consistency with the second law of thermodynamics, a still missing important part of the model.

The first goal is thus to demonstrate its coherence with the entropy principle. But, at the same time, some general aspects and problems of continuum systems with a rank-4 internal tensor variable will be discussed. The tensorial nature of such a quantity makes some of the considerations technically delicate, and there is still a number of mathematical difficulties related to this task which have not been solved in an adequate way yet.

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Therefore, it is also the subject of this article to point out these problems, propose possible solutions and to encourage further research of the remaining problems.

The key part of these considerations will be the exploitation of the entropy principle of Müller and Liu [8,10]. This formulation of the entropy principle does not make any assumptions for the constitutive behavior of the entropy flux; it does not even assume the a priori existence of an absolute temperature. This makes it particularly suitable for the consideration of a theory containing unusual degrees of freedom, which might have unexpected effects on the constitutive behavior. Finally, Liu's Lagrange multiplier method is of compelling technical elegance and beauty. Historically, the first definition of the absolute temperature was due to Kelvin, who defined it in terms of the Carnot efficiency. A mathematically more convenient (and therefore nowadays widely used) approach has been found by [1], who defined the absolute temperature as the (up to rescaling unique) integrating denominator for the inexact differential of heat, which depends only on the empirical temperature. The Müller-Liu theory adds the viewpoint that the same quantity serves as the inverse of the Lagrange multiplier of the energy equation, which pulls a theory of free variables onto the shell of energy conservation.

Usually, the exploitation of the entropy principle is done using the least possible constitutive assumptions; if possible, people try to consider a theory restricted only by the principle of frame indifference. In this work, this general path will only partly be followed. At first, the entropy inequality will be considered in as general as possible form, as well as the consequences of thermodynamic equilibrium. But then, instead of considering the most general constitutive behavior, the constitutive framework defined in part I of this paper will be used explicitly. This allows to show the existence of a suitable free energy, which achieves that the constitutive theory is in agreement with the entropy principle.

2 Free variables and kinematics

The set of free fields to be considered in the following is

$$F = \left\{\mathbf{v}, \theta, \mathbf{A}, \mathsf{Z}\right\}, \tag{1}$$

which stand for velocity, (empirical) temperature[1], Almansi tensor of delayed-elastic deformation, and rank-4 damage effect tensor. The choice of the Almansi tensor as an objective measure of delayed-elastic deformation has been explained in [5]. Neither pressure nor mass density will be treated as free fields, as a non-volume-preserving delayed elasticity will be considered. The mass density is merely a function of $\mathbf{A}$, which in the small strain approximation reads

$$\rho = \hat{\rho}\,(1 - \mathrm{tr}\mathbf{A}) + \mathscr{O}\left(\mathbf{A}^2\right), \tag{2}$$

where $\hat{\rho}$ is the mass density in the reference configuration. Of course, this approach is not as elegant as an approach with a free mass density, but it saves a considerable amount of work, without loosing any relevant information.

The constitutive quantities (stress, internal energy density, heat flux, entropy density, entropy flux, time evolution of $\mathbf{A}$, time evolution of Z) may depend on the set

$$S = \left\{\mathbf{D}, \theta, \mathbf{A}, \mathbf{g} = \nabla\theta, \mathsf{Z}\right\}, \tag{3}$$

where $\mathbf{D}$ is the strain rate tensor.

The kinematic description of a viscoelastic–viscoplastic model for a fluid is a non-trivial problem, as the coupling of the two types of deformations is not very obvious. We have considered this problem in part I and proposed that the coupling should reasonably be done in terms of strain rate tensors (instead of coupling the strains themselves). Furthermore, we have shown in part I that the relation

$$\mathbf{D} = \overset{\triangledown}{\mathbf{A}} + \mathbf{D}^v \tag{4}$$

holds, where $\overset{\triangledown}{\mathbf{A}}$ is the lower Oldroyd derivative of $\mathbf{A}$, and $\mathbf{D}^v$ the viscoplastic deformation rate. This relation can be used in order to couple viscoelastic and viscoplastic deformations.

[1] A priori θ does not need to be an absolute temperature; any empirical temperature measure (i.e., an intrinsic variable which can be determined experimentally and which satisfies the "zeroth" theorem of thermodynamics) may be used. Of course, in practice it would be very inconvenient to use anything but the absolute temperature. However, we want to stress that the existence of an absolute temperature is not a necessary assumption, but a result of the theory presented here.

In the following, we will take the kinematic coupling into account by constraining the constitutive relations in a suitable way: The constitutive relation for the time evolution function $\mathbf{f_A}$ for the delayed-elastic Almansi tensor $\mathbf{A}$ and the viscoplastic strain rate tensor $\mathbf{D^v}$ will be assumed to obey the constraint

$$\mathbf{f_A}[S] = \mathbf{D} - \mathbf{D^v}[S]. \tag{5}$$

This approach has the advantage that it only concerns the constitutive relations, instead of adding a further constraint for the free fields, which would have to be accounted for via an additional Lagrange multiplier.

The evolution of the fields F is governed by the balance equations

$$\mathfrak{V} := \rho \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v} - \nabla \cdot \boldsymbol{\sigma} - \rho \mathbf{f} = \mathbf{0}, \tag{6}$$

$$\mathfrak{E} := \rho \frac{\mathrm{d}}{\mathrm{d}t}\varepsilon + \nabla \cdot \mathbf{q} - \boldsymbol{\sigma} \cdot \mathbf{D} - \rho r = 0, \tag{7}$$

$$\mathfrak{A} := \overset{\triangledown}{\mathbf{A}} - \mathbf{f_A} = \mathbf{0}, \tag{8}$$

$$\mathfrak{Z} := \overset{\triangledown}{\mathsf{Z}} - \mathbf{f}_{\mathsf{Z}} = \mathbf{0}. \tag{9}$$

where the time derivatives are to be understood as convective derivatives, and $\mathbf{f}$, r are external source terms (force density and energy supply).

Physically, these equations represent in turn the balances of momentum and energy (6, 7), the evolution equations of the Almansi tensor and the damage effect tensor (8, 9), respectively. The quantities $\{\mathbf{v}, \boldsymbol{\sigma}, \varepsilon, \mathbf{q}\}$ are the velocity vector, the symmetric Cauchy stress tensor, the internal energy and the heat flux vector, while $\mathbf{f}$ and r are momentum and energy supply terms, and $\mathbf{f_A}$, $\mathbf{f}_{\mathsf{Z}}$ are rank-2 and rank-4 productions of $\mathbf{A}$ and Z, respectively.

The quantity $\overset{\triangledown}{\mathsf{Z}}$ is the lower Oldroyd derivative of Z, an objective time derivative defined as

$$\overset{\triangledown}{\mathsf{Z}}_{ijkl} = \dot{\mathsf{Z}}_{ijkl} + L_{im}\mathsf{Z}_{mjkl} + L_{jm}\mathsf{Z}_{imkl} + L_{km}\mathsf{Z}_{ijml} + L_{lm}\mathsf{Z}_{ijkm}, \tag{10}$$

where L_{ij} are the components of the velocity gradient. $\mathbf{f}_{\mathsf{Z}}$ is a suitable evolution function, which makes sure that Z evolves coupled to $\mathbf{A}$ as long as possible (i.e., as long as the coupling to $\mathbf{A}$ makes Z increase). For a situation with decreasing $\mathbf{A}$, Z will be either held constant, or slowly decreased according to a suitable healing law. This healing law has to be in accordance with the entropy principle; details will be discussed in a later section.

The cases for independent Z and Z coupled to $\mathbf{A}$ will a priori not be distinguished; the case distinction arises more or less automatically when evaluating explicitly the entropy production for the constitutive framework.

We mention, finally, that boundary conditions exercise no effect on the analysis of the consistency of the constitutive relations with the second law of thermodynamics, except, of course if balance laws for surface quantities (involving, e.g., flux terms such as surface tensions) are accounted for. This is not the case here.

3 Exploitation of the entropy principle

In Müller's formulation of the entropy principle, one requires that the constitutive quantities (i.e., fields that depend on S) entropy[2] η, entropy flux $\boldsymbol{\Phi}$ and an external entropy source s are such that any solution of the governing Eqs. (6)–(8) satisfies the inequality

$$\rho \frac{\mathrm{d}}{\mathrm{d}t}\eta + \nabla \cdot \boldsymbol{\Phi} - \rho s \geq 0. \tag{11}$$

In Ref. [8] it is shown that this requirement is equivalent to the existence of Lagrange multipliers $\boldsymbol{\Lambda}^{\mathfrak{V}}$, $\Lambda^{\mathfrak{E}}$, $\boldsymbol{\Lambda}^{\mathfrak{A}}$ and $\boldsymbol{\Lambda}^{\mathfrak{Z}}$ such that for any set of fields F [not necessarily solutions of Eqs. (6)–(9)] the inequality

[2] Actually specific entropy; but as with all extensive quantities (e.g., internal energy, entropy, enthalpy, ...) it will be implicitly assumed to be normalized with respect to mass.

$$\pi := \rho \frac{\mathrm{d}}{\mathrm{d}t}\eta + \nabla \cdot \boldsymbol{\Phi} - \rho s - \boldsymbol{\Lambda}^{\mathfrak{B}} \cdot \mathfrak{B} - \Lambda^{\mathfrak{E}} \mathfrak{E} - \boldsymbol{\Lambda}^{\mathfrak{A}} \cdot \mathfrak{A} - \boldsymbol{\Lambda}^{\mathfrak{Z}} \cdot \mathfrak{Z} \geq 0 \tag{12}$$

holds[3]. The quantity π is the local production rate of specific entropy.

In the following, the source terms will be omitted; material properties are assumed not to depend on external sources, and therefore, they cancel out,

$$-s + \boldsymbol{\Lambda}^{\mathfrak{B}} \cdot \mathbf{f} + \Lambda^{\mathfrak{E}} r = 0. \tag{13}$$

Following the Liu principle, inequality (12) has to be written as quasi-linear in the derivatives of F which are not in S (i.e., the constitutive quantities may not depend on them),

$$A(S) \cdot X + \beta(S) \geq 0, \tag{14}$$

where the vector X of all derivatives of F which appear linearly in (12) and are not in S reads

$$X = \left\{ W_{ij}, \partial_t D_{ij}, \nabla_i D_{jk}, \partial_t v_i, \nabla_i \nabla_j \theta, \partial_t \theta, \partial_t \nabla_i \theta, \partial_t A_{ij}, \nabla_i A_{kl}, \partial_t \mathsf{Z}_{ijkl}, \nabla_m \mathsf{Z}_{ijkl} \right\}, \tag{15}$$

in which $W_{ij} = L_{ij} - D_{ij}$ is the antisymmetric part of the velocity gradient, the so-called spin tensor. Necessary and sufficient conditions for inequality (14) to be satisfied for any X are

$$A(S) \equiv 0, \ \ \beta(S) \geq 0. \tag{16}$$

These are called Liu Identities and residual entropy inequality, respectively.

By writing inequality (14) down explicitly, we obtain

$$\begin{aligned}
0 \leq \pi = \rho & \left(\frac{\partial \eta}{\partial D_{ij}} \dot{D}_{ij} + \frac{\partial \eta}{\theta} \dot{\theta} + \frac{\partial \eta}{\partial A_{ij}} \dot{A}_{ij} + \frac{\partial \eta}{\partial g_i} \dot{g}_i \right) \\
& + \frac{\partial \Phi_i}{\partial D_{kl}} \nabla_i D_{kl} + \frac{\partial \Phi_i}{\partial \theta} \nabla_i \theta + \frac{\partial \Phi_i}{\partial A_{kl}} \nabla_i A_{kl} + \frac{\partial \Phi_i}{\partial g_j} \nabla_i g_j \\
& - \Lambda^{\mathfrak{E}} \rho \left(\frac{\partial \varepsilon}{\partial D_{ij}} \dot{D}_{ij} + \frac{\partial \varepsilon}{\partial \theta} \dot{\theta} + \frac{\partial \varepsilon}{\partial A_{ij}} \dot{A}_{ij} + \frac{\partial \varepsilon}{\partial g_i} \dot{g}_i \right) \\
& - \Lambda^{\mathfrak{E}} \left(\frac{\partial q_i}{\partial D_{kl}} \nabla_i D_{kl} + \frac{\partial q_i}{\partial \theta} \nabla_i \theta + \frac{\partial q_i}{\partial A_{kl}} \nabla_i A_{kl} + \frac{\partial q_i}{\partial g_j} \nabla_i g_j \sigma_{kl} D_{ij} \right) \\
& - \Lambda_i^{\mathfrak{B}} \left(\rho \dot{v}_i - \nabla_j \sigma_{ji} \right) - \Lambda_{ij}^{\mathfrak{A}} \left(\dot{A}_{ij} + 2 A_{ik} D_{kj} + 2 A_{ik} W_{kj} - f_{ij}^{A} \right) \\
& + \Lambda_{ijkl}^{\mathfrak{Z}} \left(\dot{\mathsf{Z}}_{ijkl} + 4 \mathsf{Z}_{ijkm} W_{ml} + 4 \mathsf{Z}_{ijkm} D_{ml} - f_{ijkl}^{\mathsf{Z}} \right).
\end{aligned} \tag{17}$$

For the sake of a more convenient notation, we will assume the Lagrange multipliers $\Lambda^{\mathfrak{A}}$ and $\Lambda^{\mathfrak{Z}}$ to have the same symmetry as the corresponding free fields. Even though this assumption is plausible from the fact that there are only as many independent evolution equations as independent tensor elements, later a rigorous proof of this fact will be given (which is not affected by its use already now).

From inequality (17) the Liu identities can be identified; they read

$$\Lambda^{\mathfrak{B}} = 0, \tag{18}$$

$$0 = \left(\Lambda_{ik}^{\mathfrak{A}} A_{kj} + \Lambda_{iklm}^{\mathfrak{Z}} \mathsf{Z}_{klmj} \right) W_{ij}, \tag{19}$$

$$\frac{\partial \Phi_i}{\partial D_{kl}} = \Lambda^{\mathfrak{E}} \frac{\partial q_i}{\partial D_{kl}}, \tag{20}$$

$$\frac{\partial \Phi_i}{\partial g_j} = \Lambda^{\mathfrak{E}} \frac{\partial q_i}{\partial g_j}, \tag{21}$$

$$\frac{\partial \Phi_i}{\partial A_{kl}} = \Lambda^{\mathfrak{E}} \frac{\partial q_i}{\partial A_{kl}}, \tag{22}$$

[3] Balance of mass does not need to enter (12) with a Lagrange multiplier, since the density in $\mathcal{B}_t$ is given by $\mathbf{A}$, see Eq. (2).

$$\frac{\partial \Phi_i}{\partial \mathsf{Z}_{jklm}} = \Lambda^{\mathfrak{E}} \frac{\partial q_i}{\partial \mathsf{Z}_{jklm}}, \tag{23}$$

$$\frac{\partial \eta}{\partial \theta} = \Lambda^{\mathfrak{E}} \frac{\partial \varepsilon}{\partial \theta}, \tag{24}$$

$$\frac{\partial \eta}{\partial g_i} = \Lambda^{\mathfrak{E}} \frac{\partial \varepsilon}{\partial g_i}, \tag{25}$$

$$\frac{\partial \eta}{\partial D_{ij}} = \Lambda^{\mathfrak{E}} \frac{\partial \varepsilon}{\partial D_{ij}}, \tag{26}$$

$$\Lambda^{\mathfrak{A}}_{ij} = -\Lambda^{\mathfrak{E}} \rho \frac{\partial \varepsilon}{\partial A_{ij}} + \rho \frac{\partial \eta}{\partial A_{ij}}, \tag{27}$$

$$\Lambda^{\mathfrak{Z}}_{ijkl} = -\Lambda^{\mathfrak{E}} \rho \frac{\partial \varepsilon}{\partial \mathsf{Z}_{ijkl}} + \rho \frac{\partial \eta}{\partial \mathsf{Z}_{ijkl}}. \tag{28}$$

An explicit representation of the residual entropy inequality $\pi = \beta(S) \geq 0$ will be given once these identities have been explored. Nevertheless, it shall be emphasized already now that, as $\nabla_i \theta = g_i \in S$, the contribution

$$\left(\frac{\partial \Phi_i}{\partial \theta} - \Lambda^{\mathfrak{E}} \frac{\partial q_i}{\partial \theta} \right) g_i \tag{29}$$

to π does not necessarily vanish (Φ_i and q_i may depend on g_i, so this is not a linear form). If, however, one takes into account Eqs. (20)–(23), the differential of the objective vector $\mathbf{k} := \boldsymbol{\Phi} - \Lambda^{\mathfrak{E}} \mathbf{q}$ can be written as

$$\begin{aligned} \mathrm{d}\mathbf{k} &= \mathrm{d}\boldsymbol{\Phi} - \Lambda^{\mathfrak{E}} \mathrm{d}\mathbf{q} - \mathbf{q} \mathrm{d}\Lambda^{\mathfrak{E}} \\ &= \left(\frac{\partial \boldsymbol{\Phi}}{\partial \theta} - \Lambda^{\mathfrak{E}} \frac{\partial \mathbf{q}}{\partial \theta} \right) \mathrm{d}\theta - \mathbf{q} \mathrm{d}\Lambda^{\mathfrak{E}}. \end{aligned} \tag{30}$$

Thus, $\mathbf{k}$ can be written purely as a function of the two objective scalars θ and $\Lambda^{\mathfrak{E}}$; as it is impossible to construct a nonzero objective vector from only objective scalars, $\mathbf{k}$ must vanish. Therefore, the identity

$$\boldsymbol{\Phi} = \Lambda^{\mathfrak{E}} \mathbf{q} \tag{31}$$

holds, i.e., entropy flux and heat flux are collinear. This relation has further consequences. Equations (20)–(26) can now be written as

$$0 = \frac{\partial \Phi_i}{\partial F_l} - \Lambda^{\mathfrak{E}} \frac{\partial q_i}{\partial F_l} = \frac{\partial k_i}{\partial F_l} + q_i \frac{\partial \Lambda^{\mathfrak{E}}}{\partial F_l} = q_i \frac{\partial \Lambda^{\mathfrak{E}}}{\partial F_l}, \tag{32}$$

where F_l is any of the fields $D_{ij}, g_i, A_{ij}, \mathsf{Z}_{ijkl}$. As q_i may in general be different from 0, we can conclude that the scalar field $\Lambda^{\mathfrak{E}}$ can only depend on $S \backslash \{D_{ij}, g_i, A_{ij}, \mathsf{Z}_{ijkl}\} = \{\theta\}$. Thus, $\Lambda^{\mathfrak{E}}$ is a function of the temperature alone. This function $\Lambda^{\mathfrak{E}}$ is exactly the "coldness function" as used by [10]. Following [10] or [3], it can be argued that

$$T(\theta) := \frac{1}{\Lambda^{\mathfrak{E}}(\theta)} \tag{33}$$

is a strictly monotonous function of θ. By postulating, furthermore, the existence of thin material walls where θ and the normal component of $\mathbf{q}$ are continuous, it can be shown that $T(\theta)$ is a universal function of θ (i.e., the function is the same in any material). Thus, it is justified to identify $T(\theta)$ with the absolute temperature, in coherence with the widely used definition of the absolute temperature as the (up to rescaling unique) integrating denominator for the inexact differential of heat which depends only on the empirical temperature [1]. In the following, for the sake of simplicity, $T(\theta) \equiv \theta$ will be assumed; i.e., the absolute temperature is used as a substitute of empirical temperature.

From the last result, we can infer consequences for the constitutive behavior of ε and η. Cross-differentiating relations (24)–(26) and eliminating of the second derivatives results in

$$\frac{\partial \Lambda^{\mathfrak{E}}}{\partial g_i} \frac{\partial \varepsilon}{\partial \theta} = \frac{\partial \Lambda^{\mathfrak{E}}}{\partial \theta} \frac{\partial \varepsilon}{\partial g_i}, \tag{34}$$

$$\frac{\partial \Lambda^{\mathfrak{E}}}{\partial D_{ij}} \frac{\partial \varepsilon}{\partial \theta} = \frac{\partial \Lambda^{\mathfrak{E}}}{\partial \theta} \frac{\partial \varepsilon}{\partial D_{ij}}. \tag{35}$$

As $\Lambda^{\mathfrak{E}}$ is a function of only θ, the left-hand sides of Eqs. (34) and (36) vanish. On the right-hand sides, the derivative $\frac{\partial \Lambda^{\mathfrak{E}}}{\partial \theta}$ is nonzero though. This implies

$$\frac{\partial \varepsilon}{\partial D_{ij}} = 0, \ \frac{\partial \varepsilon}{\partial g_i} = 0, \tag{36}$$

and the same for η. Thus, η and ε are purely functions of A_{ij}, θ and Z_{ijkl}. The same holds for the so-called free energy

$$\psi = \varepsilon - \theta\eta = \psi(A_{ij}, \theta, \mathsf{Z}_{ijkl}). \tag{37}$$

Equation (19) is the contribution of **W** to the Liu identities. It turns out that this is automatically satisfied for reasons of symmetry, if the Lagrange multipliers $\Lambda^{\mathfrak{A}}_{ij}$ and $\Lambda^{\mathfrak{Z}}_{ijkl}$ have the same symmetry as **A** and Z, respectively. We are now in a position to show that this is the case. From Eqs. (27) and (28) one can conclude that

$$\Lambda^{\mathfrak{A}}_{ij} = -\frac{\rho}{\theta}\frac{\partial \psi}{\partial A_{ij}}, \ \Lambda^{\mathfrak{Z}}_{ijkl} = -\frac{\rho}{\theta}\frac{\partial \psi}{\partial \mathsf{Z}_{ijkl}}. \tag{38}$$

It is easy to show that such a derivative always has the same symmetry as the quantity with respect to which it is differentiated.

Finally, the residual entropy inequality $\pi = \beta(S) \geq 0$ takes the form

$$\begin{aligned} 0 \leq \pi = &-\frac{q_i g_i}{\theta^2} + \frac{1}{\theta}\left(\sigma_{ij} + 2\rho\frac{\partial \psi}{\partial A_{ik}}A_{kj} + 4\rho\frac{\partial \psi}{\partial \mathsf{Z}_{imkl}}\mathsf{Z}_{jmkl}\right) D_{ij} \\ &-\frac{\rho}{\theta}\left(\frac{\partial \psi}{\partial A_{ij}} f^A_{ij} + \frac{\partial \psi}{\partial \mathsf{Z}_{ijkl}} f^{\mathsf{Z}}_{ijkl}\right). \end{aligned} \tag{39}$$

By using the self-consistency Eq. (5), this result can be written as

$$\begin{aligned} 0 \leq \pi = &-\frac{q_i g_i}{\theta^2} + \frac{1}{\theta}\sigma_{ij} D_{ij} + \frac{\rho}{\theta}\frac{\partial \psi}{\partial A_{ij}}\left(2A_{ik}D_{kj} - D_{ij} + D^v_{ij}\right) \\ &+\frac{\rho}{\theta}\frac{\partial \psi}{\partial \mathsf{Z}_{ijkl}}\left(4\mathsf{Z}_{ijkm}D_{ml} - f^{\mathsf{Z}}_{ijkl}\right). \end{aligned} \tag{40}$$

This concludes the general evaluation of the entropy production rate. Finally, using the results Eqs. (24) to (28) it is possible to explicitly write down the Gibbs relation. This reads

$$\mathrm{d}\eta = \frac{1}{\theta}\frac{\partial \varepsilon}{\partial \theta} + \left(\frac{1}{\theta}\frac{\partial \varepsilon}{\partial A_{ij}} + \frac{1}{\rho}\Lambda^{\mathfrak{A}}_{ij}\right)\mathrm{d}A_{ij} + \left(\frac{1}{\theta}\frac{\partial \varepsilon}{\partial \mathsf{Z}_{ijkl}} + \frac{1}{\rho}\Lambda^{\mathfrak{Z}}_{ijkl}\right)\mathrm{d}\mathsf{Z}_{ijkl}, \tag{41}$$

from which, on using Eqs. (37), (38), the statement

$$\eta = -\frac{\partial \psi}{\partial \theta} \tag{42}$$

ensues.

4 Consequences for the constitutive theory

In part I of this article, we have proposed a constitutive framework for a viscoelastic–viscoplastic damage theory. The key point of this is the relation for the viscoplastic deformation rate,

$$\mathbf{D}^v = \frac{1}{2\nu}\mathsf{Y}\boldsymbol{\sigma}^D, \tag{43}$$

where ν is a viscosity and Y is a rank-4 tensor function of Z^D whose structure does not matter here (but which has been proposed in the part I). Moreover, for the Cauchy stress tensor $\boldsymbol{\sigma}$ the relations

$$\mathrm{tr}\boldsymbol{\sigma} = \frac{\eta^{tr}}{\mathsf{Z}_{tr}}\left(\mathrm{tr}\mathbf{D} + \frac{K}{\eta^{tr}}\,\mathrm{tr}\mathbf{A}\right), \tag{44}$$

$$\boldsymbol{\sigma}^D = \mathsf{W}\cdot\left(\mathbf{D}^D + \frac{G}{\eta^D}\mathbf{A}^D\right), \tag{45}$$

have been proposed in the first part, where $K,\ G$ are bulk- and shear moduli, respectively, and $\eta^{tr,D}$ are the bulk- and shear viscosities for the viscoelastic part. The rank-4 tensor W is given by

$$\mathsf{W} = \left(\frac{1}{2\eta^D}\mathsf{Z}^D + \frac{1}{2\nu}\mathsf{Y}\right)^{-1}. \tag{46}$$

The resulting evolution equation for the delayed-elastic Almansi tensor is (for details see part I)

$$\mathbf{f}_{\mathbf{A}} = \mathbf{D} - \mathbf{D}^v = \frac{1}{2\eta^D}\left[\mathsf{Z}^D\boldsymbol{\sigma}^D - 2G\mathbf{A}^D\right] + \frac{1}{3\eta^{tr}}\left[\mathsf{Z}_{tr}\mathrm{tr}\,\boldsymbol{\sigma} - K\mathrm{tr}\mathbf{A}\right]\mathbb{1}_{3\times 3}. \tag{47}$$

The result (40) for the residual entropy production rate density will now be used to directly demonstrate the thermodynamic correctness of this constitutive framework (in combination with a simple Fourier-type relation for the heat flow $\mathbf{q}$). The difficult part of this consists in stating suitable constitutive relations for the entropy, η, and the internal energy, ε. This is complicated by the fact that the two are not independent; they must obey the integrability conditions resulting from cross-differentiating the Gibbs relation, Eq. (41). In order to avoid this difficulty, it is more convenient to propose a Helmholtz free energy ψ, from which the entropy can be derived via Eq. (42). As mentioned above, it would be technically extremely difficult to proceed with an approach as general as possible. One therefore has to find a smart way of successively inferring consequences for the constitutive theory, which finally leads to a constitutive relation for ψ yielding correct thermodynamics for the proposed constitutive framework.

4.1 Thermodynamic equilibrium

As a first step, the entropy production rate π close to thermodynamic equilibrium will be considered, in order to compare it with the constitutive relations.

For the sake of simplicity, only the special situation where the dynamical function $\mathbf{f}_{\mathsf{Z}}$ does not play a role will be considered. This is the case in a situation where the material has been strained up to a certain point, (i.e., a nonzero value for Z has been reached), and has then been allowed to relax to thermodynamic equilibrium, i.e., Z is present as a parameter, but not as a dynamical field ($\mathbf{f}_{\mathsf{Z}} \equiv \mathbf{0}$). Furthermore, the representation of Z proposed by [6] will be used; Z is thus assumed to be a doubly symmetric rank-4 tensor which does not mix deviatoric and hydrostatic stresses. Such a Z can be written as

$$\mathsf{Z} = \mathsf{Z}_{tr}\mathbb{1}^{tr} + \mathsf{Z}^D, \tag{48}$$

where $\mathbb{1}^{tr}_{ijkl} = \delta_{ij}\delta_{kl}$, and the deviatoric part annihilates the isotropic (i.e., non-deviatoric) part of any rank-2 tensor,

$$\mathsf{Z}^D\cdot\mathbb{1}_{3\times 3} = \mathbb{1}_{3\times 3}\cdot\mathsf{Z}^D = \mathbf{0}. \tag{49}$$

Thermodynamic equilibrium is usually defined as a state with $\mathbf{D} = \mathbf{0},\ \mathbf{g} = \mathbf{0}$. It is immediately clear from relation (5) that this requirement is too weak in the constitutive framework considered here. An additional $\mathbf{D}^v = \mathbf{0}$ is necessary. As, however, $\mathbf{D}^v \notin S$, this is not a suitable statement to define thermodynamic equilibrium. Thus, it will be replaced by $\mathbf{A}^D = \mathbf{0}$; the deviatoric part of the Almansi tensor shall thus vanish in thermodynamic equilibrium. This is a direct consequence of the fluid-like constitutive framework: Any elastic deformation causes stresses and thus viscoplastic deformation rates. The constitutive variables are consequently re-grouped in equilibrium and non-equilibrium sets,

$$S = S_e \cup S_n = \left\{\mathrm{tr}\mathbf{A}, \theta, \mathsf{Z}\right\} \cup \left\{\mathbf{D}, \mathbf{g}, \mathbf{A}^D\right\}. \tag{50}$$

The entropy production rate should vanish at $S_n = 0$ and be positive everywhere else; thus, it has a local minimum at equilibrium. Considering (40), it is easy to see that the condition $\pi|_e = 0$ is automatically satisfied, provided that $\mathbf{D}|_e = \mathbf{0}$ and $\mathbf{g}|_e = \mathbf{0}$, which is the case in the proposed constitutive theory. A necessary condition for a local minimum of π at equilibrium is

$$\frac{\partial \pi}{\partial \mathbf{g}}|_e = \mathbf{0}, \tag{51}$$

$$\frac{\partial \pi}{\partial \mathbf{D}}|_e = \mathbf{0}, \tag{52}$$

$$\frac{\partial \pi}{\partial \mathbf{A}^D}|_e = \mathbf{0}. \tag{53}$$

In the constitutive theory under consideration, the heat flow $\mathbf{q}$ is the only constitutive quantity depending on $\mathbf{g}$. Thus, Eq. (51) only concerns $\mathbf{q}$. Evaluating Eq. (52) yields

$$\sigma_{ij}|_e = -\rho \frac{\partial \psi}{\partial A_{kl}}|_e \left(2\delta_{kj} A_{li}|_e - \delta_{ki}\delta_{jl} + \frac{\partial D^v_{kl}}{\partial D_{ij}}|_e \right) - 4\rho \frac{\partial \psi}{\partial \mathsf{Z}_{klmi}}|_e \mathsf{Z}_{klmj}. \tag{54}$$

Using the fact that $\mathbf{A}^D|_e = \mathbf{0}$, this can be written as

$$\sigma_{ij}|_e = -\rho \frac{\partial \psi}{\partial A_{ij}}|_e \left(\frac{2}{3}\mathrm{tr}\mathbf{A} - 1 \right) - \rho \frac{\partial \psi}{\partial A_{kl}}|_e \frac{\partial D^v_{kl}}{\partial D_{ij}}|_e - 4\rho \frac{\partial \psi}{\partial \mathsf{Z}_{klmi}}|_e \mathsf{Z}_{klmj}. \tag{55}$$

Equation (55) defines the most general shape which the equilibrium stress may possess from the viewpoint of thermodynamics. This has to be compared now with the explicit representation of the equilibrium stress from the constitutive theory. This comparison will allow to suitably design a constitutive relation for the Helmholtz free energy ψ.

Considering the constitutive equations for the Cauchy stresses (Eqs. (44), (45)) at thermodynamic equilibrium shows that the equilibrium stress is hydrostatic. It reads simply

$$\sigma_{ij}|_e = \frac{K}{\mathsf{Z}_{tr}} \mathrm{tr}\mathbf{A}\delta_{ij}. \tag{56}$$

Thus, the deviatoric part of Eq. (55) must vanish, and the hydrostatic part must equal Eq. (56). In order to identify the deviatoric part of Eq. (55), it is useful to decompose the derivatives of ψ with respect to $\mathbf{A}$ as

$$\frac{\partial \psi}{\partial A_{ij}} = \frac{\partial \psi}{\partial \mathrm{tr}\mathbf{A}} \delta_{ij} + \frac{\partial \psi}{\partial A^D_{ij}}, \tag{57}$$

where the derivative of ψ with respect to $\mathbf{A}^D$ is in turn a deviator. A similar decomposition holds for the Z-part, if taking into account that Z does not mix deviatoric and hydrostatic stresses (see Eq. (48)):

$$\frac{\partial \psi}{\partial \mathsf{Z}_{klmi}} \mathsf{Z}_{klmj} = \frac{1}{3}\mathsf{Z}_{tr} \frac{\partial \psi}{\partial \mathsf{Z}_{tr}} \delta_{ij} + \frac{\partial \psi}{\partial \mathsf{Z}^D_{klmi}} \mathsf{Z}^D_{klmj}. \tag{58}$$

Inserting these representations into Eq. (55) yields

$$\begin{aligned} \sigma_{ij}|_e = &-\rho \left(\frac{\partial \psi}{\partial \mathrm{tr}\mathbf{A}}|_e \delta_{ij} + \frac{\partial \psi}{\partial A^D_{ij}}|_e \right) \left(\frac{2}{3}\mathrm{tr}\mathbf{A} - 1 \right) \\ &-\rho \frac{\partial \psi}{\partial A^D_{kl}}|_e \frac{\partial D^v_{kl}}{\partial D_{ij}}|_e - \frac{4}{3}\rho \frac{\partial \psi}{\partial \mathsf{Z}_{tr}}|_e \mathsf{Z}_{tr}\delta_{ij} - 4\rho \frac{\partial \psi}{\partial \mathsf{Z}^D_{klmi}}|_e \mathsf{Z}^D_{klmj} \\ &\stackrel{!}{=} -p_e \delta_{ij}. \end{aligned} \tag{59}$$

The quantity p_e is called the thermodynamic pressure. Making use of the fact that $\mathbf{D}^v$ is deviatoric (see Eq. (43)), the condition that the deviatoric part of Eq. (59) shall vanish is satisfied if ψ is stationary at $\mathbf{A}^D = \mathbf{0}$, i.e.,

$$\frac{\partial \psi}{\partial \mathbf{A}^D}|_e = \mathbf{0}, \quad \frac{\partial \psi}{\partial \mathsf{Z}^D}|_e = \mathbf{0}. \tag{60}$$

This is the case, e.g., for a ψ of the kind

$$\psi = \psi_e(\mathrm{tr}\mathbf{A}, \mathsf{Z}_{tr}, \theta) + \frac{G}{\rho}\mathbf{A}^D \cdot \left(\mathsf{Z}^D\right)^{-1} \cdot \mathbf{A}^D, \tag{61}$$

where G is the shear modulus.[4] This kind of ψ assures thus that the equilibrium stress is hydrostatic.

Moreover, comparison of the hydrostatic components of Eqs. (56) and (59) also yields a condition for ψ_e, the equilibrium part of ψ, which has to satisfy

$$-p_e = -\rho\frac{\partial\psi}{\partial\mathrm{tr}\mathbf{A}}|_e\left(\frac{2}{3}\mathrm{tr}\mathbf{A} - 1\right) - \frac{4}{3}\rho\frac{\partial\psi}{\partial\mathsf{Z}_{tr}}|_e\mathsf{Z}_{tr} \stackrel{!}{=} \frac{K}{\mathsf{Z}_{tr}}\mathrm{tr}\mathbf{A}, \tag{62}$$

suggesting ψ not to depend on Z_{tr}. As ρ behaves according to Eq. (2), this condition can be satisfied – at least to first order in tr $\mathbf{A}$ – by a ψ_e of the type

$$\psi_e = -\frac{K}{2\rho\mathsf{Z}_{tr}}\,(\mathrm{tr}\,\mathbf{A})^2 + \mathrm{o}\,(\mathrm{tr}\,\mathbf{A})^2 + \psi_e(\theta). \tag{63}$$

In order to avoid the not very handy calculus, the necessary conditions for the Hessian of π are not explored any further. Instead, the result (61) will be used directly to demonstrate the positivity of π.

4.2 Non-equilibrium part

The Helmholtz free energy ψ proposed above will now be used explicitly in order to consider its effects on the non-equilibrium part of π. At first, $\boldsymbol{\sigma}$ can be separated into equilibrium- and non-equilibrium parts by writing

$$\boldsymbol{\sigma} = \left[-p_e(\theta, \mathrm{tr}\mathbf{A}, \mathsf{Z}_{tr}) - p_n(S)\right]\mathbb{1}_{3\times 3} + \boldsymbol{\sigma}^D, \tag{64}$$

where the thermostatic pressure p_e is given by relation (62), whereas the constitutive relation for the non-equilibrium pressure p_n is (according to Eq. (44))

$$p_n = -\frac{\eta^{tr}}{3\mathsf{Z}_{tr}}\mathrm{tr}\,\mathbf{D}. \tag{65}$$

Together with the Helmholtz free energy from Eqs. (61) and (63), this has to be inserted into the residual entropy production rate π. By construction, the contributions of $\frac{\partial\psi}{\partial\mathrm{tr}\mathbf{A}}$ and $\frac{\partial\psi}{\partial\mathsf{Z}_{tr}}$ mostly cancel out with $\boldsymbol{\sigma}|_e \cdot \mathbf{D}$. The remaining entropy production reads

$$\theta\pi = -\frac{q_i g_i}{\theta} - p_n\mathrm{tr}\mathbf{D} + \sigma^D_{ij}D_{ij} + \rho\frac{\partial\psi}{\partial A^D_{ij}}\left(2A_{ik}D_{kl} - D_{ij} + D^v_{ij}\right)$$
$$+\rho\frac{\partial\psi}{\partial\mathrm{tr}\mathbf{A}}2A^D_{ij}D_{ij} + 4\rho\frac{\partial\psi}{\partial\mathsf{Z}^D_{ijkl}}\mathsf{Z}^D_{ijkm}D_{ml}. \tag{66}$$

By re-writing

$$\sigma^D_{ij}D_{ij} = \sigma^D_{ij}\left(D_{ij} - D^v_{ij}\right) + \sigma^D_{ij}D^v_{ij}, \tag{67}$$

this becomes

$$\theta\pi = -\frac{q_i g_i}{\theta} - p_n\mathrm{tr}\mathbf{D} + \sigma^D_{ij}D^v_{ij} + \left(\sigma^D_{ij} - \rho\frac{\partial\psi}{\partial A^D_{ij}}\right)\left(D_{ij} - D^v_{ij}\right)$$
$$+\rho\frac{\partial\psi}{\partial A^D_{ij}}2A_{ik}D_{kl} + \rho\frac{\partial\psi}{\partial\mathrm{tr}\mathbf{A}}2A^D_{ij}D_{ij} + 4\rho\frac{\partial\psi}{\partial\mathsf{Z}^D_{ijkl}}\mathsf{Z}^D_{ijkm}D_{ml}. \tag{68}$$

[4] The reason why the tensor $G\left(\mathsf{Z}^D\right)^{-1}$ has to arise here will become clear below.

Into this expression, the constitutive equations have to be inserted. In order to do so, it is useful to re-write the deviatoric component of the constitutive equation for $\mathbf{f}_A = \mathbf{D} - \mathbf{D}^v$, Eq. (47), as

$$\mathsf{Z}^D \boldsymbol{\sigma}^D = 2\eta^D \left(\mathbf{D} - \mathbf{D}^v\right)^D + 2G\mathbf{A}^D. \tag{69}$$

By combining this with the result of Eq. (61),

$$\rho \frac{\partial \psi}{\partial \mathbf{A}^D} = 2G \left(\mathsf{Z}^D\right)^{-1} \mathbf{A}^D, \tag{70}$$

one obtains the identity

$$\boldsymbol{\sigma}^D - \rho \frac{\partial \psi}{\partial \mathbf{A}^D} = 2\eta^D \left(\mathsf{Z}^D\right)^{-1} \left(\mathbf{D} - \mathbf{D}^v\right)^D. \tag{71}$$

Inserting Eq. (71) and Eq. (43) (inverted) for $\boldsymbol{\sigma}^D$ into the entropy production rate π, finally, yields

$$\begin{aligned} \theta\pi = &-\frac{q_i g_i}{\theta} + \frac{\eta^{tr}}{3\mathsf{Z}_{tr}} (\mathrm{tr}\mathbf{D})^2 + 2\nu D^v_{ij} \mathsf{Y}^{-1}_{ijkl} D^v_{kl} \\ &+ 2\eta^D \left(D_{ij} - D^v_{ij}\right)^D \left(\mathsf{Z}^D\right)^{-1}_{ijkl} \left(D_{kl} - D^v_{kl}\right)^D \\ &+ \rho \frac{\partial \psi}{\partial A^D_{ij}} 2A_{ik} D_{kl} + \rho \frac{\partial \psi}{\partial \mathrm{tr}\mathbf{A}} 2A^D_{ij} D_{ij} + 4\rho \frac{\partial \psi}{\partial \mathsf{Z}^D_{ijkl}} \mathsf{Z}^D_{ijkm} D_{ml}. \end{aligned} \tag{72}$$

The last line of Eq. (72) contains only contributions of at least second order in $\mathbf{A}$: Using Eqs. (61) and (63) it can easily be shown that

$$\rho \frac{\partial \psi}{\partial A^D_{ij}} = \mathcal{O}\left(\mathbf{A}^2\right), \tag{73}$$

$$\rho \frac{\partial \psi}{\partial \mathsf{Z}^D_{ijkl}} = \mathcal{O}\left(\mathbf{A}^3\right), \tag{74}$$

$$\rho \frac{\partial \psi}{\partial \mathrm{tr}\mathbf{A}} \mathbf{A}^D = \mathcal{O}\left(\mathbf{A}^2\right). \tag{75}$$

These contributions are small and can be neglected.

Thus, sufficient conditions for $\pi \geq 0$ are

- $\mathbf{q} \cdot \mathbf{g} \geq 0$,
- Z^D and Y are positive definite,
- $\nu, \eta^D, \mathsf{Z}_{tr}, \eta^{tr}$ are all positive.

These can all easily be satisfied within the constitutive framework which we have presented in part I of this work. One can thus conclude that there exists a suitable free energy ψ which allows it to be thermodynamically consistent. Note that so far a healing function has not yet been considered; this would have to be constructed in a careful way, in order not to annihilate any entropy.

5 Conclusion

The constitutive theory outlined in part I of this paper has now been subject to a rigorous investigation of its coherence with the entropy principle. The Müller-Liu entropy principle has been applied, which has proven useful in this case. Finally, it could be shown that the presented constitutive theory can be completed with a constitutive relation for a Helmholtz free energy density ψ such that it satisfies the entropy principle.

Apart from the thermodynamic consistency of the constitutive framework, several remarkable results have emerged during the evaluation. First, it turned out that the entropy flux takes the usual Clausius-Duhem shape

$$\boldsymbol{\Phi} = \frac{\mathbf{q}}{T(\theta)}, \tag{76}$$

where $\mathbf{q}$ is the heat flux and $T(\theta)$ the absolute temperature. This may seem not very surprising. Nevertheless, it is known that there are sets of constitutive variables where this is not the case (e.g., if $\dot{\theta}$ is taken as an independent constitutive variable). Therefore, it is important not to use (76) as a priori assumption (as it is done by entropy principles based on the Clausius-Duhem inequality). In this work, Eq. (76) is a *result*, not an *assumption*.

Furthermore, it has been pointed out that the conditions for thermodynamic equilibrium have to be completed with the condition $\mathbf{A}^D|_e = \mathbf{0}$; i.e., the deviatoric part of the elastic deformation in thermodynamic equilibrium should vanish. This is a consequence of the fluid-like behavior of the constitutive theory; unlike an elastic *solid*, the material considered here cannot maintain an elastic shear deformation without starting to flow, not even at low stresses.

As a step ahead, it would be desirable to exploit the entropy principle with fewer constitutive assumptions. Ideally, thermodynamics of the most general viscoelastic–viscoplastic fluid with a rank-4 damage effect variable should be considered. However, this would become technically extremely difficult, as isotropic representations involving rank-4 tensors would have to be used. These do not only have the tendency to be lengthy; more importantly, they are not even completely known yet. For rank-4 tensors, not even an irreducible representation of the isotropic invariants has been given so far [18]. Without these representations, a general consideration of the thermodynamics of rank-4 tensors is impossible. This problem should urgently be solved. This may be one of the most urgent open tasks in theoretical glaciology involving damage.

The theory presented in this article has a wide range of possible applications. The evolution of damage in a viscoelastic–viscoplastic fluid-like material is of great interest for ice sheet modelers, as the deterioration and failure of ice plays an important role for the ablation (and eventual disintegration) of the Antarctic and Greenland ice sheets. However, also the rheological consequences of damage accumulation should be taken into account. As a possible application of our theory, we suggest to implement at first a scalar bulk deformation with a scalar damage variable as a function of it into a numerical ice flow model. Following the small deformation approximation, the kinetic effect of the bulk deformation may be neglected. Later on, it would be desirable to also consider tensorial damage variables. However, this application involves further difficulties. In particular, processes which involve an approach of critical failure are delicate to treat. In this context, questions concerning the validity of a damage mechanics approach for critical processes have to be discussed, and a reasonable criterion when the model is stopped has to be defined. This is a challenging task for further research.

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