RENDICONTI
DEL SEMINARIO
MATEMATICO

Università e Politecnico di Torino

Geometry, Continua and Microstuctures, II

CONTENTS

H.J. Herrmann - W. Muschik - G. Rückner, *Constitutive theory in general relativity: basic fields, state spaces and the principle of minimal coupling* 133

H.J. Herrmann - G. Rückner - W. Muschik, *Constitutive theory in general relativity: spin-material in spaces with torsion* 141

A. Kato - W. Muschik - D. Schirrmeister, *Dynamics in quantum thermodynamics* 147

C.-S. Man - L. Noble, *Designing textured polycrystals with specific isotropic material tensors: the ODF method* 155

G.A. Maugin, *Towards an analytical mechanics of dissipative materials* 171

M. Magno - M. Musio, *An alternative interpretation of the behavior law of matter by means of a generalized stochastic process* 181

A.V. Porubov, *Strain solitary waves in an elastic rod with microstructure* 189

R. Segev, *Notes on stresses for manifolds* 199

B. Svendsen, *Non-local continuum thermodynamic extensions of crystal plasticity to include the effects of geometrically-necessary dislocations on the material behaviour* . 207

C. Trimarco, *The structure of material forces in electromagnetic materials* 237

R.W. Tucker - C. Wang, *A Cosserat detector for dynamic geometry* 245

Volume 58, N. 2 **2000**

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

H.J. Herrmann - W. Muschik - G. Rückner*

CONSTITUTIVE THEORY IN GENERAL RELATIVITY: BASIC FIELDS, STATE SPACES AND THE PRINCIPLE OF MINIMAL COUPLING

Abstract. A scheme is presented how to describe material properties under the influence of gravitation. The relativistic dissipation inequality is exploited by LIU's procedure. As an example an ideal spinning fluid is considered in the given framework.

1. Introduction

We investigate how constitutive properties can be introduced into Einstein's gravitation theory. Starting out with the balances of particle number density, spin and energy - momentum, Einstein's field equations and the relativistic dissipation inequality we consider constitutive equations and state spaces in 3-1- decomposition determining classes of materials. The set of possible constitutive equations compatible with the balances, the state space and the dissipation inequality is found out by LIU's exploitation of the dissipation inequality [1], [2].

2. Balances

We start out with the balances of particle number density, energy - momentum and spin in Einstein's gravitation theory, that means in Riemann geometry of a curved space without torsion:

$$N^{\alpha}_{;\alpha} = 0, \quad \text{1 equation,} \tag{1}$$

$$T^{\alpha\beta}{}_{;\beta} = 0, \quad \text{4 equations,} \tag{2}$$

$$S^{\alpha\beta}_{;\beta} = 0, \quad \text{3 equations.} \tag{3}$$

Here the particle flux is defined by $N^{\alpha} = nu^{\alpha}$ with the particle density n and the 4-velocity u^{α}. First of all the energy - momentum tensor is proposed to be not symmetric $T^{\alpha\beta} \neq T^{\beta\alpha}$. The spin density $S^{\alpha\beta}$ is antisymmetric $S^{\alpha\beta} = -S^{\beta\alpha}$ and satisfies the so-called Frenkel condition $u_{\alpha}S^{\alpha\beta} = 0 = S^{\alpha\beta}u_{\beta}$ which expresses that the spin tensor is purely spatial.
Because we want to describe material under the influence of gravitation in Riemann geometry we need Einstein's field equations

$$\tilde{R}_{\alpha\beta} - (1/2)g_{\alpha\beta}\tilde{R} = \kappa T_{(\alpha\beta)}, \quad \text{10 equations.} \tag{4}$$

*We would like to thank H.-H. von Borzeszkowski and Thoralf Chrobok for interesting discussions and introduction to geometries with curvature and torsion. We would also like to thank the VISHAY Company, D-95085 Selb and the Deutsche Forschungsgemeinschaft for financial support.

Here are $\tilde{R}_{\alpha\beta}$ the Ricci tensor and $\tilde{R}$ the curvature scalar due to the Riemann geometry. They are marked with a tilde because we although examine material under the framework of other geometries, so we have to distinguish between different geometric quantities. Due to the symmetry of the left hand side only the symmetric part of the energy- momentum tensor appears in the field equations.

Finally we have to take into account the dissipation inequality

$$S^{\alpha}_{;\alpha} = \sigma \geq 0. \tag{5}$$

Here $S^{\alpha} = su^{\alpha} + s^{\alpha}$, introducing the entropy density s and the entropy flux density s^{α}.

The 18 equations (1) to (4) and the dissipation inequality contain more fields than equations are. Therefore the set of equations is underdetermined. This is due to the fact, that (1) to (5) are valid for all materials and up to now no special material was taken into consideration. Hence we have to split the 37 fields appearing in (1) to (5) into the basic fields which we are looking for and into the constitutive equations describing the considered material or the class of materials. In more detail the 37 fields are:

$$\begin{array}{rl} N^{\alpha}, & \text{4 fields,} \\ T^{\alpha\beta}, & \text{16 fields,} \\ S^{\alpha\beta}, & \text{3 fields,} \\ g^{\alpha\beta}, & \text{10 fields,} \\ S^{\alpha}, & \text{4 fields.} \end{array}$$

From the energy - momentum tensor we can see, that parts of it belong to the constitutive equations, namely the 3 - stress tensor, and other parts, namely the energy density, belong to the basic fields. Therefore we perform as usual the following 3-1 decomposition

$$\begin{array}{rcll} \epsilon & := & T_{\alpha\beta}\frac{1}{c^2}u^{\alpha}u^{\beta}, & \text{energy density,} \\ t^{\alpha\beta} & := & h^{\alpha\gamma}T_{\gamma\sigma}h^{\sigma\beta}, & \text{stress tensor,} \\ q^{\alpha} & := & -h^{\alpha\sigma}T_{\gamma\sigma}u^{\gamma}, & \text{heat flux density,} \\ p^{\beta} & := & h^{\alpha\sigma}T_{\sigma\gamma}u^{\gamma}, & \text{momentum density.} \end{array}$$

Here $h^{\alpha\beta}$ is the projection tensor perpendicular to the 4-velocity:

$$h^{\alpha\gamma} := g^{\alpha\gamma} + \frac{1}{c^2}u^{\alpha}u^{\gamma} = h^{\gamma\alpha}.$$

Now we introduce the 18 basic fields:

$$\{\epsilon, n, u_{\alpha}, g_{\alpha\beta}, S_{\alpha\beta}\}(x^{\alpha}),$$

and the remaining 19 constitutive equations:

$$\{t_{\alpha\beta}, q_{\alpha}, p_{\beta}, S_{\alpha}\}(x^{\alpha}).$$

Dealing with Riemann geometry one finally have to satisfy some constraints:

$$\begin{array}{rcll} u^{\alpha}u_{\alpha} & = & -c^2, & \text{normalisation of the the 4-velocity,} \\ g_{\alpha\beta} & \stackrel{!}{=} & g_{\beta\alpha}, & \text{symmetry of the metric,} \\ g_{\alpha\beta;\gamma} & \stackrel{!}{=} & 0, & \text{vanishing of the non-metricity,} \\ \{^{\alpha}_{\beta\gamma}\} & = & F(g_{\alpha\beta}, g_{\alpha\beta,\gamma}), & \text{symmetric connection as a function of the metric} \\ & & & \text{and the first partial derivative of the metric,} \\ A_{\alpha;\beta} & = & A_{\alpha,\beta} - \{^{\sigma}_{\alpha\beta}\}A_{\sigma}, & \text{covariant derivative according to the geometry.} \end{array}$$

3. State Space

Because the system of equations (1) to (4) is underdetermined one has to introduce the constitutive equations which depend on of state space variables, which are characterizing the material.

By introducing the state space one get balances on the state space in the following form:

$$A^{\beta}_{;\beta}(Z) = a, \quad \text{or} \quad A^{\alpha\beta}_{;\beta}(Z) = a^{\alpha}.$$

Here the symbol Z represents all state space variables.

If we want to to describe material under the influence of gravitation we have to introduce a state space inducing variables which describe gravitational effects. Hence in general the state space looks like

$$Z = Z(Z_{therm}, Z_{grav})$$

Here Z_{grav} is the set of variables which describes effects of gravitation, and Z_{therm} are all other variables [3, 4, 5].

3.1. First derivative state space

First of all we have a look on state spaces which containes first derivatives:

$$Z^{I} = Z(Z^{therm}, Z^{therm}_{;\alpha}, Z^{grav}, Z^{grav}_{;\alpha}) = Z(Z^{therm}, Z^{therm}_{;\alpha}, g_{\alpha\beta}, \underbrace{g_{\alpha\beta;\gamma}}_{\equiv 0})$$

This chosen state space consists of covariant quantities. If we decompose the covariant derivative of a tensor of first order

$$A_{\alpha;\beta} = A_{\alpha,\beta} - \{^{\sigma}_{\alpha\beta}\}A_{\sigma},$$

and similary for tensors of higher order the state space writes

$$Z^{I} = Z(Z^{therm}, Z^{therm}_{,\alpha}, g_{\alpha\beta}, \{^{\alpha}_{\beta\gamma}\}).$$

Here the state space is spanned by non-covariant quantities, but the constitutive equations on it depend on covariant combinations of these non-covariant state space variables.

3.2. Second derivative state space and the principle of minimal coupling

Next a second derivative state space is discussed:

$$Z^{II} = Z(Z^{therm}, Z^{therm}_{;\alpha}, Z^{therm}_{;\alpha\beta}, g_{\alpha\beta}, \underbrace{g_{\alpha\beta;\gamma}}_{\equiv 0}, g_{\alpha\beta;\gamma\delta}, \tilde{R}_{\alpha\beta\gamma\delta}).$$

With respect to $A_{\alpha;[\beta\gamma]} = \tilde{R}^{\sigma}_{\alpha\beta\gamma}A_{\sigma}$ one can replace the skew-symmetric part of the second covariant derivatives by the Riemann curvature tensor and the quantity itself. Consequently we obtain

$$Z^{II} = Z(Z^{therm}, Z^{therm}_{;\alpha}, \underbrace{Z^{therm}_{;(\alpha\beta)}}_{\text{symmetric part}}, g_{\alpha\beta}, \tilde{R}_{\alpha\beta\gamma\delta}).$$

As done before one can rewrite this state space containing only partial derivatives

$$Z^{II} = Z(Z^{therm}, Z^{therm}_{,\alpha}, Z^{therm}_{(,\alpha\beta)}, g_{\alpha\beta}, \{^{\alpha}_{\beta\gamma}\}, \{^{\alpha}_{\beta\gamma}\}_{,\delta}).$$

By introducing this second derivative state space we are in trouble with the *principle of minimal coupling*. It states that second derivative state spaces must not include the curvature tensor or the the partial derivative of the connection (or equivalently in Riemann geometry the second derivative of the metric). The *principle of minimal coupling* guarantees that the equivalence principle holds. So we have to remove $\tilde{R}_{\alpha\beta\gamma\delta}$, $Z^{therm}_{;[\beta\gamma]}$ and $\{{}^{\alpha}_{\beta\gamma}\}_{,\delta}$ from the state space, and we get a second derivative state space obeying the *principle of minimal coupling*

$$Z^{II} = Z(Z^{therm}, Z^{therm}_{,\alpha}, Z^{therm}_{(,\alpha\beta)}, g_{\alpha\beta}, \{{}^{\alpha}_{\beta\gamma}\}).$$

With respect to the variables which are introduced to describe the effects of gravitation this state space looks like Z^{I}.

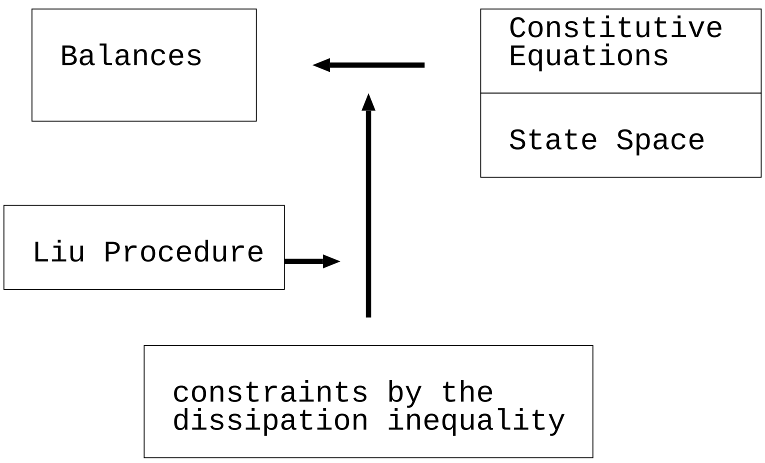
3.3. State space without derivatives

A state space which contains no derivatives is:

$$Z^{0} = Z(Z^{therm}, g_{\alpha\beta}).$$

The higher (directional) derivatives belonging to this state space are $Z^{therm}_{,\alpha}$ and $\{{}^{\alpha}_{\beta\gamma}\}$ or $g_{\alpha\beta,\gamma}$, respectively. But the Ricci tensor and the curvature scalar in Einstein's field equations depend on the partial derivatives of the Christoffel symbols or the of the connection, respectively. These quantities are no higher derivatives with respect to Z^{0}. Consequently the Einstein equations do not determine higer derivatives of the chosen state space in this case. Therefore Z^{0} does not fit to Einstein's equations and we cannot use it.
Now we have to exploit the dissipation inequality.

4. LIU's procedure



A general balance looks like

$$A_{\alpha\beta;\beta}(Z) = a_{\alpha}.$$

Applying the chain rule with respect to the chosen state space variables we obtain

$$\Longleftrightarrow \quad \underbrace{a_\alpha}_{\in \underline{B}} \quad = \quad \frac{\partial}{\partial Z}(A_{\alpha\beta})Z_{,\beta} - \underbrace{\{{}^{\sigma}_{\alpha\beta}\}A^{\beta}_{\sigma} - \{{}^{\beta}_{\sigma\beta}\}A^{\sigma}_{\alpha}}_{\in \underline{B}}.$$

Only the first term on the right hand side contains quantities which are higher higher derivatives than those included in the state space. So one can split the terms in such containing higher derivatives and such which do not. Rewriting the balances and the dissipation inequality we obtain then in the form

$$\begin{aligned} \underline{\underline{A}} \cdot \underline{y} - \underline{B} &= 0, \\ \underline{\alpha} \cdot \underline{y} - \beta &\geq 0. \end{aligned}$$

Here are $\underline{\underline{A}}$, $\underline{B}$, $\underline{\alpha}$ and β state functions depending on the constitutive properties and $\underline{y}$ represents the process direction in the chosen state space. The equations above are linear in $\underline{y}$.

DEFINITION 1. *All constitutive equations being compatible with the chosen state space and satisfying the balances and the dissipation inequality determine the* class of materials *([6], [7]).*

There exist two possibilities to find this class of materials:

- For fixed $\underline{\underline{A}}$, $\underline{B}$, $\underline{\alpha}$ and β certain $\underline{y}$ are excluded,
- For all possible $\underline{y}$ the $\underline{\underline{A}}$, $\underline{B}$, $\underline{\alpha}$ and β have to be determined in such a way, that the dissipation inequality is satisfied.

Starting out with the Coleman-Mizel formulation of the second law that all solutions of the balances are satisfying the dissipation inequality

$$\underline{\underline{A}} \cdot \underline{y} - \underline{B} = 0 \quad \Longrightarrow \quad \underline{\alpha} \cdot \underline{y} - \beta \geq 0,$$

Liu‘s proposition is valid:

$$\begin{aligned} &\underline{\alpha}(Z) = \underline{\Lambda}(Z) \cdot \underline{\underline{A}}(Z), \\ &\underline{\Lambda}(Z) \cdot \underline{B}(Z) \geq \beta(Z). \end{aligned}$$

This expresses that the entropy production $\sigma := \underline{\Lambda}(Z) \cdot \underline{B}(Z) - \beta(Z) \geq 0$ is independent of the process direction and so the second possibilty for finding the class of materials holds. These equations are the so-called LIU equations. By eliminating the lagrange parameters $\underline{\Lambda}$ from the LIU equations and inserting them into the dissipation inequality we obtain constraints restricting the possible materials.

5. Weyssenhoff fluid in Riemann geometry

A covariant description of a classical fluid with spin in Riemann spacetime can be obtained by generalising the work of Weyssenhofff and Raabe as it is done by by Obukhoy and Piskareva [8], [9] and [10].

Tensors of spin and energy-momentum for the Weyssenhoff dust are postulated to be:

$$\begin{aligned} S^{\alpha}_{\beta\gamma} &\stackrel{!}{=} u^{\alpha} S_{\beta\gamma}, \\ T_{\alpha\beta} = \hat{T}_{\alpha\beta} &\stackrel{!}{=} u_{\alpha} P_{\beta}. \end{aligned}$$

Here is $S_{\beta\gamma}$ the skew symmetric spin density, satisfying the Frenkel condition $u^\beta S_{\beta\gamma} = 0 = u^\gamma S_{\beta\gamma}$, u_α the 4-velocity and P_β the 4-vector density of energy-momentum. The explicit form of P_β can be derived from the spin conservation law $\hat{T}_{[\alpha\beta]} = 2\tilde{\nabla}_\gamma S^\gamma_{\alpha\beta}$

$$\hat{T}_{[\alpha\beta]} = u_\alpha P_\beta - u_\beta P_\alpha = 2\tilde{\nabla}_\gamma S^\gamma_{\alpha\beta}. \tag{6}$$

Taking into account the definition $u^\alpha P_\alpha = \epsilon$ where ϵ is the the energy density we obtain from (6) by contracting with the 4-velocity u^β:

$$P_\alpha = \epsilon u_\alpha + 2u^\beta 2\tilde{\nabla}_\gamma S^\gamma_{\beta\alpha}. \tag{7}$$

Inserting (7) into (6) one obtain the motion of spin, which describes the rotational dynamics of the fluid.

Assuming that the elements of the medium interact in such a way that Pascal law is valid we get the model for an ideal spinning fluid. By doing this we have to modify the stress tensor given above for the description of dust by the contribution of the isotropic pressure

$$\hat{T}^\alpha_\beta \stackrel{!}{=} u^\alpha P_\beta - p(\delta^\alpha_\beta - u^\alpha u_\beta) = -p\delta^\alpha_\beta + u^\alpha[u_\beta(\epsilon + p) + 2u^\sigma \tilde{\nabla}_\gamma u^\gamma S_{\sigma\alpha}]. \tag{8}$$

Taking the divergence of the Einstein field equations (4) one gets after 3-1-decomposition with respect to (8) the equations for the tranlational dynamics in 3-1- decomposition:

$$0 \stackrel{!}{=} \hat{T}^{(\alpha}_{\beta);\alpha}$$

$$\left\{ \begin{array}{rcl} 0 & = & (p+\epsilon)u^\alpha(u_{\beta;\alpha}) + (-\delta^\alpha_\beta + u^\alpha u_\beta)p_{;\alpha} + \\ & & +2[u^\alpha S_{\beta\gamma} u^\sigma u^\gamma_{;\sigma}]_{;\alpha} + R_{\gamma\sigma\alpha\beta} S^{\gamma\sigma} u^\alpha \\ 0 & = & (p+\epsilon)u^\alpha_{;\alpha} + u^\alpha \epsilon_\alpha \end{array} \right.$$

As it is shown above the spin enters in the spatial part of the symmetric energy-momentum tensor. So the spin is over the energy connected to the Einstein gravitation equations and in this sense connected to the geometry. But there exist no direct geometric quantity with which the spin is coupled and further on any skew symmetric parts of the balances stands alone. So one can say that Einstein gravitation field theory can deal with the physical quantity spin but say nothing about the skew symmetric parts which appear in the balances.

6. Conclusions

As usual in constitutive theory the split of the fields into basic fields and constitutive equations is also possible, if gravitation is taken into account. The non-relativistic state space is extended by geometrical variables induced by curvature which describe its influence on constitutive properties. Although the choice of the state spaces is free in principle, some restrictions appear in Riemann geometry: Because Einstein‘s field equations contain the second derivatives of the metric, its first derivatives have to be included among the state variables in form of the Christoffel symbols (connection) or the partial derivatives of the metric itself. This involves that the state space is spanned by non-covariant quantities. But nevertheless constitutive properties are described by covariant combinations of these non-covariant quantities. A second consequence is , that state spaces containing only the metric as a geometrical variable cannot be used.

The second derivative state spaces have a speciality:
They have to obey the *principle of minimal coupling*. This principle runs as follows: second derivative state spaces do not include the curvature tensor or the partial derivatives of the

Christoffel symbols (or those of the connection). From a physical point of view this principle states, that there are no materials by which the curvature of space-time can be measured by observing constitutive properties. This principle of minimal coupling is related to the equivalence principle which states, that for free falling, non-rotating observers locally the curvature of space-time vanishes.

References

[1] MUSCHIK W., PAPENFUSS C. AND EHRENTRAUT H., *Concepts of continuum thermodynamics*, Technische Universität Berlin und Kielce University of Technology, 1996.

[2] MUSCHIK W., *Aspects of non-equilibrium thermodynamics*, World Scientific, Singapore 1990.

[3] RÜCKNER G., *Materialgleichungen der erweiterten Thermodynamik in der allgemeinen Relativitätstheorie*, Studienarbeit, Institut für Theoretische Physik, TU Berlin 1999.

[4] HERRMANN H., *Verträglichkeit von Liu-Verfahren und Einstein-Gleichungen*, Diplomarbeit, Institut für Theoretische Physik, TU Berlin 1999.

[5] HERRMANN H., MUSCHIK W. PAPENFUSS C. AND RÜCKNER G, *Liu-technique for exploiting the dissipation-inequality in case of constrained state space variables*; in: "Trends in application of mathematics to mechanics", Chapman & Hall 2000.

[6] MUSCHIK W.AND EHRENTRAUT H, *An amendment to the second law*, J. Non-Equilib. Thermodyn. **21** (1976), 175.

[7] COLEMAN B.D. AND MIZEL V.J., *Existence of caloric equations of state in thermodynamics*, J. Chem. Phys. **40** (1964), 1116–1125.

[8] WEYSSENHOFF J. AND RAABE A., *Relativistic dynamics of spin-fluids and spin-particles*, Acta Phys. Polon. **9** (1947), 7–53.

[9] OBUKHOV YU. N. AND KOROTKY V.A., *The Weyssenhoff fluid in Einstein-Cartan theory*, Class. Quantum Grav. **4** (1987), 1633–1657.

[10] OBUKHOV YU. N. AND PISKAREVA O.B., *Spinning fluid in general relativity*, Class. Quantum Grav. **6** (1989), L15–L19.

[11] MISNER C.W., THORNE K.S. AND WHEELER J.A., *Gravitation*, W.H. Freeman and Company, San Francisco 1973.

[12] HEHEL F.W., MCCREA J.D., MIELKE E.W. AND NE'EMAN Y., *Metric-affine gauge theory of gravity: field equations, noether identities, world spinors, and breaking of dilation invariance*, Physics Reports **258** (1995), 1–171.

AMS Subject Classification: 83C99, 80A10.

Heiko HERRMANN, Gunnar RÜCKNER, Wolfgang MUSCHIK
Institut für Theoretische Physik
Technische Universität Berlin
D-10623 Berlin GERMANY
e-mail: `hh@itp.physik.tu-berlin.de`
e-mail: `gr@itp.physik.tu-berlin.de`
e-mail: `muschik@physik.tu-berlin.de`

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

H.J. Herrmann - G. Rückner - W. Muschik*

CONSTITUTIVE THEORY IN GENERAL RELATIVITY: SPIN-MATERIAL IN SPACES WITH TORSION

Abstract. Some of the problems arising in general relativistic constitutive theory can be solved by using the Riemann-Cartan geometry, a generalization of the Riemann geometry containing torsion. As an example the ideal spinning fluid (Weyssenhoff fluid) is discussed and different results for Einstein and Einstein-Cartan theories are compared.

1. Introduction

It is possible to formulate a relativistic constitutive theory in the framework of Einstein's theory of gravitation [1], but there are several unsatisfying points. One problem is that only symmetric energy-momentum tensors are compatible with the field equations, another problem is that the energy-momentum tensor has to have a vanishing divergence (this is also a consequence of the field equations). Other problems arise from the principle of minimal coupling. One can expect, that at least some problems can be solved by using a generalized theory of gravitation that includes spin (angular momentum) as source of gravitation. The Einstein-Cartan theory of gravitation is such a generalized theory, it is based on a spacetime with curvature and torsion, the Riemann-Cartan geometry.

2. Einstein-Cartan theory

2.1. Geometry

There is a general connection Γ, which is different from the Christoffel symbol. This connection is not symmetric, the antisymmetric part defines the torsion $\mathcal{T}$, which is a tensor of degree 3. The torsion vector is defined by a contraction of the torsion with respect to the first and third indices:

$$\begin{aligned} \mathcal{T}_{\mu\lambda\cdot}^{\cdot\,\cdot\,\kappa} &:= \Gamma^{\kappa}_{[\mu\lambda]} \\ \mathcal{T}_{\lambda} &:= \frac{3}{2}\mathcal{T}_{\mu\lambda\cdot}^{\cdot\,\cdot\,\mu} \end{aligned}$$

It is possible to represent the connection as a combination of the Christoffel symbol and the so-called contorsion:

$$\Gamma^{\kappa}_{\mu\lambda} = \underbrace{\left\{ {\kappa \atop \mu\lambda} \right\}}_{\text{Christoffel symbols}} + \underbrace{\mathcal{T}_{\mu\lambda\cdot}^{\cdot\,\cdot\,\kappa} - \mathcal{T}_{\lambda\cdot\mu}^{\cdot\,\kappa\,\cdot} + \mathcal{T}^{\kappa\,\cdot\,\cdot}_{\cdot\,\mu\lambda}}_{\text{Contorsion}}$$

*We would like to thank H.-H. von Borzeszkowski and Thoralf Chrobok for interesting discussions and introduction to geometries with curvature and torsion. We would also like to thank the VISHAY Company, D-95085 Selb and the Deutsche Forschungsgemeinschaft for financial support.

The tensor of curvature and the Ricci tensor are defined as usual:

$$\begin{aligned} R_{\nu\mu\lambda}^{\cdot\ \cdot\ \cdot\kappa} &= 2\partial_{[\nu}\Gamma^{\kappa}_{\mu]\lambda} + 2\Gamma^{\kappa}_{[\nu|\rho|}\Gamma^{\rho}_{\mu]\lambda} \\ R_{\mu\lambda} &:= R_{\kappa\mu\lambda}^{\cdot\ \cdot\ \cdot\kappa} \end{aligned}$$

The covariant derivatives are defined in the same way as in Riemann geometry, but the symmetric Christoffel symbols are replaced by the non-symmetric connection Γ:

$$\begin{aligned} u^{\nu}_{\cdot;\mu} &= u^{\nu}_{\cdot,\mu} + \Gamma^{\nu}_{\lambda\mu}u^{\lambda} \\ u_{\lambda;\mu} &= u_{\lambda,\mu} - \Gamma^{\nu}_{\lambda\mu}u_{\nu} \end{aligned}$$

2.2. Field equations

It is possible to derive field equations by a variation principle [2]. The variation of the special Lagrange density $\mathcal{L}(g_{\mu\nu}, \Gamma^{\alpha}_{\mu\nu}, \phi, \partial_m u\phi)$ given in [2] with respect to tetrades and connection results in two sets of field equations with curvature and torsion:

$$\begin{aligned} R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R &= \kappa T^{\mu\nu} \\ \mathcal{T}_{\alpha\beta}^{\cdot\ \cdot\ \mu} + 3\delta^{\mu}_{[\alpha}\mathcal{T}_{\beta]} &= \kappa S_{\alpha\beta}^{\cdot\ \cdot\ \mu} \\ \text{geometry} &\Leftrightarrow \text{material} \end{aligned} \tag{1}$$

The first set of field equations reads the same as in Einstein theory, but neither the Ricci tensor nor the energy-momentum tensor are symmetric. Both sides of this equation are not divergence-free, in contrast to Einstein's theory. The second set of the field equations connects the torsion with the spin-tensor, which is a constitutive function.

Differentiating the Einstein-Cartan tensor, i.e. the left side of the first set of field-equations (1) and contracting over the second index results in the following equations (the contracted Bianchi identity):

$$\nabla_{\kappa}(R_{\nu}^{\cdot\kappa} - \frac{1}{2}\delta^{\kappa}_{\nu}R) = 2\mathcal{T}_{\nu\kappa}^{\cdot\ \cdot\ \rho}R_{\rho}^{\cdot\kappa} - \mathcal{T}_{\kappa\mu}^{\cdot\ \cdot\ \rho}R_{\nu\rho}^{\cdot\ \cdot\ \mu\kappa}$$

Using the field equation one finds that the divergence of the energy-momentum tensor is given by:

$$\Longrightarrow \kappa\nabla_{\kappa}T_{\nu}^{\cdot\kappa} = 2\mathcal{T}_{\nu\kappa}^{\cdot\ \cdot\ \rho}R_{\rho}^{\cdot\kappa} - \mathcal{T}_{\kappa\mu}^{\cdot\ \cdot\ \rho}R_{\nu\rho}^{\cdot\ \cdot\ \mu\kappa}$$

In contrast to the Einstein theory the divergence of the energy-momentum tensor does not vanish anymore, but is geometrically determined.

2.3. Balances

It is possible to derive balances for the energy-momentum and for the spin from the field equations. This can be done by splitting the first set of field equations into a symmetric and an antisymmetric part:

$$\begin{aligned} R_{(\mu\nu)} - \frac{1}{2}g_{(\mu\nu)}R &= \kappa T_{(\mu\nu)} \\ R_{[\mu\nu]} &= \kappa T_{[\mu\nu]} \end{aligned}$$

By taking the divergence of the symmetric equation and using the contracted Bianchi identity one can derive the balance of energy-momentum:

$$(\nabla_\nu - 3\mathcal{T}_\nu)T^{\nu}_{\cdot\mu} + 2\mathcal{T}_{\mu\beta}^{\cdot\,\cdot\,\alpha}T^{\beta}_{\cdot\alpha} + S_{\alpha\beta}^{\cdot\,\cdot\,\nu}R^{\alpha\beta}_{\cdot\,\cdot\,\mu\nu} = 0 \tag{2}$$

The balance of angular momentum can be directly derived from the antisymmetric part by using a geometrical identity for the antisymmetric part of the Ricci tensor and the second set of field equations:

$$(\nabla_\alpha - 3\mathcal{T}_\alpha)\underbrace{(\mathcal{T}_{\mu\lambda}^{\cdot\,\cdot\,\alpha} + 3\delta^{\alpha}_{[\mu}\mathcal{T}_{\lambda]})}_{\kappa S_{\mu\lambda}^{\cdot\,\cdot\,\alpha}} \quad = \quad \kappa T_{[\mu\nu]} \tag{3}$$

The balance of angular momentum connects the change of the spin tensor to the antisymmetric part of the energy-momentum-tensor.

3. Weyssenhoff fluid

3.1. Heuristic description

Now the Weyssenhoff fluid [3] will be discussed as it is done by Obukhov and Korotky [4].

The Weyssenhoff fluid is defined as an ideal spinning fluid. A spin density is now introduced as a skew-symmetric tensor:

$$S^{\mu\nu} = -S^{\nu\mu}$$

The spin density is spacelike, what is ensured by the Frenkel condition:

$$S^{\mu\nu}u_\nu = 0$$

The constitutive assumptions (postulates) for a Weyssenhoff fluid are as follows:

- The spin tensor is a function of the spin density and the following constitutive equation is assumed:

$$S_{\alpha\beta}^{\cdot\,\cdot\,\mu} \quad = \quad u^\mu S_{\alpha\beta}$$

- The energy-momentum tensor should be a function of the energy-momentum density, and is defined as follows:

$$T^{\mu}_{\cdot\alpha} \quad = \quad u^\mu P_\alpha$$

Next one calculate the explicit form of the energy-momentum-density P_α. This can be done by starting out with the antisymmetric part of the energy-momentum tensor (3) and (4):

$$2T_{[\mu\nu]} = u_\mu P_\nu - u_\nu P_\mu \quad = \quad 2(\nabla_\alpha - 3\mathcal{T}_\alpha)S_{\mu\nu}^{\cdot\,\cdot\,\alpha}$$

- and with the usual definition of the internal-energy

$$u^\mu P_\mu \quad \stackrel{!}{=} \quad \epsilon$$

one obtains:

$$
\begin{aligned}
-c^2 P_\nu &= \epsilon u_\nu + 2u^\mu(\nabla_\alpha - 3\mathcal{T}_\alpha)(u^\alpha S_{\mu\nu}) \\
T^{\mu}_{\cdot\nu} &= -\frac{1}{c^2}\epsilon u^\mu u_\nu - \frac{1}{c^2}2u^\mu u^\alpha \nabla_\beta S_{\alpha\nu}^{\cdot\cdot\beta}
\end{aligned}
$$

If it is now assumed, that the interaction between the elements of the fluid is given in such a way that

- Pascal law is valid, one has to modify the equations by an isotropic pressure:

$$
\hat{T}^{\mu}_{\cdot\nu} = +\frac{1}{c^2}p\delta^\mu_\nu - \frac{1}{c^2}u^\mu(u_\nu(\epsilon + p) + 2u^\alpha \nabla_\beta S_{\alpha\nu}^{\cdot\cdot\beta})
$$

3.2. Exploiting the 2nd law

Balances

From the thermodynamical point of view the correct way would be to write down the balances and the constraints and for deriving restrictions to the constitutive equations by use of the Liu procedure.

First there is the balance of particle number density which is given in the same way as in Einstein's theory:

$$
\nabla_\mu N^\mu = 0 = (nu^\mu)_{;\mu}
$$

Next there are the balances of energy-momentum and angular momentum, which are given by the geometrical identities (2) and (3):

$$
(\nabla_\nu - 3\mathcal{T}_\nu)T^{\nu}_{\cdot\mu} + 2\mathcal{T}_{\mu\beta}^{\cdot\cdot\alpha}T^{\beta}_{\cdot\alpha} + S_{\alpha\beta}^{\cdot\cdot\nu}R^{\alpha\beta}_{\cdot\cdot\mu\nu} = 0
$$

$$
(\nabla_\alpha - 3\mathcal{T}_\alpha)S_{\mu\lambda}^{\cdot\cdot\alpha} = T_{[\mu\nu]}
$$

The next equation one needs is the balance of entropy, representing the second law of thermodynamics

$$
\nabla_\mu \Sigma^\mu = (su^\mu)_{;\mu} + s^{\mu}_{\cdot;\mu} \geq 0
$$

and the field equations are

$$
\begin{aligned}
R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R &= \kappa T^{\mu\nu} \\
\mathcal{T}_{\alpha\beta}^{\cdot\cdot\mu} + 3\delta^\mu_{[\alpha}\mathcal{T}_{\beta]} &= \kappa S_{\alpha\beta}^{\cdot\cdot\mu}
\end{aligned}
$$

Other constaints, as there are the normalization of the 4-velocity and the form of the covariant derivative have also to be taken into account.

We now choose the state space for an ideal fluid with spin. This state space has to contain the wanted fields, the metric and the connection:

$$
\mathcal{Z} = \{n, u_\alpha, \epsilon, S_{\alpha\beta}, g_{\alpha\beta}, \Gamma^\gamma_{\alpha\beta}\}
$$

Liu procedure

In order to apply Liu's procedure [5, 6, 7] one has to insert the explicit form of the covariant derivative into the balances and then use the chain rule for differentiating the constitutive quantities.

Next the balances and constraints have to be rewritten in matrix formulation:

$$\begin{aligned} \underline{\underline{A}} \cdot \underline{y} + \underline{B} &= 0, \\ \underline{\alpha} \cdot \underline{y} + \beta &\geq 0 \end{aligned}$$

PROPOSITION 1 (COLEMAN-MIZEL-FORMULATION OF THE 2$^{\text{ND}}$ LAW [8]).
If Z is no trap, the following inclusion is valid for all $\underline{y}$:

$$\underline{\underline{A}} \cdot \underline{y} = -\underline{B} \quad \Longrightarrow \quad \underline{\alpha} \cdot \underline{y} \geq -\beta$$

that means, all $\underline{y}$ which are solutions of the balances satisfy the dissipation inequality.

Then one can apply Liu's proposition, which runs as follows:

PROPOSITION 2 (LIU [5]). Starting with proposition 1 one can show:
In large state spaces exist state space functions $\underline{\Lambda}$ so that the constitutive equations satisfy the Liu relations

$$\underline{\Lambda} \cdot \underline{\underline{A}} = \underline{\alpha}, \tag{4}$$

and the residual inequality

$$-\underline{\Lambda} \cdot \underline{B} \geq -\beta. \tag{5}$$

From (4) and (5) we obtain the restrictions to the constitutive equations we are looking for. Taking these restrictions into account we obtain constitutive equations which are in accordance with the second law of thermodynamics.

4. Comparison of Einstein and Einstein-Cartan theory

We now discuss differences and similarities of Einstein and Einstein-Cartan theories with respect to coupling of constitutive properties to geometry.

In Einstein-Cartan theory with non-vanishing torsion and curvature the spin couples to torsion, and the energy-momentum tensor which is spin-dependent, non-symmetric, and not divergence-free couples to curvature. If the torsion vanishes, also the spin tensor and the skew-symme-tric part of the energy-momentum tensor vanish.

In Einstein theory with vanishing torsion and non-vanishing curvature the spin appears as in Einstein-Cartan theory in the non-symmetric and not divergence-free energy-momentum tensor which is split into its symmetric and skew-symme-tric part. The divergence-free symmetric part couples by the Einstein equations to curvature, whereas the skew-symmetric part does not couple to any geometric quantity. It represents the source in spin balance.

In Minkowski theory being flat and torsion-free there are no geometric objects to which spin and energy-momentum tensor can couple. If we regard Minkowski and Einstein theory as special cases of the Einstein-Cartan theory all having the same type of coupling, then Einstein theory has to be spin-free and Minkowski theory is only valid in vacuum. Of course, this is not the case by experience and therefore we have to regard these three theories as having different types of coupling to constitutive properties.

5. Conclusion

As dicussed above the energy-momentum tensor of the Weyssenhoff fluid was obtained by use of a variational problem without taking into account the second law of thermodynamics. This variational problem generates the balance equations of energy-momentum and spin which now are supplemented by the dissipation inequality. The Liu procedure of exploiting this dissipation inequality generates restrictions to the constitutive quantities energy-momentum and spin.

References

[1] HERRMANN H., RÜCKNER G. AND MUSCHIK W., *Constitutive theory in general relativity: spin-material in spaces with torsion*; in: "Proceedings of the 4th international seminar on geometry, continua and microstructures 2000", Rend. Sem. Mat. Univ. e Polit. Torino, **58** (2) 2000, 135–141.

[2] HEHL F.W., MCCREA J.D., MIELKE E.W. AND NE'EMAN Y., *Metric-affine Gauge theory of gravity: field equations, Noether identities, world spinors, and breaking of dilation invariance*, Physics Reports **258** (1995), 1–171.

[3] WEYSSENHOFF J. AND RAABE A., *Relativistic dynamics of spin-fluids and spin-particles*, Acta Phys. Polon. **9** (1947), 7–53.

[4] OBUKHOV YU.N. AND KOROTKY V.A., *The Weyssenhoff fluid in Einstein-Cartan theory*, Class. Quantum Grav. **4** (1987), 1633–1657.

[5] I-SHIH AND LIU, *Method of Lagrange multipliers for exploitation of the entropy principle*, Arch. Rat. Mech. Anal. **46** (1972), 131.

[6] MUSCHIK W., PAPENFUSS C. AND EHRENTRAUT H., *Concepts of continuum thermodynamics*, Technische Universität Berlin und Kielce University of Technology 1996.

[7] MUSCHIK W., *Aspects of non-equilibrium thermodynamics*, World Scientific, Singapore 1990.

[8] COLEMAN B.D. AND MIZEL V.J., *Existence of caloric equations of state in thermodynamics*, J. Chem. Phys. **40** (1964), 1116–1125.

[9] MUSCHIK W. AND EHRENTRAUT H., *An amendment to the second law*, J. Non-Equilib. Thermodyn. **21** (1996), 175.

AMS Subject Classification: 83C99, 83D05, 80A10.

Heiko HERRMANN, Gunnar RÜCKNER, Wolfgang MUSCHIK
Institut für Theoretische Physik
Technische Universität Berlin
D-10623 Berlin GERMANY
e-mail: `hh@itp.physik.tu-berlin.de`
e-mail: `gr@itp.physik.tu-berlin.de`
e-mail: `muschik@physik.tu-berlin.de`

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

A. Kato - W. Muschik - D. Schirrmeister*

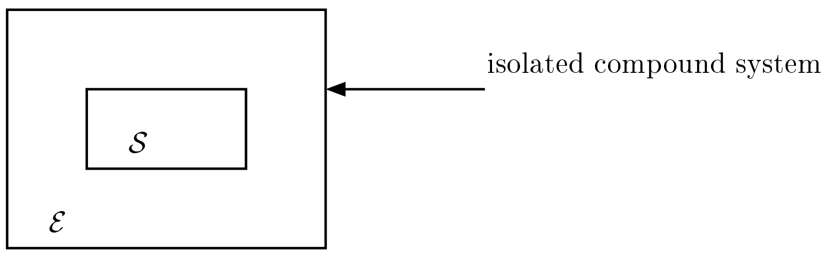
DYNAMICS IN QUANTUM THERMODYNAMICS

Abstract. A thermodynamical system being in contact with its environment is investigated by use of quantum-thermodynamical description. Since the considered system can only described by a restricted set of relevant observables, it performs an irreversible non-equilibrium process. Different statistical operators accompanying the non-equilibrium process are investigated, if their dynamics determine the expectation values of the set-variables correctly in time. The positivity of the entropy production of one of the dynamics is discussed.

1. Introduction

Thermodynamics is the theory of non-equilibrium systems. The main problem that arises, if we want a quantum mechanical description of thermodynamics, is how to get irreversibility into the reversible theory of quantum dynamics in order to get a positive entropy production. One possibility is to introduce dissipative terms into Schrödinger's equation or into the von Neumann dynamics. This leads to an irreversible quantum theory (see for instance [1]). An other possibility is this mesoscopic description of a thermodynamic system using only its restricted macroscopic information with respect to the observables. The microscopic background theory remains unchanged (see for instance [2], [3]). There is also a combination of these two methods treated in [4], [5]. We will use here the second one of the above-mentioned methods, the mesoscopic theory using conventional microscopic dynamics.

Let us consider a discrete system $\mathcal{S}$. The interaction between $\mathcal{S}$ and its environment shall be completely described by their heat exchange, power exchange and material exchange. Such systems are called Schottky systems according to [6]. Let $\mathcal{S}$ be included in an isolated system, so that we can call that part of the isolated system, that is not $\mathcal{S}$, the environment $\mathcal{E}$.



Since the isolated compound system does not interact with any environment, we can choose a quantum mechanical description using its density matrix satisfying the von Neumann dynamics.

The mesoscopic description of $\mathcal{S}$ is based on the choise of a restricted set of observables

*Financial support by the VISHAY Company, D-95085 Selb, is gratefully acknowledged.

that are relevant to the considered problem. This set of relevant observables which have to be linearily independent of each other is called *beobachtungsebene* [7]

$$\mathcal{B} := \{G_1, \ldots, G_n\}$$

$$G_i = G_i^+ \quad \textit{for all } \; i \in \{1, \ldots, n\}\,.$$

Let us introduce the abbreviation

$$\mathbf{G} := (G_1 \ldots G_n)^t\,.$$

The expectation values of those observables are given by

$$\begin{array}{rrcl} & g_i & := & \operatorname{tr}(G_i\,\varrho) \quad \textit{for all } \; i \in \{1, \ldots, n\} \\ \text{or} & \mathbf{g} & := & \operatorname{tr}(\mathbf{G}\,\varrho)\,, \end{array}$$

if ϱ is the microscopic density operator of the considered isolated compound system.

In the standard situation, the observables $\mathbf{G}$ of the beobachtungsebene depend on some work variables $a_1(t), \ldots, a_m(t)$. This is for instance the case, if we vary the volume of the considered discrete system $\mathcal{S}$ with a piston during the experiment. The abbreviation

$$\mathbf{a} := (a_1 \ldots a_m)^T$$

will be used henceforth.

On the mesoscopic level of description we are not interested in the exact microscopic state ϱ, but in the expectation values $\mathbf{g} = \operatorname{tr}(\mathbf{G}\,\varrho)$ of the observables which we are able to measure. For a chosen set of observables $\mathbf{G}(\mathbf{a})$, there exist a lot of microscopical states that are macroscopically indistinguishable, because their expectation values $\mathbf{g}$ are the same. In this context, we can define:

A density operator $\hat{\varrho}$ is called *accompanying process of ϱ with respect to $\mathcal{B}$*, if

$$\operatorname{tr}\big(\mathbf{G}(t)\,\varrho(t)\big) = \operatorname{tr}\big(\mathbf{G}(t)\,\hat{\varrho}(t)\big)$$

$$\operatorname{tr}\hat{\varrho}(t) = 1 \qquad \operatorname{tr}\dot{\hat{\varrho}}(t) = 0 \qquad \text{for } t \in \mathbb{R}.$$

We are now free to choose any of the accompanying processes for describing the original process.

2. Dynamics of accompanying processes

2.1. Canonical dynamics

The accompanying process $\hat{\varrho}$ of ϱ with respect to $\mathcal{B}$ that maximalizes the entropy of the considered system will be denoted as R:

(1) $$S_{\mathcal{B}} := -k \min_{\hat{\varrho}} (\operatorname{tr}(\hat{\varrho}\, \ln \hat{\varrho})) = -k \operatorname{tr}(R\, \ln R)\,.$$

Here k is the BOLTZMAN constant. R has the following form [8] [9]:

(2) $$R = \frac{1}{Z}\, e^{-\lambda\cdot\mathbf{G}}$$

with the partition function

(3) $$Z := \operatorname{tr}\, e^{-\lambda\cdot\mathbf{G}}\,.$$

R is called *generalized canonical operator* (with respect to $\mathcal{B}$). The λ are called Lagrangian multipliers. Dynamics which preserve the canonical form of the density operator of maximal entropy for all times are called *canonical*.

From (2) and (3) we can see that the generalized canonical operator depends on the λ and the $\mathbf{G}(\mathbf{a})$. Thus we can derive the canonical dynamics as follows:

$$\dot{R} = \frac{\partial R}{\partial \mathbf{a}} \cdot \dot{\mathbf{a}} + \frac{\partial R}{\partial \lambda} \cdot \dot{\lambda}\,,$$

and the coefficients are calculated in [2]. Inserting them we can state:

Canonical dynamics is given by

$$\dot{R} = R\,\lambda \cdot \left(\mathrm{tr} \left(R\,\frac{\partial \mathbf{G}}{\partial \mathbf{a}} \right) - \frac{\partial \mathbb{G}}{\partial \mathbb{A}} \right) \cdot \dot{\mathbf{a}} + R \left(\mathrm{tr}\,(R\,\mathbf{G}) - \mathbb{G} \right) \cdot \dot{\lambda}$$

with

$$\begin{aligned} \mathbb{G} &:= \int_0^1 e^{\mu\lambda\cdot\mathbf{G}}\,\mathbf{G}\,e^{-\mu\lambda\cdot\mathbf{G}}\,d\mu \\ \frac{\partial \mathbb{G}}{\partial \mathbb{A}} &:= \int_0^1 e^{\mu\lambda\cdot\mathbf{G}}\,\frac{\partial \mathbf{G}}{\partial \mathbf{a}}\,e^{-\mu\lambda\cdot\mathbf{G}}\,d\mu\,. \end{aligned}$$

2.2. The relevant part of the density operator

The vector space of linear operators on HILBERT space is called LIOUVILLE space $\mathcal{L}$ [10]. For instance the density matrix and the observables are elements of this space. Now we can introduce linear mappings on $\mathcal{L}$, so-called super-operators. An example of a super-operator is the LIOUVILLE operator (5). Here super-operators are interesting which enable us to derive dynamics of the generalized canonical operator.

Since the operators in a chosen beobachtungsebene do not form a complete base in the LIOUVILLE space $\mathcal{L}$, the density matrix has for this particular beobachtungsebene a relevant part, which contributes to the calculation of expectation values, and an irrelevant part, which does not show any effect on the trace in the expectation values:

$$\varrho(t) = \varrho_{rel}(t) + \varrho_{irrel}(t)$$

with

$$\begin{aligned} \mathrm{tr}\left(\mathbf{G}(t)\,\varrho(t)\right) &= \mathrm{tr}\left(\mathbf{G}(t)\,\varrho_{rel}(t)\right), \\ \mathbf{0} &= \mathrm{tr}\left(\mathbf{G}(t)\,\varrho_{irrel}(t)\right) \end{aligned}$$

$$\mathrm{tr}\,\varrho_{rel}(t) = 1 \quad , \quad \mathrm{tr}\,\dot{\varrho}_{rel}(t) = 0\,.$$

The isolation of these two parts is achieved by a linear mapping on $\mathcal{L}$. This operator transforms the VON NEUMANN equation – the quantum-mechanical dynamics of the density operator in SCHRÖDINGER's picture

(4) $$\dot{\varrho}(t) = -i L\,\varrho(t)$$

– into a mesoscopic dynamics of the generalized canonical operator. Here, L is the LIOUVILLE operator

(5) $$L\,X := \frac{1}{\hbar}\,[\mathcal{H}, X]\,.$$

(For more detailed information about the relevant/irrelevant part of ϱ see [11].)

There are two different methods to isolate the relevant part of the microscopic density operator. This mapping can be either linear or local linear.

1. relevant part by a *linear* mapping

$$\varrho_{rel}(t) = P(t)\,\varrho(t)\,, \tag{6}$$

2. relevant part by a *local linear* mapping

$$\dot{\varrho}_{rel}(t) = P(t)\,\dot{\varrho}(t)\,. \tag{7}$$

Here, $P(t)$ is supposed to be an idempotent super-operator, because it is desirable that

$$P(t)\,\varrho_{rel}(t) = \varrho_{rel}(t)$$

or

$$P(t)\,\dot{\varrho}_{rel}(t) = \dot{\varrho}_{rel}(t)$$

is valid. Let us define the operator

$$Q(t) := \underline{\underline{1}} - P(t)\,.$$

If P is idempotent, Q is idempotent, too.

We can also project an accompanying process instead of the microscopic density operator. Both procedures should yield the same relevant part, because both $\hat{\varrho}$ and ϱ describe the same macroscopic state and yield the same expectation values.

$$P(t)\,\varrho(t) \;=\; P(t)\,\hat{\varrho}(t) = \varrho_{rel}(t)\,,$$

respectively

$$P(t)\,\dot{\varrho}(t) \;=\; P(t)\,\dot{\hat{\varrho}}(t) = \dot{\varrho}_{rel}(t)\,.$$

Fick-Sauermann dynamics

The case (6) in which P maps $\varrho(t)$ specially to $R_{rel}(t)$ (cf. [8] [9]) has been treated by FICK and SAUERMANN [10]. Starting out with the VON NEUMANN equation (4) they derived the *Fick-Sauermann dynamics*

$$\begin{aligned}\dot{R}_{rel}(t) &= -i\big(P(t)\,L(t) + i\,\dot{P}(t)\big)\,R_{rel}(t)\\ &- \int_{t_0}^{t}\big(P(t)\,L(t) + i\,\dot{P}(t)\big)\,T(t,s)\,\big(Q(s)\,L(s)\\ &- i\,\dot{P}(s)\big)\,R_{rel}(s)\,ds\end{aligned} \tag{8}$$

with

$$\begin{aligned}\frac{\partial}{\partial s}\,T(t,s) &= i\,T(t,s)\,\big(Q(s)\,L(s) - i\,\dot{P}(s)\big)\,,\\ T(t,t) &= 1\,,\end{aligned}$$

and

$$\varrho(t_0) = R_{rel}(t_0)\,.$$

One possible operator P for this dynamics is the *Kawasaki-Gunton operator* [12]

$$P^{KG} : \mathcal{L} \to \mathcal{L}$$

$$P^{KG}\, X := R_{rel}\, \mathrm{tr} X + \frac{\partial R_{rel}}{\partial \mathbf{g}} \cdot (\mathrm{tr}\,(\mathbf{G}\, X) - \mathbf{g}\, \mathrm{tr} X)\ . \tag{9}$$

In this case, the dynamics (8) is an implicit differential equation, because $\dot{R}_{rel}$ is included in $\dot{P}^{KG}(t)$, which appears on the right hand side of the equation.

Robertson dynamics

Let us consider the dynamics using the local linear mapping (7). This case has been treated by ROBERTSON [13]. He started out with the VON NEUMANN equation (4) and assumed that $\varrho_{rel}(t)$ preserves the form of the generalized canonical operator for all time:

$$\dot{R}_{rel}(t) = P(t)\, \dot{\varrho}(t)\,. \tag{10}$$

Then he derived the so-called *Robertson dynamics*

$$\dot{R}_{rel}(t) = -i\, P(t)\, L(t)\, R_{rel}(t) - \int_{t_0}^{t} P(t)\, L(t)\, T(t,s)\, Q(s)\, L(s)\, R_{rel}(s)\, ds \tag{11}$$

with

$$\frac{\partial}{\partial s} T(t,s) = i\, T(t,s)\, Q(s)\, L(s)\,, \tag{12}$$

$$T(t,t) = 1\,, \tag{13}$$

$$\varrho(t_0) = R_{rel}(t_0)\,. \tag{14}$$

Although ROBERTSON derived this dynamics only for constant work variables, the dynamics remains its form also for time dependent work variables. However, we must now use an another mapping $P(t)$ than the ROBERTSON operator [13] or the KAWASAKI-GUNTON operator (9), which are used in ROBERTSON dynamics, because they only satisfy (10) if the work variables are constant in time. This problem is treated in [14] and partly in [15], too.

3. Positivity of entropy production

From (1) and (2) we get for the rate of entropy in canonical dynamics [2]:

$$\dot{S} = -k\, \mathrm{tr}\,(\dot{R}\, \ln R) = k\, \mathrm{tr}\,(\lambda \cdot \mathbf{G}\, \dot{R})\,. \tag{15}$$

The rate of entropy in an isolated system is called *entropy production* σ:

$$\sigma := \dot{S}\,\Big|_{\dot{\mathbf{a}}=\mathbf{0},\ \dot{Q}=0,\ \dot{\mathbf{n}}=\mathbf{0}}\,. \tag{16}$$

Considering a system $\mathcal{S}$ in contact with its environment $\mathcal{E}$ during a contact time Δt, that is sufficiently short, conduction problems are out of scope and exclusively the contact problem can be treated. If all the quantum mechanical drift terms [5] are vanishing in the chosen beobachtungsebene

$$\mathbf{v} := -i\, \mathrm{tr}\,(\mathbf{G} L R) = \mathbf{0}$$

and if we make a short time approximation (Taylor-expansion and neglecting quadratic and higher powers of Δt), the FICK-SAUERMANN dynamics using the KAWASAKI-GUNTON operator transforms into *contact time dynamics* [15]

$$\dot{R}_{rel} = P^{KG}\, R_{rel} - (P^{KG}\, L + i\, \dot{P}^{KG})(L - i\, \dot{P}^{KG})\, R_{rel}\, \Delta t\,.$$

The corresponding rate of entropy $\dot{S}$ and the entropy production σ of $\mathcal{S}$ can be calculated by inserting (8) into (15) and (16):

$$\sigma = \dot{S}\,\Big|_{\dot{\mathbf{a}}=\mathbf{0},\ \dot{Q}=0,\ \dot{\mathbf{n}}=\mathbf{0}} = k\,(i\,\lambda \cdot L\,\mathbf{G}\,\big|\,i\,\lambda \cdot L\,\mathbf{G})\,\Delta t \geq 0\,.$$

Here, the parentheses stand for the generalized MORI product [16]

$$(F\,\big|\,G) := \int_0^1 \mathrm{tr}\,(R_{rel}\, F^{+}\, R_{rel}^{u}\, G\, R_{rel}^{-u})\, du$$

which is a scalar product.

So it is possible to show the positivity of entropy production using this formalism.

4. Outlook

The question we are investigating is, if the maximum entropy principle is valid for systems in non-equilibrium, too. At this point, we can say that there are good prospects to answer this question in the near future using the formalism of quantum thermodynamics presented here.

References

[1] BERETTA G.P., GYFTOPOULOS E.P., PARK J.L. AND HATSOPOULOS G.N., *Quantum thermodynamics. A new equation of motion for a single constituent of matter*, Il Nuovo Cimento **82** B (1984), 169–191.

[2] MUSCHIK W. AND KAUFMANN M., *Quantum-thermodynamical description of discrete non-equilibrium systems*, Journal of Non-Equilibrium Thermodyn. **19** (1994), 76–94.

[3] ALIAGRA J., OTERO D., PLASTINO A. AND PROTO A.N. *Quantum thermodynamics and information theory*, Physical Review **38** A (1988), 918–929.

[4] KAUFMANN M., *Quantum thermodynamics of discrete systems endowed with time dependent work variables and based on a dissipative v. Neumann equation*, Wissenschaft und Technik Verlag, Berlin 1996.

[5] SCHIRRMEISTER D., *Unterschiedliche mikroskopische Dynamiken zur Quantenthermodynamik unter Berücksichtigung explizit zeitabhängiger thermodynamischer Zustände*, Diplomarbeit, TU Berlin 1999.

[6] SCHOTTKY W., *Thermodynamik*, Verlag von Julius Springer, Berlin 1929.

[7] SCHWEGLER H., *Verallgemeinerte physikalische Entropien auf informationstheoretischer Grundlage*, Zeitschrift für Naturforschung **20** (1965), 1543–1553.

[8] JAYNES E.T., *Information theory and statistical mechanics*, Physical Review **106** (1957), 620–630.

[9] JAYNES E.T., *Information theory and statistical mechanics II*, Physical Review **108** (1957), 171–190.

[10] FICK E. AND SAUERMANN G., *Quantum statistics of dynamic processes*, Springer, Heidelberg 1990.

[11] BALIAN R., ALHASSID Y. AND REINHARDT H., *Dissipation in many-body systems: a geometric approach based on information theory*, Physics Reports **131** (1986), 1–146.

[12] KAWASAKI K. AND GUNTON J.D., *Theory of nonlinear transport processes: nonlinear shear viscosity and normal stress effects*, Physical Review **8** A (1973), 2048–2064.

[13] ROBERTSON B., *Equations of motion in nonequilibrium statistical mechanics*, Physical Review **144** (1966), 151–161.

[14] KATO A., *Dynamics of statistical operators and entropy production in nonisolated discrete nonequilibrium systems*, Diplomarbeit, TU Berlin 1999.

[15] KATO A., KAUFMANN M., MUSCHIK W. AND SCHIRRMEISTER D., *Different dynamics and entropy rates in quantum-thermodynamics*, Journal of Non-Equilibrium Thermod. **25** (2000), 63–86.

[16] MORI H., *A continued-fraction representation of the time-correlation functions*, Progress of Theoretical Physics **34** (1965), 399–416.

AMS Subject Classification: 94A17, 62B05.

Akiko KATO, Wolfgang MUSCHIK, Dirk SCHIRRMEISTER
Institut für Theoretische Physik
Technische Universität Berlin
Sekretariat PN7-1, Hardenbergstrasse 36
D-10623 Berlin, GERMANY
e-mail: akiko@itp.physik.tu-berlin.de
e-mail: muschik@physik.tu-berlin.de

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

C.-S. Man - L. Noble*

DESIGNING TEXTURED POLYCRYSTALS WITH SPECIFIC ISOTROPIC MATERIAL TENSORS: THE ODF METHOD

Abstract. Herein we study the following problem: Suppose we are given a supply of grains, which are of the same material and have equal volume. Given a finite set of material tensors $\mathbb{H}^{(i)}$, can we find an arrangement of grains in an aggregate so that all the tensors $\mathbb{H}^{(i)}$ pertaining to this aggregate are isotropic? In this paper we examine the preceding problem within the special context of physical theories where material anisotropy of polycrystalline aggregates is determined by crystallographic texture, and we restrict our attention to tensors whose anisotropic part is linear in the texture coefficients. A method is developed by which the preceding problem is answered positively for tensors of various orders and grains of various crystal symmetries. Our method uses the machinery developed in quantitative texture analysis. It is based on the symmetry properties of the orientation distribution function (ODF) and appeals to some recent findings on how crystallographic texture affects material tensors of weakly textured polycrystals. As illustration, explicit solutions are worked out for the fourth-order elasticity tensor and for the sixth-order acoustoelastic tensor.

1. Introduction

Consider an aggregate $\mathcal{A}$ of N linearly elastic cubic crystallites $\mathcal{B}_\alpha$, which are of the same material and have equal volume. Let a reference crystallite $\mathcal{B}_o$ be chosen, and let $\mathbb{C}^o$ be its elasticity tensor. For a rotation R and fourth-order tensor $\mathbb{H}$, let $R^{\otimes 4}$ be the linear transformation on the space of fourth-order tensors such that $\widetilde{\mathbb{H}} \equiv R^{\otimes 4}\mathbb{H}$ has its Cartesian components given by

$$\widetilde{H}_{ijkl} = R_{ip}R_{jq}R_{kr}R_{ls}H_{pqrs},$$

where R_{ij} and H_{pqrs} denote the components of R and of $\mathbb{H}$, respectively, and repeated suffixes mean summation from 1 to 3. Under the Voigt model, the effective elasticity tensor of the aggregate $\mathcal{A}$ is given by

$$\overline{\mathbb{C}} = \frac{1}{N}\sum_{\alpha=1}^{N} R_\alpha^{\otimes 4}\mathbb{C}^o, \tag{1}$$

where the rotation R_α defines the orientation of $\mathcal{B}_\alpha$ with respect to $\mathcal{B}_o$. Recently Bertram et al. [1, 2], in the course of their work on texture-induced elastic anisotropy that results from finite

*Man first learnt of the work of Bertram et al. when he visited Dr. Roberto Paroni at Carnegie Mellon in December 1998. He thanks Dr. Paroni for the stimulating discussions. We are grateful to Professor Albrecht Bertram for sending us preprints of their papers [1, 2]. The findings reported here were obtained in the course of work supported in part by a grant from the National Science Foundation (No. DMS-9803441) and by a DoD EPSCoR grant from AFOSR (No. F49620-98-1-0469).

plastic deformations of polycrystals, raised and answered the following question: What is the smallest number N of cubic grains required and how should they be arranged (i.e., determine R_α for $\alpha = 1, 2, ..., N$) so that $\overline{\mathbb{C}}$ is isotropic? They proved that the smallest N is 4 and determined R_1, ..., R_4 for $\overline{\mathbb{C}}$ in Eq. (1) to be isotropic. In their papers Bertram et al. showed also that each arrangement R_α ($\alpha = 1, ..., N$) which delivers an isotropic $\overline{\mathbb{C}}$ under the Voigt model also renders the effective elasticity tensor isotropic under the Reuss model and under the "geometric mean" estimate [3, 4].

For broader applications, naturally one would ask analogous questions that pertain to aggregates of grains of other crystalline symmetries and to other material tensors. For example, the sixth-order acoustoelastic tensor [5, 6] figures prominently in problems that concern wave propagation in prestressed solids; in some formulations [7], yield functions and flow rules in plasticity involve not only fourth-order tensors but also sixth-order and even higher order tensors. For definiteness, let us paraphrase the problem that we shall investigate in this paper as follows: Suppose we are given an unlimited supply of grains $\mathcal{B}_\alpha$, which are of the same material, have equal volume, and have crystal symmetry characterized by the group $\mathcal{G}_{\text{cr}}$. We consider aggregates $\mathcal{A}$ made up of a finite number N of grains $\mathcal{B}_\alpha$. Given a finite set of material tensors $\mathbb{H}^{(1)}, \ldots, \mathbb{H}^{(s)}$, find a number N and an arrangement of grains $\mathcal{B}_\alpha$ for which the N-grain aggregate $\mathcal{A}$ has all its tensors $\mathbb{H}^{(i)}$ ($i = 1, \ldots, s$) isotropic. To reduce the foregoing to a manageable mathematical problem, we shall restrict our discussion to a special class of physical theories where material anisotropy of polycrystalline aggregates is determined by crystallographic texture (i.e., the preferred orientations of the constituting grains), and we shall only consider what we call tensor functions of class (*) (see Definition 2 in Section 3 for a precise definition). Prime examples are tensors of polycrystals defined by orientational averaging (e.g., $\overline{\mathbb{C}}$ in Eq. (1)) and material tensors of "weakly textured" polycrystals [8, 9].

In their papers [1, 2], Bertram et al. restricted their attention to fourth-order tensors and to aggregates of grains with cubic symmetry. As far as we can discern, the methods that they developed are applicable only for those special circumstances. To tackle our more general problem, we shall appeal to the machinery developed in quantitative texture analysis [10, 11, 12], in particular the restrictions that crystal and texture symmetry impose on the orientation distribution function (ODF), and draw on some recent findings of Man [8, 13] with regard to how crystallographic texture affects material tensors of weakly textured polycrystals. Since the expansion coefficients c^l_{mn} of the ODF (see Eq. (9) in Section 2.2) play a crucial role in the present work, we call the approach developed in this paper for designing polycrystals with specific isotropic material tensors the *ODF method*.

As the reader will see in detail below, this method relies on finding suitable combinations of crystal and texture symmetries which produce solvable systems of equations where specific texture coefficients c^l_{mn} of an aggregate are set equal to zero. In this paper we take $\mathcal{G}_{\text{cr}}$ to be a finite rotation group which satisfies the crystallographic restriction, i.e., $\mathcal{G}_{\text{cr}} = C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T$, or O in the Schoenflies notation. Let $\mathcal{G}_{\text{tex}}$ be a group of texture symmetry. Unlike $\mathcal{G}_{\text{cr}}$, $\mathcal{G}_{\text{tex}}$ need not observe the crystallographic restriction. The only requirement on $\mathcal{G}_{\text{tex}}$ is that it be a subgroup of the rotation group. Since we shall use various $\mathcal{G}_{\text{tex}}$'s for building aggregates that consist of a finite number of crystallites, in this paper we use only those $\mathcal{G}_{\text{tex}}$ which are finite. In what follows, for a finite group G, we write $|G|$ for the order of G.

2. Preliminaries

In this section we recapitulate some facts about orientation measures and tensor representations of the rotation group, which we shall use below. Throughout this paper, when we talk about orientations of crystallites, it is understood that a reference crystallite has been chosen. The orientation of a crystallite is then specified by a rotation with respect to the reference.

2.1. Tensor representations of the rotation group

Let V be the translation space of the three-dimensional Euclidean space, and V^r the r-fold tensor product $V \otimes V \cdots \otimes V$. A rotation Q on V induces a linear transformation $Q^{\otimes r}$ on V^r defined by

$$(Q^{\otimes r}\mathbb{H})_{i_1\cdots i_r} = Q_{i_1 j_1} Q_{i_2 j_2} \cdots Q_{i_r j_r} H_{j_1\cdots j_r}, \tag{2}$$

where repeated suffixes mean summation from 1 to 3. The map $Q \mapsto Q^{\otimes r}$ defines [14] a linear representation of the rotation group SO(3) on V^r. A subspace $Z \subset V^r$ is said to be invariant under the action of the rotation group if it remains invariant under $Q^{\otimes r}$ for each rotation Q. Let $Q^{\otimes r}|Z$ be the restriction of $Q^{\otimes r}$ on Z. Then $Q \mapsto Q^{\otimes r}|Z$ defines a linear representation of the rotation group on Z. We refer to these representations of SO(3) on tensor spaces as tensor representations. By formally introducing the complexification V_c of V and Z_c of Z (see Miller [14], p. 105), we shall henceforth regard the tensor representations as complex representations. For simplicity, we shall suppress the subscript "c" and continue to write the complex representations as $Q \mapsto Q^{\otimes r}|Z$.

In what follows we shall be concerned only with tensor spaces Z which remain invariant under the action of the rotation group and, to specify the various types of tensors, we shall adopt a system of notation advocated by Jahn [15] and Sirotin [16]. In this notation, V^2 stands for the tensor product $V \otimes V$, $[V^2]$ the space of symmetric second-order tensors, $V[V^2]$ the tensor product of V and $[V^2]$, $[[V^2]^2]$ the symmetric square of $[V^2]$ (i.e., the symmetrized tensor product of $[V^2]$ and $[V^2]$), $[[V^2]^3]$ the symmetric cube of $[V^2]$, $[V^2][[V^2]^2]$ the tensor product of $[V^2]$ and $[[V^2]^2]$, ..., etc. For instance, the fourth-order elasticity tensor is of type $[[V^2]^2]$, and the sixth-order acoustoelastic tensor of type $[V^2][[V^2]^2]$.

Following usual practice [16], we shall use the notation for each type of tensor space (e.g., $[[V^2]^2]$) to denote also the corresponding tensor representation (e.g., $Q \mapsto Q^{\otimes 4}|[[V^2]^2]$). Whether we really mean the tensor space or the corresponding tensor representation should be clear from the context. The rotation group has a complete set of absolutely irreducible unitary representations $\mathcal{D}_l$ ($l = 0, 1, 2, ...$) of dimension $2l + 1$. Tensor representations of the rotation group are, in general, not irreducible. Each tensor representation $Q \mapsto Q^{\otimes r}|Z$ can be decomposed as a direct sum of subrepresentations, each of which is equivalent to some $\mathcal{D}_l$:

$$Z = n_0\mathcal{D}_0 + n_1\mathcal{D}_1 + \cdots + n_r\mathcal{D}_r, \tag{3}$$

where n_k is the multiplicity of $\mathcal{D}_k$ in the decomposition. When $Z = V^r$, we always have $n_r = 1$ in the decomposition formula. When Z is a proper subspace of V^r, some n_k's in Eq. (3) may be equal to zero, but we must have $\dim Z = \sum_{k=0}^{r} n_k(2k + 1)$. For example, we have

$$[[V^2]^2] = 2\mathcal{D}_0 + 2\mathcal{D}_2 + \mathcal{D}_4, \tag{4}$$

$$[V^2][[V^2]^2] = 4\mathcal{D}_0 + 2\mathcal{D}_1 + 7\mathcal{D}_2 + 3\mathcal{D}_3 + 4\mathcal{D}_4 + \mathcal{D}_5 + \mathcal{D}_6, \tag{5}$$

and $\dim [[V^2]^2] = 21$, $\dim [V^2][[V^2]^2] = 126$. Here a term such as $\mathcal{D}_6$ in Eq. (5) denotes a $2 \times 6 + 1 = 13$ dimensional subspace of $[V^2][[V^2]^2]$, over which the subrepresentation of

$Q \mapsto Q^{\otimes 6}$ is equivalent to the irreducible representation $\mathcal{D}_6$. Decomposition formulae such as Eqs. (4) and (5) above can be derived by computing the character of the tensor representation in question [15, 17] or by other methods [16].

A tensor $\mathbb{H} \in Z \subset V^r$ is isotropic if and only if it takes value in the subspace $n_0\mathcal{D}_0$, which is a direct sum of n_0 1-dimensional subspaces invariant under $Q^{\otimes r}$. Thus we can read from Eqs. (4) and (5) that isotropic elasticity and acoustoelastic tensors in $[[V^2]^2]$ and $[V^2][[V^2]^2]$ are specified by two and four material constants, respectively.

In what follows we shall refer to formula (3) as the decomposition of the tensor space Z into its irreducible parts.

2.2. Orientation measures

For brevity, henceforth we write $\mathcal{G}$ for the rotation group SO(3), which is a compact topological group. Let $C(\mathcal{G})$ be the space of continuous complex functions on $\mathcal{G}$. It is a Banach space under the supremum norm. The elements of $C(\mathcal{G})^*$, the dual space of $C(\mathcal{G})$, are the Radon measures on $\mathcal{G}$. For $f \in C(\mathcal{G})$ and $\mu \in C(\mathcal{G})^*$, we denote by $\langle \mu, f \rangle$ the complex number that results when μ is applied to f. Anticipating the applications that we shall investigate, we call positive Radon measures $\wp$ with $\wp(\mathcal{G}) = 1$ orientation measures, and we denote by $\mathcal{M}(\mathcal{G})$ the set of orientation measures on $\mathcal{G}$. Under the weak* topology, $\mathcal{M}(\mathcal{G})$ is compact in $C(\mathcal{G})^*$ (cf. [18], p. 19).

For $Q \in \mathcal{G}$, the orientation measure δ_Q defined by

$$\langle \delta_Q, f \rangle = f(Q) \qquad \text{for each } f \in C(\mathcal{G})$$

is called the Dirac measure concentrated at Q. Discrete orientation measures are finite linear combinations of Dirac measures $\sum_i a_i \delta_{Q_i}$, where $a_i > 0$ for each i and $\sum_i a_i = 1$.

For orientation measures $\wp$ and a fixed $\mathbb{H}^o \in Z \subset V^r$, we consider (cf. Eq. (1))

$$\overline{\mathbb{H}}(\wp) = \int_{\mathcal{G}} R^{\otimes r}\mathbb{H}^o d\wp(R). \tag{6}$$

When the orientation measure $\wp$ is absolutely continuous with respect to the Haar measure $\wp_H$ (with $\wp_H(\mathcal{G}) = 1$), the Radon-Nikodym derivative $d\wp/d\wp_H$ is well defined. Following common practice, we call

$$w = \frac{1}{8\pi^2}\frac{d\wp}{d\wp_H} \tag{7}$$

the orientation distribution function (ODF), and we may recast Eq. (6) in terms of the ODF as

$$\overline{\mathbb{H}}(w) = 8\pi^2 \int_{\mathcal{G}} R^{\otimes r}\mathbb{H}^o w(R) d\wp_H(R). \tag{8}$$

If w is square integrable on $\mathcal{G}$ with respect to $\wp_H$, we may choose a spatial Cartesian coordinate system and expand w in an infinite series as follows:

$$w(R(\psi,\theta,\phi)) = \frac{1}{8\pi^2} + \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c^l_{mn} D^l_{mn}(R(\psi,\theta,\phi)), \tag{9}$$

$$c^l_{mn} = (-1)^{m+n}\overline{c^l_{\bar{m}\bar{n}}}. \tag{10}$$

Here D^l_{mn} are the Wigner D-functions [19, 20]; (ψ, θ, ϕ) are the Euler angles [11] corresponding to the rotation R; $\bar{z}$ denotes the complex conjugate of the complex number z, and $\bar{m} = -m$. We call the expansion coefficients

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \int_{\mathcal{G}} \overline{D^l_{mn}(R)} d\wp(R) \tag{11}$$

the texture coefficients; they are related to Roe's [11] coefficients W_{lmn} by the formula

$$W_{lmn} = (-1)^{m-n} \sqrt{\frac{2}{2l+1}}\, c^l_{mn}.$$

Let $\mathcal{M}_2(\mathcal{G})$ be the set of orientation measures which are absolutely continuous and have their corresponding ODF square integrable. Under the weak* topology, $\mathcal{M}_2(\mathcal{G})$ is dense in $\mathcal{M}(\mathcal{G})$, because discrete orientation measures lie (see, e.g. [21]) in the weak* closure of $\mathcal{M}_2(\mathcal{G})$ and they are dense in $\mathcal{M}(\mathcal{G})$ (see [18], p. 27).

For any sequence ${}^{(k)}w$ of square-integrable ODF's whose corresponding orientation measures ${}^{(k)}\wp$ converge weakly* to the Dirac measure δ_Q, by Eq. (11) their texture coefficients ${}^{(k)}c^l_{mn}$ converge to

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \overline{D^l_{mn}(Q(\psi, \theta, \phi))}. \tag{12}$$

We call the c^l_{mn}'s given by Eq. (12) the texture coefficients pertaining to the Dirac measure δ_Q. Likewise, we associate a unique set of texture coefficients c^l_{mn} to each orientation measure $\wp$. Thus the texture coefficients c^l_{mn}, originally defined on $\mathcal{M}_2(\mathcal{G})$ by Eq. (11), are extended by continuity to become weakly* continuous functions on $\mathcal{M}(\mathcal{G})$.

Now consider an aggregate $\mathcal{A}$ which consists of a single crystallite $\mathcal{B}$ with crystal symmetry specified by a point group $\mathcal{G}_{\text{cr}}$ which is a subgroup of the rotation group $\mathcal{G}$. Let N_{cr} be the order of $\mathcal{G}_{\text{cr}}$, and let $\check{Q}_k$ $(k = 1, ..., N_{\text{cr}})$ be the elements of $\mathcal{G}_{\text{cr}}$. Suppose $\mathcal{B}$ assumes an orientation specified by the rotation R_0. The orientation measure of $\mathcal{A}$ is given by

$$\wp = \frac{1}{N_{\text{cr}}} \sum_{k=1}^{N_{\text{cr}}} \delta_k,$$

where δ_k is the Dirac measure concentrated at $R_0 \check{Q}_k$. The texture coefficients of $\mathcal{A}$ are then given by

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_{\text{cr}}} \cdot \sum_{k=1}^{N_{\text{cr}}} \overline{D^l_{mn}(R_0 \check{Q}_k)}. \tag{13}$$

Let $\mathcal{G}^{(1)}$ be a finite subgroup of $\mathcal{G}$ with elements $Q^{(1)}_j$, $j = 1, ..., N_1$, where N_1 is the order of $\mathcal{G}^{(1)}$. Let $\mathcal{A}^{(1)}$ be an aggregate of N_1 crystallites $\mathcal{B}_j$ of equal volume, which have crystal symmetry $\mathcal{G}_{\text{cr}}$ and orientations specified by $Q^{(1)}_j R_0$. The texture coefficients of $\mathcal{A}^{(1)}$ are:

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_1} \cdot \frac{1}{N_{\text{cr}}} \cdot \sum_{j=1}^{N_1} \sum_{k=1}^{N_{\text{cr}}} \overline{D^l_{mn}(Q^{(1)}_j R_0 \check{Q}_k)}. \tag{14}$$

If the entire aggregate $\mathcal{A}^{(1)}$ is rotated by R_1, the rotated aggregate $\mathcal{A}_R^{(1)}$ will have texture coefficients

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_1} \cdot \frac{1}{N_{\mathrm{cr}}} \cdot \sum_{j=1}^{N_1} \sum_{k=1}^{N_{\mathrm{cr}}} \overline{D^l_{mn}(R_1 Q_j^{(1)} R_0 \check{Q}_k)}. \tag{15}$$

Let $\mathcal{G}^{(2)}$ be a finite subgroup of $\mathcal{G}$ with elements $Q_i^{(2)}$, $i = 1, \ldots, N_2$, where N_2 is the order of $\mathcal{G}^{(2)}$. Let $\mathcal{A}^{(2)}$ be the aggregate of $N_1 \times N_2$ crystallites formed by replacing each crystallite $\mathcal{B}_j$ in the aggregate $\mathcal{A}_R^{(1)}$, whose orientation is $R_1 Q_j^{(1)} R_0$, with N_2 copies whose orientations are $Q_i^{(2)} R_1 Q_j^{(1)} R_0$ ($i = 1, \ldots, N_2$). The texture coefficients of aggregate $\mathcal{A}^{(2)}$ are:

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_2} \cdot \frac{1}{N_1} \cdot \frac{1}{N_{\mathrm{cr}}} \cdot \sum_{i=1}^{N_2} \sum_{j=1}^{N_1} \sum_{k=1}^{N_{\mathrm{cr}}} \overline{D^l_{mn}(Q_i^{(2)} R_1 Q_j^{(1)} R_0 \check{Q}_k)}. \tag{16}$$

Let $\mathcal{G}_{\mathrm{cr}} = \mathcal{G}^{(0)}$, where $\mathcal{G}^{(0)} \subset \mathcal{G}$ is a specific point group. We call $\mathcal{A}^{(1)}$, and $\mathcal{A}^{(2)}$ aggregates of type $\mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$, and $\mathcal{G}^{(2)} R_1 \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$, respectively. (We shall take aggregate $\mathcal{A}_R^{(1)}$ to be of the same type as that of $\mathcal{A}^{(1)}$.) In general, for $p \geq 1$, for a set of rotations $R_0, \ldots, R_{p-1}$, and finite subgroups $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(p)}$ of the rotation group $\mathcal{G}$, we can easily write down the formula for the texture coefficients c^l_{mn} that pertain to the aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} \ldots \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$, which consists of $N_p \times N_{p-1} \times \cdots \times N_1$ crystallites of equal volume and with $\mathcal{G}_{\mathrm{cr}} = \mathcal{G}^{(0)}$, namely:

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_p} \cdot \ldots \cdot \frac{1}{N_1} \cdot \frac{1}{N_0} \cdot \sum_{i_p=1}^{N_p} \ldots \sum_{i_1=1}^{N_1} \sum_{i_0=1}^{N_0} \overline{D^l_{mn}(Q_{i_p}^{(p)} R_{p-1} \cdots Q_{i_1}^{(1)} R_0 Q_{i_0}^{(0)})}, \tag{17}$$

where the order and elements of $\mathcal{G}^{(0)}$ are denoted by N_0 and $Q_{i_0}^{(0)}$ ($i_0 = 1, \ldots, N_0$), respectively.

3. The ODF method

Let $w_{\mathrm{iso}} = 1/(8\pi^2)$, the ODF when all texture coefficients are zero. Let $m = 8\pi^2 \wp_H$, and let $L^2(\mathcal{G}, m)$ be the space of complex functions on $\mathcal{G}$ which are square integrable with respect to the measure m. Let

$$\mathcal{H}_0 = \{f \in L^2(\mathcal{G}, m) : \int_{\mathcal{G}} f \, dm = 0\}, \tag{18}$$

$$\mathcal{H} = \{w \in L^2(\mathcal{G}, m) : w = w_{\mathrm{iso}} + f, \text{ where } f \in \mathcal{H}_0\}. \tag{19}$$

All orientation distribution functions w fall in $\mathcal{H}$.

Let w be the ODF which characterizes the crystallographic texture of a polycrystalline aggregate $\mathcal{A}$. After $\mathcal{A}$ undergoes a rotation Q, its texture is described by a new ODF $\mathcal{T}_Q w$, which is related to w, the ODF before rotation, by the formula

$$\mathcal{T}_Q w(R) = w(Q^T R) \tag{20}$$

for each rotation R.

The tensor function $\overline{\mathbb{H}} : \mathcal{M}(\mathcal{G}) \longrightarrow V^r$, as defined in Eq. (6) by orientational averaging, is weakly* continuous. When restricted to $\mathcal{M}_2(\mathcal{G})$, the function $\overline{\mathbb{H}}(\cdot)$ can be taken as a function of the ODF. This function is defined by Eq. (8), which makes sense for any argument f in $L^2(\mathcal{G}, m)$. As is apparent from Eq. (8), the extended function $f \mapsto \overline{\mathbb{H}}(f)$ is strongly continuous on $L^2(\mathcal{G}, m)$. Substituting Eq. (9) into Eq. (8), we observe that

$$\overline{\mathbb{H}}(w) = \overline{\mathbb{H}}_{\text{iso}} + \overline{\mathbb{H}}'[w - w_{\text{iso}}], \tag{21}$$

where

$$\overline{\mathbb{H}}_{\text{iso}} = \int_{\mathcal{G}} R^{\otimes r} \mathbb{H}^o d\wp_H(R)$$

is the isotropic part of $\overline{\mathbb{H}}$, and

$$\overline{\mathbb{H}}'[w - w_{\text{iso}}] = 8\pi^2 \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^l_{mn} \int_{\mathcal{G}} R^{\otimes r} \mathbb{H}^o D^l_{mn}(R) d\wp_H(R),$$

the anisotropic part, is linear and strongly continuous on $\mathcal{H}_0$. From the invariance of the Haar measure $\wp_H$, we observe immediately that $\overline{\mathbb{H}}'$ satisfies the constraint

$$\overline{\mathbb{H}}'[\mathcal{T}_Q w - w_{\text{iso}}] = Q^{\otimes r} \left(\overline{\mathbb{H}}'[w - w_{\text{iso}}]\right) \tag{22}$$

for each rotation Q.

Tensor functions defined by orientational averaging are prime examples of the class (*) of material tensors that we study in this paper. We formalize this class with a definition.

DEFINITION 2. *Let Z be a subspace of V^r which is invariant under $Q^{\otimes r}$ for each rotation Q. We say that a tensor function $\mathbb{B} : \mathcal{M}(\mathcal{G}) \longrightarrow Z$ is of class (*) if*

(i) $\mathbb{B}$ *is weakly* continuous;*

(ii) when restricted to $\mathcal{M}_2(\mathcal{G})$,

$$\mathbb{B}(w) = \mathbb{B}_{\text{iso}} + \mathbb{B}'[w - w_{\text{iso}}], \tag{23}$$

where $\mathbb{B}_{\text{iso}}$ is isotropic and $\mathbb{B}'[\cdot]$ is linear and strongly continuous on $\mathcal{H}_0$;

(iii) $\mathbb{B}[\cdot]$ *observes the constraint*

$$\mathbb{B}'[\mathcal{T}_Q w - w_{\text{iso}}] = Q^{\otimes r} \left(\mathbb{B}'[w - w_{\text{iso}}]\right) \tag{24}$$

for each rotation Q.

Besides tensors defined by orientational averaging, class (*) includes material tensors pertaining to "weakly textured" polycrystals [8, 9]. Henceforth we shall consider only tensor functions of class (*).

Let $\mathbb{B} : \mathcal{M}(\mathcal{G}) \longrightarrow Z \subset V^r$ be a tensor function of class (*). In our method for designing aggregates with an isotropic $\mathbb{B}$, the following observation is instrumental:

(#) Let $Z = n_0\mathcal{D}_0 + n_1\mathcal{D}_1 + \cdots + n_r\mathcal{D}_r$ be the decomposition of the tensor space Z into its irreducible parts. Let $\mathbb{B}(\wp) = \mathbb{B}_0(\wp) + \mathbb{B}_1(\wp) + \mathbb{B}_2(\wp) + \ldots + \mathbb{B}_r(\wp)$, where $\mathbb{B}_k(\cdot)$ ($k = 0, 1, \ldots, r$) takes values in the $n_k \times (2k+1)$ dimensional subspace $n_k\mathcal{D}_k$ of Z. For $k \geq 1$, the components of $\mathbb{B}_k(\wp)$ are linear combinations of only those texture coefficients c^l_{mn} with $l = k$.

Observation (#) is an immediate corollary of a theorem due to Man [13].

REMARK 1. The tensor $\mathbb{B}(\wp)$ is isotropic if and only if $\mathbb{B}_k(\wp) = 0$ for $k = 1, 2, ..., r$. Hence, to design an aggregate with an isotropic $\mathbb{B}$, it suffices to find an orientation measure $\wp$ which has its $c^l_{mn} = 0$ for those $1 \leq l \leq r$ with $n_l \neq 0$ in the decomposition formula for Z above.

REMARK 2. Let $\mathcal{G}^{(0)}$ and $\mathcal{G}^{(p)}$ be finite rotation groups that satisfy the crystallographic restriction, and let $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(p-1)}$ be finite rotation groups. Let $\mathcal{A}$ and $\hat{\mathcal{A}}$ be aggregates of type $\mathcal{G}^{(p)}R_{p-1}\mathcal{G}^{(p-1)}...\mathcal{G}^{(1)}R_0\mathcal{G}^{(0)}$ and type $\mathcal{G}^{(0)}R_0^T\ \mathcal{G}^{(1)}...\mathcal{G}^{(p-1)}R^T_{p-1}\mathcal{G}^{(p)}$, respectively, and let c^l_{mn} and $\hat{c}^l_{mn}$ be their texture coefficients. Since $D^l_{mn}(R^T) = \overline{D^l_{nm}(R)}$ for each rotation R, we see that $\hat{c}^l_{mn} = \overline{c^l_{nm}}$. Hence, if all $c^l_{mn} = 0$ for a specific set of l's, then all $\hat{c}^l_{mn} = 0$ for the same set of l's, and vice versa. Thus, if we can find an aggregate of type $\mathcal{G}^{(p)}R_{p-1}\mathcal{G}^{(p-1)}...\mathcal{G}^{(1)}R_0\ \mathcal{G}^{(0)}$ which has an isotropic $\mathbb{B}$, we obtain at once another aggregate of type $\mathcal{G}^{(0)}R_0^T\ \mathcal{G}^{(1)}...\mathcal{G}^{(p-1)}R^T_{p-1}\mathcal{G}^{(p)}$ which has an isotropic $\mathbb{B}$.

By Remark 1, the problem of designing aggregates with their elasticity tensors isotropic reduces to that of designing aggregates with all their c^2_{mn}'s and c^4_{mn}'s zero. By the same token, an aggregate with all its $c^l_{mn} = 0$ for $1 \leq l \leq 6$ has both its elasticity and acoustoelastic tensors isotropic. In any case, to design an aggregate which has a finite set of specific material tensors isotropic, we just need to determine an arrangements of grains so that the resulting aggregate has all its $c^l_{mn} = 0$ for an appropriate finite set of l's. Let us now proceed to examine this problem.

With the original formulation of the problem of Bertram et al. [1, 2] in mind, here we seek only aggregates whose constituting crystallites all have equal volume. For simplicity, whenever no confusion should arise, we shall simply say "identical grains" or just "grains" when we really mean crystallites of the same material that have equal volume. In fact, all solutions reported in Sections 4 and 5 below are aggregates of "identical grains".

Consider a polycrystalline aggregate $\mathcal{A}$, which undergoes a rotation Q. Let c^l_{mn} and $\tilde{c}^l_{mn}$ be the texture coefficients of the aggregate before and after the rotation. These two sets of texture coefficients are related by the formula [8, 11]

$$\tilde{c}^l_{mn} = \sum_{p=-l}^{l} c^l_{pn} D^l_{pm}(Q^{-1}). \tag{25}$$

For a fixed l and n, if $c^l_{mn} = 0$ for all $-l \leq m \leq l$, then $\tilde{c}^l_{mn} = 0$ for all $-l \leq m \leq l$, irrespective of the rotation Q. This observation suggests a procedure for constructing an aggregate of crystallites with $\mathcal{G}_{\mathrm{cr}} = \mathcal{G}^{(0)}$ which has all its $c^l_{mn} = 0$ for a specific finite set of l's (say, for $l = l_1, ..., l_a$):

1. For $l = l_1$ and an n_i between $-l_1$ and l_1, find an aggregate $\mathcal{A}^{(1)}$ of type $\mathcal{G}^{(1)}R_0\mathcal{G}^{(0)}$ (see Section 2.2 above) which has $c^{l_1}_{mn_i} = 0$ for $-l_1 \leq m \leq l_1$. The job here is to seek an appropriate rotation R_0 and a finite rotation group $\mathcal{G}^{(1)}$ which meet the requirement. The aggregate $\mathcal{A}^{(1)}$ has $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(0)}$ as its group of texture symmetry and crystal symmetry, respectively. This knowledge will facilitate the search for an appropriate R_0 and $\mathcal{G}^{(1)}$, as we shall see from the specific examples in the next two sections.
2. Depending on the specific l_1 and $\mathcal{G}^{(0)}$, the aggregate $\mathcal{A}^{(1)}$ may already have its $c^{l_1}_{mn} = 0$ for all $-l_1 \leq m \leq l_1$ and $-l_1 \leq n \leq l_1$. If that is the case, for $l = l_2$ and an

n_i between $-l_2$ and l_2, find an aggregate $\mathcal{A}^{(2)}$ of type $\mathcal{G}^{(2)} R_1 \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$ which has $c^{l_2}_{mn_i} = 0$ for $-l_2 \le m \le l_2$. Since R_0 and $\mathcal{G}^{(1)}$ have already been determined, the task here is to find an appropriate rotation R_1 and a suitable finite rotation group $\mathcal{G}^{(2)}$. The aggregate $\mathcal{A}^{(2)}$ has $\mathcal{G}^{(2)}$ and $\mathcal{G}^{(0)}$ as its group of texture symmetry and crystal symmetry, respectively. Because of the transformation formula (25), aggregate $\mathcal{A}^{(2)}$ still has its $c^{l_1}_{mn} = 0$, irrespective of our choice of R_1 and $\mathcal{G}^{(2)}$ which renders the texture coefficients $c^{l_2}_{mn_i}$ of $\mathcal{A}^{(2)}$ null for all $-l_2 \le m \le l_2$. If there is an $n_j \ne n_i$ such that $c^{l_1}_{mn_j} \ne 0$ for some m, find an aggregate $\mathcal{A}^{(2)}$ of type $\mathcal{G}^{(2)} R_1 \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$ such that $c^{l_1}_{mn_j} = 0$ for all $-l_1 \le m \le l_1$.

3. Repeat the preceding procedure iteratively to find an aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} \ldots \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$ which has all its $c^l_{mn} = 0$ for $l = l_1, \ldots, l_a$.

We shall work out a few concrete examples in the next two sections to illustrate the procedure described above.

4. Example: elasticity tensor

As our first example, let us consider the elasticity tensor $\mathbb{C}$. By decomposition formula (3) and observation (#), if we wish to design an aggregate with an isotropic elasticity tensor of class (*), we need only to find an aggregate whose c^2_{mn} and c^4_{mn} coefficients are zero. We begin our discussion by revisiting the problem solved by Bertram et al. [1, 2], namely, that of cubic grains.

In what follows we always assume that a fixed spatial Cartesian coordinate system has been chosen. We write e_1, e_2, and e_3 for the orthonormal basis vectors that define this coordinate system. For a unit vector e and an angle $\omega \in [0, \pi]$, we denote by $R(e, \omega)$ the rotation about e by angle ω. All angles given below are in radians.

4.1. Cubic grains

Here $\mathcal{G}_{\mathrm{cr}} = O$. We choose a reference crystallite which has its three four-fold axes of cubic symmetry in line with the three spatial coordinate axes. This is tantamount to choosing $R(e_1, \pi/2)$, $R(e_2, \pi/2)$, and $R(e_3, \pi/2)$ to be the generators of the group O of crystal symmetry. With this choice of reference, the texture coefficients of any aggregate of cubic grains satisfy [10, 11] the equation

$$c^l_{mn} = \sum_{p=-l}^{l} c^l_{mp} D^l_{np}(Q), \tag{26}$$

for each of the 24 rotations Q in the symmetry group of the reference crystallite. As a result, any aggregate of cubic grains has [22] their c^2_{mn} coefficients all zero. Moreover, of the c^4_{mn} coefficients, only one coefficient is independent for each fixed m $(-4 \le m \le 4)$, and c^4_{m0} $(-4 \le m \le 4)$ may be chosen as the independent coefficients. An aggregate of cubic grains with $c^4_{m0} = 0$ for each m has all its c^2_{mn} and c^4_{mn} coefficients vanish and thence has an isotropic $\mathbb{C}$.

For an aggregate of one grain, there are nine equations (i.e., $c^4_{\bar{4}0}(R_0) = 0$, $c^4_{\bar{3}0}(R_0) = 0$, $c^4_{\bar{2}0}(R_0) = 0, \ldots, c^4_{20}(R_0) = 0$, $c^4_{30}(R_0) = 0$, $c^4_{40}(R_0) = 0$, where each texture coefficient is in the form of Eq. (13)) to be solved for one orientation $R_0(\psi_0, \theta_0, \phi_0)$. Clearly there need not be a solution. In fact, thanks to the work of Bertram et al. [1], we already know that this system of nine equations has no solution for R_0. By adding additional identical grains in specific orientations dictated by a group $\mathcal{G}^{(1)}$ of texture symmetry, we can place additional restrictions on the texture coefficients and reduce the number of equations which must be satisfied.

Suppose we add three identical cubic grains and arrange them so that the aggregate has orthorhombic texture symmetry with the coordinate axes being the axes of two-fold rotational symmetry (i.e., $\mathcal{G}^{(1)} = D_2$ with $R(e_2, \pi)$ and $R(e_3, \pi)$ as generators). The texture coefficients must be calculated as in Eq. (14) but there are fewer independent coefficients. For $Q \in D_2$, Eq. (25) implies that

$$c^l_{mn} = \sum_{p=-l}^{l} c^l_{mp} D^l_{np}(Q^{-1}) \tag{27}$$

holds. By considering $Q(\psi, \theta, \phi) = (0, \pi, 0)$ and $Q(\psi, \theta, \phi) = (0, 0, \pi)$, we determine that $c^l_{mn} = 0$ if m is odd, and $c^l_{\bar{m}n} = (-1)^l c^l_{mn}$ if m is even. Hence, under this texture symmetry/crystal symmetry combination, the only independent c^4_{m0} coefficients can be chosen to be c^4_{00}, c^4_{20}, and c^4_{40}, and by making these coefficients zero, all c^4_{mn} vanish.

The result is a system of three equations:

$$c^4_{00}(R_0) = 0, \qquad c^4_{20}(R_0) = 0, \qquad c^4_{40}(R_0) = 0, \tag{28}$$

where each texture coefficient is of the form given in Eq. (14). Since R_0 is parametrized by Euler angles, the equations need only be solved for $(\psi_0, \theta_0, \phi_0)$. We used the computer algebra system Maple to find solutions to the three simultaneous equations. Because of the D_2 texture symmetry and O crystal symmetry, two solutions R_0 and $R_0^{\#}$ of system (28) describe the same arrangement of grains if

$$R_0^{\#} = \widetilde{Q} R_0 \check{Q}$$

for some $\widetilde{Q} \in D_2$ and $\check{Q} \in O$. Surely we should regard such an R_0 and $R_0^{\#}$ as equivalent solutions. Since $|D_2| = 4$, $|O| = 24$, and D_2 is a subgroup of O, given a solution R_0 there will be 96, 48, or 24 solutions equivalent to it if R_0 commutes with none, one, or both of the generators of D_2. From our Maple solutions of (28), we identified the following four, which are not equivalent in the preceding sense:

$$R_0^{(1)}(\psi_0, \theta_0, \phi_0) = (0.59549275, 0.52174397, 0.59549275), \tag{29}$$

$$R_0^{(2)}(\psi_0, \theta_0, \phi_0) = (2.16628908, 0.52174397, 0.59549275), \tag{30}$$

$$R_0^{(3)}(\psi_0, \theta_0, \phi_0) = (0.97530358, 0.52174397, 0.97530358), \tag{31}$$

$$R_0^{(4)}(\psi_0, \theta_0, \phi_0) = (2.54609990, 0.52174397, 0.97530358), \tag{32}$$

where the angles are given in radians. The preceding solutions are clearly related by the equations

$$R_0^{(2)} = R(e_3, \pi/2) R_0^{(1)}, \qquad R_0^{(4)} = R(e_3, \pi/2) R_0^{(3)}. \tag{33}$$

Solution $R_0^{(1)}$ is none other than the 4-grain solution found by Bertram et al. [1, 2].

Let $\mathcal{A}_i$ ($i = 1, 2, 3, 4$) be the aggregate described by solution $R_0^{(i)}$. Since

$$R(e_3, \pi/2) D_2 = D_2 R(e_3, \pi/2),$$

we observe from (33) that $\mathcal{A}_2$ and $\mathcal{A}_4$ result if we rotate aggregates $\mathcal{A}_1$ and $\mathcal{A}_3$ by $R(e_3, \pi/2)$, respectively. We take aggregates $\mathcal{A}_2$ and $\mathcal{A}_4$ to be of the same type as $\mathcal{A}_1$ and $\mathcal{A}_3$, respectively.

For brevity, let us simply write R_0 for $R_0^{(1)}$. Then aggregate $\mathcal{A}_1$ is of type $D_2 R_0 O$. If we write $R_0(\psi_0, \theta_0, \phi_0) = (\alpha, \beta, \alpha)$, then $R_0^{(3)}(\psi_0, \theta_0, \phi_0) = (\pi/2 - \alpha, \beta, \pi/2 - \alpha)$. Construct an aggregate $\widetilde{\mathcal{A}}$ by rearranging the grains in $\mathcal{A}_1$ so that R_0 is replaced by R_0^T, which has Euler angles $(\pi - \alpha, \beta, \pi - \alpha)$ and is equivalent to $(\pi - \alpha, \beta, \pi/2 - \alpha)$ for a $D_2 R_0^T O$ aggregate. If we rotate $\widetilde{\mathcal{A}}$ by $R(e_3, -\pi/2)$, we obtain aggregate $\mathcal{A}_3$ because $R(e_3, -\pi/2)D_2 = D_2 R(e_3, -\pi/2)$. Hence $\mathcal{A}_3$ is of type $D_2 R_0^T O$.

4.2. Grains of other crystal symmetries

In Eq. (29) we obtain an aggregate $\mathcal{A}^{(1)}$ of type $D_2 R_0 O$, which has its elasticity tensor $\mathbb{C}$ isotropic. From this solution we can construct, for crystallites of any $\mathcal{G}_{\mathrm{cr}} \subset \mathcal{G}$, an aggregate with an isotropic $\mathbb{C}$.

The method is as follows: Let R_1 be any rotation and $\mathcal{G}^{(2)}$ be any finite subgroup of $\mathcal{G}$ which satisfies the crystallographic restriction. If we rotate the aggregate $\mathcal{A}^{(1)}$ by R_1, the rotated aggregate $\mathcal{A}_R^{(1)}$ still has its $\mathbb{C}$ isotropic. Now append grains to $\mathcal{A}_R^{(1)}$ to obtain an aggregate of type $\mathcal{G}^{(2)} R_1 D_2 R_0 O$, which is simply an assembly of N_2 (the order of $\mathcal{G}^{(2)}$) rotated copies of $\mathcal{A}_R^{(1)}$. Clearly the new assembly has an isotropic $\mathbb{C}$. By Remark 2, we conclude that the aggregate of type $O R_0^T D_2 R_1^T \mathcal{G}^{(2)}$, which consists of $24 \times 4 = 96$ grains with $\mathcal{G}_{\mathrm{cr}} = \mathcal{G}^{(2)}$, also has an isotropic $\mathbb{C}$. In other words, for crystallites with its $\mathcal{G}_{\mathrm{cr}}$ being a finite rotation group, including triclinic crystallites with $\mathcal{G}_{\mathrm{cr}} = C_1$, we can always design an aggregate with 96 identical grains which has an isotropic elasticity tensor.

The appearance of an arbitrary rotation R_1 in the preceding scheme suggests that this recipe generally will not lead to a solution with the least possible number of grains. Indeed for many crystal symmetries we can achieve our goal using less grains. Let us now present one other solution for each $\mathcal{G}_{\mathrm{cr}} \subset \mathcal{G}$ other than C_1.

$\underline{\mathcal{G}_{\mathrm{cr}} = D_2, D_4, D_6}$

By Remark 2, $O R_0^T D_2$ is a solution with 24 orthorhombic grains. Moreover, if $\mathcal{G}^{(1)}$ contains D_2 as a subgroup, then the 24-grain aggregate of type $O R_0^T\, \mathcal{G}^{(1)}$ also has an isotropic $\mathbb{C}$. Indeed, let $q = |\mathcal{G}^{(1)}|/|D_2|$ and

$$\mathcal{G}^{(1)} = \bigcup_{i=1}^{q} g_i D_2, \qquad \text{(disjoint union)} \tag{34}$$

where $\{g_i : i = 1, ..., q\}$ is a set of left coset representatives of D_2 in $\mathcal{G}^{(1)}$. An aggregate of type $\mathcal{G}^{(1)} R_0 O$ can be taken as a "super-aggregate" of q rotated copies of the aggregate of type $D_2 R_0 O$, where g_i $(i = 1, ..., q)$ describe the rotations in question. Since each rotated copy has an isotropic $\mathbb{C}$, so does the super-aggregate. It follows from Remark 2 that an aggregate of type $O R_0^T \mathcal{G}^{(1)}$ also has an isotropic $\mathbb{C}$.

The same argument in fact proves a general assertion, which we put as the next remark.

REMARK 3. Let $\mathcal{G}_a$ and $\mathcal{G}_b$ be point groups such that $\mathcal{G}_a \subset \mathcal{G}_b \subset \mathcal{G} = \mathrm{SO}(3)$. If an aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0 \mathcal{G}_a$ has its material tensors $\mathbb{H}^{(1)}, ..., \mathbb{H}^{(p)}$ isotropic, so does an aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0 \mathcal{G}_b$.

By the preceding remark, cubic aggregates of 24 tetragonal and hexagonal crystallites which are of type $OR_0^T D_4$ and $OR_0^T D_6$, respectively, have their elasticity tensor isotropic; here we take rotations $R(e_2, \pi)$ and $R(e_3, \pi/2)$ as the two generators of group D_4 and rotations $R(e_2, \pi)$ and $R(e_3, \pi/3)$ as the two generators of group D_6.

$\underline{\mathcal{G}_{\mathrm{cr}} = C_2, C_4, C_6}$

Let $C_2^{(1)} = \{I, R(e_3, \pi)\}$ and $C_2^{(2)} = \{I, R(e_2, \pi)\}$, where I is the identity in $\mathcal{G}$. The solution of type $D_2 R_0 O$ can be looked upon as of type $C_2^{(1)} I C_2^{(2)} R_0 O$. By Remark 2, we obtain a solution of type $OR_0^T C_2^{(2)} I C_2^{(1)}$, which consists of $24 \times 2 = 48$ C_2-grains of equal volume.

Let $R(e_3, \pi/2)$ and $R(e_3, \pi/3)$ be the generator of group C_4 and C_6, respectively. Since both C_4 and C_6 include $C_2^{(1)}$ as a subgroup, by Remark 3 we conclude that aggregates of type $OR_0^T C_2^{(2)} I C_4$ and $OR_0^T C_2^{(2)} I C_6$ are also solutions. These aggregates are made up of 48 C_4- and C_6-grains, respectively.

$\underline{\mathcal{G}_{\mathrm{cr}} = C_3}$

First we present a solution of hexagonal grains which exhibits C_3 texture symmetry. To start with, we arrange an aggregate of 8 identical hexagonal grains so that it has tetragonal texture symmetry (i.e. $\mathcal{G}^{(1)} = D_4$, where $R(e_2, \pi)$ and $R(e_3, \pi/2)$ are taken as generators). Then, by determining the independent coefficients for $l = 4$ and solving the resulting equations with texture coefficients of form shown in Eq. (14), we find that the orientation

$$R_0(\psi_0, \theta_0, \phi_0) = (0.39269908, 1.22389959, 0) \tag{35}$$

generates an aggregate of type $D_4 R_0 D_6$ which has all its c_{mn}^4 coefficients zero.

By placing three copies of this aggregate in such a way that the super-aggregate has C_3 texture (i.e. $\mathcal{G}^{(2)} = C_3$, with $R(e_3, 2\pi/3)$ as generator), we are able to determine that among the c_{mn}^2 coefficients of the super-aggregate only the coefficient c_{00}^2 is independent, and $c_{00}^2 = 0$ renders all c_{mn}^2 coefficients zero. Moreover, we find that

$$R_1(\psi_1, \theta_1, \phi_1) = (0, 0.95531662, 0)$$

is a solution of $c_{00}^2 = 0$, where the texture coefficient is of form Eq. (16) with R_0 given by Eq. (35). Thus we obtain an aggregate of type $C_3 R_1 D_4 R_0 D_6$, which has an isotropic elasticity tensor $\mathbb{C}$.

By Remark 2, aggregates of type $D_6 R_0^T D_4 R_1^T C_3$, which consist of $12 \times 8 = 96$ C_3-grains of equal volume, have their elasticity tensor isotropic.

$\underline{\mathcal{G}_{\mathrm{cr}} = D_3}$

We found an arrangement of 24 D_3-grains, for which the elasticity tensor $\mathbb{C}$ of the aggregate is isotropic. The arrangement is of type $OR_0 D_3$, where

$$R_0(\psi_0, \theta_0, \phi_0) = (0.55357436, \pi/2, 0).$$

$\mathcal{G}_{\text{cr}} = T$

In paper [1] Bertram et al. have presented a solution of type TR_0O, where

$$R_0(\psi_0, \theta_0, \phi_0) = (0.24002358,\ 2.67480609,\ 2.90156907). \tag{36}$$

Hence there is a solution of type $OR_0^T T$ with 24 tetrahedral grains. In fact, $R_0^T = R_0$ in this case.

In summary, we have presented at least one solution for each $\mathcal{G}_{\text{cr}}$ which is a finite rotation group that satisfies the crystallographic restriction. For each $\mathcal{G}_{\text{cr}}$, our best solution at present (where using a smaller number of grains means better) requires 4 grains for $\mathcal{G}_{\text{cr}} = O$; 24 grains for $\mathcal{G}_{\text{cr}} = D_2, D_3, D_4, D_6$, or T; 48 grains for $\mathcal{G}_{\text{cr}} = C_2, C_4$, or C_6; 96 grains for $\mathcal{G}_{\text{cr}} = C_1$, or C_3. Except for the case of cubic grains, where a proof was given by Bertram et al. [1], it remains unclear whether the solution we presented would be a minimal solution, i.e., one with the least possible number of identical grains for the $\mathcal{G}_{\text{cr}}$ in question. In fact, we believe that many of our present "best solutions" can be improved upon.

5. Example: acoustoelastic tensor

In a similar manner, it is possible to build textured aggregates which have isotropic tensors of higher order. As an example, here we seek designs which render the sixth-order acoustoelastic tensor $\mathbb{D}$ [5, 6] isotropic. A glance at decomposition formula (5) reveals that we should design aggregates with their c^l_{mn} coefficients all zero for $1 \le l \le 6$. A solution in this regard will not only have its acoustoelastic tensor $\mathbb{D}$ isotropic, but will also attain (cf. Section 2.1) isotropy for all its material tensors of order $l \le 6$, including the fourth-order elasticity tensor $\mathbb{C}$.

For all the finite rotation groups that appear below, we have already specified their generators in the preceding section. For groups of crystal symmetry, the generators help specify the orientation of the reference crystallite with respect to the chosen spatial Cartesian coordinate system.

5.1. Cubic grains

With our choice of reference crystallite and spatial coordinate system, the restrictions imposed by crystal symmetry (see Eq. (26)) dictate [10, 22] that any aggregate of cubic grains must have all their c^l_{mn} coefficients vanish for $l = 1, 2, 3, 5$. Hence we just need to worry about the c^4_{mn} and c^6_{mn} coefficients.

Consider an arrangement of 8 identical cubic grains so that the aggregate $\mathcal{A}^{(1)}$ has tetragonal texture symmetry (i.e. $\mathcal{G}_{\text{cr}} = O$ and $\mathcal{G}^{(1)} = D_4$). From the fact that Eqs. (26) and (27) should hold for $Q \in O$ and $Q \in D_4$, respectively, we observe that all the c^6_{mn} coefficients will vanish if c^6_{00} and c^6_{40} are null. Using Maple to solve the equations $c^6_{00}(R_0) = 0$ and $c^6_{40}(R_0) = 0$, where the texture coefficients are in the form of Eq. (14), we found that

$$R_0(\psi_0, \theta_0, \phi_0) = (0.08033115,\ 2.63923776,\ 0.99945255) \tag{37}$$

is an orientation which makes all the c^6_{mn} coefficients vanish for the aggregate $\mathcal{A}^{(1)}$ of type D_4R_0O.

Place 4 identical copies of this $\mathcal{A}^{(1)}$ aggregate so that the new super-aggregate $\mathcal{A}^{(2)}$ has orthorhombic texture symmetry D_2. Equation (25) reminds us that the c^6_{mn} coefficients of $\mathcal{A}^{(2)}$

vanish since all the c^6_{mn} coefficients of $\mathcal{A}^{(1)}$ are zero. Because of the D_2 texture symmetry, we only need to solve a system of three equations:

$$c^4_{00}(R_1) = 0, \qquad c^4_{20}(R_1) = 0, \qquad c^4_{40}(R_1) = 0, \tag{38}$$

where each texture coefficient is of the form given in Eq. (16).

Using Maple, we found a solution

$$R_1(\psi_1, \theta_1, \phi_1) = (0.10523426, 0.47936161, 0.28647879). \tag{39}$$

Thus we have constructed an aggregate of type $D_2R_1D_4R_0O$ consisting of $4 \times 8 = 32$ identical cubic grains which has all its material tensors of order $l \le 6$ isotropic.

5.2. Grains of other crystal symmetries

By the argument given in Section 4.2, we know that for any rotation R_2 and point group $\mathcal{G}^{(3)} \subset \mathcal{G}$, an aggregate $\mathcal{A}^{(3)}$ of type $OR_0^TD_4R_1^TD_2R_2^T\mathcal{G}^{(3)}$, where R_0 and R_1 are given by Eqs. (37) and (39), respectively, has all its material tensors of order $l \le 6$ isotropic. Such an aggregate consists of $24 \times 8 \times 4 = 768$ identical grains of crystal symmetry $\mathcal{G}_{\rm cr} = \mathcal{G}^{(3)}$.

For most crystal symmetries, we expect that we can achieve the same goal with a smaller number of grains. For instance, by Remark 2 and 3, aggregates of types $OR_0^TD_4R_1^TD_2$, $OR_0^TD_4R_1^TD_4$, and $OR_0^TD_4R_1^TD_6$, where R_0 and R_1 are given by Eqs. (37) and (39), respectively, have all their material tensors of order $l \le 6$ isotropic. These aggregates are made up of $24 \times 8 = 192$ identical orthorhombic, tetragonal, and hexagonal grains, respectively.

Likewise, by treating an aggregate of type $D_2R_1D_4R_0O$ as of type $C_2^{(1)}IC_2^{(2)}R_1D_4R_0O$, where $C_2^{(1)}$ and $C_2^{(2)}$ are defined in Sec. 4.2, we obtain a solution of type $OR_0^TD_4R_1^TC_2^{(2)}IC_2^{(1)}$, which consists of $24 \times 8 \times 2 = 384$ C_2-grains of equal volume. By Remark 3, aggregates of type $OR_0^TD_4R_1^TC_2^{(2)}IC_4$ and of type $OR_0^TD_4R_1^TC_2^{(2)}IC_6$ are also solutions. These aggregates are made up of 384 C_4- and C_6-grains, respectively.

6. Discussion

The outlined method allows the construction of aggregates having isotropic tensors of various orders. So long as $\mathcal{G}_{\rm cr}$ is a finite subgroup of the rotation group $\mathcal{G}$, the specific crystal symmetry of the crystallites is of no concern. Indeed we have shown in Sections 4 and 5 that once a design of any type is found for an aggregate of identical grains which has a specific set of material tensors isotropic, it generates for each such $\mathcal{G}_{\rm cr}$ a solution which has the same set of tensors isotropic. Our ODF method can be easily implemented using any software which can solve (nonlinear) systems of equations.

But there are limitations. At each step, say the p-th, the method requires finding a rotation $R_{p-1}(\psi_{p-1}, \theta_{p-1}, \phi_{p-1})$ which satisfies a system of nonlinear equations $c^l_{mn}(R_{p-1}) = 0$, where c^l_{mn} is of the form (17), l and n are given, and m runs over those indices between $-l$ and l for which the texture coefficients c^l_{mn} are independent for aggregates with $\mathcal{G}^{(p)}$ as the group of texture symmetry. When the number of independent indices is bigger than three, there are more equations than the number of unknowns. While nothing can be said for sure because the equations are nonlinear, it is likely that the method would break down when that happens. To reduce the number of independent m's, we could take $\mathcal{G}^{(p)}$ to be a group of larger order. For example, for $\mathcal{G}^{(p)} = O$, the number of independent m's is not bigger than three when $l \le 34$.

Of course, we hardly need to worry about tensors of order higher than 34 in practice. But taking $\mathcal{G}^{(p)} = O$ at every step is also impractical. The equations describing the c^l_{mn} coefficients quickly become unwieldy as l is increased or when the orders of the symmetry groups involved are large. In this case, it may be infeasible to find solutions even if they exist. Using $\mathcal{G}_{\rm cr}$ and $\mathcal{G}^{(p)}$ $(p \geq 1)$ of smaller orders will simplify the equations. A smaller $\mathcal{G}_{\rm cr}$, however, will increase the number of steps required because for each l there will be more (l, n) pairs for which the c^l_{mn} coefficients must be considered. A smaller $\mathcal{G}^{(p)}$ will increase the number of equations at the p-th step. Hence the method relies on finding a suitable combination of $\mathcal{G}_{\rm cr}$ and $\mathcal{G}^{(p)}$ $(p \geq 1)$ which produces solvable systems of equations at all the necessary steps that lead to the design of a suitable aggregate. This requires some trial-and-error until a more systematic approach is worked out. In fact, some texture and crystal symmetry combinations do not have solutions to produce $\mathcal{A}^{(1)}$ aggregates with isotropic elasticity tensor. (For example, $\mathcal{G}_{\rm cr} = D_6$ with $\mathcal{G}^{(1)} = C_2$ has no solution for $c^2_{00}(R_0) = 0$, $c^2_{02}(R_0) = 0$.) Finally, even if our method successfully produces a solution for a given $\mathcal{G}_{\rm cr}$ and a given set of material tensors $\mathbb{H}^{(i)}$ $(i = 1, ..., s)$, the solution found need not be a minimal solution, i.e., there might still be other arrangements involving a smaller number of $\mathcal{G}_{\rm cr}$-grains for which all the $\mathbb{H}^{(i)}$ tensors of the aggregate are isotropic.

Our ODF method seeks solutions which exhibit texture symmetry. Carrying texture symmetry is clearly not a necessary condition for a solution. A more basic question, which remains to be answered, is whether the set of minimal solutions for a particular $\mathcal{G}_{\rm cr}$ and set of material tensors $\mathbb{H}^{(i)}$, if non-empty, would always include some member that exhibits texture symmetry.

References

[1] Bertram A., Bölke T., Gaffke N., Heiligers B. and Offinger R., *On the generation of discrete isotropic orientation distributions for linear elastic cubic crystals*, Elasticity **58** (2000), 233–248.

[2] Bölke T., Bertram A., *On isotropic orientation distributions of cubic crystals*, J. Mech. Phys. Solids **49** (2001), 2459–2470.

[3] Aleksandrov K. and Aisenberg L., *A method of calculating the physical constants of polycrystalline materials*, Soviet Physics Doklady **11** (1966), 323–325.

[4] Matthies S. and Humbert M, *On the principle of a geometric mean of even-rank symmetric tensors for textured polycrystals*, J. Appl. Cryst. **28** (1995), 254–266.

[5] Man C.-S. and Paroni R., *On the separation of stress-induced and texture-induced birefringence in acoustoelasticity*, J. Elasticity **45** (1996), 91–116.

[6] Man C.-S., *Effects of crystallographic texture on the acoustoelastic coefficients of polycrystals*, Nondestructive Testing and Evaluation **15** (1999), 191–214.

[7] Man C.-S. and Huang M., *Identification of material parameters in yield functions and flow rules for weakly textured sheets of cubic metals*, Int. J. Non-Linear Mech. **36** (2001), 501–514.

[8] Man C.-S., *On the constitutive equations of some weakly-textured materials*, Arch. Rational Mech. Anal. **143** (1998), 77–103.

[9] Paroni R. and Man C.-S., *Constitutive equations of elastic polycrystalline materials*, Arch. Rational Mech. Anal. **150** (1999), 153–177.

[10] Bunge H.J. *Texture analysis in materials science*, Butterworth's, London 1982.

[11] ROE R.-J., *Description of crystallite orientation in polycrystalline materials*, III. *General solution to pole figures*, J. Appl. Phys. **36** (1965), 2024–2031.

[12] MATTHIES S., VINEL G.W. AND HELMING K, *Standard distributions in texture analysis*, Vol. 1, Akademie-Verlag, Berlin 1987.

[13] MAN C.-S., *Material tensors of weakly-textured polycrystals*; in: "Proceedings of the third international conference on nonlinear mechanics" (Eds. W. Chien, C. Chang and S. Dai), Shanghai University Press, Shanghai 1998, 87–94.

[14] MILLER W., *Symmetry groups and their applications*, Academic Press, New York 1972.

[15] JAHN H.A., *Note on the Bhagavantam-Suryanarayana method of enumerating the physical constants of crystals*, Acta Cryst. **2** (1949), 30–33.

[16] SIROTIN YU. I., *Decomposition of material tensors into irreducible parts*, Sov. Phys. Crystallogr. **19** (1975), 565–568.

[17] TISZA L., *Zur Deutung der Spektren mehratomiger Moleküle*, Z. Physik **82** (1933), 48–72.

[18] TJUR T., *Probability based on radon measures*, Wiley, Chichester 1980.

[19] VARSHALOVICH D.A., MOSKALEV A.N., AND KHERSONSKII V.K. *Quantum theory of angular momentum*, World Scientific, Singapore 1988.

[20] BIEDENHARN L.C. AND LOUCK J.D., *Angular momentum in quantum physics*, Cambridge University Press, Cambridge 1984.

[21] PARONI R., *Optimal bounds on texture coefficients*, J. Elasticity **60** (2000), 19–34.

[22] ROE R.J., *Inversion of pole figures for materials having cubic crystal symmetry*, J. Appl. Phys. **37** (1966), 2069–2072.

AMS Subject Classification: 74A20, 74E25, 74Q99.

Chi-Sing MAN, Leigh NOBLE
Department of Mathematics
University of Kentucky
Lexington, KY 40506-0027, USA
e-mail: `mclxyh@ms.uky.edu`

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

G.A. Maugin*

TOWARDS AN ANALYTICAL MECHANICS OF DISSIPATIVE MATERIALS

Abstract. A Lagrangian-Hamiltonian variational formulation is proposed for the thermoelasticity of heat conductors and its generalization to anelasticity - described by means of internal-state variables- by using a gauge-theoretical technique (introduction of an additional variable of state - the gradient of thermacy - that renders the system apparently Hamiltonian). Projecting the equations resulting from the Euler-Lagrange equations and the equations deduced from the application of Noether's theorem back on the original space provides all local balance equations of the dissipative theory, including the entropy equation and the equation of canonical momentum in material space (which are not strict conservation laws). A canonical structure clearly emerges for the anelasticity of conductors in finite strains.

1. Introduction

A recurrent dream of many mathematical physicists is to construct a variational formulation for all field equations of continuum physics *including in the presence of dissipative effects.* We all know that this is not possible unless one uses special tricks such as introducing complex-valued functions and adjoint fields (e.g., for heat conduction). But we do present here a variational and canonical formulation for the nonlinear continuum theory of *thermoelastic conductors* and then generalize this to the case of anelastic conductors of heat. This is made possible through the introduction of a rather old notion, clearly insufficiently exploited, that of *thermacy* introduced by Van Danzig (cf. [9]), a field of which the time derivative is the thermodynamical temperature. It happens that we used such a notion in relativistic studies in the late 60s-early 70s, (Pre-general exam Seminar at Princeton University, Spring 1969; [10], [11]), a time at which we found that thermacy is nothing but the *Lagrange multiplier* introduced to account for *isentropy* in a Lagrangian variational formulation. But , completely independently and much later, Green and Naghdi ([4]) formulated a strange "thermoelasticity without dissipation". Dascalu and I ([1]) identified thermacy as the unknowingly used notion by Green and Naghi (unaware of works in relativistic variational formulations), and we formulated the corresponding *canonical balance laws of momentum and energy* - of interest in the design of fracture criteria - which, contrary to the expressions of the classical theory, indeed present *no* source of dissipation and canonical momentum, e.g., no thermal source of quasi-inhomogeneities (cf. [2]). In recent works ([14], [21]), we have shown the consistency between the expressions of intrinsic dissipation and source of canonical momentum in dissipative continua. This is developed within the framework of so-called *material* or *configurational forces*, "Eshelbian mechanics", that world of forces which, for instance, drive structural rearrangements and material defects of different types on the material

*Enlightening discussions with Prof. Ernst Binz (Mannheim, Germany) during the Torino International Seminar are duly acknowledged.

manifold (for these notions see [12], [13], [5] and [7]). The road to the analytical continuum mechanics was explored in particular by P.Germain (1992) in [3], but not in a variational framework.

Herebelow we first present a consistent variational formulation for thermoelastic conductors of heat, which, with the use of Noether's theorem, delivers all equations of interest, that is, the balance of linear momentum, the equation of entropy, the balance of canonical momentum, and the energy equation, all in the apparently"dissipationless form". But these equations can be transformed to those of the classical theory of (obviously thermally dissipative) nonlinear elastic conductors (cf. [20]). Therefore, we have a good starting point for a true canonical formulation of dissipative continuum mechanics. The possible extension of the formulation to anelastic conductors of heat is also presented when the anelastic behavior is accounted for through the introduction of internal variables of state. Elements of the present work were given in a paper by Kalpakides and Maugin ([6]).

2. Direct Variational formulation and its results.

We use classical elements of field theory as enunciated in several books (e.g. [12], [14], [21]). The reader is referred to these works for the abstract equations.

Consider Hamiltonian-Lagrangian densities (per unit volume of the undeformed configuration K_R of nonlinear continuum mechanics given by the following general expression:

$$L = \bar{L}\,(\mathbf{v}, \mathbf{F}, \theta, \beta; \mathbf{X}) = K\,(\mathbf{v}; \mathbf{X}) - W\,(\mathbf{F}, \theta, \beta; \mathbf{X})\,, \tag{1}$$

where

$$K(\mathbf{v}; \mathbf{X}) = \frac{1}{2}\rho_0\,(\mathbf{X})\,\mathbf{v}^2, \quad \theta = \dot{\gamma}, \quad \beta = \nabla_{\mathbf{R}}\gamma.$$

Here, K is the kinetic energy, W is the free energy density, ρ_0 is the mass density at the reference configuration, a superimposed dot denotes time differentiation at constant fixed material point $\mathbf{X}$, ∇_R denotes the material gradient, the scalar function β is called the *thermacy*, and $\mathbf{v}$ and $\mathbf{F}$ are the physical velocity and direct deformation gradient such that

$$\mathbf{v} = \left.\frac{\partial \chi}{\partial t}\right|_X, \qquad \mathbf{F} = \left.\frac{\partial \chi}{\partial \mathbf{X}}\right|_t \equiv \nabla_R \chi,$$

if

$$\mathbf{x} = \chi\,(\mathbf{X}, t\,)\,, \qquad det\,\mathbf{F} > 0,$$

is the smooth placement of $\mathbf{X}$ at Newtonian time t. The explicit dependence of ρ_0 and W on $\mathbf{X}$ indicates material inhomogeneity (direct smooth dependence on the material point $\mathbf{X}$).

In the Lagrangian density (1), the *basic fields* are the *placement* $\mathbf{x}$ and the thermacy γ, both being assumed sufficiently smooth functions of the *space-time parametrization* $(\mathbf{X}, t)$, which is the one favored in the Piola-Kirchhoff formulation of nonlinear continuum mechanics (cf.Truesdell and Noll, 1965). Notice that L is not an explicit function of $\mathbf{x}$ by virtue of Galilean invariance (translations in physical space of placements). Neither is it an explicit function of γ itself, this implying a sort of *gauge invariance* very similar to that of electrostatic for the electric potential. Since the focus is on field equations rather than on boundary conditions and initial conditions, the density (1) may be integrated over a Newtonian space-time volume of infinite extent with proper limit behavior of the various involved functions at infinity in space and at time limits. According to the general field theory, in the absence of external sources (these would be explicit functions of the fields themselves), the **field equations** , i.e, the Euler-Lagrange equations (cf. eqns. (A.7) in Maugin, 1999a) associated with χ and γ, are immediately given by

$$\left.\frac{\partial \mathbf{p}}{\partial t}\right|_X - div_R \mathbf{T} = \mathbf{0}, \tag{2}$$

$$\left.\frac{\partial S}{\partial t}\right|_X + \nabla_R.\mathbf{S} = 0, \tag{3}$$

wherein

$$\begin{aligned} \mathbf{p} &:= \rho_0 \mathbf{v} = \frac{\partial L}{\partial \dot{\chi}}, \quad \mathbf{T} := \frac{\partial W}{\partial \mathbf{F}} = -\frac{\partial L}{\partial(\nabla_R \chi)}, \\ S &:= -\frac{\partial W}{\partial \theta} = \frac{\partial L}{\partial \dot{\gamma}}, \quad \mathbf{S} := -\frac{\partial W}{\partial \beta} = \frac{\partial L}{\partial(\nabla_R \gamma)}, \end{aligned} \tag{4}$$

are, respectively, the *linear momentum vector* in physical space, the *first Piola-Kirchhoff stress*, the *entropy density* (by appealing to the axiom of local state and assuming that entropy density has the same general functional definition as in thermostatics), and, accordingly, the *entropy flux* in material form.

Invoking now Noether's theorem (cf. eqns. (A.11) in Maugin, 1999a) for the Lagrangian (1) with respect to the space-time parametrization $(\mathbf{X}, t)$, we obtain the following two, respectively co-vectorial and scalar, equations:

$$\left.\frac{\partial P_L^{th}}{\partial t}\right|_X - \left(div_R \mathbf{b}^{th}\right)_L = \left(\mathbf{f}^{inh}\right)_L, \tag{5}$$

and

$$\left.\frac{\partial H}{\partial t}\right|_X - \nabla_R.\mathbf{U} = 0, \tag{6}$$

where we have defined the *canonical momentum* (material-covariant) vector $\mathbf{P}^{th}$ of the present approach, the corresponding *canonical material stress* tensor $\mathbf{b}^{th}$, *the material force* of true inhomogeneities $\mathbf{f}^{inh}$, the *Hamiltonian density* (total energy density) H, and the material Umov-Poynting energy-flux vector $\mathbf{U}$ by [15] (compare the general definitions given in eqns. (A.16), (A.17), (A.14) and (A.15)).

$$\mathbf{P}^{th} = -\nabla_R \chi . \frac{\partial L}{\partial \mathbf{v}} - \nabla_R \gamma \frac{\partial L}{\partial \dot{\gamma}} = -\mathbf{p}.\mathbf{F} - S\beta = \mathbf{P}^{\mathbf{mech}} - \mathbf{S}\beta, \tag{7}$$

$$\begin{aligned} \mathbf{b}^{th} \ : \ &= \left\{ b^K_{.L} := -\left(L\delta^K_L - \left(\gamma_{,L} \frac{\partial L}{\partial \gamma_{,K}} + \chi_{,L} \frac{\partial L}{\partial \chi_{,K}} \right) \right) \right. \\ &= \left. -\left(L\delta^K_L - S^K \beta_{\mathbf{L}} + \mathbf{T}^{\mathbf{K}}_{\mathbf{.i}} \mathbf{F}^{\mathbf{i}}_{\mathbf{.L}} \right) \right\}, \end{aligned} \tag{8}$$

$$\mathbf{f}^{inh} := \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{\exp l} = \left(\frac{\mathbf{v}^2}{2}\right)(\nabla_R \rho_0) - \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{\exp l},$$

$$H = \dot{\gamma}\frac{\partial L}{\partial \dot{\gamma}} + \mathbf{v}.\frac{\partial L}{\partial \mathbf{v}} - L \; = S\theta + 2K - L = K + E, \tag{9}$$

$$U^K = -\left(\dot{\gamma}\frac{\partial L}{\partial \gamma_{,K}} + v^i \frac{\partial L}{\partial \chi^i_{.K}}\right) = T^K_{.i} v^i - S^K \theta,$$

where we have defined the *mechanical canonical* (material) momentum $\mathbf{P}^{mech}$ and the *internal energy* per unit reference volume by

$$\begin{aligned} \mathbf{P}^{mech} &= -\mathbf{p}.\mathbf{F}, \\ E &= W + S\theta. \end{aligned} \tag{10}$$

For the first of these sometimes referred to as the *pseudomomentum,* see, for instance [12], [13], eq. (10) is the usual Legendre transformation of thermodynamics between internal and free energies. As a matter of fact, the definition (9) contains two Legendre transformations, one related to mechanical fields, and the other to thermal ones.

If we assume, as in standard continuum thermodynamics, that entropy and heat flux are related by the usual relation

$$\mathbf{S} = \mathbf{Q}/\theta, \tag{11}$$

we have

$$\mathbf{Q} = -\theta \frac{\partial W}{\partial \beta}, \tag{12}$$

and eqn. (6 takes on the classical form of the energy-conservation equation (cf. Maugin and Berezovski, 1999)

$$\left.\frac{\partial H}{\partial t}\right|_{\mathbf{X}} - \nabla_R . (\mathbf{T}.\mathbf{v} - \mathbf{Q}) = 0. \tag{13}$$

Summing up, we have deduced from the Hamiltonian-Lagrangian density (1) all field equations, balance laws and constitutive relations for the theory of materially inhomogeneous, finitely deformable, thermoelastic conductors of heat. As a matter of fact, eqns. (2) and (13) are the local balance equations of linear momentum (in physical space) and energy, respectively. This is completed by the balance equation of mass which here trivially reads

$$\left.\frac{\partial \rho_0}{\partial t}\right|_X = 0. \tag{14}$$

These are all formally identical to those of the classical thermoelasticity of conductors (e.g., as recalled in [18]). Another balance law if that of *moment of momentum* (in physical space). This is deduced from (1) by considering the action of the infinitesimal rotational component of the connected group SO(3) in physical space. A classical derivation yields then (in components in order to avoid any confusion in notation)

$$\frac{\partial W}{\partial F^{[i}_{.K}} F^{\,j]}_{.L} = 0 \quad or \quad T^K_{.[i} F^{\,j]}_{.L} = 0, \tag{15}$$

as the action of this group is inoperative on the material vector β. Apart from the functional dependence of W, eqn. (15) is also formally identical to the classical counterpart. Only the equation of canonical momentum (5) differs from the one originally obtained in [2] material thermoelasticity. But, abstraction being made of material inhomogeneities, it is the same as the one obtained by direct algebraic manipulations in [1] in the "dissipationless" formulation of thermoelasticity. Indeed, canonical momentum (7) is made of two parts, a strictly mechanical part - which is none other than the pull back, changed of sign, of the physical momentum - and a purely thermal part given by the constitutive behavior. In addition, the canonical stress tensor (8) - also called *Eshelby stress tensor* by the present author - contains a contribution of β because, from its very definition, its captures material gradients of all fields. One should note that the source term in eqn. (5) has no energetic contents. Furthermore, contrary to common use, even the entropy equation (3) is source free so that, surprisingly, in the absence of material inhomogeneities, all equations obtained here are *strict conservation laws*, hence the qualification of "*dissipationless theory*". In this rather strange -we admit it - approach, the entropy flux and heat flux are derived from the free energy, on the same footing as entropy density , and stress (eqns. (4) and (12)).

3. Correspondence with the classical theory

Since eqns. (2), (13), (14) and (15) are formally the same as in the classical theory, the limit where W does not depend on β is trivial for these. What about eqns. (3) and (5) which are of utmost importance for crack and phase-transition front studies (cf. [18]). We need to isolate the contributions of β in order to get some "classical" limit (this means *projecting* onto the classical state space of the thermoelasticity of conductors). First we expand eqn. (5) by accounting for the expressions (7) and (8). After some rearrangements, we obtain the following equation (note that $curl_R \beta = 0$; T =transposed)

$$\left.\frac{\partial\, \mathbf{P}^{mech}}{\partial\, t}\right|_{\mathbf{X}} - div_R \bar{\mathbf{b}}^{mech} = S\,\nabla_R \theta\; + \mathbf{S}.\,(\nabla_R \beta)^T\; + \mathbf{f}^{inh}, \tag{16}$$

where $\bar{\mathbf{b}}^{mech} = \bar{\mathbf{b}}^{th} - \mathbf{S} \otimes \beta$. But this is not all because L in $\mathbf{b}^{th}$ still depends on β. We must isolate this dependency by writing

$$\frac{\partial\, W}{\partial\, \mathbf{X}} = \frac{\partial\, W^{mech}}{\partial\, \mathbf{X}} + \frac{\partial\, W}{\partial\, \beta}.\,(\nabla_R \beta)^T = \frac{\partial\, W^{mech}}{\partial\, \mathbf{X}} - \mathbf{S}.\,(\nabla_R \beta)^T\;, \tag{17}$$

where, in essence, $W^{mech} = W(F, \theta\,,\; \beta\; = \;0; X)$. On substituting (17) into the material divergence of $\mathbf{b}^{mech}$, we finally transform (16) to

$$\left.\frac{\partial\, \mathbf{P}^{mech}}{\partial\, t}\right|_{\mathbf{X}} - div_R \mathbf{b}^{mech} = \mathbf{f}^{inh} + \mathbf{f}^{th}, \tag{18}$$

where

$$\mathbf{b}^{mech} = -(L\mathbf{1}_R + \mathbf{T}.\mathbf{F}), \quad L = K - W^{mech}(\mathbf{F}, \theta; \mathbf{X}), \quad \mathbf{f}^{th} := S\nabla_R \theta.$$

The last introduced quantity is the material *thermal force of quasi-inhomogeneity* clearly defined by Epstein and Maugin [2] in their general theory of *material uniformity and inhomogeneity*. Thus equation (18) has recovered its "classical" form, the quotation marks here emphasizing that, in fact , while "classical" from our viewpoint, this equation is practically unknown to most people, although it is the one on which thermoelastic generalizations of the J-integral of fracture must be based (cf. [18], [21]). As to eqn. (3) we use the following trick. Multiplying (3) by $\theta \neq 0$ and accounting for (11) we obtain the "heat-propagation" equation in the form

$$\theta \frac{\partial S}{\partial t} + \nabla_R . \mathbf{Q} = \mathbf{S} . \dot{\beta}, \tag{19}$$

or else, by integration by parts,

$$\left. \frac{\partial (\theta S)}{\partial t} \right|_{\mathbf{X}} + \nabla_R . \mathbf{Q} = S \dot{\theta} + \mathbf{S} . \dot{\beta}. \tag{20}$$

This equation is interesting by itself because of its structure - especially the right-hand side - which is similar to that of eqn. (16), time derivatives replacing material space derivatives. The "classical" limit is obtained in (19) or (20) by ignoring the β term, i.e., restricting W to W^{mech}. The other terms then acquire their usual significance with $\mathbf{Q}$ and $\mathbf{S}$ no longer derivable from a potential. Working then in reverse, one recovers in this approximation the equations

$$\theta \frac{\partial S}{\partial t} + \nabla_R . \mathbf{Q} = 0, \qquad \frac{\partial S}{\partial t} + \nabla_R . \mathbf{S} = \sigma^{th},$$

where $\sigma^{th} = -S.\ \nabla_R\ (\ln \theta)$ is the *thermal entropy source*. $\mathbf{S}$ and $\mathbf{Q} = \mathbf{S}/\theta$ are now given by a constitutive equation obtained by invoking the noncontradiction of the formulation with the second law of thermodynamics, which here locally reads $\sigma^{th} \geq 0$. This yields, for instance, Fourier's law of heat conduction.

4. Accounting for anelasticity

At this point we have effectively formulated a canonical theory of the thermoelasticity of conductors. All field equations, balance laws , and constitutive equations follow from it. The relationship with the "classical" formulation was established. To proceed further, one must envisage the case where nonthermal *dissipative processes* (e.g., anelasticity) are present. Considering the theory of *internal variables of state* to describe these phenomena is a sufficiently general approach as demonstrated in a recent book [15]. The only *a priori* change should be accounting for the dependency of the free energy W on a new set of variables collectively represented by the symbol α The corresponding equation of state reads

$$A + (\partial\, W / \partial \alpha) = 0.$$

The main problem, however, remains to build the evolution equation of α, normally a relationship between $\dot{\alpha}$ and the thermodynamical force A constrained by the second law of thermodynamics. Thus the very presence of α is related to *dissipative processes* and a priori not amenable by means of a *canonical variational* formulation; $\alpha(X, t)$ is *not* a classical field; neither does it possess inertia, nor is its gradient introduced to account for some nonlocality). But it was recently shown how variables α and θ could play parallel roles in a certain reformulation of the anelasticity of thermoconductors ([14] , [17] (2000)). This is the trend to be followed. In effect, now we propose the following variational formulation in symbolic form:

$$\lim_{\beta \to \mathbf{0}} \delta \int_{E^3 \times T} L\, (\mathbf{v}, \mathbf{F}, \alpha, \theta = \dot{\gamma}, \beta = \nabla_{\mathbf{R}} \gamma; \mathbf{X})\ d^4 X = 0 \tag{21}$$

where L is the Hamiltonian-Lagrangian density per unit reference volume. The *limit* symbolism used in eqn. (21) means that the limit as β goes to zero must be taken *in the equations* resulting from the variational formulation, this applying to both field equations and other consequences of the principle such as the results of the application of Noether's theorem. We claim that in this limit *all equations of the "classical" theory of anelastic conductors of heat* are obtained, including the entropy equation and heat-propagation equation in this quite general case, a rather surprising result, we admit it. The only change compared to (1) is that the free energy W now depends on α, i.e., we have the following general expression

$$L = \bar{L}\,(\mathbf{v}, \mathbf{F}, \alpha, \theta, \beta; \mathbf{X}) = K\,(\mathbf{v}; \mathbf{X}) - W\,(\mathbf{F}, \alpha, \theta, \beta; \mathbf{X})\,.$$

Equations (2), (3), (5) and (6) hold true but for the additional dependence of W on α. The intrinsic dissipation necessary for the expression of the dissipative nature of this variable becomes visible only after performing manipulations of the type of those made in Section 3. We need to isolate the contributions due to the "dissipative" variables in eqns. (3) and (15). Equation (17) is modified due to the dependence on α:

$$\begin{aligned} \frac{\partial W}{\partial \mathbf{X}} &= \frac{\partial W^{mech}}{\partial \mathbf{X}} + \frac{\partial W}{\partial \alpha}\,(\nabla_R \alpha)^T + \frac{\partial W}{\partial \beta}\,(\nabla_R \beta)^T \\ &= \frac{\partial W^{mech}}{\partial \mathbf{X}} - A.\,(\nabla_R \alpha)^T - S.\,(\nabla_R \beta)^T \end{aligned} \tag{22}$$

where, in essence, $W^{mech} = W(F, \theta, \alpha = const., \beta = 0; X)$. The equation of canonical momentum first yields

$$\left.\frac{\partial\, \mathbf{P}^{mech}}{\partial t}\right|_{\mathbf{X}} - div_R \bar{\mathbf{b}}^{mech} = S\,\nabla_R \theta + \mathbf{S}.\,(\nabla_R \beta)^T + \mathbf{f}^{inh}.$$

But on substituting from (22) into this equation, it comes

$$\left.\frac{\partial\, \mathbf{P}^{mech}}{\partial t}\right|_{X} - div_R \mathbf{b}^{mech} = \mathbf{f}^{inh} + \mathbf{f}^{th} + \mathbf{f}^{intr} \tag{23}$$

where

$$\begin{aligned} \mathbf{b}^{mech} &= -\,(L \mathbf{1_R} + \mathbf{T}.\mathbf{F}) \\ L &= K - W^{mech}\,(\mathbf{F}, \theta, \alpha = const.; \mathbf{X})\,, \\ \mathbf{f}^{th} : &= S \nabla_R \theta, \\ \mathbf{f}^{intr} : &= A\,(\nabla_R \alpha)^T\,, \end{aligned}$$

The last two introduced quantities are material *forces of quasi-inhomogeneity* due to a nonuniform temperature field (cf. [2]) and to a nonuniform α field, respectively ([14]). The presence of those terms on an equal footing with $\mathbf{f}^{inh}$ means that, insofar as the material manifold is concerned, spatially nonuniform fields of α or θ are equivalent to distributed material inhomogeneities (also continuously distributed defects such as dislocations) ; they are *quasi-plastic effects* (cf. [13]). As to eqn. (3), accounting for the kinetic-energy theorem (obtained by multiplying scalarly eqn. (2) by $\mathbf{v}$ after multiplication by $\theta \neq 0$ and accounting for (6) and finally making $\beta =$ const. (this is equivalent to discarding β in the resulting equation and loosing the connection of $\mathbf{S}$ and $\mathbf{Q}$ with β) we arrive at the "*heat-propagation" equation* in the form

$$\left.\frac{\partial\,(S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R.\mathbf{Q} = S\dot{\theta} + A.\dot{\alpha} \equiv \bar{\Phi}^{th} + \Phi^{intr}. \tag{24}$$

Then working in reverse, in this approximation one recovers the equations (compare to [14])

$$\theta \frac{\partial S}{\partial t} + \nabla_R . \mathbf{Q} = \Phi^{intr},$$
$$\frac{\partial S}{\partial t} + \nabla_R . \mathbf{S} = \sigma^{th} + \sigma^{intr},$$

where $\sigma^{th} = -S\nabla_R(\ln\theta)$ is the *thermal entropy source* and

$$\sigma^{intr} = \theta^{-1} A . \dot{\alpha},$$
$$\Phi^{intr} = \theta\, \sigma^{intr}$$

are the *intrinsic* entropy source and the *intrinsic* dissipation , respectively. In the present classical limit, $bf\,S$ and $bf\,S = bf\,S\theta$ are now given by a constitutive equation obtained by invoking the noncontradiction with the second law of thermodynamics which here locally reads

$$\sigma = \sigma^{th} + \sigma^{intr} \geq 0.$$

We have recovered all equations or constraints of the "classical theory" by applying the scheme proposed in eqn. (21).

5. Canonical four-dimensional space-time formulation

Equations (23) and (24) present an obvious space-time symmetry (see the two right-hand sides). This obviously suggest considering these two equations as space and time-like components of a unique *four-dimensional equation* in the appropriate space and the canonical momentum $\mathbf{P}^{mech}$ and the quantity θS (an energy which is the difference between internal and free energies) as dual space-time quantities, i.e., they together form a four-dimensional canonical momentum

$$\mathbf{P}_{(4)} = \left(\mathbf{P}^{mech},\, P_4 = \theta\, S\right).$$

We let the reader check that eqns. (23) and (24) can in fact be rewritten in the following pure 4-dimensional or 4×4 formalism in an Euclidean 4-dim space (compare to World-invariant kinematics in [20])

$$(25) \qquad \frac{\partial}{\partial X^\beta} B^{\beta}_{.\alpha} = f_\alpha \equiv \bar{A} . \frac{\partial}{\partial X^\alpha}\mu \; - \left.\frac{\partial W}{\partial X^\alpha}\right|_{\exp l} = \left.\frac{\partial L}{\partial X^\alpha}\right|_{(\mathbf{F},\mathbf{v}\, fixed)}$$

$$\bar{A} = (A, S) \quad \mu = (\alpha,\, \theta),$$
$$X^\alpha(\alpha = 1, 2, 3, 4) = \left\{X^K\,(K = 1, 2, 3)\,,\; X^4 = t\right\}$$

$$B^{\beta}_{.\alpha} = \left\{ \begin{array}{cc} B^{K}_{.L} = -b^{K}_{L} & B^{4}_{.L} = P^{mech}_{L} \\ B^{K}_{.4} = Q^{K} & B^{4}_{.4} = \theta\, S \end{array} \right\},\; P_{(4)} = \left(B^{4}_{.L}\,,\; B^{4}_{.4}\right)$$

or, introducing intrinsically four-dimensional gradients and divergence in E^4 for eqn. (25),

$$(26) \qquad div_{E^4}\, \mathbf{B}^{mech} = \nabla_{E^4} L\, |_{mech}$$

where the right-hand side means the gradient computed keeping the "mechanical" fields (**F**,**v**) *fixed.* Equation (26) represents the canonical form of the balance of canonical momentum and the heat-propagation equation for anelastic, anisotropic, finitely deformable solid heat conductors. The 4-dimensional formalism introduced is somewhat different from that used by Maugin ([17]) or Herrmann and Kienzler ([7]). However, in the absence of intrinsic dissipative processes and for isothermal processes, eqns. (23) and (24) - or eqn. (26) reduce to those of Kijowski and Magli ([8]) in isothermal thermoelasticity, the second equation reducing obviously to the simple equation

$$\partial(\theta\, S)/\partial\, t = 0.$$

This shows the closedness of the present approach with the general relativistic Hamiltonian scheme.

6. Conclusion

The procedure used in this paper is essentially that of a *gauge theory* as practiced in modern physics. We have artificially enlarged the state space of the theory by adding one coordinate (the material gradient of the "potential" γ) to this space and then projected the resulting equations back onto the original state space. The latter could not accommodate dissipative processes, but the enlarged one does. Recurring to the classical dissipative formulation then requires this projection or "return to reality". In the mean time, a variational formulation has indeed been proposed.

References

[1] DASCALU C. AND MAUGIN G A., *The thermal material momentum equation*, J. Elasticity **39** (1994), 201–212.

[2] EPSTEIN M. AND MAUGIN G A., *Thermal materials forces: definition and geometric aspects*, C. R. Acad. Sci. Paris **320** II (1995), 63–68.

[3] GERMAIN P., *Toward an analytical mechanics of materials*, in: "Nonlinear thermodynamical processes in continua" (Eds. W. Muschik and G.A. Maugin), TUB-Dokumentation und Tagungen, Heft 61, Berlin 1992, 198–212.

[4] GREEN A.E. AND NAGHDI P.M., *Thermoelasticity without energy dissipation*, J. Elasticity **31** (1993), 189–208.

[5] GURTIN M.E., *Configurational forces as basic concepts of continuum physics*, Springer, New York 1999.

[6] KALPAKIDES V. AND MAUGIN G.A., *Canonical formulation of thermoelasticity without dissipation*, J. Elasticity (2002).

[7] KIENZLER R. AND HERRMANN G., *Mechanics in material space*, Springer, Berlin 2000.

[8] KIJOWSKI J. AND MAGLI G., *Unconstrained Hamiltonian formulation of general relativity with thermoelastic sources,* Class. Quant. Gravity **15** (1988), 3891–3916.

[9] LAUE M. VON, *Relativitätstheorie*, Vol.1, Vieweg-Verlag, Leipzig 1921.

[10] MAUGIN G.A., *Magnetized deformable media in general relativity*, Ann. Inst. Henri Poincaré **15** A (1971), 275–302.

[11] MAUGIN G.A., *An action principle in general relativistic magnetohydrodynamics*, Ann. Inst. Henri Poincaré **16** A (1972), 133–169.

[12] MAUGIN G.A. *Material inhomogeneities in elasticity*, Chapman and Hall, London 1993.

[13] MAUGIN G.A., *Material forces: concepts and applications*, Appl. Mech. Rev. **48** (1995), 213–245.

[14] MAUGIN G.A., *Thermomechanics of inhomogeneous-heterogeneous systems: application to the irreversible progress of two- and three-dimensional defects*, ARI Springer **50** (1997), 43–56.

[15] MAUGIN G.A., *Nonlinear waves in elastic crystals*, Oxford University Press, Oxford 1999.

[16] MAUGIN G.A., *Thermomechanics of nonlinear irreversible behaviors,* World Scientific, Singapore and River Edge 1999.

[17] MAUGIN G.A., *On the universality of the thermomechanics of forces driving singular sets*, Arch. Appl. Mech. **70** (2000), 31–45.

[18] MAUGIN G.A. AND BEREZOVSKI A., *Material formulation of finite-strain thermoelasticity*, J. Thermal Stresses **22** (1999), 421–449.

[19] MAUGIN G.A. AND TRIMARCO C., *Elements of field theory in inhomogeneous and defective materials*; in: "Configurational mechanics of materials", (Eds. R. Kienzler and G.A. Maugin) CISM Udine 2000, Springer-Verlag, Wien 2001, 55–128.

[20] TRUESDELL C.A. AND TOUPIN R.A., *Classical field theories*; in: "Handbuch der Physik, III/1", (Ed. S. Flügge) Springer-Verlag, Berlin 1960.

[21] TRUESDELL C.A. AND NOLL W., *Nonlinear field theories of mechanics*; in: "Handbuch der Physik", (Ed. S. Flügge), Bd.III/3, Springer-Verlag, Berlin 1965.

AMS Subject Classification: 74A15, 70S05.

Gérard A. MAUGIN
Laboratoire de Modélisation en Mécanique (UMR 7607)
Université Pierre et Marie Curie
Case 162, 4 place Jussieu
75252 Paris Cedex 05, FRANCE
e-mail: `gam@ccr.jussieu.fr`

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

M. Magno - M. Musio

AN ALTERNATIVE INTERPRETATION OF THE BEHAVIOR LAW OF MATTER BY MEANS OF A GENERALIZED STOCHASTIC PROCESS

Abstract. Discrepancy between discrete models and continuous theoretical ones is a common concern with the behavior laws of matter. We propose an alternative frame in which the transition from a discrete to a continuous model becomes very natural. A statistical description of matter laws is given in this contexte.

1. Introduction

The aim of this paper is to present a new mathematical background which allows to modelize in a natural way the mechanical behavior of matter. In such a model the transition from the discrete microscopic structure to the macroscopic behavior is very easy. This point of view, involves an alternative mathematical theory called "Radically Frequentist Statistics" (RFS), based on an idealized concept of *very large finite sequence of outcomes*. Such an idealization cannot be performed within the classical mathematical frame based on Zermelo-Fraenkel's set theory. Therefore we use an extended frame based on a conservative extensions with a double scale of magnitude order of ZF, where the concepts of large numbers and small fluctuations can be formalized in a way which is very close to the statistical language. The use of a conservative extentions of ZF with one scale of magnitude order as a mathematical background for modelisation is not news in mechanics (see [2], [3], [4], [5]).

The structure of the paper is the following: first we present roughly an intuitive statistical description of matter; then we present the mathematical model considered . In section 3 we introduced the RFS theory; we end in section 4 with the description of matter laws within RFS.

2. Intuitive statistical description

Consider a number s of macroscopically identical samples of some matter, say plates of concrete or a generalized composite. Divide each sample into adjacent cells of the same size (this last hypothesis is not essential).

Let $X_{i,j,k}$ be a mechanical parameter of interest (Young modulus, shear modulus...).and $x^a_{i,j,k}$ its value for the a^{th} sample. The range of $X_{i,j,k}$ is discretized into finite numbers of little intervals. Thus we may suppose that $X_{i,j,k}$ takes its values in a finite set E. For $a \in E$, we define the frequency

$$fr\left(X_{i,j,k} = a\right) = \frac{1}{s} card\left\{a \leqslant s, x^a_{i,j,k} = a\right\}$$

and the conditional frequency

$$fr\left(X_{i,j,k}=a \mid X_{i_1,j_1,k_1}=a_1, X_{i_2,j_2,k_2}=a_2,\cdots, X_{i_r,j_r,k_r}=a_r\right)=$$
$$=\frac{fr\left(X_{i,j,k}=aX_{i_1,j_1,k_1}=a_1, X_{i_2,j_2,k_2}=a_2,\cdots, X_{i_r,j_r,k_r}=a_r\right)}{fr\left(X_{i_1,j_1,k_1}=a_1, X_{i_2,j_2,k_2}=a_2,\cdots, X_{i_r,j_r,k_r}=a_r\right)}$$

which measures the dependence of the mechanical properties of one cell with respect to the r other cells.

The knowledge of all these frequencies gives an approximative description of the statistical behavior law of this material.

A first way to transform this description into a mathematical model is to introduce a family of random variables $X^{\varepsilon}_{i,j,k}$ where ε is the size of the cells and $f^{\varepsilon}_{i,j,k}$ denotes the associated conditional probabilities relying each cell to the others. For $\varepsilon \to 0$ the corresponding continuous model is rather to manage since we must handle the intricacies of continuous stochastic processes with moderate parameter space. In the present work we introduce an alternative mathematical model, which remains in the ream of finite combinatorics but replaced limit procedures by perfect approximations. This is possible in a slight extension of classical mathematics where absolute orders of magnitude are formalized.

3. The mathematical framework ZFL$_2$

Scientists often deal in an intuitive way with orders of magnitude, large, little, very large, near, very near... and they manipulate informally these fuzzy concepts in order to support their reasoning about real integers. But these concepts have no counterpart within classical mathematics. This is a fundamental weakness of mathematics, in particular as concerns modelisation where the link between micro et macroscopic levels has to be described. Fortunately there are now, since the emergence of A.Robinson's *Non Standard Analysis* [10] in the sixties, various conservative extensions of ZF where absolute orders of magnitude can be introduced in a very natural way. The most famous is E.Nelson's *Internal Set Theory* (IST) [8], an axiomatic setting of *Non Standard Analysis*. Weaker extensions may also be useful to the probabilist, as Nelson showed in his book on *Radically Elementary Probability Theor* y [9] (see also [1]).

In the present paper we introduce an elementary conservative extension of ZF with a double hierarchy of orders of magnitude in which we develop the theory of Radically Frequentist Statistics. Classical mathematics may be formalized in the context of Zermelo-Freankel's set theory (called here ZF). To get the extension ZFL$_2$ (second order Leibniz extension of ZF),we call internal the formulas of ZF we add to the language of ZF the two unary external predicates moderate and weakly moderate and the following axiom rule:

1) 1 is moderate

2) every integer which is lower than a moderate integer is moderate;

3) every integer which is lower than a weakly moderate integer is weakly moderate;

4) if n and m are moderate integers, so are $n+m$, nm and nm;

5) all moderate integers are weakly moderate;

6) there exists a weakly moderate integer which is not moderate;

7) there exists an integer which is not weakly moderate;

It is possible to prove (see [1]) that ZFL$_2$ is a conservative extension of ZF. This means that
:

(i) every internal statement which is a theorem in ZFL_2 is also a theorem in ZF;

(ii) all theorems of ZF are theorems within ZFL_2.

Thus ZFL_2 enriches classical mathematics with new concepts, but does not alter the status of internal statements: they are neither more nor less theorems in ZFL_2 than in ZF. This legitimates, from the logical point of view the use of ZFL_2 as a basis for the mathematical practice. But we have external theorems which may be of help in modelisation procedures. Among all external concepts expressible in the language of ZFL_2 we have the following:

DEFINITION 1. *A real number is called moderate (resp. weakly moderate) if and only if its absolute value has a moderate (resp. weakly moderate) integral part. A positive real number which is not moderate (resp weakly moderate) is called large (write $\sim \infty$) (resp. very large (write $\approx \infty$)). A real number is called small (resp. very small) if and only if it is* 0 *or its inverse is not moderate (resp. weakly moderate). Two real numbers x and y are called close (write $x \sim y$) (resp. very close (write $x \approx y$)) if their difference is small (resp. very small)*

The orders of magnitude satisfy the following generalized Leibniz rules:
Concerning the first scale:

THEOREM 1. *Moderate + moderate = moderate,*
moderate × moderate =moderate,
small + small = small,
small × moderate = small.

Concerning the second scale:

THEOREM 2. *Weakly moderate + weakly moderate = weakly moderate,*
weakly moderate × weakly moderate = weakly moderate,
very small + very small = very small,
very small × weakly moderate = very small.

The two scales are linked by the following relations:

THEOREM 3. *Very small ⇒ small,*
very large ⇒ large,
moderate ⇒ weakly moderate.

The proofs are easy consequences of the external axioms (see [1]).
Notice that a good model for the macroscopic continuous is a finite set $x_1 < x_2 < \cdots < x_n$ with $x_{1\approx}x_{2\approx\ldots\approx}x_n$ where $x_1 \approx -\infty$ and $x_n \approx +\infty$. If we use the weak scale, we have an intermediate near-continuous where a very large numbers of x_i remain at a small distance.

4. The theory RFS

In a ZFL_2 context we introduce the Radically Frequentist Statistics (RFS) theory which can be considered as an alternative mathematical foundation of statistics (see [6], [7]). The mean fact about RFS is that all results of Probability Theory which are relevant in statistics have a more general counterpart in RFS. Moreover, these probabilistic statements can be deduced from their RFS counterpart through a purely logical procedure. Thus RFS contains the whole scientific power of Probability Theory as concerns statistical modelisation.

The fundamental concept of RFS is that of *random number,* i.e. a finite sequence $X = (x_1, ..., x_s) \in \mathbf{R}^s$ with very large size s and such that $fr\{|X| > m\} \approx 0$ for every $m \approx \infty$.. Its *mean value* $M(X)$, *variance* $V(X)$, *deviation* $\sigma(X)$ and *distribution function* are defined as usual by the formulas

$$\begin{aligned} M(X) &= \frac{1}{s}\sum_{j=1}^{s} x_j \\ V(X) &= M((X - M(X))^2) = M(X^2) - (M(X))^2, \\ \sigma(X) &= \sqrt{V(X)}, \\ F_X(t) &= fr\{X \le t\}. \end{aligned}$$

We say that *t*wo random numbers X and Y *have common distribution* if and only if $fr\{X \in I\} \approx fr\{Y \in I\}$ for each interval I. Starting from the concept of random number, we define a *large random sample* as a finite sequence of random numbers $S = (X_1, ..., X_n)$ with n large but not very large. In other words we have a matrix (s_{ij}) with n rows and s columns, where each column is a *sample realization*. Then write $\mu(S)$ for the average of S, $\mu(S) = \frac{\sum X_i}{n}$.

The concept of large random sample can be interpreted as an idealization of the informal discourse which is usual in statistics: if very long independent sampling could be performed repeatedly a large number of times, we would know the phenomenon nearly perfectly.

Let $T = \{t_0, \cdots, t_n\}$ be a set of n real numbers with $t_0 < \cdots < t_n$ and n weakly moderate. A one-dimensional stochastic process indexed by T is a sequence of random numbers $X_{t_0}, \cdots, X_{t_n}$ with the same very large size s. As a random sample, also a stochastic process can be visualized by a nxs matrix, whose columns are the trajectories of the process.

In order to express the low of matter we have introduce the *characteristic function* $\Phi_X(t) = M(\exp(itX))$ of a random number X which satisfies :

(i) if X and Y have common (resp. weakly common) distribution, then $\Phi_X(t) \approx \Phi_Y(t)$ (resp. $\sim$) for every weakly moderate (resp. moderate) t;

(ii) inversion formula:

$$\begin{aligned} fr(a < X \le b) &+ \frac{1}{2}fr\{X = a\} - \frac{1}{2}fr\{X = b\} \\ &\approx \frac{1}{2\pi}\int_{-T}^{+T} \frac{exp(-ita) - exp(-itb)}{it}\Phi_X(t)dt \end{aligned}$$

for every $a < b$, every very large T ;

(iii) for every continuous probability density f with

$$\int_{-\infty}^{+T} f(x)dx \approx \int_{T}^{\infty} f(x)dx \approx 0$$

for all very large T, there is a random number X such that

$$\int_{-\infty}^{x_j} f(x)\,dx = \frac{j}{s+1}.$$

Then

$$\Phi_X(t) \approx \int_{-\infty}^{+\infty} exp(itx)f(x)dx$$

for all weakly moderate t;

(iv) if X is LL^n for some weakly moderate n, then

$$\Phi_X(t+h) = \Phi_X(t) + \sum_{k=1}^{n} \frac{h^k}{k!} M((iX)^k exp(itX)) + h^n \varepsilon$$

where $\varepsilon \approx 0$ for all $h \approx 0$ and weakly moderate t;

(v) if $S = (X_1, ..., X_n)$ is a sample of independent random numbers then

$$\Phi_{X_1+\cdots+X_n}(t) \approx \Phi_{X_1}(t) \cdots \Phi_{X_n}(t).$$

For the proof we refer to [6].

5. Theoretic model inside the RFS context

To formalize the empirical statistical description of §1 we introduce a random number $X_{i,j,k}$ for every cell (i, j, k) where $1 \leqslant i \leqslant n$, $1 \leqslant j \leqslant p$, $1 \leqslant k \leqslant q$. These random numbers take their values in a discrete finite set E and the numbers n, p, q are large while s is a very large. The cells are supposed to be of small size. Thus the model can be visualized by a multidimensional table $x^a_{i,j,k}$, $1 \leqslant a \leqslant s$.

We have then the following cases:

a linear material is represented by a nxs matrix;

a bidimensional material is represented by a cubic $nxpxs$ matrix;

a tridimensional material is represented by an hypercubic $nxpxqxs$ matrix.

The statistical matter behavior law can be expressed by means of the following conditional frequencies:

$$fr(X_{i,j,k} = a \mid X_{i_1,j_1,k_1} = a_1, X_{i_2,j_2,k_2} = a_2, \cdots, X_{i_r,j_r,k_r} = a_r).$$

The model suggests the following rough classification of behaviors:

A) Local behaviors: among them we distinguish between the independent case

$\forall a \in E$, $\forall a_1, \cdots, a_r \in E$

$$\left| \begin{array}{c} fr\left(X_{i,j,k} = a \mid X_{i_1,j_1,k_1} = a_1, X_{i_2,j_2,k_2} = a_2, \cdots, X_{i_r,j_r,k_r} = a_r\right) - \\ fr\left(X_{i,j,k} = a\right) \end{array} \right| \approx 0$$

and the weakly dependence case expressed by the conditions

$\forall a \in E$, $\forall a_1, \cdots, a_r \in E$

$$\left| \begin{array}{c} fr\left(X_{i,j,k} = a \mid X_{i_1,j_1,k_1} = a_1, X_{i_2,j_2,k_2} = a_2, \cdots, X_{i_r,j_r,k_r} = a_r\right) - \\ fr\left(X_{i,j,k} = a\right) \end{array} \right| \sim 0$$

B) Non local behavior, where we distinguish between the short range dependence expressed by the two conditions

$\forall a \in E$, $\forall a_1, \cdots, a_r \in E$

$\left| fr\left(X_{i,j,k} = a\right) - fr\left(X_{i,j,k} = a \mid X_{i_r,j_r,k_r} = a_r\right) \right| not \approx 0$

$$\left| \begin{array}{c} fr\left(X_{i,j,k} = a \mid X_{i_1,j_1,k_1} = a_1, X_{i_2,j_2,k_2} = a_2, \cdots, X_{i_r,j_r,k_r} = a_r\right) - \\ fr\left(X_{i,j,k} = a \mid X_{i_r,j_r,k_r} = a_r\right) \end{array} \right| \approx 0$$

and the weak short range dependence case expressed by:

$\left| fr\left(X_{i,j,k} = a\right) - fr\left(X_{i,j,k} = a \mid X_{i_r,j_r,k_r} = a_r\right) \right| not \approx 0$

$$\left| \begin{array}{c} fr\left(X_{i,j,k} = a \mid X_{i_1,j_1,k_1} = a_1, X_{i_2,j_2,k_2} = a_2, \cdots, X_{i_r,j_r,k_r} = a_r\right) - \\ fr\left(X_{i,j,k} = a \mid X_{i_r,j_r,k_r} = a_r\right) \end{array} \right| \sim 0$$

the cells (i_r, j_r, k_r) range into the neighborhood of the (i, j, k)cell;

C) the long range dependence case expressed by the conditions:

$\forall a \in E$, $\forall a_1, \cdots, a_r \in E$

$\left|fr\left(X_{i,j,k} = a\right) - fr\left(X_{i,j,k} = a \mid X_{i_r,j_r,k_r} = a_r\right)\right|$ *not* ≈ 0

and

$\left|fr\left(X_{i,j,k} = a\right) - fr\left(X_{i,j,k} = a \mid X_{i_r,j_r,k_r} = a_r\right)\right| \not\sim 0$

where the cells $(i_r, j_r, k_r)$are not necessary in the neighborhood of the (i, j, k)cell.

This classification may be refined if one relates the dependences with the distances. The inversion formula of the characteristic function may be useful to treat the information in order to eliminate the white noise and to put in evidence the intrinsic characteristic distances of the concerned matter.

6. Conclusion

This model gives a formal tool to characterize the behavior of matter in terms of local and non-local interactions.

A theoretical model inside the probabilistic context would replace the random numbers by the random variable and frequency by the probabilities. Such a modelization hides the intuitive interpretation of the model since the probability is a mathematical concept, which has no direct statistical interpretation. However, in the statistical context of RFS, which works within the mathematical framework of ZFL_2 the description of the behavior is at the same time intuitive and formal.

References

[1] LUTZ R. AND ALBUQUERQUE L G. *Modern infinitesimals as tools to Mach intuitive and formal reasoning in analysis*, to appear.

[2] MAGNO M., *Buckling of generalized beams*, Quaderni del dip. di Matem. dell'Univ. di Torino **27** (1999).

[3] GANGHOFFER J.F. AND MAGNO M., *Mechanics of planar beams focusing on buckling phenomena*, C. R. Acad. Sci. Paris **328** II b (2000), 283–288.

[4] GANGHOFFER J.F. AND MAGNO M., *From microscopic to macroscopic mechanics of beams*, Rend. Sem. Matem. Univ. e Polit. di Torino **57** 4 (1999).

[5] GANGHOFFER J.F. AND MAGNO M., *La mécanique des tissu*, Pour la Science (french edition of "Scientific American"), December 1999.

[6] MUSIO M. AND LUTZ R., *Radically frequentist statistics: a new background for statistics* (2000), preprint.

[7] MUSIO M., *Radically frequentist statistics: an intermediate theory between statistics and probability* (2000), preprint.

[8] NELSON E., *Internal set theory*, Bull. Amer. Math. Soc. **83** 6 (1977).

[9] NELSON E. *Radically elementary probability theory*, Ann. Math. Studies **117**, Princeton Univ. Press N.J. 1987.

[10] ROBINSON A., *Non-standard analysis*, North-Holland, Amsterdam 1966.

AMS Subject Classification: 74A25, 74A60.

Massimo MAGNO
Laboratoire de Physique et Mécanique des Textiles ENSITM
11, rue Alfred Werner
68093 Mulhouse, FRANCE
e-mail: `massimo.magno@mageos.com`

Monica MUSIO
Laboratoire des Mathématiques
Université de Haute Alsace
4, rue des frères Lumière
68093 Mulhouse, FRANCE

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

A.V. Porubov*

STRAIN SOLITARY WAVES IN AN ELASTIC ROD WITH MICROSTRUCTURE

Abstract. The nonlinear longitudinal strain solitary waves are studied inside cylindrical elastic rod with microstructure. The problem is solved using the pseudo-continuum Cosserat model and the Le Roux continuum model. A procedure is developed for derivation of a governing equation for longitudinal nonlinear strain waves. Exact solution of the equation has the form of a travelling bell-shaped solitary wave. The influence of microstructure on the solitary wave propagation is studied. Possible experimental determination of the parameters of the microstructure is discussed.

1. Introduction

Sometimes classic elastic theory cannot account for phenomenon caused by the microstructure of a material. A particular case is a dispersion of strain waves in an elastic medium. The influence of microstructure may provide dissipative effects [14, 6, 2], however, here consideration is restricted by non-dissipative case. The theory of microstructure has been developed recently, see [6, 7, 15, 17] and references therein. Most of results belong to the linear theory of elasticity, however, there are findings in the field of the nonlinear theory [6, 7]. Strain waves were studied mainly in the linear approximation [7, 15, 17]. Only a few works are devoted to the nonlinear waves in microstructured non-dissipative media [6, 19, 20, 10, 9]. Waves in elastic *wave-guides* with microstructure were out of considerable investigation. Also the values of the parameters characterizing microstructure, are unknown as a rule, only a few data may be mentioned [20].

It is known that the balance between nonlinearity and dispersion may result in an appearance of bulk localized long bell-shaped strain waves of permanent form (solitary waves or solitons) which may propagate and transfer energy over the long distance along an elastic wave guide. The amplification of them may cause the appearance of plasticity zones or microcracks in a wave guide. This is of importance for an assessment of durability of elastic materials and structures, methods of nondestructive testing, determination of the physical properties of elastic materials, particularly, polymeric solids, and ceramics. Bulk waves provide better suited detection requirements than surface strain waves in setting up a valuable nondestructive test for pipelines.

Recently, the theory has been developed to account for long longitudinal strain solitary waves propagating in a free lateral surface elastic rod [5, 21, 22]. The procedure has been proposed to obtain model equations using boundary conditions on the rod surface [18]. The nonlinearity, caused by both the finite stress values and elastic material properties, and the dispersion resulting from the finite transverse size of the rod, when in balance allow the propagation of

*This research has been supported by the INTAS under Grant 99-0167.

strain solitary waves v. The equation governing this process is of Boussinesq type, namely, a double dispersive equation

$$v_{tt} - \alpha_1 v_{xx} - \alpha_2 (v^2)_{xx} + \alpha_3 v_{xxtt} - \alpha_4 v_{xxxx} = 0.$$

The coefficients α_i depend upon the elastic parameters of the rod material. Exact solution of the equation has the form of a travelling bell-shaped solitary wave. The amplitude and the velocity of the solitary wave are explicitly connected with the elastic moduli. It allows to propose the estimation of the Murnaghan third order elastic moduli using measurement of the solitary wave parameters [1]. Motivated by analytical theoretical predictions, there has been successful experimental generation of strain solitons in a polystyrene free lateral surface rod using holographic interferometry [3]. The procedure developed in Ref.[18], has been successfully applied for the more complicated modelling of strain waves in a narrowing rod[4] and in a rod interacting with an another external elastic medium [1].

The present paper refers to the study of nonlinear solitary waves inside cylindrical rod with microstructure. The problem is solved using the "pseudocontinuum" Cosserat model and the Le Roux continuum model. A procedure is developed for derivation of the model equation for long longitudinal strain waves inside the rod. The influence of the microstructure on the solitary wave propagation is studied. Possible experimental determination of the parameters of the microstructure is discussed.

2. Modelling of elastic medium with microstructure

Recall some basic ideas following Eringen [7]. Suppose the macroelement of an elastic body contains discrete micromaterial elements. At any time the position of a material point of the αth microelement may be expressed as

$$\mathbf{x}^{(\alpha)} = \mathbf{x} + \xi^{(\alpha)},$$

where $\mathbf{x}$ is the position vector of the center of mass of the macroelement, $\xi^{(\alpha)}$ is the position of a point in the microelement relative to the center of mass. The motion of the center of mass depends upon the initial position $\mathbf{X}$ and time t, $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$, while for $\xi^{(\alpha)}$ the axiom of affine motion is assumed,

$$\xi^{(\alpha)} = \chi_K(\mathbf{X}, t)\ \Xi_K^{(\alpha)},$$

where $\Xi^{(\alpha)}$ characterizes initial position of a point relative to the center of mass. Then the square of the arc length is $(ds^{(\alpha)})^2 = d\mathbf{x}^{(\alpha)} d\mathbf{x}^{(\alpha)}$, and the difference between the squares of arc length in the deformed and undeformed body is

$$\begin{aligned}(ds^{(\alpha)})^2 - (dS^{(\alpha)})^2 &= (x_{k,K}\, x_{k,L} - \delta_{KL} + 2x_{k,K}\, \chi_{kM,L}\, \Xi_M \\ &+ \chi_{kM,K}\, \chi_{kN,L}\, \Xi_M\, \Xi_N) dX_K\, dX_L \\ &+ 2\left(x_{k,K}\, \chi_{kL} - \delta_{KL} + \chi_{kL}\, \chi_{kM}\, \Xi_M\right) dX_K\, d\Xi_L \\ &+ \chi_{kK}\, \chi_{kL} d\Xi_K\, d\Xi_L.\end{aligned} \tag{1}$$

where δ_{KL} is the Kronecker delta. Let us introduce vector of macrodisplacements, $\mathbf{U}(\mathbf{X}, t)$ and tensor of microdisplacements, $\Phi(\mathbf{X}, t)$,

$$\begin{aligned} x_{k,K} &= (\delta_{LK} + U_{L,K})\delta_{kL}, \\ \chi_{kK} &= (\delta_{LK} + \Phi_{LK})\delta_{kL} \end{aligned}$$

Then three tensors characterizing the behavior of microstructured medium follow from (1),

$$\begin{aligned}C_{KL} &= \frac{1}{2}\left(U_{K,L} + U_{L,K} + U_{M,K}U_{M,L}\right),\\ E_{KL} &= \Phi_{KL} + U_{L,K} + U_{M,K}\,\Phi_{ML},\\ \Gamma_{KLM} &= \Phi_{KL,M} + U_{N,K}\,\Phi_{NL,M},\end{aligned}$$

where C_{KL} is the Cauchy-Green macrostrain tensor, E_{KL} is the tensor of a reference distortion, Γ_{KLM} is the tensor of microdistortion. Tensor of the second rank E_{KL} accounts for the microelements motion relative to the center of mass of the macroelement, while tensor of the third rank Γ_{KLM} characterizes relative motion of the microelements of one another.

The density of the potential energy Π should be the function of these tensors, $\Pi = \Pi(C_{KL}, E_{KL}, \Gamma_{KLM})$, more precisely upon the invariants of them. The bulk density of the kinetic energy has the form [15]

(2) $$K = \frac{1}{2}\rho_0\left(U^2_{M,t} + J_{KN}\,\Phi_{KM,t}\,\Phi_{NM,t}\right),$$

where ρ_0 is macrodensity of the elastic material, J_{KN} is the inertia tensor. Elastic media with central symmetry posses simpler representation, $J_{KN} = J^*\delta_{KN}$.

One of the main problem is to define integrity basis of three tensors C_{KL}, E_{KL}, Γ_{KLM} [23, 8]. Moreover, the basic invariants of the third and higher rank tensors have not been studied. That is why the models were developed based on the additional assumption on a relationship between $\mathbf{U}$ and Φ. One of them is the pseudocontinuum Cosserat model. According to it

(3) $$\Phi_{KL} = -\varepsilon_{KLM}\Phi_M, \;\; \Phi_M = \frac{1}{2}\varepsilon_{MLK}U_{K,L},$$

where ε_{KLM} is the alternating tensor. The first relationship represents to the classic Cosserat model when only rotations of solid microelements are possible. The last expression in (3) accounts for the pseudocontinuum Cosserat model when micro rotation vector Φ coincides with the macro rotation vector. In this case the density of the potential energy my be either $\Pi = \Pi(C_{KL}, \Gamma_{KLM})$ or $\Pi = \Pi(C_{KL}, \Phi_{K,L})$ [17, 20]. Tensor E_{KL} has the form

$$E_{KL} = \frac{1}{2}\left(U_{K,L} + U_{L,K} + U_{M,K}U_{M,L} - U_{M,K}U_{L,M}\right),$$

and only linear part of E_{KL} coincides with those of C_{KL}. Assume the microstructure is sufficiently weak to be considered in the linear approximation[17, 20], and the Murnaghan model [5, 12, 16] is valid for macro motion. Then the density of the potential energy may be written as

(4) $$\begin{aligned}\Pi &= \frac{\lambda + 2\mu}{2}I_1^2 - 2\mu I_2 + \frac{l + 2m}{3}I_1^3 - 2mI_1I_2 + nI_3\\ &+ 2\mu M^2(\Phi_{K,L}\Phi_{K,L} + \eta\Phi_{K,L}\Phi_{L,K} + \beta\Phi_{K,K}\Phi_{L,L}),\end{aligned}$$

where λ and μ are the Lamé coefficients, (l, m, n) are the third order elastic moduli, or the Murnaghan moduli, M, η and β are the microstructure constants, I_p, $p = 1, 2, 3$ are the invariants of the tensor $\mathbf{C}$:

(5) $$I_1(\mathbf{C}) = tr\mathbf{C}, \;\; I_2(\mathbf{C}) = [(tr\mathbf{C})^2 - tr\mathbf{C}^2]/2, \;\; I_3(\mathbf{C}) = \det\mathbf{C}.$$

Another simplified microstructure model was used by some authors, see [15, 19, 10]. Sometimes it is referred to as the Le Roux continuum [9]. According to it

$$\Phi_{KL} = -U_{L,K}, \ \Gamma_{KLM} = -U_{L,KM}.$$

When microstructure is weak and may be considered in the linear approximation the linear part of E_{KL} is zero tensor. It means that there is no difference between deformation of elastic microelement and elastic macrostructure. In this case $\Pi = \Pi(C_{KL}, \Gamma_{KLM})$. Assume again the Murnaghan model for the macro part of the energy density and use the linear Mindlin's model [15] for its micro part one can obtain

$$\begin{aligned} \Pi \ &= \ \frac{\lambda+2\mu}{2} I_1^2 - 2\mu I_2 + \frac{l+2m}{3} I_1^3 - 2m I_1 I_2 + n I_3 + a_1 \Gamma_{KKM}\Gamma_{MLL} + \\ &\quad a_2\Gamma_{KLL}\Gamma_{KMM} + a_3\Gamma_{KKM}\Gamma_{LLM} + a_4\Gamma^2_{KLM} + a_5\Gamma_{KLM}\Gamma_{MLK}. \end{aligned} \tag{6}$$

where a_i, $i = 1-5$, are the constant microstructure parameters.

3. Nonlinear waves in a rod with pseudocontinuum Cosserat microstructure

Let us consider the propagation of a longitudinal strain wave in an isotropic cylindrical *compressible* nonlinearly elastic rod. We take cylindrical Lagrangian coordinates (x, r, φ) where x is directed along the axis of the rod, $-\infty < x < \infty$; r is the coordinate along the rod radius, $0 \le r \le R$; φ is a polar angle, $\varphi \, \epsilon[0, 2\pi]$. Neglecting torsions the displacement vector is $\mathbf{U} = (u, w, 0)$. Then nonzero components of the macrostrain tensor $\mathbf{C}$ are

$$\begin{aligned} C_{xx} \ &= \ u_x + \frac{1}{2}(u_x^2 + w_x^2), C_{rr} = w_r + \frac{1}{2}(u_r^2 + w_r^2), C_{\varphi\varphi} = \frac{w}{r} + \frac{w^2}{2r^2}, \\ C_{rx} \ &= \ C_{xr} = \frac{1}{2}\left(u_r + w_x + u_x u_r + w_x w_r\right). \end{aligned} \tag{7}$$

while nonzero components of the rotation tensor Φ_{KL} are

$$\Phi_{\varphi,x} = w_{xx} - u_{rx}, \qquad \Phi_{\varphi,r} = w_{xr} - u_{rr}. \tag{8}$$

The governing equations together with the boundary conditions are obtained using the Hamilton variational principle, i.e., setting to zero the variation of the action functional,

$$\delta S \ = \ \delta \int_{t_0}^{t_1} dt \left[2\pi \int_{-\infty}^{\infty} dx \int_0^R r \, \mathcal{L} dr \right] = 0, \tag{9}$$

where the Lagrangian density per unit volume, $\mathcal{L}$=$K - \Pi$, with K and Π defined by Eqs.(2) (4) correspondingly. The integration in brackets in (9) is carried out at the initial time $t = t_0$. Initially, the rod is supposed to be in its natural, equilibrium state.

The following boundary conditions (b.c.) are imposed:

$$w \ \to \ 0, \qquad \text{at } r \ \to \ 0, \tag{10}$$

$$P_{rr} \ = \ 0, \qquad \text{at } r \ = \ R, \tag{11}$$

$$P_{rx} \ = \ 0, \qquad \text{at } r \ = \ R, \tag{12}$$

where the components P_{rr}, P_{rx} of the modified Piola - Kirchhoff stress tensor $\mathbf{P}$ are defined from (9) with (4), (2), (7) and (8) being taken into account:

$$\begin{aligned} P_{rr} = \;& (\lambda+2\mu)\, w_r + \lambda\, \frac{w}{r} + \lambda\, u_x + \frac{\lambda+2\mu+m}{2}\, u_r^2 + \\ & \frac{3\lambda+6\mu+2l+4m}{2}\, w_r^2 + (\lambda+2l)\, w_r \frac{w}{r} + \frac{\lambda+2l}{2} \frac{w^2}{r^2} + \\ & (\lambda+2l)\, u_x w_r + (2l-2m+n)\, u_x \frac{w}{r} + \frac{\lambda+2l}{2}\, u_x^2 + \\ & \frac{\lambda+2\mu+m}{2}\, w_x^2 + (\mu+m)\, u_r w_x + 4\mu M^2\, (u_{rrx} - w_{xxr}), \end{aligned} \tag{13}$$

$$\begin{aligned} P_{rx} = \;& \mu\, (u_r + w_x) + (\lambda+2\mu+m)\, u_r w_r + (2\lambda+2m-n)\, u_r \frac{w}{r} + \\ & (\lambda+2\mu+m)\, u_x u_r + \frac{2m-n}{2}\, w_x \frac{w}{r} + (\mu+m)\, w_x w_r + \\ & (\mu+m)\, u_x w_x + 4\mu M^2 [w_{xxx} - u_{xxr} + \frac{1}{r}\, (r(w_{xr} - u_{rr}))_r - \\ & \frac{1}{2} J^* (u_{rtt} - w_{xtt})]. \end{aligned} \tag{14}$$

Exception of torsions provides transformation of the initial 3D problem into a 2D one. Subsequent simplification is caused by the consideration of only long elastic waves with the ratio between the rod radius R and typical wavelength L is $R/L \ll 1$. The typical elastic strain magnitude B is also small, $B \ll 1$. The Hamilton principle (9) yields a set of coupled equations for u and w together with the b.c. (11), (12). To obtain a solution in universal way one usually proceeds to the dimensionless form of the equations and looks for the unknown displacement vector components in the form of power series in the small parameters of the problem (for example R/L), hence, leading to an asymptotic solution of the problem. However, this procedure has some disadvantages. In particular, comparison of the predictions from the dimensionless solution to the experiments suffers from the fact that both B and L, are not well defined. Further, the coefficients of the nonlinear terms usually contain combinations of elastic moduli which may be also small in addition to the smallness of B [21, 22] something not predicted beforehand. Finally, this procedure gives equations of only first order in time, t, while general equations for displacements u and w are of the second order in time. Therefore the solution of the model equation will not satisfy two independent initial conditions on longitudinal strains or displacements [21].

An alternative is to simplify the problem making some assumptions about the behavior of longitudinal and/or shear displacements and/or strains in the elastic wave-guide. Referring to the elastic rod these relationships give explicit dependence of u and w upon the radius, while their variations along the rod axis are described by some unknown function and its derivatives along the axis of the rod. Then the application of Hamilton's principle (9) yields the governing equation in dimensional form for this function. This equation is of the second order of time, hence its solution can satisfy two independent initial conditions. Any combinations of elastic moduli appear in the coefficients of the equation, hence, subsequent scaling may take into account their orders when introducing small parameters.

For an elastic rod, the simplest assumption is the plane cross section hypothesis [13]: the longitudinal deformation process is similar to the beards movement on the thread. Then every cross-section of the rod remains flat, hence, $u = U(x,t)$ does not change along the radius

r. However, this assumption is not enough due to the Poisson effect, i.e., longitudinal and shear deformations are related. That is why Love proposed to use a relationship between w and u: $w = -r\,\nu\, U_x$, with ν the Poisson coefficient[11]. Unfortunately, the plane cross-section hypothesis and Love's hypothesis do not satisfy the boundary conditions that demand vanishing of both the normal and tangential stresses, P_{rr} and P_{rx}, at the lateral surface of the rod with prescribed precision.

Another theory has been proposed in [18] to find the relationships between displacement vector components satisfying b.c. on the lateral surface of the rod (11), (12) as well as the condition for w (10).

Since pure elastic wave are studied, $B \ll 1$, the "linear" and "nonlinear" parts of the relationships may be obtained separately. A power series approximations is used, as generally done for long wave processes. An additional parameter $\gamma = M^2/R^2$ is introduced to characterize the microstructure contribution. Accordingly, the longitudinal and shear displacement in *dimensional* form are:

$$\begin{aligned} u &= u_L + u_{NL}, \\ u_L &= u_0(x,t) + r\,u_1(x,t) + r^2 u_2(x,t) + ..., \\ u_{NL} &= u_{NL0}(x,t) + r\,u_{NL1}(x,t) + ..., \end{aligned} \tag{15}$$

$$\begin{aligned} w &= w_L + w_{NL}, \\ w_L &= w_0(x,t) + r\,w_1(x,t) + r^2 w_2(x,t) + ..., \\ w_{NL} &= w_{NL0}(x,t) + r\,w_{NL1}(x,t) + ... \end{aligned} \tag{16}$$

Substituting the linear parts u_L and w_L (15), (16) into the b.c. (10) and in the linear parts of b.c. (11), (12), and equating to zero terms at equal powers of r one obtains u_k and w_k. Using these results the nonlinear parts u_{NL} , w_{NL} are similarly obtained from the full b.c. We get

$$u = U(x,t) + \frac{\nu r^2}{2}\frac{1+4\gamma}{1-4\gamma}U_{xx}, \tag{17}$$

$$\begin{aligned} w &= -\nu r U_x - \frac{\nu}{2(3-2\nu)(1-4\gamma)}\left[\nu + 4\gamma(2+\nu)\right] r^3 U_{xxx} - \\ &\left[\frac{\nu(1+\nu)}{2} + \frac{(1-2\nu)(1+\nu)}{E}\Big(l(1-2\nu)^2 + 2m(1+\nu) - n\nu\Big)\right] r U_x^2, \end{aligned} \tag{18}$$

where ν is the Poisson ratio, E is the Young modulus. Other terms from the series (15), (16) for $i > 3$ may be found in the same way, however, they are omitted here because of no influence on the final model equation for the strain waves. Substituting (17), (18) into (9), and using Hamilton's principle we obtain that longitudinal strains, $v = U_x$, obey a double dispersive nonlinear equation:

$$v_{tt} - \alpha_1\, v_{xx} - \alpha_2 (v^2)_{xx} + \alpha_3\, v_{xxtt} - \alpha_4\, v_{xxxx} = 0, \tag{19}$$

where $\alpha_1 = c_*^2 = E/\rho_0$, $\alpha_2 = \beta/(2\rho_0)$, $\beta = (3E + 2l(1-2\nu)^3 + 4m(1+\nu)^2(1-2\nu) + 6n\nu^2)$, $\alpha_3 = \nu(1-\nu)R^2/2$,

$$\alpha_4 = \frac{\nu E R^2}{2\rho_0}\frac{1+4\gamma}{1-4\gamma}.$$

Hence the microstructure affects only dispersion in Eq.(19). The solitary wave solution of Eq.(19) is

$$v = \frac{6\nu E R^2 k^2}{\beta}\left(\frac{1+4\gamma}{1-4\gamma} - \frac{(1-\nu)V^2}{c_*^2}\right)\cosh^{-2}(k\,(x - Vt)), \tag{20}$$

where V is a free parameter while the wave number k is defined by

$$k^2 = \frac{2\rho_0(V^2 - c_*^2)}{\nu E R^2\left(\frac{1+4\gamma}{1-4\gamma} - \frac{(1-\nu)V^2}{c_*^2}\right)}. \tag{21}$$

Therefore the contribution of the microstructure results in the widening of the permitted solitary wave velocities,

$$1 < \frac{V^2}{c_*^2} < \frac{1}{1-\nu}\frac{1+4\gamma}{1-4\gamma}.$$

Also the characteristic width of the solitary wave proportional to $1/k$ becomes larger relative to the wave width in pure elastic case, $\gamma = 0$. We consider γ to be rather small due to the experimental data from Ref. [20]. Then the type of the solitary wave (compression/tensile) is defined by the sign of the nonlinearity parameter β like in case without microstructure.

4. Nonlinear waves in a rod with Le Roux continuum microstructure

The procedure of obtaining the governing equations is similar to those used in previous section. The nonzero components of the tensor Γ_{KLM} are

$$\begin{aligned}
\Gamma_{xxx} &= -u_{xx}, \Gamma_{xxr} = \Gamma_{rxx} = -u_{xr}, \Gamma_{xrx} = -w_{xr},\\
\Gamma_{xrr} &= \Gamma_{rrx} = -w_{xr}, \Gamma_{rxr} = -u_{rr}, \Gamma_{rrr} = -w_{rr}.
\end{aligned}$$

The b.c. (11), (12) are satisfied for the strain tensor components

$$\begin{aligned}
P_{rr} = {} & (\lambda + 2\mu)\, w_r + \lambda\, \frac{w}{r} + \lambda\, u_x + \frac{\lambda + 2\mu + m}{2}\, u_r^2 + \frac{3\lambda + 6\mu + 2l + 4m}{2}\, w_r^2 + \\
& (\lambda + 2l)\, w_r \frac{w}{r} + \frac{\lambda + 2l}{2}\frac{w^2}{r^2} + (\lambda + 2l)\, u_x w_r + (2l - 2m + n)\, u_x \frac{w}{r} + \\
& \frac{\lambda + 2l}{2}\, u_x^2 + \frac{\lambda + 2\mu + m}{2}\, w_x^2 + (\mu + m)\, u_r w_x + 2J^*(2u_{xtt} + w_{rtt}) - \\
& 2a_1 u_{xxx} - 2(a_1 + 2a_2) w_{xxr} - 2(a_1 + a_2)\frac{1}{r}\,(r(w_{rr}))_r - a_1 \frac{1}{r}\,(r(u_{xr}))_r\,,
\end{aligned} \tag{22}$$

$$\begin{aligned}
P_{rx} = {} & \mu\,(u_r + w_x) + (\lambda + 2\mu + m)\, u_r w_r + (2\lambda + 2m - n)\, u_r \frac{w}{r} + \\
& (\lambda + 2\mu + m)\, u_x u_r + \frac{2m - n}{2}\, w_x \frac{w}{r} + (\mu + m)\, w_x w_r + \\
& (\mu + m)\, u_x w_x + 2J^* u_{rtt} - a_1 w_{xrr} - 2(a_1 + 2a_2) u_{xxr} - 2a_2 \frac{1}{r}\,(r(u_{rr}))_r\,.
\end{aligned} \tag{23}$$

Then the approximations for the components of the displacement vector have the form

$$u = U(x,t) + \frac{\nu r^2}{2}\frac{1}{1-N}U_{xx}, \tag{24}$$

$$
\begin{aligned}
w \;=\; & -\nu r U_x \;-\; \frac{4J^*(2-\nu)(1+\nu)(1-2\nu)}{E(3-2\nu)R^2} r^3 U_{xtt} - \\
& \frac{\nu^2-(1-2\nu)(1-N)(G(1-\nu)-2\nu N)}{2(3-2\nu)(1-N)} r^3 U_{xxx} - \\
& \left[\frac{\nu(1+\nu)}{2}+\frac{(1-2\nu)(1+\nu)}{E}\Big(l(1-2\nu)^2+2m(1+\nu)-n\nu\Big)\right] r U_x^2, \qquad (25)
\end{aligned}
$$

where $G = 2a_1/\mu R^2$, $N = 2a_2/\mu R^2$. Like in previous section the governing equation for longitudinal strain $v = U_x$ is the double dispersive equation (19) whose coefficients are defined now as

$$
\alpha_1 = c_*^2, \alpha_2 = \frac{\beta}{2\rho_0}, \alpha_3 = \frac{\nu R^2}{2(1-N)} - \frac{\nu^2 R^2}{2} + 2J^*\nu(2-\nu), \alpha_4 = \frac{\nu c_*^2 R^2}{2(1-N)}.
$$

Solitary wave solution has the form

$$
v = \frac{6\nu E R^2 k^2}{\beta}\left(\frac{1}{1-N} - \left[\frac{1}{1-N} - \nu + \frac{4J^*(2-\nu)}{R^2}\right]\frac{V^2}{c_*^2}\right)\cosh^{-2}(k\,(x-Vt)), \qquad (26)
$$

where V is a free parameter, and the wave number k is defined by

$$
k^2 = \frac{2(1-N)\rho_0(V^2-c_*^2)}{\nu E R^2\left[c_*^2 - V^2\left(1-\nu(1-N)+4J^*(1-N)(2-\nu)/R^2\right)\right]}. \qquad (27)
$$

Physically reasonable case corresponds to rather small N, $N < 1$. Then the influence of the microstructure yields an alteration of the permitted solitary wave velocities interval,

$$
1 < \frac{V^2}{c_*^2} < \frac{1}{1-\nu(1-N)+4J^*(1-N)(2-\nu)/R^2}.
$$

The widening or narrowing of the interval depends upon the relationship between N and the parameter of microinertia J^*. Like in previous section the type of the solitary wave is governed by the sign of the nonlinearity parameter β. At the same time the characteristic width of the solitary wave proportional to $1/k$ turns out smaller than the wave width in a pure macroelastic case, $N = 0$, $J^* = 0$.

5. Discussion

It is found that the double dispersive equation (19) accounts for longitudinal strain wave propagation inside the rod even in presence of the microstructure, and only dispersion term coefficients alter in comparison with the pure macroelastic case. The procedure proposed in [18] is profitably applied for the derivation of the governing equation in dimensional form for both the Cosserat and the Le Roux models. The assumption of the linear contribution of the microstructure is correct since its nonlinear contribution, being weaker, may provide alterations only in the neglected higher order nonlinear and dispersion terms in the governing equation. Hence we don't need in an additional nonlinear terms in the density of the potential energy Π thus avoiding the additional unknown parameters (like Murnaghan's third order moduli) describing the nonlinear contribution of the microstructure.

The alterations of the amplitude and the wave width, caused by the microstructure, have been found in both case under study. The important result is in the opposite changing of the wave width which gives a possibility to distinguish the Cosserat and the Le Roux models in possible experiments.

The dispersion caused by the microstructure may be observed experimentally, and numerical data on microstructure parameters my be obtained[20]. In experiments on solitary waves propagation [3] the amplitude and the velocity of the wave may be measured. Therefore expressions (20), (21) provide possible estimation of the parameter M in the pseudocontinuum Cosserat model. In case of the Le Roux continuum there is an extra parameter J^*, see (26), (27), and parameters N and J^* cannot be estimated separately.

References

[1] PORUBOV A.V., SAMSONOV A.M., VELARDE M.G. AND BUKHANOVSKY A.V., *Strain solitary waves in an elastic rod embedded in another elastic external medium with sliding*, Phys. Rev. **58** E (1998), 3854–3864.

[2] CERMELLI P. AND PASTRONE F., *Growth and decay of waves in microstructured solids*, Proc. Estonian Acad. Sci. Phys. Math. **46** (1997), 32–40.

[3] DREIDEN G.V., PORUBOV A.V., SAMSONOV A.M., SEMENOVA I.V. AND SOKURINSKAYA E.V., *Experiments in the propagation of longitudinal strain solitons in a nonlinearly elastic rod*, Tech. Phys. Lett. **21** (1995), 415–417.

[4] SAMSONOV A.M., DREIDEN G.V., PORUBOV A.V. AND SEMENOVA I.V., *Longitudinal-strain soliton focusing in a narrowing nonlinearly elastic rod*, Phys. Rev. B **57** (1998), 5778–5787.

[5] ENGELBREGHT J., *Nonlinear wave processes of deformation in solids*, Pitman, Boston 1983.

[6] ENGELBREGHT J. AND BRAUN M., *Nonlinear waves in nonlocal media*, Appl. Mech. Rev. **51** 8 (1998), 475–488.

[7] ERINGEN A.C., *Theory of micropolar elasticity*, in: "Fracture. An advanced treatise" (Ed. H. Liebowitz), Mathematical Fundamentals **2**, Academic Press, New York 1968, 622–729.

[8] ERINGEN A.C. AND SUHUBI E.S., *Nonlinear theory of micro-elastic solids*, Intern. J. Eng. Sci. **2** (1964), Part I 189–203, Part II 389–404.

[9] EROFEEV V.I., *Wave processes in solids with microstructure*, Moscow University Publ., Moscow 1999, 328.

[10] EROFEEV V.I. AND POTAPOV A.I., *Longitudinal strain waves in non-linearly elastic media with couple stresses*, Int. J. Nonlin. Mech. **28** 4 (1993), 483–488.

[11] LOVE A.E.H., *A Treatise on the mathematical theory of elasticity*, University Press, Cambridge 1927.

[12] LURIE A.I., *Nonlinear theory of elasticity,* Elsevier, Amsterdam 1990.

[13] MCNIVEN H.D. AND MCCOY J.J., *Vibrations and wave propagation in rods*; in: "R. Mindlin and applied mechanics" (Ed. G. Herrmann), Pergamon, New York 1974, 197–226.

[14] MAUGIN G.A. AND MUSCHIK W., *Thermodynamics with internal variables*; part I: *General concepts*, part II: *Applications*, J. Non-Equil. Thermodyn. **19** (1994), 217–289.

[15] MINDLIN R.D., *Microstructure in linear elasticity*, Archive of Rat. Mech. and Anal. **1** (1964), 51–78.

[16] MURNAGHAN F.D., *Finite deformations of an elastic solid*, J. Wiley, New York 1951.

[17] NOWACKI W., *Theory of elasticity*, Mir, Moscow 1975.

[18] PORUBOV A.V. AND SAMSONOV A.M., *Refinement of the model for the propagation of longitudinal strain waves in a rod with nonlinear elasticity*, Tech. Phys. Lett. **19** (1993), 365–366.

[19] SAVIN G.N., LUKASHEV A.A. AND LYSKO A.A., *Elastic wave propagation in a solid with microstructure*, Soviet Appl. Mech. **15** (1973), 725.

[20] SAVIN G.N., LUKASHEV A.A., LYSKO A.A., VEREMEEENKO S.V. AND AGASIEV G.G., *Elastic wave propagation in the Cosserat continuum with constrained particle rotation*, Soviet Appl. Mech. **15** (1973).

[21] SAMSONOV A.M., *Nonlinear strain waves in elastic waveguides*; in: "Nonlinear Waves in Solids" (Eds. A. Jeffrey and J. Engelbrecht), Springer, New York 1994.

[22] SAMSONOV A.M., *How to predict, generate and observe strain solitons in solids*, Acta Tech. CSAV **42** (1997), 93–113.

[23] SPENCER A.J.M., *Theory of invariants,* New York 1971.

AMS Subject Classification: 74A60, 74B20, 74J30.

Alexey V. PORUBOV
Ioffe Physical Technical Institute of the Russian Academy of Sciences
Polytechnicheskaya st., 26
St.Petersburg, 194021 RUSSIA
e-mail: `porubov@soliton.ioffe.rssi.ru`

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

R. Segev*

NOTES ON STRESSES FOR MANIFOLDS

Abstract. The geometric structure of stress theory on differentiable manifolds is considered. Mechanics is assumed to take place on an m-dimensional and no additional metric or parallelism structure is assumed. Two different approaches are described. The first is a generalisation of the traditional Cauchy approach where the resulting stresses are represented mathematically as vector valued $(m-1)$-forms. The second approach is variational and stresses are represented by densities valued in the dual of the first jet bundle. It is shown how a variational stress induces a Cauchy stress.

1. Introduction

This work describes some issues related to the formulation of stress theory on manifolds. In previous works (see [1, 2, 3, 4]), stress theory for the case where both body and space are modeled by differentiable manifolds rather the traditional Euclidean spaces was developed. In [1] a general weak formulation of stress theory was presented. On the basis of some general guidelines (see the motivation for the introduction of variational stresses below), stresses were presented as measures on the body manifold valued in the dual of a jet bundle. Such a stress measure represents a force using a representation theorem for the force functional. In that work, assuming that the stress measures may be represented by smooth densities, the additional geometric structure of a connection was used in order to allow the representation of a force by a body force field and a surface force field. In the sequel, we will refer to this approach as the variational approach. In the more recent works, [2, 3] stress theory was presented on manifolds without any additional geometric structure (e.g., a connection) from a point of view that is analogous to the classical Cauchy theory of stresses. In [2] the theory was presented for the case of scalar valued quantities and in [3] the theory was extended to forces. We will refer to this method as the generalized Cauchy approach. In [4], some aspects of the relation between the Cauchy approach and the variational approach were considered.

After a presentation of the generalized Cauchy approach in Section 2, Section 3 is concerned with the Cauchy postulates given in [3]. It is shown that the boundedness postulate in [3], that is a generalization of the balance of momentum in the traditional formulation, is not general enough. A revised version of the boundedness postulate is suggested and it is shown that the weaker assumption does not alter the proof of the generalized Cauchy theorem in the aforementioned paper.

Sections 4 and 5 review the variational approach and its relation to the generalized Cauchy approach presented in [4]. Section 6 extends this relation and shows how the representation of

*The research leading to this paper was partially supported by the Paul Ivanier Center for Robotics Research and Production Management at Ben-Gurion University.

forces by body forces and surface forces in the Cauchy approach is completely equivalent to the representation of forces by variational stress densities in the variational approach.

2. Cauchy's stress theory for manifolds

Let $\pi : W \to \mathcal{U}$ be a vector bundle over the m-dimensional orientable manifold $\mathcal{U}$. It is assumed that a particular orientation is chosen on $\mathcal{U}$. The vector bundle is interpreted as the bundle of generalized velocities over $\mathcal{U}$. The manifold $\mathcal{U}$ is interpreted as the universal body and the vector bundle is interpreted as the bundle of generalized velocities over $\mathcal{U}$. Cauchy's stress theory for manifolds, presented in [3], considers for each compact m-dimensional submanifold with boundary $\mathcal{R}$ of $\mathcal{U}$ linear functionals of the generalized velocity fields containing a volume term and a boundary term of the form

$$F_{\mathcal{R}}(w) = \int_{\mathcal{R}} \mathbf{b}_{\mathcal{R}}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w).$$

Here, using the notation $\bigwedge^p(T^*X)$ for the bundle of p-forms on a manifold X, w is a section of W, $\mathbf{b}_{\mathcal{R}}$, the *body force*, is a section of $L\big(W, \bigwedge^m(T^*\mathcal{R})\big)$ and $\mathbf{t}_{\mathcal{R}}$ the *boundary force* is a section of $L\big(W, \bigwedge^{m-1}(T^*\partial\mathcal{R})\big)$. The functional $F_{\mathcal{R}}$ is interpreted as the force, or power, functional and the value $F_{\mathcal{R}}(w)$ is classically interpreted as the power of the force for the generalized velocity field w.

Cauchy's postulates for the force system $\{F_{\mathcal{R}} = (\mathbf{b}_{\mathcal{R}}, \mathbf{t}_{\mathcal{R}})\}$ presented in [3] may be summarized as follows.

- (*i*) For every $x \in \mathcal{U}$ and every body $\mathcal{R}$, $\mathbf{b}_{\mathcal{R}}(x) = \mathbf{b}(x)$, that is, the value of the body force at a point is independent of the body containing it. Accordingly, we will omit the subscript $\mathcal{R}$.
- (*ii*) Let us consider the Grassmann bundle of hyperplanes $G_{m-1}(T\mathcal{U}) \to \mathcal{U}$ whose fiber $G_{m-1}(T_x\mathcal{U})$ at any point $x \in \mathcal{U}$ is the Grassmann manifold of hyperplanes, i.e., $(m-1)$-dimensional subspaces of the tangent space $T_x\mathcal{U}$. Let

$$L\big(W, \bigwedge^{m-1} G_{m-1}(T\mathcal{U})^*\big) \to G_{m-1}(T\mathcal{U})$$

  be the vector bundle over $G_{m-1}(T\mathcal{U})$ whose fiber over a hyperplane $H \subset T_x\mathcal{U}$ is the vector space of linear mappings $L\big(W_x, \bigwedge^{m-1} H^*\big)$. Then, the dependence of $\mathbf{t}_{\mathcal{R}}$ on $\mathcal{R}$ is via a smooth section

$$\Sigma : G_{m-1}(T\mathcal{U}) \to L\big(W, \bigwedge^{m-1} G_{m-1}(T\mathcal{U})^*\big),$$

  the *Cauchy section*, such that $\mathbf{t}_{\mathcal{R}} = \Sigma(H)$ where $H = T_x\partial\mathcal{R}$.
- (*iii*) The Cauchy section Σ is continuous.
- (*iv*) There is a section ζ of $L\big(W, \bigwedge^m(T^*\mathcal{U})\big)$ such that

$$\big|F_{\mathcal{R}}(w)\big| = \left|\int_{\mathcal{R}} \mathbf{b}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)\right| \leq \int_{\mathcal{R}} \zeta(w)$$

  for every body $\mathcal{R}$.

Using the results of [2], it is shown in [3] that there is a unique section σ of $L\big(W, \bigwedge^{m-1}(T^*\mathcal{U})\big)$ called the *Cauchy stress* such that

$$\mathbf{t}_{\mathcal{R}}(w)(v_1, \ldots, v_{m-1}) = \sigma(w)(v_1, \ldots, v_{m-1}),$$

for any collection of $m-1$ vectors $(v_1, \ldots, v_{m-1}) \in T_x\partial\mathcal{R},\ x \in \partial\mathcal{R}$, where the dependence on x was omitted in order to simplify the notation. Using the notation $\iota\colon \partial\mathcal{R} \to \mathcal{U}$ for the natural inclusion mapping, so that $\iota^*\colon \bigwedge^{m-1}(T^*\mathcal{U}) \to \bigwedge^{m}-1\big(T^*\partial\mathcal{R}\big)$ is the restriction of forms, we may write $\mathbf{t}_{\mathcal{R}}(w) = \iota^*\big(\sigma(w)\big)$ which we will also write as $\mathbf{t}_{\mathcal{R}} = \iota^*(\sigma)$—the generalized Cauchy formula. We will refer to this result as the *generalized Cauchy theorem*.

Assume that (x^i, w^α) are local vector bundle coordinates in a neighborhood $\pi^{-1}(U) \subset W$, $U \subset \mathcal{U}$ with local basis elements $\{W^\alpha e_\alpha\}$ so a section of W is represented locally by $w^\alpha W^\alpha e_\alpha$. Then, denoting the dual base vectors by $\{W^\alpha e_\alpha\}$ a stress σ is represented locally by

$$\sigma_{\alpha 1\ldots\hat{k}\ldots m} W^\alpha e_\alpha \otimes dx^1 \wedge \ldots \wedge \widehat{dx^k} \wedge \ldots \wedge dx^m,$$

where a "hat" indicates the omission of an item (an index or a factor). The value of $\sigma(w)$ is represented locally by

$$\sigma_{\alpha 1\ldots\hat{k}\ldots m} w^\alpha dx^1 \wedge \ldots \wedge \widehat{dx^k} \wedge \ldots \wedge dx^m.$$

3. The revised boundedness postulate

If we substitute the generalized Cauchy formula into the expression for $F_{\mathcal{R}}(w)$ we obtain

$$\begin{aligned} F_{\mathcal{R}}(w) &= \int_{\mathcal{R}} \mathbf{b}_{\mathcal{R}}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w) \\ &= \int_{\mathcal{R}} \mathbf{b}_{\mathcal{R}}(w) + \int_{\partial\mathcal{R}} \iota^*\big(\sigma(w)\big) \\ &= \int_{\mathcal{R}} \mathbf{b}_{\mathcal{R}}(w) + \int_{\mathcal{R}} d\big(\sigma(w)\big), \end{aligned}$$

where Stokes' theorem was used in the last line. It is clear form the local expression for $\sigma(w)$ that the exterior derivative $d\sigma(w)$ depends on the derivative of w an not only on the local value of w. In other words, $F_{\mathcal{R}}(w)$ is a local linear functional on the first order jet $j^1(w)$.

Using the observation that $F_{\mathcal{R}}$ should be a local linear functional on the first jet of w, we replace the boundedness postulate (*iv*) by the following

Revised boundedness postulate

There is a section S of $L\big(J^1(W), \bigwedge^m(T^*\mathcal{U})\big)$ such that

$$\big|F_{\mathcal{R}}(w)\big| = \left|\int_{\mathcal{R}} \mathbf{b}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)\right| \le \int_{\mathcal{R}} \left|S\big(j^1(w)\big)\right|,$$

where the absolute value of an m-form θ, $S\big(j^1(w)\big)$ in this case, is given as

$$|\theta(x)| = \begin{cases} \theta(x) & \text{if } \theta(x) \text{ is positively oriented,} \\ -\theta(x) & \text{if } \theta(x) \text{ is negatively oriented} \end{cases}$$

relatively to the orientation chosen on $\mathcal{U}$.

It is noted that the revised boundedness postulate may also be written as

$$\Big|\int\limits_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)\Big| \leq \int\limits_{\mathcal{R}} \Big|S_0\big(j^1(w)\big)\Big|,$$

for some section S_0 of $L\big(J^1(W), \bigwedge^m(T^*\mathcal{U})\big)$. This follows from

$$-\Big|\int\limits_{\mathcal{R}} \mathbf{b}(w)\Big| + \Big|\int\limits_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)\Big| \leq \Big|\int\limits_{\mathcal{R}} \mathbf{b}(w) + \int\limits_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)\Big| \leq \int\limits_{\mathcal{R}} \Big|S\big(j^1(w)\big)\Big|$$

so

$$\begin{aligned}\Big|\int\limits_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)\Big| &\leq \int\limits_{\mathcal{R}} \Big|S\big(j^1(w)\big)\Big| + \Big|\int\limits_{\mathcal{R}} \mathbf{b}(w)\Big| \\ &\leq \int\limits_{\mathcal{R}} \Big|S\big(j^1(w)\big)\Big| + \int\limits_{\mathcal{R}} \Big|\mathbf{b}(w)\Big| \\ &= \int\limits_{\mathcal{R}} \Big(\Big|S\big(j^1(w)\big)\Big| + \Big|\mathbf{b}(w)\Big|\Big) \\ &\leq \int\limits_{\mathcal{R}} \Big|S_0\big(j^1(w)\big)\Big|,\end{aligned}$$

for some S_0.

For an arbitrary $x \in \mathcal{U}$ we want to show that

$$\mathbf{t}_{\mathcal{R}}(w) = \Sigma(T_x\partial\mathcal{R})(w) = \iota^*\big(\sigma(w)\big),$$

for a unique element of $L\big(W_x, \bigwedge^m -1(T_x\mathcal{U})\big)$, where in the equation above we omitted the dependence on x.

Just as in [3], the proof the generalized Cauchy theorem is based on the following points:

(a) The assertion is local and written in an invariant form and hence it may be proved in any vector bundle chart.

(b) Using a local basis $\{W^\alpha e_\alpha\}$ for the neighbohood where the vector bundle chart is used, any vector $w \in W_x$ may be expressed in the form $w = w^\alpha W^\alpha e_\alpha$, so $\mathbf{t}_{\mathcal{R}}(w) = w^\alpha \tau_{\mathcal{R}\alpha}$, where, $\tau_{\mathcal{R}\alpha} = \mathbf{t}_{\mathcal{R}}(W^\alpha e_\alpha)$.

(c) For the local vector field $W^\alpha e_\alpha$ in the chart neighborhood of x, the scalar valued extensive property given by the volume term $\beta_\alpha = \mathbf{b}(W^\alpha e_\alpha)$, the flux density term $\tau_{\mathcal{R}\alpha} = \mathbf{t}_{\mathcal{R}}(W^\alpha e_\alpha)$, and the source term $s_\alpha = \big|S\big(j^1(Wase_\alpha)\big)\big|$ satisfies the generalized Cauchy postulates for scalar valued quantities (see [2]). In particular, it is noted that if $S\big(j^1(w)\big)$ is represented locally by

$$S\big(j^1(w)\big)_{\alpha 1\dots m}dx^1\wedge\dots\wedge dx^m = \big(S_{\alpha 1\dots m}w^\alpha + S^i_{\alpha 1\dots m}w^\alpha_{,i}\big)dx^1\wedge\dots\wedge dx^m$$

(the components dual to w^α and those dual to w^α_i differ in notation only by the number of indices), then, $s_\alpha = |S_{\alpha 1\dots m}|$. Hence, by the Cauchy theorem for scalars [2], there is a unique collection of (dim W_x) $(m-1)$-forms σ_α such that $\tau_{\mathcal{R}\alpha} = \iota^*(\sigma_\alpha)$. These forms represent $\sigma(x) \in L\big(W_x, \bigwedge^{m-1} T_x\partial\mathcal{R}\big)$ in the given chart.

4. Variational stress densities

Let $\pi : W \to \mathcal{U}$ be a vector bundle as in the previous section. A *variational stress density* is a section of $L\big(J^1(W)_1 \bigwedge^m (T^*\mathcal{U})\big)$, where $J^1(W)$ is the first jet bundle associated with W.

For the vector bundle coordinate system (x^i, w^α), $i = 1, \dots, m$, $\alpha = 1, \dots, \dim(W_x)$, the jet of a section is represented locally by the functions $\{w^\alpha(x^i), w^\beta_{,j}(x^k)\}$, where a subscript following a comma indicates partial differentiation. A variational stress density will be represented locally by the functions $\{S_{\alpha 1\dots m}, S^j_{\beta 1\dots m}\}$ so that the single component of the m-form $S\big(j^1(w)\big)$ in this coordinate system is

$$S\big(j^1(w)\big)_{1\dots m} = S_{\alpha 1\dots m} w^\alpha + S^j_{\beta 1\dots m} w^\beta_{,j}.$$

Note that the notation distinguishes between the components of S that are dual to the values of the section and those dual to the derivatives by the number of indices only. The next few paragraphs motivate the introduction of variational stress densities.

The rational behind the generalized variational formulation of stress theory is the framework for mechanical theories where a configuration manifold is constructed for the system under consideration, generalized velocities are defined as elements of the tangent bundle to the configuration manifold, and generalized forces are defined as elements of the cotangent bundle of the configuration space. For the mechanics of continuous bodies, a configuration is an embedding of the body $\mathcal{R}$ in space $\mathcal{M}$. The natural topology for the collection of embeddings is the C^1-topology for which the collection of embeddings is open in the collection of all C^1-mappings of the body into space. Using this topology, the tangent space to the configuration manifold at the configuration $\kappa : \mathcal{R} \to \mathcal{M}$ is $C^1\big(\kappa^*(T\mathcal{M})\big)$, the Banachable space of C^1-sections of the pullback $\kappa^*(T\mathcal{M})$. Thus forces in continuum mechanics are elements of $C^1\big(\kappa^*(T\mathcal{M})\big)^*$ – linear functionals on the space of differentiable vector fields equipped with the C^1-topology.

The basic representation theorem (see [1]) states that a force functional $F \in C^1\big(\kappa^*(T\mathcal{M})\big)^*$ may be represented by measures on $\mathcal{U}$ - the *variational stress measures* - valued in $J^1(\kappa^*(T\mathcal{M}))^*$, the dual of the first jet bundle $J^1(\kappa^*(T\mathcal{M})) \to \mathcal{U}$. Thus, the evaluation of a force $F_\mathcal{R}$ on the generalized velocity w is

$$F_\mathcal{R}(w) = \int_\mathcal{R} d\mu\big(j^1(w)\big),$$

where μ is the $J^1(\kappa^* T\mathcal{M})^*$-valued measure – a section Schwartz distribution.

Assuming that κ is defined on all the material universe $\mathcal{U}$, we use the notation W for $\kappa^*(T\mathcal{M})$. This vector bundle can be restricted to the individual bodies, and with some abuse of notation, we use the same notation for both the bundle and its restriction to the individual bodies.

Thus, in the smooth case, a variational stress measure is given in terms of a section S of the vector bundle of linear mappings $L\big(J^1(W), \bigwedge^{m-1}(T^*\mathcal{U})\big)$ so

$$F_\mathcal{R}(w) = \int_\mathcal{R} S(j^1(w)).$$

This expression makes sense as $S(j^1(w))$, is an $(m-1)$-form whose value at a point $x \in \mathcal{R}$ is $S(x)\big(j^1(w)(x)\big)$.

Since in the sequel we consider only the smooth case, we will use "variational stresses" to refer to the densities.

5. The Cauchy stress induced by a variational stress

In [4] we defined a canonical mapping

$$p_\sigma : L\big(J^1(W), \bigwedge^m (T^*\mathcal{U})\big) \to L\big(W, \bigwedge^{m-1} (T^*\mathcal{U})\big),$$

that assigns to a variational stress density S a Cauchy stress σ satisfying the following relation. At every $x \in \mathcal{U}$ (we suppress the evaluation at x in the notation)

$$\phi \wedge \sigma(w) = S(j_{\phi\otimes w}).$$

Here, $j_{\phi\otimes w}$ is roughly the jet at x of a section whose value is $0 \in W_x$ and its derivative is $\phi \otimes w$. More precisely, if $u\colon \mathcal{U} \to W$ is the section whose first jet at x is $j_{\phi\otimes w}$, then, u satisfies the following conditions: $u(x) = 0$; denoting the zero section of W by 0, $T_x u - T_x 0 \in L\big(T_x\mathcal{U}, T_{0(x)} W_x\big)$ induces the linear mapping $\phi \otimes w$ through the isomorphism of $T_{0(x)} W_x$ with W_x. The local representative of p_σ is as follows. If $\sigma = p_\sigma(S)$, then, using the local representatives of σ and S as in the previous sections,

$$\sigma_{\beta 1 \ldots \hat{\imath} \ldots m} = (-1)^{i-1} S^{+i}_{\beta 1 \ldots m}, \quad \text{(no sum over } i\text{)}.$$

The mapping p_σ is clearly linear and surjective.

6. The divergence of a variational stress

Given a variational stress density S its generalized divergence Div S is the section of the bundle $L\big(W, \bigwedge^m (T^*\mathcal{U})\big)$ defined by

$$\mathrm{Div} S(w) = d\big(p_\sigma(S)(w)\big) - S\big(J^1(w)\big).$$

The local expression for Div $S(w)$ is

$$\big(S^i_{\alpha 1 \ldots m,i} - S_{\alpha 1 \ldots m}\big) w^\alpha dx^1 \wedge \ldots \wedge dx^m,$$

which shows that Div S depends only on the values of w and not its derivative. With these definitions one obtains for the case where

$$F_{\mathcal{R}}(w) = \int_{\mathcal{R}} S\big(j^1(w)\big)$$

that

$$F_{\mathcal{R}}(w) = \int_{\mathcal{R}} \mathbf{b}_{\mathcal{R}}(w) + \int_{\partial\mathcal{R}} \mathbf{t}_{\mathcal{R}}(w)$$

where $\mathbf{t}_{\mathcal{R}}(w) = \iota^*_{\mathcal{R}}\big(\sigma(w)\big)$ and Div $S + \mathbf{b}_{\mathcal{R}} = 0$. We conclude that every variational stress induces a unique force system $\{(\mathbf{b}_{\mathcal{R}}, \mathbf{t}_{\mathcal{R}})\}$ through the Cauchy stress it induces and its divergence. Actually, we obtained a decomposition of $S\big(j^1(w)\big)$ into an exact differential and a term that is linear in the values of w. The converse is also true. If we have a force system that satisfies Cauchy's postulates, then, the induced Cauchy stress enables us to define a section S of $L\big(J^1(W), \bigwedge^{m-1}(T^*\mathcal{U})\big)$ by $S\big(j^1(w)\big) = \mathbf{b}(w) + d\sigma(w)$. Clearly, writing the local expression for S, it is linear in the jet of w. Hence,

$$F_{\mathcal{R}}(w) = \int_{\mathcal{R}} \mathbf{b}(w) + \int_{\mathcal{R}} d\sigma(w) = \int_{\mathcal{R}} S\big(j^1(w)\big).$$

If for a given variational stress Div $S = 0$, then $S\big(j^1(w)\big) = d\sigma(w)$, for $\sigma = p_\sigma \circ S$.

References

[1] SEGEV R., *Forces and the existence of stresses in invariant continuum mechanics*, J. of Math. Phys. **27** (1986), 163–170.

[2] SEGEV R., *The geometry of Cauchy's fluxes*, Archive for Rat. Mech. and Anal. **154** (2000), 183–198.

[3] SEGEV R. AND RODNAY G., *Cauchy's theorem on manifolds*, Journal of Elasticity **56** (2000), 129–144.

[4] SEGEV R. AND RODNAY G., *Divergences of stresses and the principle of virtual work on manifolds*, Technische Mechanik **20** (2000), 129–136.

AMS Subject Classification: 73A05, 58A05.

Reuven SEGEV
Department of Mechanical Engineering
Ben-Gurion University
P. O. Box 653
Beer-Sheva 84105, ISRAEL
e-mail: `rsegev@bgumail.bgu.ac.il`

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

B. Svendsen*

NON-LOCAL CONTINUUM THERMODYNAMIC EXTENSIONS OF CRYSTAL PLASTICITY TO INCLUDE THE EFFECTS OF GEOMETRICALLY-NECESSARY DISLOCATIONS ON THE MATERIAL BEHAVIOUR

Abstract. The purpose of this work is the formulation of constitutive models for the inelastic material behaviour of single crystals and polycrystals in which geometrically-necessary dislocations (GNDs) may develop and influence this behaviour. To this end, we focus on the dependence of the development of such dislocations on the inhomogeneity of the inelastic deformation in the material. More precisely, in the crystal plasticity context, this is a relation between the density of GNDs and the inhomogeneity of inelastic deformation in glide systems. In this work, two models for GND density and its evolution, i.e., a glide-system-based model, and a continuum model, are formulated and investigated. As it turns out, the former of these is consistent with the original two-dimensional GND model of Ashby (1970), and the latter with the more recent model of Dai and Parks (1997). Since both models involve a dependence of the inelastic state of a material point on the (history of the) inhomogeneity of the glide-system inelastic deformation, their incorporation into crystal plasticity modeling necessarily implies a corresponding non-local generalization of this modeling. As it turns out, a natural quantity on which to base such a non-local continuum thermodynamic generalization, i.e., in the context of crystal plasticity, is the glide-system (scalar) slip deformation. In particular, this is accomplished here by treating each such slip deformation as either (1), a generalized "gradient" internal variable, or (2), as a scalar internal degree-of-freedom. Both of these approaches yield a corresponding generalized Ginzburg-Landau- or Cahn-Allen-type field relation for this scalar deformation determined in part by the dependence of the free energy on the dislocation state in the material. In the last part of the work, attention is focused on specific models for the free energy and its dependence on this state. After summarising and briefly discussing the initial-boundary-value problem resulting from the current approach as well as its algorithmic form suitable for numerical implementation, the work ends with a discussion of additional aspects of the formulation, and in particular the connection of the approach to GND modeling taken here with other approaches.

*I thank Paolo Cermelli for helpful discussions and for drawing my attention to his work and that of Morton Gurtin on gradient plasticity and GNDs.

1. Introduction

Standard micromechanical modeling of the inelastic material behaviour of metallic single crystals and polycrystals (e.g., Hill and Rice, 1972; Asaro, 1983; Cuitiño and Ortiz, 1992) is commonly based on the premise that resistance to glide is due mainly to the random trapping of mobile dislocations during locally homogeneous deformation. Such trapped dislocation are commonly referred to as statistically-stored dislocations (SSDs), and act as obstacles to further dislocation motion, resulting in hardening. As anticipated in the work of Nye (1953) and Kröner (1960), and discussed by Ashby (1970), an additional contribution to the density of immobile dislocations and so to hardening can arise when the continuum lengthscale (e.g., grain size) approaches that of the dominant microstructural features (e.g., mean spacing between precipitates relative to the precipitate size, or mean spacing between glide planes). Indeed, in this case, the resulting deformation incompatibility between, e.g., "hard" inclusions and a "soft" matrix, is accomodated by the development of so-called geometrically-necessary dislocations (GNDs). Experimentally-observed effects in a large class of materials such as increasing material hardening with decreasing (grain) size (i.e., the Hall-Petch effect) are commonly associated with the development of such GNDs.

These and other experimental results have motivated a number of workers over the last few years to formulate various extensions (e.g., based on strain-gradients: Fleck and Hutchinson, 1993, 1997) to existing local models for phenomenological plasticity, some of which have been applied to crystal plasticity (e.g., the strain-gradient-based approach: Shu and Fleck, 1999; Cosserat-based approach: Forest et al., 1997) as well. Various recent efforts in this direction based on dislocation concepts, and in particular on the idea of Nye (1953) that the incompatibility of local inelastic deformation represents a continuum measure of dislocation density (see also Kröner, 1960; Mura, 1987), include Steinmann (1996), Dai and Parks (1997), Shizawa and Zbib (1999), Menzel and Steinmann (2000), Acharya and Bassani (2000), and most recently Cermelli and Gurtin (2001). In addition, the recent work of Ortiz and Repetto (1999) and Ortiz et al. (2000) on dislocation substructures in ductile single crystals demonstrates the fundamental connection between the incompatibility of the local inelastic deformation and the lengthscale of dislocation microstructures in FCC single crystals. In particular, the approaches of Dai and Parks (1997), Shizawa and Zbib (1999), and Archaya and Bassani (2000) are geared solely to the modeling of additional hardening due to GNDs and involve no additional field relations or boundary conditions. For example, the approach of Dai and Parks (1997) was used by Busso et al. (2000) to model additional hardening in two-phase nickel superalloys, and that of Archaya and Bassani (2000) by Archaya and Beaudoni (2000) to model grain-size effects in FCC and BCC polycrystals up to moderate strains. Except for the works of Acharya and Bassani (2000) and Cermelli and Gurtin (2001), which are restricted to kinematics, all of these presume directly or indirectly a particular dependence of the (free) energy and/or other dependent constitutive quantities (e.g., yield stress) on the gradients of inelastic state variables, and in particular on that of the local inelastic deformation, i.e., that determine its incompatibility. Yet more general formulations of crystal plasticity involving a (general) dependence of the free energy on the gradient of the local inelastic deformation can be found in, e.g., Naghdi and Srinivasa (1993, 1994), Le and Stumpf (1996), or in Gurtin (2000).

From the constitutive point of view, such experimental and modeling work clearly demonstrates the need to account for the dependence of the constitutive relations, and so material behaviour, on the inhomogeneity or "non-locality" of the internal fields as expressed by their gradients. In the phenomenological or continuum field context, such non-locality of the material behaviour is, or can be, accounted for in a number of existing approaches (e.g., Maugin, 1980;

Capriz, 1989; Maugin, 1990; Fried and Gurtin, 1993, 1994; Gurtin, 1995; Fried, 1996; Valanis, 1996, 1998) for broad classes of materials. It is not the purpose of the current work to compare and contrast any of these with each other in detail (in this regard, see, e.g., Maugin and Muschik, 1994; Svendsen, 1999); rather, we wish to apply two of them to formulate continuum thermodynamic models for crystal plasticity in which gradients of the inelastic fields in question influence the material behaviour. To this end, we must first identify the relevant internal fields. On the basis of the standard crystal plasticity constitutive relation for the local inelastic deformation $\boldsymbol{F}_{\mathrm{P}}$, a natural choice for the principal inelastic fields of the formulation is the set of glide-system deformations. In contrast, Le and Stumpf (1996) worked in their variational formulation directly with $\boldsymbol{F}_{\mathrm{P}}$, and Gurtin (2000) in his formulation based on configurational forces with the set of glide-system slip rates. In both of these works, a principal result takes the form of an extended or generalized Euler-Lagrange-, Ginzburg-Landau- or Cahn-Allen-type field relation for the respective principal inelastic fields. Generalized forms of such field relations for the glide-system deformations are obtained in the current work by modeling them in two ways. In the simplest approach, these are modeled as "generalized" internal variables (GIVs) via a generalization of the approach of Maugin (1990) to the modeling of the entropy flux. Alternatively, and more generally, these are modeled here as internal degrees-of-freedom (DOFs) via the approach of Capriz (1989) in the extended form discussed by Svendsen (2001a). In addition, as shown here, these formulations are general enough to incorporate in particular a number of models for GNDs (e.g., Ashby, 1970; Dai and Parks, 1997) and so provide a thermodynamic framework for extended non-local crystal plasticity modeling including the effects of GNDs on the material behaviour.

After some mathematical preliminaries (§2), the paper begins (§3) with a brief discussion and formulation of basic kinematic and constitutive issues and relations relevant to the continuum thermodynamic approach to crystal plasticity taken in this work. In particular, as mentioned above, the standard constitutive form for $\boldsymbol{F}_{\mathrm{P}}$ in crystal plasticity determines the glide-system slip deformations ("slips") as principal constitutive unknowns here. Having then established the corresponding constitutive class for crystal plasticity, we turn next to the thermodynamic field formulation and analysis (§§4-5), depending on whether the glide-system slips are modeled as generalized internal variables (GIVs) (§4), or as internal degrees-of-freedom (DOFs) (§5). Next, attention is turned to the formulation of two (constitutive) classes of GND models (§6), yielding in particular expressions for the glide-system effective (surface) density of GNDs. The first class of such models is based on the incompatibility of glide-system local deformation. To this class belong for example the original model of Ashby (1970) and the recent dislocation density tensor of Shizawa and Zbib (1999). The second is based on the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ and is consistent with the model of Dai and Parks (1997). With such models in hand, the possible dependence of the free energy on quantities characterising the dislocation state of the material (e.g., dislocation densities) and the corresponding consequences for the formulation are investigated (§7). Beyond the GND models formulated here, examples are also given of existing SSD models which can be incorporated into models for the free energy, and so into the current approach. After discussing simplifications arising in the formulation for the case of small deformation (§8), as well as the corresponding algorithmic form, the paper ends (§9) with a discussion of additional general aspects of the current approach and a comparison with other related work.

2. Mathematical preliminaries

If W and Z represent two finite-dimensional linear spaces, let $\mathrm{Lin}(W, Z)$ represent the set of all linear mappings from W to Z. If W and Z are inner product spaces, the inner products on W and Z induce the transpose $\mathcal{A}^{\mathrm{T}} \in \mathrm{Lin}(Z, W)$ of any $\mathcal{A} \in \mathrm{Lin}(W, Z)$, as well as the inner product $\mathcal{A} \cdot \mathcal{B} := \operatorname{tr}_W(\mathcal{A}^{\mathrm{T}}\mathcal{B}) = \operatorname{tr}_Z(\mathcal{A}\mathcal{B}^{\mathrm{T}})$ on $\operatorname{Lin}(W, Z)$ for all $\mathcal{A}, \mathcal{B} \in \operatorname{Lin}(W, Z)$. The main linear space of interest in this work is of course three-dimensional Euclidean vector space V. Let $\operatorname{Lin}(V, V)$ represent the set of all linear mappings of V into itself (i.e., second-order Euclidean tensors). Elements of V and $\operatorname{Lin}(V, V)$, or mappings taking values in these spaces, are denoted here as usual by bold-face, lower-case $\boldsymbol{a}, \ldots$ and upper-case $\boldsymbol{A}, \ldots$, italic letters, respectively. In particular, $\boldsymbol{I} \in \operatorname{Lin}(V, V)$ represents the second-order identity tensor. As usual, the tensor product $\boldsymbol{a} \otimes \boldsymbol{b}$ of any two $\boldsymbol{a}, \boldsymbol{b} \in V$ can be interpreted as an element $\boldsymbol{a} \otimes \boldsymbol{b} \in \operatorname{Lin}(V, V)$ of $\operatorname{Lin}(V, V)$ via $(\boldsymbol{a} \otimes \boldsymbol{b})\boldsymbol{c} := (\boldsymbol{b} \cdot \boldsymbol{c})\boldsymbol{a}$ for all $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in V$. Let $\operatorname{sym}(\boldsymbol{A}) := \frac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^{\mathrm{T}})$ and $\operatorname{skw}(\boldsymbol{A}) := \frac{1}{2}(\boldsymbol{A} - \boldsymbol{A}^{\mathrm{T}})$ represent the symmetric and skew-symmetric parts, respectively, of any $\boldsymbol{A} \in \operatorname{Lin}(V, V)$. The axial vector $\operatorname{axi}(\boldsymbol{W}) \in V$ of any skew tensor $\boldsymbol{W} \in \operatorname{Lin}(V, V)$ is defined by $\operatorname{axi}(\boldsymbol{W}) \times \boldsymbol{a} := \boldsymbol{W}\boldsymbol{a}$. Let $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in V$ be constant vectors in what follows.

Turning next to field relations, the definition

$$\operatorname{curl} \boldsymbol{u} := 2 \operatorname{axi}(\operatorname{skw}(\nabla \boldsymbol{u})) \tag{1}$$

for the curl of a differentiable Euclidean vector field $\boldsymbol{u}$ is employed in this work, ∇ being the standard Euclidean gradient operator. In particular, (1) and the basic result

$$\nabla(f\boldsymbol{u}) = \boldsymbol{u} \otimes \nabla f + f(\nabla \boldsymbol{u}) \tag{2}$$

for all differentiable functions f and vector fields $\boldsymbol{u}$ yield the identity

$$\operatorname{curl}(f\boldsymbol{u}) = \nabla f \times \boldsymbol{u} + f(\operatorname{curl} \boldsymbol{u}) \quad . \tag{3}$$

In addition, (1) yields the identity

$$\operatorname{curl} \boldsymbol{u} \cdot \boldsymbol{a} \times \boldsymbol{b} = \nabla_{\boldsymbol{a}} \boldsymbol{u} \cdot \boldsymbol{b} - \nabla_{\boldsymbol{b}} \boldsymbol{u} \cdot \boldsymbol{a} \tag{4}$$

for $\operatorname{curl} \boldsymbol{u}$ in terms of the directional derivative

$$\nabla_{\boldsymbol{a}} \boldsymbol{u} := (\nabla \boldsymbol{u})\boldsymbol{a} \tag{5}$$

of $\boldsymbol{u}$ in the direction $\boldsymbol{a} \in V$. Turning next to second-order tensor fields, we work here with the definition*

$$(\operatorname{curl} \boldsymbol{T})^{\mathrm{T}} \boldsymbol{a} := \operatorname{curl}(\boldsymbol{T}^{\mathrm{T}} \boldsymbol{a}) \tag{6}$$

for the curl of a differentiable second-order Euclidean tensor field $\boldsymbol{T}$ as a second-order tensor field. From (3) and (6) follows in particular the identity

$$\operatorname{curl}(f\boldsymbol{T}) = \boldsymbol{T}(\boldsymbol{I} \times \nabla f) + f(\operatorname{curl} \boldsymbol{T}) \tag{7}$$

for all differentiable f and $\boldsymbol{T}$, where $(\boldsymbol{I} \times \boldsymbol{a})\boldsymbol{b} := \boldsymbol{b} \times \boldsymbol{a}$. Note that $(\boldsymbol{I} \times \boldsymbol{a})^{\mathrm{T}} = \boldsymbol{a} \times \boldsymbol{I}$ with $(\boldsymbol{a} \times \boldsymbol{I})\boldsymbol{b} := \boldsymbol{a} \times \boldsymbol{b}$. Likewise, (1) and (6) yield the identity

$$(\operatorname{curl} \boldsymbol{T})(\boldsymbol{a} \times \boldsymbol{b}) := (\nabla_{\boldsymbol{a}} \boldsymbol{T})\boldsymbol{b} - (\nabla_{\boldsymbol{b}} \boldsymbol{T})\boldsymbol{a} \tag{8}$$

for $\operatorname{curl} \boldsymbol{T}$ in terms of the directional derivative

$$\nabla_{\boldsymbol{a}} \boldsymbol{T} (\nabla \boldsymbol{T})\boldsymbol{a}$$

*This is of course a matter of convention. Indeed, in contrast to (6), Cermelli and Gurtin (2001) define $(\operatorname{curl} \boldsymbol{T})\boldsymbol{a} := \operatorname{curl}(\boldsymbol{T}^{\mathrm{T}} \boldsymbol{a})$.

of $\boldsymbol{T}$ in the direction $\boldsymbol{a} \in V$. Here, $\nabla\boldsymbol{T}$ represents a third-order Euclidean tensor field. Let $\boldsymbol{H}$ be a differentiable invertible tensor field. From (8) and the identity

$$\boldsymbol{A}^{\mathrm{T}}(\boldsymbol{A}\boldsymbol{b} \times \boldsymbol{A}\boldsymbol{c}) = \det(\boldsymbol{A})\,(\boldsymbol{b} \times \boldsymbol{c}) \tag{9}$$

for any second-order tensor $\boldsymbol{A} \in \mathrm{Lin}(V, V)$, we obtain

$$\mathrm{curl}\,(\boldsymbol{T}\boldsymbol{H}) = \det(\boldsymbol{H})\,(\mathrm{curl}^{\boldsymbol{H}}\boldsymbol{T})\boldsymbol{H}^{-\mathrm{T}} + \boldsymbol{T}\,(\mathrm{curl}\,\boldsymbol{H}) \tag{10}$$

for the curl of the product of two second-order tensor fields. Here, $\mathrm{curl}^{\boldsymbol{H}}$ represents the curl operator induced by the Koszul connection $\nabla^{\boldsymbol{H}}$ induced in turn by the invertible tensor field $\boldsymbol{H}$, i.e.,

$$\nabla^{\boldsymbol{H}}\boldsymbol{T} := (\nabla\boldsymbol{T})\boldsymbol{H}^{-1} \quad . \tag{11}$$

The corresponding curl operation then is defined in an analogous fashion to the standard form (8) relative to ∇.

Third-order tensors such as $\nabla\boldsymbol{T}$ are denoted in general in this work by A, B, ... and interpreted as elements of either $\mathrm{Lin}(V, \mathrm{Lin}(V, V))$ or $\mathrm{Lin}(\mathrm{Lin}(V, V), V)$. Note that any third-order tensor A induces one A^{S} defined by

$$(\mathsf{A}^{\mathrm{S}}\boldsymbol{b})\boldsymbol{c} := (\mathsf{A}\boldsymbol{c})\boldsymbol{b} \quad . \tag{12}$$

In particular, this induces the split

$$\mathsf{A} = \mathrm{sym}_{\mathrm{S}}(\mathsf{A}) + \mathrm{skw}_{\mathrm{S}}(\mathsf{A}) \tag{13}$$

of any third-order tensor A into "symmetric"

$$\mathrm{sym}_{\mathrm{S}}(\mathsf{A}) := \tfrac{1}{2}(\mathsf{A} + \mathsf{A}^{\mathrm{S}}) \tag{14}$$

and "skew-symmetric"

$$\mathrm{skw}_{\mathrm{S}}(\mathsf{A}) := \tfrac{1}{2}(\mathsf{A} - \mathsf{A}^{\mathrm{S}}) \tag{15}$$

parts. In addition, the latter of these induces the linear mapping

$$\mathrm{axi}_{\mathrm{S}} : \mathrm{Lin}(V, \mathrm{Lin}(V, V)) \longrightarrow \mathrm{Lin}(V, V) \quad | \quad \mathsf{A} \longmapsto \boldsymbol{A} = \mathrm{axi}_{\mathrm{S}}(\mathsf{A}) \tag{16}$$

defined by

$$\mathrm{axi}_{\mathrm{S}}(\mathsf{A})(\boldsymbol{b} \times \boldsymbol{c}) := 2\,(\mathrm{skw}_{\mathrm{S}}(\mathsf{A})\boldsymbol{b})\boldsymbol{c} = (\mathsf{A}\boldsymbol{b})\boldsymbol{c} - (\mathsf{A}\boldsymbol{c})\boldsymbol{b} \quad . \tag{17}$$

With the help of (12)–(17), one obtains in particular the compact form

$$\mathrm{curl}\,\boldsymbol{T} = \mathrm{axi}_{\mathrm{S}}(\nabla\boldsymbol{T}) \tag{18}$$

for the curl of a differentiable second-order tensor field $\boldsymbol{T}$ as a function of its gradient $\nabla\boldsymbol{T}$ from (8). The transpose $\mathsf{A}^{\mathrm{T}} \in \mathrm{Lin}(\mathrm{Lin}(V, V), V)$ of any third-order tensor $\mathsf{A} \in \mathrm{Lin}(V, \mathrm{Lin}(V, V))$ is defined here via $\mathsf{A}^{\mathrm{T}}\boldsymbol{B} \cdot \boldsymbol{c} = \boldsymbol{B} \cdot \mathsf{A}\boldsymbol{c}$.

Finally, for notational simplicity, it proves advantageous to abuse notation in this work and denote certain mappings and their values by the same symbol. Other notations and mathematical concepts will be introduced as they arise in what follows.

3. Basic kinematic, constitutive and balance relations

Let B represent a material body, $p \in B$ a material point of this body, and E Euclidean point space with translation vector space V. A motion of the body with respect to E in some time interval $I \subset \mathbb{R}$ takes as usual the form

$$\boldsymbol{x} = \xi(t, p)$$

relating each p to its (current) time $t \in I$ position $\boldsymbol{x} \in E$ in E. On this basis, $\dot{\xi}$ represents the material velocity, and

$$\boldsymbol{F}_\kappa(t, p) := (\nabla^\kappa \xi)(t, p) \in \mathrm{Lin}^+(V, V) \tag{19}$$

the deformation gradient relative to the (global) reference placement κ of B into E. Here, we are using the notation

$$\nabla^\kappa \xi := \kappa^*(\nabla(\kappa_* \xi))$$

for the gradient of ξ with respect to κ in terms of push-forward and pull-back, where $(\kappa_*\xi)(t, \boldsymbol{r}_\kappa) := \xi(t, \kappa^{-1}(\boldsymbol{r}_\kappa))$ for push-forward by κ, with $\boldsymbol{r}_\kappa = \kappa(p)$, and similarly for κ^*. Like ξ, $\dot{\xi}$ and $\boldsymbol{F}_\kappa$, all fields to follow are represented here as time-dependent fields on B. And analogous to that of ξ in (19), the gradients of these fields are all defined relative to κ. More precisely, these are defined at each $p \in B$ relative to a corresponding local reference placement† at each $p \in B$, i.e., an equivalence class of global placements κ having the same gradient at p. Since κ and the corresponding local reference placement at each $p \in B$ is arbitrary here, and the dependence of $\boldsymbol{F}_\kappa$ and the gradients of other fields, as well as that of the constitutive relations to follow, on κ does not play a direct role in the formulation in this work, we suppress it in the notation for simplicity.

In the case of phenomenological crystal plasticity, any material point $p \in B$ is endowed with a "microstructure" in the form of a set of n glide systems. The geometry and orientation of each such glide system is described as usual by an orthonormal basis $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$ ($\mathfrak{a} = 1, \ldots, n$). Here, $\boldsymbol{s}_\mathfrak{a}$ represents the direction of glide in the plane, $\boldsymbol{n}_\mathfrak{a}$ the glide-plane normal, and $\boldsymbol{t}_\mathfrak{a} := \boldsymbol{s}_\mathfrak{a} \times \boldsymbol{n}_\mathfrak{a}$ the direction transverse to $\boldsymbol{s}_\mathfrak{a}$ in the glide plane. Since we neglect in this work the effects of any processes involving a change in or evolution of either the glide direction $\boldsymbol{s}_\mathfrak{a}$ or the glide-system orientation $\boldsymbol{n}_\mathfrak{a}$ (e.g., texture development), these referential unit vectors, and so $\boldsymbol{t}_\mathfrak{a}$ as well, are assumed constant with respect to the reference placement. With respect to the glide-system geometry, then, the (local) deformation $\boldsymbol{F}_\mathfrak{a}$ of each glide system takes the form of a simple shear‡

$$\boldsymbol{F}_\mathfrak{a} = \boldsymbol{I} + \gamma_\mathfrak{a}\, \boldsymbol{s}_\mathfrak{a} \otimes \boldsymbol{n}_\mathfrak{a} \quad , \tag{20}$$

$\gamma_\mathfrak{a}$ being its magnitude in the direction $\boldsymbol{s}_\mathfrak{a}$ of shear. For simplicity, we refer to each $\gamma_\mathfrak{a}$ as the (scalar) glide-system slip (deformation). The orthogonality of $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$ implies $\boldsymbol{F}_\mathfrak{a}^{\mathrm{T}} \boldsymbol{n}_\mathfrak{a} = \boldsymbol{n}_\mathfrak{a}$ and $\boldsymbol{F}_\mathfrak{a}\, \boldsymbol{s}_\mathfrak{a} = \boldsymbol{s}_\mathfrak{a}$, as well as $\gamma_\mathfrak{a} = \boldsymbol{s}_\mathfrak{a} \cdot \boldsymbol{F}_\mathfrak{a}\, \boldsymbol{n}_\mathfrak{a}$. In addition,

$$\dot{\boldsymbol{F}}_\mathfrak{a} = \boldsymbol{s}_\mathfrak{a} \otimes \boldsymbol{n}_\mathfrak{a}\, \dot{\gamma}_\mathfrak{a} =: \boldsymbol{L}_\mathfrak{a} \boldsymbol{F}_\mathfrak{a} \tag{21}$$

follows from (20). As such, the evolution of the glide-system deformation tensor $\boldsymbol{F}_\mathfrak{a}$ is determined completely by that of the corresponding scalar slip $\gamma_\mathfrak{a}$.

† Refered to by Noll (1967) as local reference configuration of $p \in B$ in E.

‡ As discussed in §6, like $\boldsymbol{F}_{\mathrm{P}}$, and unlike $\boldsymbol{F}$, $\boldsymbol{F}_\mathfrak{a}$ is in general not compatible.

From a phenomenological point of view, the basic local inelastic deformation at each material point in the material body in question is represented by an invertible second-order tensor field $\boldsymbol{F}_{\mathrm{P}}$ on $I \times B$. The evolution of $\boldsymbol{F}_{\mathrm{P}}$ is given by the standard form

$$\dot{\boldsymbol{F}}_{\mathrm{P}} = \boldsymbol{L}_{\mathrm{P}} \boldsymbol{F}_{\mathrm{P}} \tag{22}$$

in terms of the plastic velocity "gradient" $\boldsymbol{L}_{\mathrm{P}}$. The connection to crystal plasticity is then obtained via the *constitutive* assumption

$$\boldsymbol{L}_{\mathrm{P}} \mathrel{\widehat{=}} \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{L}_{\mathfrak{a}} = \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}\, \dot{\gamma}_{\mathfrak{a}} \tag{23}$$

for $\boldsymbol{L}_{\mathrm{P}}$ via (21), where $m \leq n$ represents the set[§] of *active* glide-systems, i.e., those for which $\dot{\gamma}_{\mathfrak{a}} \neq 0$. Combining this last constitutive relation with (22) then yields the basic constitutive expression

$$\dot{\boldsymbol{F}}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{L}_{\mathfrak{a}}\, \boldsymbol{F}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{m} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}) \boldsymbol{F}_{\mathrm{P}}\, \dot{\gamma}_{\mathfrak{a}} \tag{24}$$

for the evolution of $\boldsymbol{F}_{\mathrm{P}}$. In turn, this basic constitutive relation implies that

$$\dot{\overline{\nabla \boldsymbol{F}_{\mathrm{P}}}} = \sum\nolimits_{\mathfrak{a}=1}^{m} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})(\nabla \boldsymbol{F}_{\mathrm{P}})\, \dot{\gamma}_{\mathfrak{a}} + (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}) \boldsymbol{F}_{\mathrm{P}} \otimes \nabla \dot{\gamma}_{\mathfrak{a}} \tag{25}$$

for the evolution of $\nabla \boldsymbol{F}_{\mathrm{P}}$, and so that

$$\dot{\overline{\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}}} = \sum\nolimits_{\mathfrak{a}=1}^{m} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})(\operatorname{curl} \boldsymbol{F}_{\mathrm{P}})\, \dot{\gamma}_{\mathfrak{a}} + \boldsymbol{s}_{\mathfrak{a}} \otimes (\nabla \dot{\gamma}_{\mathfrak{a}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}) \tag{26}$$

for the evolution of $\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}$ via (7) and (8). On this basis, the evolution relation for $\boldsymbol{F}_{\mathrm{P}}$ is *linear* in the set $\dot{\gamma} := (\dot{\gamma}_1, \ldots, \dot{\gamma}_m)$ of active glide-system slip rates. Similarly, the evolution relations for $\nabla \boldsymbol{F}_{\mathrm{P}}$ and $\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}$ are *linear* in $\dot{\gamma}$ and $\nabla \dot{\gamma}$. Generalizing the case of $\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}$ slightly, which represents one such measure, the dislocation state in the material is modeled phenomenologically in this work via a general inelastic state/dislocation measure α whose evolution is assumed to depend *quasi-linearly* on $\dot{\gamma}$ and $\nabla \dot{\gamma}$, i.e.,

$$\dot{\alpha} = \mathcal{K} \dot{\gamma} + \mathcal{J}\, \nabla \dot{\gamma} \tag{27}$$

in terms of the dependent constitutive quantities $\mathcal{K}$ and $\mathcal{J}$. In particular, on the basis of (24), $\boldsymbol{F}_{\mathrm{P}}$ is considered here to be an element of α. In turn, the dependence of this evolution relation on $\nabla \dot{\gamma}$ requires that we model the γ as time-dependent *fields* on B. As such, in the current thermomechanical context, the absolute temperature θ, the motion ξ, and the set γ of glide-system slips, represent the principal time-dependent fields, $\boldsymbol{F}_{\mathrm{P}}$ and α being determined constitutively by the history of γ and $\nabla \dot{\gamma}$ via (24) and (27), respectively. On the basis of determinism, local action, and short-term mechanical memory, then, the material behaviour of a given material point $p \in B$ is described by the general material frame-indifferent constitutive form

$$\mathfrak{R} = \mathfrak{R}(\theta, \boldsymbol{C}, \alpha, \nabla \theta, \dot{\gamma}, \nabla \dot{\gamma}, p) \tag{28}$$

for all dependent constitutive quantities (e.g., stress), where $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}} \boldsymbol{F}$ represents the right Cauchy-Green deformation as usual. In particular, since the motion ξ, as well as the material

---

[§] In standard crystal plasticity models, the number m of active glide system is determined among other things by the glide-system "flow rule," loading conditions, and crystal orientation. As such, it is constitutive in nature, and in general variable.

velocity $\dot{\xi}$, are not Euclidean frame-indifferent, $\mathfrak{R}$ is independent of these to satisfy material frame-indifference. As such, (28) represents the basic reduced constitutive form of the constitutive class of interest for the continuum thermodynamic formulation of crystal plasticity to follow. Because it plays no direct role in the formulation, the dependence of the constitutive relations on $p \in B$ is suppressed in the notation until needed.

The derivation of balance and field relations relative to the given reference configuration of B is based in this work on the local forms for total energy and entropy balance, i.e.,

$$\begin{aligned} \dot{e} &= \operatorname{div} \boldsymbol{h} + s \ , \\ \dot{\eta} &= \pi - \operatorname{div} \phi + \sigma \ , \end{aligned} \tag{29}$$

respectively. Here, e represents the total energy density, $\boldsymbol{h}$ its flux density, and s its supply rate density. Likewise, π, ϕ, and σ represent the production rate, flux, and supply rate, densities, respectively, of entropy, with density η. In particular, the mechanical balance relations follow from $(29)_1$ via its invariance with respect to Euclidean observer. And as usual, the thermodynamic analysis is based on $(29)_2$; in addition, it yields a field relation for the temperature, as will be seen in what follows.

This completes the synopsis of the basic relations required for the sequel. Next, we turn to the formulation of field relations and the thermodynamic analysis for the constitutive class determined by the form (28).

4. Generalized internal variable model for glide-system slips

The modeling of the γ as generalized internal variables (GIVs) is based in particular on the standard continuum forms

$$\begin{aligned} e &= \varepsilon &+& \tfrac{1}{2}\varrho\, \dot{\xi} \cdot \dot{\xi} \ , \\ \boldsymbol{h} &= -\boldsymbol{q} &+& \boldsymbol{P}^{\mathrm{T}}\dot{\xi} \ , \\ s &= r &+& \boldsymbol{f} \cdot \dot{\xi} \ , \end{aligned} \tag{30}$$

for total energy density e, total energy flux density $\boldsymbol{h}$, and total energy supply rate density s, respectively, hold. Here, ϱ represents the referential mass density, $\boldsymbol{P}$ the first Piola-Kirchhoff stress tensor, and $\boldsymbol{f}$ the momentum supply rate density. Further, ε represents the internal energy density, and $\boldsymbol{q}$ the heat flux density. As in the standard continuum case, $\boldsymbol{P}$, ε, $\boldsymbol{q}$, η and ϕ represent dependent constitutive quantities in general. Substituting the forms (30) for the energy fields into the local form $(29)_1$ for total energy balance yields the result

$$\dot{\varepsilon} + \operatorname{div} \boldsymbol{q} - r = \boldsymbol{P} \cdot \nabla\dot{\xi} - \boldsymbol{z} \cdot \dot{\xi} + \tfrac{1}{2}\, c\, \dot{\xi} \cdot \dot{\xi} \tag{31}$$

for this balance. Appearing here are the field

$$c := \dot{\varrho} \tag{32}$$

associated with mass balance, and that

$$\boldsymbol{z} := \dot{\boldsymbol{m}} - \operatorname{div} \boldsymbol{P} - \boldsymbol{f} \tag{33}$$

associated with momentum balance, where

$$\boldsymbol{m} := \varrho\dot{\xi}$$

represents the usual continuum momentum density. As discussed by, e.g., Šilhavý (1997, Ch. 6), in the context of the usual transformation relations for the fields appearing in (31) under change of Euclidean observer, one can show that necessary conditions for the Euclidean frame-indifference of $(29)_1$ in the form (31) are the mass

$$c = 0 \qquad \Longrightarrow \qquad \dot{\varrho} = 0 \tag{34}$$

via (32), momentum

$$\boldsymbol{z} = \boldsymbol{0} \qquad \Longrightarrow \qquad \dot{\boldsymbol{m}} = \operatorname{div} \boldsymbol{P} + \boldsymbol{f} \tag{35}$$

via (33), and moment of momentum

$$\boldsymbol{S}^{\mathrm{T}} = \boldsymbol{S} \tag{36}$$

balances, respectively, the latter with respect to the second Piola-Kirchhoff stress $\boldsymbol{S} = \boldsymbol{F}^{-1}\boldsymbol{P}$. As such, beyond a constant (i.e., in time) mass density, we obtain the standard forms

$$\begin{array}{rclclcl} \dot{\boldsymbol{m}} & = & \boldsymbol{0} & + & \operatorname{div} \boldsymbol{P} & + & \boldsymbol{f}\,, \\ \dot{\varepsilon} & = & \frac{1}{2}\boldsymbol{S}\cdot\dot{\boldsymbol{C}} & - & \operatorname{div} \boldsymbol{q} & + & r\,, \end{array} \tag{37}$$

for local balance of continuum momentum and internal energy, respectively, in the current context via (31), (35) and (36).

We turn next to thermodynamic considerations. As shown in effect by Maugin (1990), one approach to the formulation of the entropy principle for material behaviour depending on internal variables and their gradients can be based upon a weaker form of the dissipation (rate) inequality than the usual Clausius-Duhem relation. This form follows from the local entropy (29) and internal energy $(37)_2$ balances via the Clausius-Duhem form

$$\sigma = r/\theta \tag{38}$$

for the entropy supply rate σ density in terms of the internal energy supply rate density r and temperature θ. Indeed, this leads to the expression

$$\delta = \tfrac{1}{2}\boldsymbol{S}\cdot\dot{\boldsymbol{C}} - \dot{\psi} - \eta\,\dot{\theta} + \operatorname{div}(\theta\boldsymbol{\phi} - \boldsymbol{q}) - \boldsymbol{\phi}\cdot\nabla\theta \tag{39}$$

for the dissipation rate density

$$\delta := \theta\pi \tag{40}$$

via $(37)_2$, where

$$\psi := \varepsilon - \theta\,\eta \tag{41}$$

represents the referential free energy density. Substituting next the form (28) for ψ into (39) yields that

$$\begin{array}{rcl} \delta & = & \{\tfrac{1}{2}\boldsymbol{S} - \psi_{,\boldsymbol{C}}\}\cdot\dot{\boldsymbol{C}} - \{\eta + \psi_{,\theta}\}\,\dot{\theta} - \psi_{,\nabla}\cdot\nabla\dot{\theta} - \psi_{,\dot{\gamma}}\cdot\ddot{\gamma} - \psi_{,\nabla\dot{\gamma}}\cdot\nabla\ddot{\gamma} \\ & + & \operatorname{div}(\theta\boldsymbol{\phi} - \boldsymbol{q} - \Phi_{\mathrm{V}}^{\mathrm{T}}\dot{\gamma}) + (\varpi_{\mathrm{V}} + \operatorname{div}\Phi_{\mathrm{V}})\cdot\dot{\gamma} - \boldsymbol{\phi}\cdot\nabla\theta \end{array} \tag{42}$$

for δ via (27). Here,

$$\varpi_{\mathrm{V}} := -\,K^{\mathrm{T}}\psi_{,\alpha} \quad , \tag{43}$$

$\varpi_V := (\varpi_{V1}, \ldots, \varpi_{Vm})$, and

$$\Phi_V := \mathcal{J}^T \psi_{,\alpha} \quad , \tag{44}$$

with $\Phi_V := (\varphi_{V1}, \ldots, \varphi_{Vm})$. Now, on the basis of (27) and (28), δ in (42) is linear in the fields $\dot{\boldsymbol{C}}$, $\dot{\theta}$, $\nabla\dot{\theta}$, $\ddot{\gamma}$ and $\nabla\ddot{\gamma}$. Consequently, the Coleman-Noll approach to the exploitation of the entropy inequality implies that $\delta \geq 0$ is insured for all thermodynamically-admissible processes iff the corresponding coefficients of these fields in (42) vanish, yielding the restrictions

$$\begin{aligned} \boldsymbol{S} &= 2\psi_{,\boldsymbol{C}} , \\ \eta &= -\psi_{,\theta} , \\ \mathbf{0} &= \psi_{,\nabla\theta} , \\ 0 &= \psi_{,\dot{\gamma}_\mathfrak{a}} , \quad \mathfrak{a} = 1, \ldots, m , \\ \mathbf{0} &= \psi_{,\nabla\dot{\gamma}_\mathfrak{a}} , \quad \mathfrak{a} = 1, \ldots, m , \end{aligned} \tag{45}$$

on the form of the referential free energy density ψ, as well as the reduced expression

$$\delta = \operatorname{div}(\theta\phi - \boldsymbol{q} - \Phi_V^T\dot{\gamma}) + (\varpi_V + \operatorname{div}\Phi_V)\cdot\dot{\gamma} - \theta\phi\cdot\nabla\ln\theta \tag{46}$$

for δ as given by (42), representing its so-called residual form for the current constitutive class. In this case, then, the reduced form

$$\psi = \psi(\theta, \boldsymbol{C}, \alpha) \tag{47}$$

of ψ follows from (28) and (45).

On the basis of the residual form (46) for δ, assume next that, as dependent constitutive quantities, $\varpi_V + \operatorname{div}\Phi_V$ and ϕ are defined on convex subsets of the non-equilibrium part of the state space, representing the set of all admissible $\nabla\theta$, $\dot{\gamma}$ and $\nabla\dot{\gamma}$. If $\varpi_V + \operatorname{div}\Phi_V$ and ϕ, again as dependent constitutive quantities, are in addition continuously differentiable in $\nabla\theta$, $\dot{\gamma}$ and $\nabla\dot{\gamma}$ on the subset in question, one may generalize the results of Edelen (1973, 1985) to show[¶] that the requirement $\delta \geq 0$ on δ given by (46) yields the constitutive results

$$\begin{aligned} \varpi_V + \operatorname{div}\Phi_V &= d_{V,\dot{\gamma}} - \operatorname{div} d_{V,\nabla\dot{\gamma}} + \zeta_{V\dot{\gamma}} , \\ -\theta\phi &= d_{V,\nabla\ln} + \zeta_{V\nabla\ln} , \end{aligned} \tag{48}$$

for $\varpi_V + \operatorname{div}\Phi_V$ and ϕ, respectively, in terms of the dissipation potential

$$d_V = d_V(\theta, \boldsymbol{C}, \alpha, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma}) \tag{49}$$

and constitutive quantities

$$\begin{aligned} \zeta_{V\dot{\gamma}} &= \zeta_{V\dot{\gamma}}(\theta, \boldsymbol{C}, \alpha, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma}) , \\ \zeta_{V\nabla\ln} &= \zeta_{V\nabla\ln}(\theta, \boldsymbol{C}, \alpha, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma}) , \end{aligned}$$

which satisfy

$$\zeta_{V\dot{\gamma}}\cdot\dot{\gamma} + \zeta_{V\nabla\ln}\cdot\nabla\ln\theta = 0 \quad , \tag{50}$$

[¶] In fact, this can be shown for the weaker case of simply-connected, rather than convex, subsets of the dynamic part of state space via homotopy (see, e.g., Abraham et al. 1988, proof of Lemma 6.4.14).

i.e., they do not contribute to δ. To simplify the rest of the formulation, it is useful to work with the stronger constitutive assumption that d_{V} exists, in which case $\zeta_{\mathrm{V}\,\dot{\gamma}}$ and $\zeta_{\mathrm{V}\,\nabla\ln}$ vanish identically. On the basis then of the *constitutive form*

$$\phi \mathrel{\widehat{=}} \theta^{-1}\boldsymbol{q} + \theta^{-1}(\Phi_{\mathrm{V}} + d_{\mathrm{V},\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} \tag{51}$$

for the entropy flux density, δ is determined by the form of d_{V} alone, i.e.,

$$\delta = d_{\mathrm{V},\,\dot{\gamma}} \cdot \dot{\gamma} + d_{\mathrm{V},\,\nabla\dot{\gamma}} \cdot \nabla\dot{\gamma} + d_{\mathrm{V},\,\nabla\ln} \cdot \nabla\ln\theta \quad . \tag{52}$$

Among other things, (52) implies that a convex dependence of d_{V} on the non-equilibrium fields is sufficient, but not necessary, to satisfy $\delta \geq 0$. Indeed, with $d_{\mathrm{V}}(\theta, \boldsymbol{C}, \alpha, \mathbf{0}, \mathbf{0}, \mathbf{0}) = 0$, d_{V} is convex in $\nabla\theta$, $\dot{\gamma}$ and $\nabla\dot{\gamma}$ if $\delta \geq d_{\mathrm{V}}$ (i.e., with δ given by (52)) for given values of the other variables. So, if d_{V} is convex in $\nabla\theta$ and $\dot{\gamma}$, and $d_{\mathrm{V}} \geq 0$, then $\delta \geq 0$ is satisfied. On the other hand, even if $d_{\mathrm{V}} \geq 0$, $\delta \geq 0$ does not necessarily require $\delta \geq d_{\mathrm{V}}$, i.e., d_{V} convex.

Lastly, in the context of the entropy balance $(29)_2$, the constitutive assumption (38), together with (40) and the results $(45)_{1,2}$, (46) and (48), lead to the expression

$$c\,\dot{\theta} = \tfrac{1}{2}\,\theta\boldsymbol{S}_{,\,\theta} \cdot \dot{\boldsymbol{C}} + \omega_{\mathrm{V}} + \operatorname{div} d_{\mathrm{V},\,\nabla\ln} + r \tag{53}$$

for the evolution of θ via (47) and (49). Here,

$$c \,:=\, -\,\theta\psi_{,\,\theta\theta} \tag{54}$$

represents the heat capacity at constant γ, $\boldsymbol{C}$, and so on, $\frac{1}{2}\,\theta\boldsymbol{S}_{,\,\theta} \cdot \dot{\boldsymbol{C}} = \theta\psi_{,\,\theta\boldsymbol{C}} \cdot \dot{\boldsymbol{C}}$ the rate (density) of heating due to thermoelastic processes, and

$$\omega_{\mathrm{V}} \,:=\, (d_{\mathrm{V},\,\dot{\gamma}} + \theta\, K^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \dot{\gamma} + (d_{\mathrm{V},\,\nabla\dot{\gamma}} + \theta\,\mathcal{J}^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \nabla\dot{\gamma} \tag{55}$$

that due to inelastic processes via (27). In addition, $(48)_1$ implies the result

$$d_{\mathrm{V},\,\dot{\gamma}} = \operatorname{div}(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} + d_{\mathrm{V},\,\nabla\dot{\gamma}}) - K^{\mathrm{T}}\psi_{,\,\alpha} \tag{56}$$

for the evolution of γ via (43) and (44). Finally,

$$-\boldsymbol{q} = d_{\mathrm{V},\,\nabla\ln} + (\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} + d_{\mathrm{V},\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} \tag{57}$$

follows for the heat flux density $\boldsymbol{q}$ from (51) and $(48)_2$. As such, the dependence of ψ on α, as well as that of d_{V} on $\nabla\dot{\gamma}$, lead in general to additional contributions to $\boldsymbol{q}$ in the context of the modeling of the γ as GIVs.

This completes the formulation of balance relations and the thermodynamic analysis for the modeling of the γ as GIVs. Next, we carry out such a formulation for the case that the γ are modeled as internal DOFs.

5. Internal degrees-of-freedom model for glide-system slips

Alternative to the model for the glide-system slips as GIVs in the sense of the last section is that in which they are interpreted as so-called internal degrees-of-freedom (DOFs). In this case, the degrees-of-freedom[‖] of the material consist of (i), the usual "external" continuum DOFs

[‖]This entails a generalization of the classical concept of "degree-of-freedom" to materials with structure.

represented by the motion ξ, and (ii), the "internal" DOFs γ. Or to use the terminology of Capriz (1989), the γ are modeled here as scalar-valued continuum microstructural fields. Once established as DOFs, the modeling of the γ proceeds by formal analogy with that of ξ, the only difference being that, in contrast to external DOFs represented by ξ, each internal DOF $\gamma_{\mathfrak{a}}$ is (i.e., by assumption) Euclidean frame-indifferent. Otherwise, the analogy is complete. In particular, each $\gamma_{\mathfrak{a}}$ is assumed to contribute to the total energy, the total energy flux and total energy supply, of the material in a fashion formally analogous to ξ, i.e.,

$$\begin{array}{rclclcl} e & = & \varepsilon & + & \frac{1}{2}\dot{\xi}\cdot\varrho\dot{\xi} & + & \frac{1}{2}\dot{\gamma}\cdot\varrho\mathbf{I}\dot{\gamma}\ , \\ \boldsymbol{h} & = & -\boldsymbol{q} & + & \boldsymbol{P}^{\mathrm{T}}\dot{\xi} & + & \Phi_{\mathrm{F}}^{\mathrm{T}}\dot{\gamma}\ , \\ s & = & r & + & \boldsymbol{f}\cdot\dot{\xi} & + & \varsigma\cdot\dot{\gamma}\ , \end{array} \tag{58}$$

for total energy density e, total energy flux density $\boldsymbol{h}$, and total energy supply rate density s. Here,

$$\mathbf{I} := \begin{bmatrix} \iota_{11} & \cdots & \iota_{1m} \\ \vdots & \ddots & \vdots \\ \iota_{m1} & \cdots & \iota_{mm} \end{bmatrix}$$

is the (symmetric, positive-definite) matrix of microinertia coefficients, $\Phi_{\mathrm{F}} := (\varphi_{\mathrm{F}1}, \ldots, \varphi_{\mathrm{F}m})$ the array of flux densities, and $\varsigma := (\varsigma_1, \ldots, \varsigma_m)$ the array of external supply rate densities, associated with γ. For simplicity, we assume that $\mathbf{I}$ is constant in this work. Next, substitution of (58) into the general local form $(29)_1$ of total energy balance yields

$$\dot{\varepsilon} + \operatorname{div}\boldsymbol{q} - r = \boldsymbol{P}\cdot\nabla\dot{\xi} + \Phi_{\mathrm{F}}\cdot\nabla\dot{\gamma} - \boldsymbol{z}\cdot\dot{\xi} - \varpi_{\mathrm{F}}\cdot\dot{\gamma} + \tfrac{1}{2}c\,(\dot{\xi}\cdot\dot{\xi} + \dot{\gamma}\cdot\mathbf{I}\dot{\gamma}) \tag{59}$$

via (32) and (33). Here,

$$\varpi_{\mathrm{F}} := \dot{\mu} - \operatorname{div}\Phi_{\mathrm{F}} - \varsigma \tag{60}$$

is associated with the evolution of γ,

$$\mu := \varrho\,\mathbf{I}\,\dot{\gamma} \tag{61}$$

being the corresponding momentum density. Consider now the usual transformation relations for the field appearing in (58) and (59) under change of Euclidean observer, and in particular the assumed Euclidean frame-indifference of the elements of γ, $\mathbf{I}$, and Φ_{F}. As discussed in the last section, using these, one can show that necessary conditions for the Euclidean frame-indifference of $(29)_1$ in the form (59) are the mass (34), momentum (35), and moment of momentum (36) balances, respectively. As such, beyond a constant (i.e., in time) mass density, we obtain the set

$$\begin{array}{rclclclc} \dot{\boldsymbol{m}} & = & \mathbf{0} & + & \operatorname{div}\boldsymbol{P} & + & \boldsymbol{f}\ , \\ \dot{\mu} & = & \varpi_{\mathrm{F}} & + & \operatorname{div}\Phi_{\mathrm{F}} & + & \varsigma\ , \\ \dot{\varepsilon} & = & \frac{1}{2}\boldsymbol{S}\cdot\dot{\boldsymbol{C}} + \Phi_{\mathrm{F}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{F}}\cdot\dot{\gamma} & - & \operatorname{div}\boldsymbol{q} & + & r\ , \end{array} \tag{62}$$

of field relations via (35), (36), (59) and (60).

Since we are modeling the γ as (internal) DOFs in the current section, the relevant thermodynamic analysis is based on the usual Clausius-Duhem constitutive forms

$$\begin{array}{rcl} \phi & = & \boldsymbol{q}/\theta\ , \\ \sigma & = & r/\theta\ , \end{array} \tag{63}$$

for the entropy flux ϕ and supply rate σ densities, respectively. Substituting these into the entropy balance $(29)_2$, we obtain the result

$$\delta = \tfrac{1}{2}\,\boldsymbol{S}\cdot\dot{\boldsymbol{C}} + \Phi_{\mathrm{F}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{F}}\cdot\dot{\gamma} - \dot{\psi} - \eta\,\dot{\theta} - \theta^{-1}\boldsymbol{q}\cdot\nabla\theta \tag{64}$$

for the dissipation rate density $\delta := \theta\pi$ via $(62)_3$ via (41). In turn, substitution of the constitutive form (28) for the free energy ψ into (64), and use of that (27) for α, yields

$$\begin{aligned} \delta &= \{\tfrac{1}{2}\,\boldsymbol{S} - \psi_{,\boldsymbol{C}}\}\cdot\dot{\boldsymbol{C}} - \{\eta + \psi_{,\theta}\}\,\dot{\theta} - \psi_{,\nabla\theta}\cdot\nabla\dot{\theta} - \theta^{-1}\boldsymbol{q}\cdot\nabla\theta \\ &+ \Phi_{\mathrm{FN}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{FN}}\cdot\dot{\gamma} - \psi_{,\dot{\gamma}}\cdot\ddot{\gamma} - \psi_{,\nabla\dot{\gamma}}\cdot\nabla\ddot{\gamma}\ , \end{aligned} \tag{65}$$

with

$$\begin{aligned} \Phi_{\mathrm{FN}} &:= \Phi_{\mathrm{F}} - \mathcal{J}^{\mathrm{T}}\psi_{,\alpha}\ , \\ \varpi_{\mathrm{FN}} &:= \varpi_{\mathrm{F}} + K^{\mathrm{T}}\psi_{,\alpha}\ , \end{aligned} \tag{66}$$

the non-equilibrium parts of Φ_{F} and ϖ_{F}, respectively. On the basis of (28), δ is linear in the independent fields $\dot{\boldsymbol{C}}, \dot{\theta}, \nabla\dot{\theta}, \ddot{\gamma}$ and $\nabla\ddot{\gamma}$. As such, in the context of the Coleman-Noll approach to the exploitation of the entropy inequality, $\delta \geq 0$ is insured for all thermodynamically-admissible processes iff the corresponding coefficients of these fields in (65) vanish, yielding

$$\begin{aligned} \boldsymbol{S} &= 2\,\psi_{,\boldsymbol{C}}\ , \\ \eta &= -\psi_{,\theta}\ , \\ \mathbf{0} &= \psi_{,\nabla\theta}\ , \\ 0 &= \psi_{,\dot{\gamma}_{\mathfrak{a}}}\ , \quad \mathfrak{a} = 1,\dots,m\ , \\ \mathbf{0} &= \psi_{,\nabla\dot{\gamma}_{\mathfrak{a}}}\ , \quad \mathfrak{a} = 1,\dots,m\ . \end{aligned} \tag{67}$$

As in the last section, these restrictions also result in the reduced form (47) for ψ. Consequently, the constitutive fields $\boldsymbol{S}$, ε and η are determined in terms of ψ as given by (47). On the other hand, the Φ_{FN}, ϖ_{FN} as well as $\boldsymbol{q}$ still take the general form (28). These are restricted further in the context of the residual form

$$\delta = \Phi_{\mathrm{FN}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{FN}}\cdot\dot{\gamma} - \theta^{-1}\boldsymbol{q}\cdot\nabla\theta$$

for δ in the current constitutive class from (67). Treating Φ_{FN}, ϖ_{FN} and $\boldsymbol{q}$ constitutively in a fashion analogous to $\varpi_{\mathrm{V}} + \operatorname{div}\Phi_{\mathrm{V}}$ and ϕ from the last section in the context of (48), the requirement $\delta \geq 0$ results in the constitutive forms

$$\begin{aligned} \Phi_{\mathrm{FN}} &= d_{\mathrm{F},\nabla\dot{\gamma}} + \zeta_{\mathrm{F}\nabla\dot{\gamma}}\ , \\ -\varpi_{\mathrm{FN}} &= d_{\mathrm{F},\dot{\gamma}} + \zeta_{\mathrm{F}\dot{\gamma}}\ , \\ -\boldsymbol{q} &= d_{\mathrm{F},\nabla\ln} + \zeta_{\mathrm{F}\nabla\ln}\ , \end{aligned} \tag{68}$$

for these in terms of a dissipation potential d_{F} and corresponding constitutive quantities $\zeta_{\mathrm{F}\nabla\dot{\gamma}}$, $\zeta_{\mathrm{F}\dot{\gamma}}$ and $\zeta_{\mathrm{F}\nabla\ln}$, all of the general reduced material-frame-indifferent form (28). As in the last section, the latter three are dissipationless, i.e.,

$$\zeta_{\mathrm{F}\dot{\gamma}}\cdot\dot{\gamma} + \zeta_{\mathrm{F}\nabla\dot{\gamma}}\cdot\nabla\dot{\gamma} + \zeta_{\mathrm{F}\nabla\ln}\cdot\nabla\ln\theta = 0 \tag{69}$$

analogous to (50) in the GIV case. Consequently, δ reduces to

$$\delta = d_{\mathrm{F},\,\dot\gamma} \cdot \dot\gamma + d_{\mathrm{F},\,\nabla\dot\gamma} \cdot \nabla\dot\gamma + d_{\mathrm{F},\,\nabla\ln} \cdot \nabla\ln\theta$$

via (68) and (69), analogous to (52) in the GIV case. In what follows, we again, as in the last section, work for simplicity with the stronger constitutive assumption that d_{F} exists, in which case $\zeta_{\mathrm{F}\,\dot\gamma}$, $\zeta_{\mathrm{F}\,\nabla\dot\gamma}$ and $\zeta_{\mathrm{F}\,\nabla\ln}$ vanish identically.

On the basis of the above assumptions and results, then, the field relation

$$c\,\dot\theta = \tfrac{1}{2}\,\theta\boldsymbol{S}_{,\,\theta} \cdot \dot{\boldsymbol{C}} + \omega_{\mathrm{F}} + \operatorname{div} d_{\mathrm{F},\,\nabla\ln} + r \tag{70}$$

for temperature evolution analogous to (53) is obtained in the current context via (54), with

$$\omega_{\mathrm{F}} := (d_{\mathrm{F},\,\dot\gamma} + \theta\,\mathcal{K}^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \dot\gamma + (d_{\mathrm{F},\,\nabla\dot\gamma} + \theta\,\mathcal{J}^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \nabla\dot\gamma \tag{71}$$

the rate of heating due to inelastic processes analogous to ω_{V} from (55). Finally, $(68)_{1,2}$ lead to the form

$$\varrho\mathbf{I}\ddot\gamma + d_{\mathrm{F},\,\dot\gamma} = \operatorname{div}(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} + d_{\mathrm{F},\,\nabla\dot\gamma}) - \mathcal{K}^{\mathrm{T}}\psi_{,\,\alpha} + \varsigma \tag{72}$$

for the evolution of γ via (61), $(62)_2$ and (66).

With the general thermodynamic framework established in the last two sections now in hand, the next step is the formulation of specific models for GND development and their incoporation into this framework, our next task.

6. Effective models for GNDs

The first model for GNDs to be considered in this section is formulated at the glide-system level. As it turns out, this model represents a three-dimensional generalization of the model of Ashby (1970), who showed that the development of GNDs in a given glide system is directly related to the inhomogeneity of inelastic deformation in this system. In particular, in the current finite-deformation context, this generalization is based on the incompatibility of $\boldsymbol{F}_{\mathfrak{a}}$ with respect to the reference placement. To this end, consider the vector measure**

$$\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C) := \oint_C \boldsymbol{F}_{\mathfrak{a}}\,\boldsymbol{t}_C = \oint_C \gamma_{\mathfrak{a}}\,(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{t}_C)\,\boldsymbol{s}_{\mathfrak{a}} \tag{73}$$

of the length of glide-system GNDs around an *arbitrary* closed curve or circuit C in the reference configuration, the second form following from (20). Here, $\boldsymbol{t}_C$ represents the unit tangent to C oriented *clockwise*. Alternatively, $\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C)$ is given by††

$$\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C) := \oint_C \boldsymbol{F}_{\mathfrak{a}}\,\boldsymbol{t}_C = \int_S (\operatorname{curl}\boldsymbol{F}_{\mathfrak{a}})\boldsymbol{n}_S \tag{74}$$

with respect to the material surface S bounded by C via Stokes theorem. Here,

$$\operatorname{curl}\boldsymbol{F}_{\mathfrak{a}} = (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})(\boldsymbol{I} \times \nabla\gamma_{\mathfrak{a}}) = \boldsymbol{s}_{\mathfrak{a}} \otimes (\nabla\gamma_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}}) \tag{75}$$

**Volume dv, surface da and line $d\ell$ elements are suppressed in the corresponding integrals appearing in what follows for notational simplicity. Unless otherwise stated, all such integrals to follow are with respect to line, surfaces and/or parts of the arbitrary global reference placement of the material body under consideration.

††Note that curl $\boldsymbol{F}_{\mathfrak{a}}$ appearing in (74) is consistent with the form (8) for the curl of a second-order Euclidean tensor field.

from (7), (20), and the constancy of $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$. On the basis of (74), $\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C)$ can also be interpreted as a vector measure of the total length of GNDs piercing the material surface S enclosed by C. The quantity curl $\boldsymbol{F}_\mathfrak{a}$ determines in particular the dislocation density tensor $\alpha^{(I)}$ worked with recently by Shizawa and Zbib (1999) as based on the incompatibility of their slip tensor $\gamma^{(I)} := \sum_{\mathfrak{a}=1}^{n} \gamma_\mathfrak{a}\, \boldsymbol{s}_\mathfrak{a} \otimes \boldsymbol{n}_\mathfrak{a}$. Indeed, we have $\alpha^{(I)} := \operatorname{curl} \gamma^{(I)} = \sum_{\mathfrak{a}=1}^{n} \operatorname{curl} \boldsymbol{F}_\mathfrak{a}$ in the current notation.

Now, from (73) and the constancy of $\boldsymbol{s}_\mathfrak{a}$, note that $\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C)$ is parallel to the slip direction $\boldsymbol{s}_\mathfrak{a}$, i.e.,

$$\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C) = l_{\mathrm{G}\mathfrak{a}}\, \boldsymbol{s}_\mathfrak{a}$$

with

$$l_{\mathrm{G}\mathfrak{a}}(C) := \oint_C \gamma_\mathfrak{a}\, \boldsymbol{n}_\mathfrak{a} \cdot \boldsymbol{t}_C = \int_S (\operatorname{curl} \boldsymbol{F}_\mathfrak{a})^{\mathrm{T}} \boldsymbol{s}_\mathfrak{a} \cdot \boldsymbol{n}_S \tag{76}$$

the scalar length of GNDs piercing S via (74). With the help of a characteristic Burgers vector magnitude b, this length can be written in the alternative form

$$l_{\mathrm{G}\mathfrak{a}}(C) = b \int_S \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} \cdot \boldsymbol{n}_S \tag{77}$$

in terms of the vector field $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ determined by

$$\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} := b^{-1} (\operatorname{curl} \boldsymbol{F}_\mathfrak{a})^{\mathrm{T}} \boldsymbol{s}_\mathfrak{a} = b^{-1}\, \nabla\gamma_\mathfrak{a} \times \boldsymbol{n}_\mathfrak{a} \quad . \tag{78}$$

From the dimensional point of view, $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ represents a (vector-valued) GND surface (number) density. As such, the projection $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} \cdot \boldsymbol{n}_S$ of $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ onto S gives the (scalar) surface (number) density of such GNDs piercing S. The projection of (78) onto the glide-system basis $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$ yields

$$\begin{aligned} \boldsymbol{s}_\mathfrak{a} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} &= -b^{-1}\, \boldsymbol{t}_\mathfrak{a} \cdot \nabla\gamma_\mathfrak{a} \,, \\ \boldsymbol{t}_\mathfrak{a} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{s}_\mathfrak{a} \cdot \nabla\gamma_\mathfrak{a} \,, \\ \boldsymbol{n}_\mathfrak{a} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} &= 0 \,, \end{aligned} \tag{79}$$

for the case of constant b. In particular, the first two of these expressions are consistent with two-dimensional results of Ashby (1970) for the GND density with respect to the slip direction and that perpendicular to it in the glide plane generalized to three dimensions. Such three-dimensional relations are also obtained in the recent crystallographic approach to GND modeling of Arsenlis and Parks (1999). Likewise in agreement with the model of Ashby (1970) is the fact that $(79)_3$ implies that there is no GND development perpendicular to the glide plane (i.e., parallel to $\boldsymbol{n}_\mathfrak{a}$) in this model. ¿From another point of view, if $\nabla\gamma_\mathfrak{a}$ were parallel to $\boldsymbol{n}_\mathfrak{a}$, there would be no GND development at all in this model; indeed, as shown by (75), in this case, $\boldsymbol{F}_\mathfrak{a}$ would be compatible.

The second class of GND models considered in this work is based on the vector measure

$$\boldsymbol{l}_{\mathrm{G}}(C) := \oint_C \boldsymbol{F}_{\mathrm{P}}\, \boldsymbol{t}_C = \int_S (\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}) \boldsymbol{n}_S \tag{80}$$

of the length of GNDs from all glide systems around C in the material as measured by the incompatibility of the local inelastic deformation $\boldsymbol{F}_{\mathrm{P}}$. In particular, the phenomenological GND model of Dai and Parks (1997), utilized by them to model grain-size effects in polycrystalline metals, applied as well recently by Busso et al. (2000) to model size effects in nickel-based superalloys, is of this type. In a different context, the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ has also been used recently by Ortiz and Repetto (1999), as well as by Ortiz et al. (2000), to model in an effective fashion the contribution of the dislocation self- or core energy to the total free energy of ductile single crystals. In what follows, we refer to the GND model based on the measure (80) as the continuum (GND) model. To enable comparison of this continuum GND model with the glide-system model discussed above, it is useful to express the former in terms of glide-system quantities formally analogous to those appearing in the latter. To this end, note that the evolution relation (24) for $\boldsymbol{F}_{\mathrm{P}}$ induces the glide-system decomposition

$$\boldsymbol{l}_{\mathrm{G}}(C) = \sum\nolimits_{\mathfrak{a}=1}^{n} l_{\mathrm{G}\mathfrak{a}}(C)\, \boldsymbol{s}_{\mathfrak{a}}$$

of $\boldsymbol{l}_{\mathrm{G}}(C)$ in terms of the set $l_{\mathrm{G}1}(C), \ldots, l_{\mathrm{G}n}(C)$ of glide-system GND lengths with respect to C formally analogous to those (76) in the context of the glide-system GND model. In contrast to this latter case, however, each $l_{\mathrm{G}\mathfrak{a}}$ here is determined by an evolution relation, i.e.,

$$\dot{l}_{\mathrm{G}\mathfrak{a}}(C) = \oint_C \dot{\gamma}_{\mathfrak{a}}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{t}_C = \int_S \mathrm{curl}\, (\dot{\boldsymbol{F}}_{\mathfrak{a}} \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{n}_S \quad , \tag{81}$$

with

$$\mathrm{curl}\, (\dot{\boldsymbol{F}}_{\mathfrak{a}} \boldsymbol{F}_{\mathrm{P}}) = (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}})(\boldsymbol{I} \times \nabla \dot{\gamma}_{\mathfrak{a}}) + \boldsymbol{s}_{\mathfrak{a}} \otimes (\mathrm{curl}\, \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}\, \dot{\gamma}_{\mathfrak{a}}$$

via (7) and (20). Alternatively, we can express $l_{\mathrm{G}\mathfrak{a}}(C)$ as determined by (81) in the form (77) involving the vector-valued GND surface density $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$, with now

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = b^{-1}\, \mathrm{curl}\, (\dot{\boldsymbol{F}}_{\mathfrak{a}} \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{s}_{\mathfrak{a}} = b^{-1}\, \nabla \dot{\gamma}_{\mathfrak{a}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} + b^{-1}\, (\mathrm{curl}\, \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}\, \dot{\gamma}_{\mathfrak{a}} \tag{82}$$

in the context of (80). As implied by the notation, $\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}}$ from (82) in the current context is formally analogous to the time-derivative of (78) in the glide-system GND model. Now, from the results (26) and (82), we have

$$\dot{\overline{\mathrm{curl}\, \boldsymbol{F}_{\mathrm{P}}}} = b \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{s}_{\mathfrak{a}} \otimes \dot{\boldsymbol{g}}_{\mathfrak{a}}$$

and so the expression[‡‡]

$$\mathrm{curl}\, \boldsymbol{F}_{\mathrm{P}} = b \sum\nolimits_{\mathfrak{a}=1}^{n} \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{g}_{\mathfrak{a}}$$

for the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ in terms of the set $(\boldsymbol{g}_1, \ldots, \boldsymbol{g}_n)$ of vector-valued GND densities. Substituting this result into (82) then yields

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \sum\nolimits_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} + b^{-1}\, \nabla \dot{\gamma}_{\mathfrak{a}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}$$

with $\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{a}} = 0$ and $\sum_{\mathfrak{b}\neq\mathfrak{a}} := \sum_{\mathfrak{b}=1,\mathfrak{b}\neq\mathfrak{a}}^{m}$. Relative to $(\boldsymbol{s}_{\mathfrak{a}}, \boldsymbol{n}_{\mathfrak{a}}, \boldsymbol{t}_{\mathfrak{a}})$, note that

$$\begin{aligned}
\boldsymbol{s}_{\mathfrak{a}} \cdot \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{s}_{\mathfrak{a}} \cdot \nabla \dot{\gamma}_{\mathfrak{a}} &+& \sum\nolimits_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}}\, , \\
\boldsymbol{t}_{\mathfrak{a}} \cdot \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{t}_{\mathfrak{a}} \cdot \nabla \dot{\gamma}_{\mathfrak{a}} &+& \sum\nolimits_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{t}_{\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}}\, , \\
\boldsymbol{n}_{\mathfrak{a}} \cdot \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}} \cdot \nabla \dot{\gamma}_{\mathfrak{a}} &+& \sum\nolimits_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}}\, ,
\end{aligned}$$

via (8) and (21), analogous to (79). In contrast to the glide-system GND model, then, this approach does lead to a development of (edge) GNDs perpendicular to the glide plane (i.e., parallel to $\boldsymbol{n}_{\mathfrak{a}}$).

[‡‡]Assuming the integration constant to be zero for simplicity, i.e., that there is no initial inelastic incompatibility.

To summarize then, we have the expressions

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \begin{cases} b^{-1}\,\dot{\overline{\nabla\gamma_{\mathfrak{a}}}} \times \boldsymbol{n}_{\mathfrak{a}} & \text{glide-system model} \\ b^{-1}\,\dot{\overline{\nabla\gamma_{\mathfrak{a}}}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} + \sum_{\mathfrak{b}\neq\mathfrak{a}}(\boldsymbol{n}_{\mathfrak{a}}\cdot\boldsymbol{s}_{\mathfrak{b}})\,\boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\,\dot{\gamma}_{\mathfrak{a}} & \text{continuum model} \end{cases} \tag{83}$$

for the evolution of the vector-valued measure $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ of GND density from the glide-system and continuum models discussed above. With these in hand, we are now ready to extend existing models for crystal plasticity to account for the effects of GNDs on their material behaviour, and in particular their effect on the hardening behaviour of the material. In the current thermodynamic context, such extensions are realized via the constitutive dependence of the free energy on GND density, and more generally on the dislocation state in the material, our next task.

7. Free energy and GNDs

With GND models such as those from the last section in hand, the question arises as to how these can be incoporated into the thermodynamic formulation for crystal plasticity developed in the previous sections. Since this formulation is determined predominantly by the free energy density ψ and dissipation potential d, this question becomes one of (i), which quantities characterize effectively (i.e., phenomenologically) the GND, and more generally dislocation, state of each material point $p \in B$, and (ii), how do ψ and d depend on these? The purpose of this section is to explore these issues for the case of the referential free energy density ψ. In particular, this involves the choice for α.

Among the possible measures of the inelastic/dislocation state of each material point, we have the arrays $\rho_{\mathrm{S}} = (\rho_{\mathrm{S}1}, \ldots, \rho_{\mathrm{S}n})$ and $g_{\mathrm{G}} = (\boldsymbol{g}_{\mathrm{G}1}, \ldots, \boldsymbol{g}_{\mathrm{G}n})$ of glide-system effective SSD and GND densities, respectively. Choosing then $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \rho_{\mathrm{S}}, g_{\mathrm{G}})$, ψ takes the form

$$\psi(\theta, \boldsymbol{C}, \alpha) = \psi_{\mathrm{D}}(\theta, \boldsymbol{C}, \boldsymbol{F}_{\mathrm{P}}, \rho_{\mathrm{S}}, g_{\mathrm{G}})$$

for ψ from (47), with

$$\begin{aligned} \dot{\rho}_{\mathrm{S}\mathfrak{a}} &= \textstyle\sum_{\mathfrak{b}=1}^{m} K_{\mathrm{S}\mathfrak{a}\mathfrak{b}}\,\dot{\gamma}_{\mathfrak{b}}\,, \\ \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= \textstyle\sum_{\mathfrak{b}=1}^{m} \boldsymbol{k}_{\mathrm{G}\mathfrak{a}\mathfrak{b}}\,\dot{\gamma}_{\mathfrak{b}} + \boldsymbol{J}_{\mathrm{G}\mathfrak{a}\mathfrak{b}}\nabla\dot{\gamma}_{\mathfrak{b}}\,, \end{aligned} \tag{84}$$

from (27). This choice induces the decompositions

$$\begin{aligned} \mathcal{K}^{\mathrm{T}}\psi_{,\,\alpha} &= (\dot{\boldsymbol{F}}_{\mathrm{P},\,\dot{\gamma}})^{\mathrm{T}}\psi_{\mathrm{D},\,\boldsymbol{F}_{\mathrm{P}}} &+\quad& \mathcal{K}_{\mathrm{S}}^{\mathrm{T}}\psi_{\mathrm{D},\,\rho_{\mathrm{S}}} &+\quad& \mathcal{K}_{\mathrm{G}}^{\mathrm{T}}\psi_{\mathrm{D},\,g_{\mathrm{G}}}\,, \\ \mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} &= 0 &+\quad& 0 &+\quad& \mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\psi_{\mathrm{D},\,g_{\mathrm{G}}}\,, \end{aligned} \tag{85}$$

from (24) of the constitutive quantities $\mathcal{K}^{\mathrm{T}}\psi_{,\,\alpha}$ and $\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha}$ determining the form (56) or (72) of the field relation for γ. In particular, the models (83) for $\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}}$ yield

$$\boldsymbol{k}_{\mathrm{G}\mathfrak{a}\mathfrak{b}} = \begin{cases} 0 & \text{glide-system model} \\ \delta_{\mathfrak{a}\mathfrak{b}}\sum_{\mathfrak{c}\neq\mathfrak{b}}(\boldsymbol{n}_{\mathfrak{b}}\cdot\boldsymbol{s}_{\mathfrak{c}})\,\boldsymbol{g}_{\mathrm{G}\mathfrak{c}} & \text{continuum model} \end{cases} \tag{86}$$

and

$$\boldsymbol{J}_{\mathrm{G}\mathfrak{a}\mathfrak{b}} = b^{-1}\,\delta_{\mathfrak{a}\mathfrak{b}} \begin{cases} \boldsymbol{I}\times\boldsymbol{n}_{\mathfrak{b}} & \text{glide-system model} \\ \boldsymbol{I}\times\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{b}} & \text{continuum model} \end{cases} \tag{87}$$

for $\boldsymbol{k}_{\mathrm{G}\mathfrak{a}\mathfrak{b}}$ and $\boldsymbol{J}_{\mathrm{G}\mathfrak{a}\mathfrak{b}}$, respectively. And from (87), we have

$$(88)\qquad (\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha})_{\mathfrak{a}} = (\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{D},\,g_{\mathrm{G}}})_{\mathfrak{a}} = b^{-1}\begin{cases} \boldsymbol{n}_{\mathfrak{a}} \times \psi_{\mathrm{D},\,\boldsymbol{g}_{\mathfrak{a}}} & \text{glide-system model} \\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times \psi_{\mathrm{D},\,\boldsymbol{g}_{\mathfrak{a}}} & \text{continuum model} \end{cases}$$

for the flux contribution appearing in the evolution relation (56) or (72) for γ. From (84), $(85)_1$ and (86), we have

$$(K^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} = -\tau_{\mathfrak{a}} + x_{\mathfrak{a}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\, r_{\mathfrak{a}}$$

where

$$(89)\qquad \tau_{\mathfrak{a}} = -((\dot{\boldsymbol{F}}_{\mathrm{P},\,\dot{\gamma}})^{\mathrm{T}}\psi_{,\,\boldsymbol{F}_{\mathrm{P}}})_{\mathfrak{a}} = -(\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})\boldsymbol{F}_{\mathrm{P}} \cdot \psi_{,\,\boldsymbol{F}_{\mathrm{P}}}$$

represents the glide-system Schmid stress via (24),

$$(90)\qquad x_{\mathfrak{a}} := \begin{cases} 0 & \text{glide-system model} \\ \sum_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \psi_{\mathrm{D},\,\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}} & \text{continuum model} \end{cases}$$

(a contribution to) the glide-system back stress, and

$$(91)\qquad r_{\mathfrak{a}} := \sum\nolimits_{\mathfrak{b}=1}^{m} I_{\mathrm{S}\mathfrak{b}\mathfrak{a}}\, \psi_{\mathrm{D},\,\rho_{\mathrm{S}\mathfrak{b}}}$$

the glide-system yield stress, with $K_{\mathrm{S}\mathfrak{b}\mathfrak{a}} = I_{\mathrm{S}\mathfrak{b}\mathfrak{a}}\operatorname{sgn}(\dot{\gamma}_{\mathfrak{b}})$. Note that $\operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})$ is a constitutive quantity in existing crystal plasticity models. For example, in the case of the (non-thermodynamic) glide-system flow rule

$$(92)\qquad \dot{\gamma}_{\mathfrak{a}} = \dot{\gamma}_{\mathfrak{a}0}\left|\frac{\tau_{\mathfrak{a}}}{\tau_{\mathrm{C}\mathfrak{a}}}\right|^{n} \operatorname{sgn}(\tau_{\mathfrak{a}})$$

of Teodosiu and Sideroff (1976) (similar to the form used by Asaro and Needleman, 1985; see also Teodosiu, 1997), we have $\operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}}) \mathrel{\widehat{=}} \operatorname{sgn}(\tau_{\mathfrak{a}})$. Here, $\tau_{\mathrm{C}\mathfrak{a}}$ represents the critical Schmid stress for slip. In particular, such a constitutive assumption insures that the contribution $\tau_{\mathfrak{a}}\dot{\gamma}_{\mathfrak{a}} = |\tau_{\mathfrak{a}}||\dot{\gamma}_{\mathfrak{a}}| = |\tau_{\mathfrak{a}}|\dot{\nu}_{\mathfrak{a}}$ to the dissipation rate density remains greater than or equal to zero for all $\mathfrak{a} \in \{1, \ldots, m\}$. Such a constitutive assumption is made for other types of glide-system flow rules, e.g., the activation form

$$\dot{\gamma}_{\mathfrak{a}} = \dot{\gamma}_{\mathfrak{a}0}\,\exp\left\{-\frac{\Delta G_{\mathfrak{a}}(|\tau_{\mathfrak{a}}|,\,\tau_{\mathrm{C}\mathfrak{a}})}{k_{\mathrm{B}}\,\theta}\right\}\operatorname{sgn}(\tau_{\mathfrak{a}})$$

used by Anand et al. (1997) to model the inelastic behaviour of tantalum over a much wider range of strain rates and temperatures than possible with (92). Here, $\Delta G_{\mathfrak{a}}(|\tau_{\mathfrak{a}}|,\,\tau_{\mathrm{C}\mathfrak{a}})$ represents the activation Gibbs free energy for thermally-induced dislocation motion.

Consider next the dependence of $\dot{\rho}_{\mathrm{S}\mathfrak{a}}$ on $\dot{\gamma}_{\mathfrak{b}}$, i.e., $K_{\mathrm{S}\mathfrak{a}\mathfrak{b}}$. As it turns out, a number of existing approaches model this dependence. For example, in the approach of Estrin (1996, 1998) to dislocation-density-based constitutive modeling (see also * Estrin et al., 1998; Sluys and Estrin, 2000), this dependence follows from the constitutive relation

$$(93)\qquad \dot{\rho}_{\mathrm{S}\mathfrak{a}} = \left\{\sum\nolimits_{\mathfrak{b}=1}^{n} j_{\mathrm{S}\mathfrak{a}\mathfrak{b}}\sqrt{\rho_{\mathrm{S}\mathfrak{b}}} - k_{\mathrm{S}\mathfrak{a}}\,\rho_{\mathrm{S}\mathfrak{a}}\right\}\operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\dot{\gamma}_{\mathfrak{a}}$$

*Because their model for SSD flux includes a Fickian-diffusion-like contribution due to dislocation cross-slip proportional to $\boldsymbol{n}_{\mathfrak{a}} \cdot \nabla\rho_{\mathrm{S}\mathfrak{a}}$, the approach of Sluys and Estrin (2000) does not fit into the current framework as it stands. The necessary extension involves treating the SSD densities ρ_{S} as, e.g., (independent) GIVs, analogous to the γ.

for the evolution of $\rho_{S\mathfrak{a}}$ in terms of magnitude $|\dot{\gamma}_{\mathfrak{a}}| = \mathrm{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\dot{\gamma}_{\mathfrak{a}}$ of $\dot{\gamma}_{\mathfrak{a}}$ for $\mathfrak{a} = 1, \ldots, m$. In (93), $j_{S11}, j_{S12}, \ldots$ represent the elements of the matrix of athermal dislocation storage coefficients, which in general are functions of ρ_S, and $k_{\mathfrak{a}}$ the glide-system coefficient of thermally-activated recovery. In this case, then,

$$I_{S\mathfrak{a}\mathfrak{b}} = \delta_{\mathfrak{a}\mathfrak{b}} \left\{ \sum\nolimits_{\mathfrak{c}=1}^{n} j_{S\mathfrak{b}\mathfrak{c}} \sqrt{\rho_{S\mathfrak{c}}} - k_{S\mathfrak{b}}\, \rho_{S\mathfrak{b}} \right\}$$

holds, and so

$$(K_S^{\mathrm{T}} \psi_{D,\,\rho_S})_{\mathfrak{a}} = K_{S\mathfrak{a}\mathfrak{a}}\, \psi_{D,\,\rho_{S\mathfrak{a}}} = \mathrm{sgn}(\dot{\gamma}_{\mathfrak{a}})\, I_{S\mathfrak{a}\mathfrak{a}}\, \psi_{D,\,\rho_{S\mathfrak{a}}}$$

from (91). Other such models for $K_{S\mathfrak{a}\mathfrak{b}}$ can be obtained analogously from existing ones for $\dot{\rho}_{S\mathfrak{a}}$ in the literature, e.g., from the dislocation-density-based approach of Teodosiu (1997).

Models such as those $(83)_2$ for $\boldsymbol{g}_{G\mathfrak{a}}$, or that (93) in the case of $\rho_{S\mathfrak{a}}$, account in particular for dislocation-dislocation interactions. At least in these cases, then, such interactions are taken into account in the evolution relations for the dislocation measures, and so need not (necessarily) be accounted for in the form of ψ. From this point of view, ψ_D could take for example the simple "power-law" form

$$\begin{array}{rccccc} \psi_D = & \frac{1}{2}\,\boldsymbol{E}_E \cdot \mathcal{C}_E \boldsymbol{E}_E & + & s^{-1}\, c_S\, \mu \sum\nolimits_{\mathfrak{a}=1}^{n} \epsilon_{S\mathfrak{a}}^{2s} & + & g^{-1}\, c_G\, \mu \sum\nolimits_{\mathfrak{a}=1}^{n} \epsilon_{G\mathfrak{a}}^{2g} \\ =: & \psi_{DE} & + & \psi_{DS} & + & \psi_{DG} \end{array} \tag{94}$$

in the case of ductile single crystals, perhaps the simplest possible. Here, $\mathcal{C}_E$ represents the referential elasticity tensor, and

$$\boldsymbol{E}_E := \tfrac{1}{2}(\boldsymbol{C}_E - \boldsymbol{I})$$

the elastic Green strain determined by the corresponding right Cauchy-Green tensor

$$\boldsymbol{C}_E := \boldsymbol{F}_P^{-\mathrm{T}} \boldsymbol{C} \boldsymbol{F}_P^{-1} \quad . \tag{95}$$

Further, c_S and c_G are (scaling) constants, s and g exponents, μ the average shear modulus, and

$$\begin{array}{rcl} \epsilon_{S\mathfrak{a}} & := & \ell_S \sqrt{\rho_{S\mathfrak{a}}}\ , \\ \epsilon_{G\mathfrak{a}} & := & \ell_G \sqrt{|\boldsymbol{g}_{G\mathfrak{a}}|}\ , \end{array}$$

non-dimensional deformation-like internal variables associated with SSDs and GNDs, respectively, involving the characteristic lengths ℓ_S and ℓ_G, respectively. In particular, the GND contribution ψ_{DG} to ψ_D appearing in (94) is motivated by and represents a power-law generalization of the model of Kuhlmann-Wilsdorf (1989) for dislocation self-energy (see also Ortiz and Repetto, 1999) as based on the notion of dislocation line-length. From (94), we have in particular the simple expression

$$\tau_{\mathfrak{a}} = \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}} \cdot 2\, \boldsymbol{C}_E\, \psi_{DE,\,\boldsymbol{C}_E}$$

for the Schmid stress $\tau_{\mathfrak{a}}$ from (89) in terms of the Mandel stress $-\psi_{D,\,\boldsymbol{F}_P} \boldsymbol{F}_P^{\mathrm{T}} = 2\, \boldsymbol{C}_E\, \psi_{DE,\,\boldsymbol{C}_E}$. In addition,

$$\begin{array}{rcl} \psi_{D,\,\rho_{\mathfrak{a}}} & = & c_S\, \mu\, \ell_S^{2s}\, \rho_{S\mathfrak{a}}^{s-1}\ , \\ \psi_{D,\,\boldsymbol{g}_{\mathfrak{a}}} & = & c_G\, \mu\, \ell_G^{2g}\, |\boldsymbol{g}_{G\mathfrak{a}}|^{g-2}\, \boldsymbol{g}_{G\mathfrak{a}}\ , \end{array}$$

then hold. From these, we obtain in turn

$$x_{\mathfrak{a}} = \begin{cases} 0 & \text{glide-system model} \\ c_G\, \mu\, \ell_G^{2g}\, |\boldsymbol{g}_{G\mathfrak{a}}|^{g-2} \sum\nolimits_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{g}_{G\mathfrak{a}} \cdot \boldsymbol{g}_{G\mathfrak{b}} & \text{continuum model} \end{cases} \tag{96}$$

from (90) for $x_{\mathfrak{a}}$,

$$(97) \qquad (\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{D},\,g_{\mathrm{G}}})_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,b^{-1}\,\ell_{\mathrm{G}}^{2g}\,|\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}|^{g-2}\begin{cases} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} & \text{glide-system model} \\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} & \text{continuum model} \end{cases}$$

from (88), as well as the result

$$(98) \qquad r_{\mathfrak{a}} = c_{\mathrm{S}}\,\mu\,\ell_{\mathrm{S}}^{2s}\sum\nolimits_{\mathfrak{b}=1}^{m} I_{\mathrm{S}\mathfrak{b}\mathfrak{a}}\,\rho_{\mathrm{S}\mathfrak{b}}^{s-1}$$

from (91) for $r_{\mathfrak{a}}$. On the basis of models like that (93) of Estrin (1998) for $\dot{\rho}_{\mathrm{S}\mathfrak{a}}$, this last form for $r_{\mathfrak{a}}$ is consistent with and represents a generalization of distributed dislocation strength models (e.g., Kocks, 1976, 1987) to account for the effects of GNDs on glide-system (isotropic) hardening. Indeed, for $s = 1$, $r_{\mathfrak{a}}$ becomes proportional to $\sqrt{\rho_{\mathrm{S}\mathfrak{b}}}$ in the context of (93).

The simplest case of the formulation as based on (94) arises in the context of the glide-system model for GNDs when we set $s = 1$ and $g = 2$. Then

$$(99) \qquad (\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{D},\,g_{\mathrm{G}}})_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{4}\,b^{-1}\begin{cases} b^{-1}\boldsymbol{n}_{\mathfrak{a}} \times (\nabla\gamma_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}}) & \text{glide-system model} \\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} & \text{continuum model} \end{cases}$$

follows from (87) for the flux contribution via (78) and (83). Note that $(99)_1$ follows from the fact that $(83)_1$ is integrable. Then, the corresponding reduction of $r_{\mathfrak{a}}$ from (98), (56) and $(99)_1$ implies in particular the evolution-field relation

$$(100) \qquad d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{4}\,b^{-2}\,\mathrm{div}_{\mathfrak{a}}(\nabla\gamma_{\mathfrak{a}}) + \tau_{\mathfrak{a}} - c_{\mathrm{S}}\,\mu\,\ell_{\mathrm{S}}^{2}\sum\nolimits_{\mathfrak{b}=1}^{m} K_{\mathrm{S}\mathfrak{b}\mathfrak{a}}$$

for $\gamma_{\mathfrak{a}}$ modeled as a GIV via (56), again in the context of the glide-system GND model, assuming c_{G}, μ and ℓ_{G} constant. The perhaps simplest possible non-trivial form of (100) for the evolution of $\gamma_{\mathfrak{a}}$ in the current context follows in particular from the corresponding simplest (i.e., quasi-linear) form* $d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}} = \beta_{\mathfrak{a}}\,\dot{\gamma}_{\mathfrak{a}}$ for $d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}}$ in terms of the glide-system damping modulus $\beta_{\mathfrak{a}} \geq 0$ with units of J s m^{-3} or Pa s (i.e., viscosity-like). In addition,

$$\mathrm{div}_{\mathfrak{a}}(\nabla\gamma_{\mathfrak{a}}) := (\boldsymbol{I} - \boldsymbol{n}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}) \cdot \nabla(\nabla\gamma_{\mathfrak{a}}) = (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{s}_{\mathfrak{a}} + \boldsymbol{t}_{\mathfrak{a}} \otimes \boldsymbol{t}_{\mathfrak{a}}) \cdot \nabla(\nabla\gamma_{\mathfrak{a}})$$

represents the projection of the divergence operator onto the glide plane spanned by $(\boldsymbol{s}_{\mathfrak{a}}, \boldsymbol{t}_{\mathfrak{a}})$. Given suitable forms for the constitutive quantities, then, the field relation (100) can in principal be solved (i.e., together with the momentum balance in the isothermal case) for $\gamma_{\mathfrak{a}}$. On the other hand, since $\boldsymbol{F}_{\mathrm{P}}$ does not depend explicitly on γ, and, in contrast to the glide-system model, $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ does not depend explicitly on γ and $\nabla\gamma$ in the continuum GND model, no "simple" expression like (100) for the evolution of $\gamma_{\mathfrak{a}}$ is obtainable in this case. Indeed, in all other cases, one must proceed more generally to solve initial-boundary-value problems for ξ, the γ, and θ. We return to this issue in the next section.

A second class of free energy models can be based on the choice $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \nu, \mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})$, i.e.,

$$(101) \qquad \psi(\theta, \boldsymbol{C}, \alpha) = \psi_{\mathrm{C}}(\theta, \boldsymbol{C}, \boldsymbol{F}_{\mathrm{P}}, \nu, \mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}) \quad ,$$

with

$$\dot{\nu}_{\mathfrak{a}} = |\dot{\gamma}_{\mathfrak{a}}|$$

*The coupling with ∇ in d_{V} and the dependence of d_{V} on $\nabla\dot{\gamma}_{\mathfrak{a}}$, is neglected here.

the glide-system accumulated slip rate. In this case, we have

$$
\begin{aligned}
(K^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} &= -\tau_{\mathfrak{a}} + x_{\mathfrak{a}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\, r_{\mathfrak{a}}\ ,\\
(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} &= \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times (\psi_{\mathrm{C,\,curl}\,\boldsymbol{F}_{\mathrm{P}}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}}\ ,
\end{aligned}
\tag{102}
$$

via (26) and (89), where now

$$
x_{\mathfrak{a}} := \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}} \cdot \psi_{\mathrm{C,\,curl}\,\boldsymbol{F}_{\mathrm{P}}}(\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \tag{103}
$$

and

$$
r_{\mathfrak{a}} := \psi_{\mathrm{C},\,\nu_{\mathfrak{a}}}
$$

Consider for example the particular form

$$
\begin{array}{ccccccc}
\psi_{\mathrm{C}} & = & \frac{1}{2}\,\boldsymbol{E}_{\mathrm{E}}\cdot\mathcal{C}_{\mathrm{E}}\boldsymbol{E}_{\mathrm{E}} & + & \psi_{\mathrm{CS}}(\nu) & + & g^{-1}\,c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{g}\,|\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}|^{g}\\
 & =: & \psi_{\mathrm{CE}} & + & \psi_{\mathrm{CS}} & + & \psi_{\mathrm{CG}}
\end{array}
\tag{104}
$$

for ψ_{C} analogous to (94) for ψ_{D}. In this context, the choice

$$
\psi_{\mathrm{CS}} = \frac{(\tau_S - \tau_0)^2}{h_0}\,\ln\left[\cosh\left(\frac{h_0}{\tau_S - \tau_0}\,\nu\right)\right]
$$

yields the simple model for isotropic or Taylor hardening (i.e., due to SSDs) proposed by Hutchinson (1976), with

$$
\nu := \textstyle\sum_{\mathfrak{a}=1}^{n} \nu_{\mathfrak{a}}
$$

the total accumulated inelastic slip in all glide systems. Here, τ_S represents a characteristic saturation strength, τ_0 a characteristic initial critical resolved shear stress, and h_0 a characteristic initial hardening modulus, for all glide systems. Another possibility for ψ_{CS} is the form

$$
\psi_{\mathrm{CS}} = \textstyle\sum_{\mathfrak{a}=1}^{n} r_{\mathfrak{a}0}\,\nu_{\mathfrak{a}} + s^{-1}\,h_0\,\nu^{s}
$$

consistent with the model of Ortiz and Repetto (1999) for latent hardening in single crystals, with now

$$
\nu := \sqrt{\textstyle\sum_{\mathfrak{a},\mathfrak{b}=1}^{n} \iota_{\mathfrak{s}\mathfrak{a}\mathfrak{b}}\,\nu_{\mathfrak{a}}\,\nu_{\mathfrak{b}}}
$$

the effective total accumulated slip in all glide systems in terms of the interaction coefficients $\iota_{\mathfrak{s}\mathfrak{a}\mathfrak{b}}$, $\mathfrak{a}, \mathfrak{b} = 1, \ldots, n$. In particular, this model is based on the assumptions that (i), hardening is parabolic in single slip (i.e., for $s = 2/3$), and (ii), the hardening matrix $\psi_{\mathrm{CS},\,\nu_{\mathfrak{a}}\,\nu_{\mathfrak{b}}}$ is dominated by its off-diagonal components. Beyond such models for glide-system (isotropic) hardening, (104) yields the expression

$$
x_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{g}\,|\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}|^{g-2}\,\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}} \cdot (\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})(\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}}
$$

for glide-system back-stress from (103), as well as that

$$
(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{g}\,|\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}|^{g-2}\,\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times (\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}}
$$

for $(\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{C,\,curl}\,\boldsymbol{F}_{\mathrm{P}}})_{\mathfrak{a}}$ from $(102)_2$. Analogous to $\boldsymbol{F}_{\mathrm{P}}$ and $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ in the case of the continuum GND model, because $\boldsymbol{F}_{\mathrm{P}}$ and curl $\boldsymbol{F}_{\mathrm{P}}$ do not depend explicitly on γ and $\nabla\gamma$, no field relation for $\gamma_{\mathfrak{a}}$ of the type (100) follows from (104), and we are again forced to proceed numerically.

8. The case of small deformation

Clearly, the formulation up to this point is valid for large deformation. For completeness, consider in this section the simplifications arising in the formulation under the assumption of small deformation. In particular, such a simplification is relevant to comparisons of the current approach with other modeling approaches such as the dislocation computer simulation of Van der Giessen and Needleman (1995). This has been carried out recently (Svendsen & Reese, 2002) in the context of the (isothermal) simple shear of a crystalline strip containing one or two glide planes. This model problem has been used in the recent work of Shu et al.(2001) in order to compare the predictions of the discrete dislocation computer simulation with those of the nonlocal strain-gradient approach of Fleck and Hutchinson (1997) and applied to crystal plasticity (e.g., Shu and Fleck, 1999). As dicusssed by them, it represents a model problem for the type of plastic constraint found at grain boundaries of a polycrystal, or the surface of a thin film, or at interfaces in a composite.

In the crystal plasticity context, the small-deformation formulation begins with the corresponding form

$$\boldsymbol{H}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{n} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})\, \gamma_{\mathfrak{a}} \tag{105}$$

for the local inelastic displacement "gradient" $\boldsymbol{H}_{\mathrm{P}}$ assuming no initial inelastic deformation in the material. Note that this measure is in effect equivalent to the slip tensor $\gamma^{(I)} := \sum_{\mathfrak{a}=1}^{n} \gamma_{\mathfrak{a}}\, \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}$ of Shizawa and Zbib (1999). In addition, note that $\boldsymbol{H}_{\mathrm{P}}$ can be considered as a function of γ in this case. In turn, (105) yields the expression

$$\operatorname{curl} \boldsymbol{H}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{n} \boldsymbol{s}_{\mathfrak{a}} \otimes (\nabla\gamma_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}}) \tag{106}$$

for the incompatibility of $\boldsymbol{H}_{\mathrm{P}}$. This is equivalent to the dislocation density tensor $\alpha^{(I)} := \operatorname{curl} \gamma^{(I)}$ of Shizawa and Zbib (1999). Note that either $\operatorname{curl} \boldsymbol{H}_{\mathrm{P}}$ or this latter measure may be considered a function of $\nabla\gamma$. In this context, then, rather than for example with the choice $(\boldsymbol{H}_{\mathrm{P}}, \nu, \operatorname{curl} \boldsymbol{H}_{\mathrm{P}})$, we could work alternatively with that $\alpha = (\gamma, \nu, \nabla\gamma)$ as a measure for the inelastic/dislocation state in the material at any material point $p \in B$. In fact, it would appear to be the simplest possible choice. Indeed, any such choice based alternatively on the small-deformation form

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \begin{cases} b^{-1}\, \dot{\overline{\nabla\gamma_{\mathfrak{a}}}} \times \boldsymbol{n}_{\mathfrak{a}} & \text{glide-system model} \\ b^{-1}\, \dot{\overline{\nabla\gamma_{\mathfrak{a}}}} \times \boldsymbol{n}_{\mathfrak{a}} + \sum_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} & \text{continuum model} \end{cases}$$

of (83) for the development of vector-valued glide-system GND density $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ would appear, at least in the context of the continuum model, to be more complicated since $\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}}$ is not exactly integrable, i.e., even in the small-strain case. On this basis, the general constitutive form (28) reduces to

$$\mathfrak{R} = \mathfrak{R}(\theta, \boldsymbol{E}, \gamma, \nu, \nabla\gamma, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma}, p)$$

for all dependent constitutive quantities (e.g., stress) in the small-deformation context, again with $\alpha = (\gamma, \nu, \nabla\gamma)$. Here,

$$\boldsymbol{E} := \operatorname{sym}(\nabla\boldsymbol{u})$$

represents the symmetric part of the displacement gradient. By analogy, the results of the thermodynamic formulations in §§4–5 for γ modeled as GIVs or as internal DOFs can used to obtain those for the case of small strain. Further, the reduced form (47) of ψ becomes

$$\psi = \psi(\theta, \boldsymbol{E}, \gamma, \nu, \nabla\gamma).$$

Consider for example the class

$$\psi(\theta, \boldsymbol{E}, \gamma, \nu, \nabla\gamma) = \psi_{\mathrm{C}}(\theta, \boldsymbol{E}, \boldsymbol{E}_{\mathrm{P}}(\gamma), \nu, \operatorname{curl} \boldsymbol{H}_{\mathrm{P}}(\nabla\gamma)) \tag{107}$$

of forms for ψ analogous to (101), with

$$\boldsymbol{E}_{\mathrm{P}} := \operatorname{sym}(\boldsymbol{H}_{\mathrm{P}}) \tag{108}$$

the inelastic strain. From (107) follow

$$\begin{array}{rclcl} (K^{\mathrm{T}}\psi_{,\alpha})_{\mathfrak{a}} & = & \psi_{,\gamma_{\mathfrak{a}}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{C},\,\nu_{\mathfrak{a}}} & = & -\tau_{\mathfrak{a}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{C},\,\nu_{\mathfrak{a}}}\,, \\ (\mathcal{J}^{\mathrm{T}}\psi_{,\alpha})_{\mathfrak{a}} & = & \psi_{,\nabla\gamma_{\mathfrak{a}}} & = & \boldsymbol{n}_{\mathfrak{a}} \times (\psi_{\mathrm{C},\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}}\,, \end{array}$$

by analogy with (102) via (108) and (106), with now

$$\tau_{\mathfrak{a}} := -\,\boldsymbol{s}_{\mathfrak{a}} \cdot \psi_{\mathrm{C},\,\boldsymbol{E}_{\mathrm{P}}}\boldsymbol{n}_{\mathfrak{a}}$$

for the Schmid stress. In the case of small deformation, then, the contribution $x_{\mathfrak{a}}$ from inhomogeneity to the glide-system back stress vanishes identically. On the basis of these results, the form

$$d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}} = \operatorname{div}[\boldsymbol{n}_{\mathfrak{a}} \times (\psi_{\mathrm{C},\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}} + d_{\mathrm{V},\,\nabla\dot{\gamma}_{\mathfrak{a}}}] + \tau_{\mathfrak{a}} - \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{C},\,\nu_{\mathfrak{a}}} \tag{109}$$

of the evolution relation for the γ from (56) in the context of their modeling as GIVs, holds.

Further insight into (109) can be gained by introducing concrete forms for ψ_{C} and d_{V}. For example, consider that

$$\psi_{\mathrm{C}} = \tfrac{1}{2}\,\boldsymbol{E}_{\mathrm{E}} \cdot \mathcal{C}_{\mathrm{E}}\boldsymbol{E}_{\mathrm{E}} + \psi_{\mathrm{CS}}(\nu) + g^{-1}\mu\,\ell^{g}\,|\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}|^{g} \tag{110}$$

for ψ_{C} analogous to (104), with $\boldsymbol{E}_{\mathrm{E}} := \boldsymbol{E} - \boldsymbol{E}_{\mathrm{P}}$ now the (small) elastic strain, and $\boldsymbol{E}_{\mathrm{P}} := \operatorname{sym}(\boldsymbol{H}_{\mathrm{P}})$ the (small) inelastic strain. Further, the power-law form

$$d_{\mathrm{V}} = \frac{n}{n+1}\,\varsigma\,\dot{\nu}_0 \sum\nolimits_{\mathfrak{a}=1}^{m} \left\{\frac{|\dot{\gamma}_{\mathfrak{a}}|}{\dot{\nu}_0}\right\}^{(n+1)/n} \tag{111}$$

for the dissipation potential d_{V} is perhaps the simplest one for d_{V} of practical relevance. Here, ς represents a characteristic energy scale for activation of dislocation glide motion with units of J m^{-3} or Pa, and $\dot{\nu}_0$ a characteristic value of $|\dot{\gamma}_{\mathfrak{a}}|$. Substituting (110) and (111) into (109) results in the evolution/field relation

$$\varsigma\,\dot{\nu}_0^{-1}\dot{\gamma}_{\mathfrak{a}} = \mu\,\ell^2 \sum\nolimits_{\mathfrak{b}=1}^{m} \boldsymbol{A}_{\mathfrak{ab}} \cdot \nabla(\nabla\gamma_{\mathfrak{b}}) \;+\; \boldsymbol{s}_{\mathfrak{a}} \cdot (\mathcal{C}_{\mathrm{E}}\boldsymbol{E}_{\mathrm{E}})\boldsymbol{n}_{\mathfrak{a}} - \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{CS},\,\nu_{\mathfrak{a}}}$$

for the glide system slip $\gamma_{\mathfrak{a}}$ via the $g = 2$ and $n = 1$, with $\boldsymbol{A}_{\mathfrak{ab}} := (\boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,[(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{n}_{\mathfrak{b}})\,\boldsymbol{I} - \boldsymbol{n}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{b}}]$. In particular, note that $\boldsymbol{A}_{\mathfrak{aa}} \cdot \nabla(\nabla\gamma_{\mathfrak{a}}) = [\boldsymbol{I} - \boldsymbol{n}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}] \cdot \nabla(\nabla\gamma_{\mathfrak{a}}) = [\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{s}_{\mathfrak{a}} + \boldsymbol{t}_{\mathfrak{a}} \otimes \boldsymbol{t}_{\mathfrak{a}}] \cdot \nabla(\nabla\gamma_{\mathfrak{a}})$ represents the divergence of $\nabla\gamma_{\mathfrak{a}}$ projected onto the $\mathfrak{a}^{\text{th}}$ glide plane. It is worth emphasizing that the form of this projection results from the dependence of ψ on $\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}$. For comparison, note that $\boldsymbol{A}_{\mathfrak{ab}} := (\boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{n}_{\mathfrak{b}})\boldsymbol{I}$, and so $\boldsymbol{A}_{\mathfrak{ab}} \cdot \nabla(\nabla\gamma_{\mathfrak{b}}) = (\boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{n}_{\mathfrak{b}})\operatorname{div}(\nabla\gamma_{\mathfrak{b}})$, would hold if ψ depended on the inhomogeneity $\nabla\boldsymbol{H}_{\mathrm{P}}$ instead of on the incompatibility $\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}$ of $\boldsymbol{H}_{\mathrm{P}}$. In the crystal plasticity and current context, at least, the distinction is significant in the sense that no additional hardening results in the current context when ψ depends directly on $\nabla\boldsymbol{H}_{\mathrm{P}}$.

9. Discussion

Consider the results of the two approaches to the modeling of the glide-system slips γ from §§4-5. Formally speaking, these differ in (i), the respective forms (56) and (72) for the evolution of the γ, (ii), those (55) and (71) for the rate of heating ω due to inelastic processes, and (iii), those (57) and $(68)_3$ for the heat flux density $\boldsymbol{q}$. In particular, in view of the corresponding forms (53) and (70) for temperature evolution, this latter difference is of no consequence for the field relations. Indeed, except for the contribution $\zeta_{\mathrm{F}\nabla\dot{\gamma}}$ to Φ_{N} in the internal DOF model for the γ, the total energy flux density $\boldsymbol{h}$ has the same form in both cases, i.e.,

$$\begin{aligned} \boldsymbol{h} &= -\boldsymbol{q} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi} = d_{\mathrm{V},\,\nabla\ln} + \zeta_{\mathrm{V}\,\nabla\ln} + (\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha} + d_{\mathrm{V},\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi}\ , \\ &= -\boldsymbol{q} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi} + \Phi_{\mathrm{F}}^{\mathrm{T}}\dot{\gamma} = d_{\mathrm{F},\,\nabla\ln} + \zeta_{\mathrm{F}\,\nabla\ln} + (\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha} + d_{\mathrm{F},\,\nabla\dot{\gamma}} + \zeta_{\mathrm{F}\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi}\ , \end{aligned}$$

from $(30)_2$, (57), $(66)_1$ and $(68)_1$. This fact is related to the observation of Gurtin (1971, footnote 1) in the context of classical mixture theory concerning the interpretation of "entropy flux" and "heat flux" in phenomenology and the relation between these two. There, the issue was one of whether diffusion flux is to be interpreted as a flux of energy (e.g., Eckhart, 1940; Gurtin, 1971) or a flux of entropy (e.g., Meixner and Reik, 1959; DeGroot and Mazur, 1962; Müller, 1968). In the current context, the flux (density) of interest is that $(\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha} + d_{,\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma}$. In the GIV approach, the constitutive form (51) shows that this flux (i.e., divided by θ) is being interpreted as an entropy flux. On the other hand, $(58)_2$ and $(63)_2$ imply that it is being interpreted as an energy flux in the internal DOF approach. In this point, then, both approaches are consistent with each other.

As it turns out, the field relation (56) for the γ derived on the basis of the modeling of these as generalized internal variables, represents a generalized form of the Cahn-Allen field relation (e.g., Cahn, 1960; Cahn and Allen, 1977) for non-conservative phase fields, itself in turn a generalization of the Ginzburg-Landau model for phase transitions. In particular, (56) would reduce to the Cahn-Allen form (i), if d_{V} were proportional to a quadratic form in $\dot{\gamma}$ and independent of $\nabla\dot{\gamma}$, and (ii), if $\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha}$ and $\mathcal{K}^{\mathrm{T}}\psi_{,\,\alpha}$ were reduceable to $\psi_{,\,\nabla\gamma}$ and $\psi_{,\,\gamma}$, respectively. In particular, this latter case arises only for monotonic loading and small deformation. The Cahn-Allen relation has been studied quite extensively from the mathematical point of view (see, e.g., Brokate and Sprekels, 1996). As such, one may profit from the corresponding literature on the solution of specific initial-boundary value problems in applications of the approach leading to (56), or more generally that leading to (72), which are currently in progress.

From a phenomenological point of view, the concrete form (94) for ψ_{D}, and in particular that of ψ_{DE}, or that of ψ_{CE} in (104), is contingent upon the modeling of $\boldsymbol{F}_{\mathrm{P}}$ as an elastic material isomorphism (e.g., Wang and Bloom, 1974; Bertram, 1993; Svendsen, 1998), i.e., inelastic processes represented by $\boldsymbol{F}_{\mathrm{P}}$ do not change the form of the elastic constitutive relation. Such an assumption, quite appropriate and basically universal for single-crystal plasticity, may be violated in the case of strong texture development, induced anisotropy and/or anisotropic damage in polycrystals. As discussed by Svendsen (1998), one consequence of the modeling of $\boldsymbol{F}_{\mathrm{P}}$ as an elastic isomorphism is the identification of

$$\boldsymbol{F}_{\mathrm{E}} := \boldsymbol{F}\boldsymbol{F}_{\mathrm{P}}^{-1} \tag{112}$$

as the local (elastic) deformation in the material, and in particular that of the crystal lattice in single-crystal plasticity. More generally, $\boldsymbol{F}_{\mathrm{P}}$ can be modeled as a material uniformity (Maugin and Epstein, 1998; Svendsen, 2001b) in the case of simple materials. In the current context,

(112) implies the connection

$$\mathrm{curl}^{F_\mathrm{P}} F_\mathrm{E} = -\det(F_\mathrm{P}^{-1}) F_\mathrm{E} (\mathrm{curl}\, F_\mathrm{P}) F_\mathrm{P}^\mathrm{T}$$

via (9) and (8) between incompatibility of the local lattice deformation F_E with respect to the intermediate (local) "configuration" and that of F_P with respect to the reference (local) "configuration" (i.e., placement) at each $p \in B$ via (10), (11), and the compatibility of F. Alternatively, we have

$$\mathrm{curl}^{F_\mathrm{P}} F_\mathrm{E} = -F_\mathrm{E}\, G_\mathrm{I},$$

where*

$$G_\mathrm{I} := \det(F_\mathrm{P})^{-1}\,(\mathrm{curl}\, F_\mathrm{P}) F_\mathrm{P}^\mathrm{T} = \det(F_\mathrm{E})\,(\mathrm{curl}^{F} F_\mathrm{E}^{-1}) F_\mathrm{E}^{-\mathrm{T}} \tag{113}$$

represents the geometric dislocation tensor recently introduced by Cermelli and Gurtin (2001). As shown by them, G_I represents the incompatibility of F_P relative to the surface element

$$n_\mathrm{I}\, da_\mathrm{I} := \det(F_\mathrm{P})\, F_\mathrm{P}^{-\mathrm{T}} n_S\, da_S$$

in the intermediate configuration. Indeed, relative to this element, the equivalence

$$(\mathrm{curl}\, F_\mathrm{P}) n_S\, da_S = G_\mathrm{I} n_\mathrm{I}\, da_\mathrm{I}$$

holds. As such, curl F_P gives the same measure of GNDs with respect to surface elements in the reference configuration as does G_I with respect to such elements in the intermediate configuration. Note that G_I, like curl F_P, has units of inverse length. The definition $(113)_1$ implies the form

$$\dot{G}_\mathrm{I} = \mathrm{curl}^{F_\mathrm{P}} L_\mathrm{P} + L_\mathrm{P} G_\mathrm{I} + G_\mathrm{I} L_\mathrm{P}^\mathrm{T} - G_\mathrm{I}\,(I \cdot L_\mathrm{P}) \tag{114}$$

for the evolution of G_I via (22). Alternatively, this can be expressed "objectively" as

$$\det(F_\mathrm{P})^{-1}\, F_\mathrm{P}\, \overline{[\det(F_\mathrm{P})\, F_\mathrm{P}^{-1} G_\mathrm{I} F_\mathrm{P}^{-\mathrm{T}}]}^{\boldsymbol{\cdot}}\, F_\mathrm{P}^\mathrm{T} = \det(F_\mathrm{P})^{-1}\, F_\mathrm{P}\, \dot{G}_\mathrm{R} F_\mathrm{P}^\mathrm{T} = \mathrm{curl}^{F_\mathrm{P}} L_\mathrm{P} \tag{115}$$

relative to the "upper" Oldroyd-Truesdell derivative of G_I with respect to F_P, where

$$G_\mathrm{R} := \det(F_\mathrm{P})\, F_\mathrm{P}^{-1} G_\mathrm{I} F_\mathrm{P}^{-\mathrm{T}} = F_\mathrm{P}^{-1}(\mathrm{curl}\, F_\mathrm{P})$$

represents the referential form of G_I via (113). In the current crystal plasticity context, the right-hand side of (115) reduces to

$$\mathrm{curl}^{F_\mathrm{P}} L_\mathrm{P} = b \sum\nolimits_{\mathfrak{a}=1}^{n} s_\mathfrak{a} \otimes F_\mathrm{P}^{-\mathrm{T}} \dot{g}_{\mathrm{G}\mathfrak{a}} = \sum\nolimits_{\mathfrak{a}=1}^{n} s_\mathfrak{a} \otimes F_\mathrm{P}^{-\mathrm{T}} [\nabla \dot{\gamma}_\mathfrak{a} \times n_\mathfrak{a}]$$

via (6) and (23) in terms of the evolution of the vector-valued GND surface density $g_{\mathrm{G}\mathfrak{a}}$ for the glide-system GND model from (78). As such, (114) implies

$$\dot{G}_\mathrm{I} = \sum\nolimits_{\mathfrak{a}=1}^{m} [(s_\mathfrak{a} \otimes n_\mathfrak{a}) G_\mathrm{I} + G_\mathrm{I}(n_\mathfrak{a} \otimes s_\mathfrak{a})]\, \dot{\gamma}_\mathfrak{a} + \sum\nolimits_{\mathfrak{a}=1}^{m} s_\mathfrak{a} \otimes F_\mathrm{P}^{-\mathrm{T}} [\nabla \dot{\gamma}_\mathfrak{a} \times n_\mathfrak{a}]$$

for the evolution of G_I in the case of crystal plasticity via (23) and the fact that $I \cdot L_\mathrm{P} = 0$ in this context. So, another class of specific forms for ψ from (47) can be based on the choice $\alpha = (F_\mathrm{P}, \nu, G_\mathrm{I}$, implying

$$\psi(\theta, C, \alpha, p) = g(\theta, C_\mathrm{E}, \nu, G_\mathrm{I}, p)$$

*Recall that we have defined the curl of a second-order tensor field in (6) via $(\mathrm{curl}\, T)^\mathrm{T} a := \mathrm{curl}\,(T^\mathrm{T} a)$, rather than in the form $(\mathrm{curl}\, T) a := \mathrm{curl}\,(T^\mathrm{T} b)$ used by Cermelli and Gurtin (2001).

via (95). In turn, g itself is a member of the class defined by the choice $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \nu, \nabla\boldsymbol{F}_{\mathrm{P}})$, as can be concluded directly from (25) and the fact that curl $\boldsymbol{F}_{\mathrm{P}}$ is a function of $\nabla\boldsymbol{F}_{\mathrm{P}}$ via (18). As shown by Cermelli and Gurtin (2001), constitutive functions for any $p \in B$ depending on $\nabla\boldsymbol{F}_{\mathrm{P}}$ must reduce to a dependence on $\boldsymbol{G}_{\mathrm{I}}$ for their form to be independent of change of compatible local reference placement at $p \in B$, i.e., one induced by a change* of global reference placement. This requirement is in turn based on the result of Davini (1986), and Davini and Parry (1989) that such changes leave dislocation measures such as $\boldsymbol{G}_{\mathrm{I}}$ unchanged, representing as such "elastic" changes of local reference placement. As it turns out, one can show more generally (Svendsen, 2001c) that ψ reduces to g for all $p \in B$, i.e., for B as a whole, under the assumption that $\boldsymbol{F}_{\mathrm{P}}$ represents a particular kind of material uniformity.

References

[1] Abraham R., Marsden J.E. and Ratiu T., *Manifolds, tensor analysis and applications*, Appl. Mat. Sc. **75**, Springer, New York 1988.

[2] Acharya A. and Bassani J.L., *Lattice incompatibility and a gradient theory of crystal plasticity*, J. Mech. Phys. Solids **48** (2000), 1565–1595.

[3] Acharya A. and Beaudoin A.J., *Grain-size effect in viscoplastic polycrystals at moderate strains*, J. Mech. Phys. Solids **48** (2000), 2213–2230.

[4] Anand L., Balasubramanian S. and Kothari M., *Constitutive modeling of polycrystalline metals at large strains, application to deformation processes*; in: "Large plastic deformation of crystalline aggregates" (Ed. C. Teodosiu), CISM **376**, Springer 1997, 109–172.

[5] Arsenlis A. and Parks D.M., *Crystallographic aspects of geometrically-necessary and statistically-stored dislocation density*, Acta Mater. **47** (1999), 1597–1611.

[6] Asaro R.J., *Micromechanics of crystals and polycrystals*, Adv. Appl. Mech. **23** (1983), 1–115.

[7] Asaro R.J. and Needleman A., *Texture development and strain hardening in rate-dependent polycrystals*, Acta Metall. **33** (1985), 923–953, 1985.

[8] Ashby M.F., *The deformation of plastically non-homogeneous materials*, Phil. Mag. **21** (1970), 399–424.

[9] Bertram A., *Description of finite inelastic deformations*; in: "MECAMAT '92 Multiaxial Plasticity" (Eds. A. Benallal, R. Billardon and D. Marquis), 1993, 821–835.

[10] Brokate M. and Sprekels J., *Hysteresis and phase transitions*, App. Mat. Sciences **121**, Springer, New York 1996.

[11] Busso E.F., Meissonnier F.T. and O'Dowd N.P., *Gradient-dependent deformation of two-phase single crystals*, J. Mech. Phys. Solids **48** (2000), 2333–2361.

[12] Cahn J.W., *Theory of crystal growth and interface motion in crystalline materials*, Acta Metall. **8** (1960), 554–562.

[13] Cahn J.W. and Allen S.M., *A microscopic theory for domain wall motion and its experimental verification in Fe-Al alloy domain growth kinetics*, J. de Physique **38** (1977), 51–54.

*Since local changes of reference placement for any $p \in B$ represent equivalence classes of corresponding changes of global reference placement there, any local change of reference placement for $p \in B$ is induced by a corresponding change of global placement.

[14] CAPRIZ G., *Continua with microstructure*, Tracts in Natural Philosophy **37**, Springer, New York 1989.

[15] CERMELLI P. AND GURTIN M.E., *On the characterization of geometrically necessary dislocations in finite plasticity*, J. Mech. Phys. Solids (2001).

[16] CUITIÑO A.M. AND ORTIZ M., *Computational modeling of single crystals*, Modelling Simul. Mater. Sci. Eng. **1** (1992), 225–263.

[17] DAI H. AND PARKS D.M., *Geometrically-necessary dislocation density and scale-dependent crystal plasticity*; in: "Proceedings of Plasticity" (Ed. A.S. Khan), Neat Press 1997, 17–18.

[18] DAVINI C., *A proposal for a continuum theory of defective crystals*, Arch. Rat. Mech. Anal. **96** (1986), 295–317.

[19] DAVINI C. AND PARRY G.P., *On defect-preserving deformations in crystals*, Int. J. Plast. **5** (1989), 337–369.

[20] DEGROOT S.R. AND MAZUR P., *Non-equlibrium thermodynamics*, Wiley-Interscience 1962.

[21] ECKHART C., *The thermodynamics of irreversible processes; II. Fluid mixtures*, Phys. Rev. **58** (1940), 269–275.

[22] EDELEN D.G.B., *On the existence of symmetry relations and dissipation potential*, Arch. Rat. Mech. Anal. **51** (1973), 218–227.

[23] EDELEN D.G.B., *Applied exterior calculus*, John Wiley & Sons, New York 1985.

[24] ESTRIN Y., *Dislocation-density related constitutive modelling*, in: "Unified constitutive laws of plastic deformation", (Eds. A.S. Krausz and K. Krausz), Academic Press 1996, 69–106.

[25] ESTRIN Y., *Dislocation-theory-based constitutive modelling: foundations and applications*, J. Mater. Processing Tech. **80-81** (1998), 33–39.

[26] ESTRIN Y., SLUYS L.J., BRECHET Y. AND MOLINARI A., *A dislocation-based gradient plasticity model*, J. de Physique **8** (1998), 135–141.

[27] FRIED E., *Continua described by a microstructural field*, Z. Angew. Math. Phys. **47** (1996), 168–175.

[28] FRIED E. AND GURTIN M., *Continuum theory of thermally-induced phase transitions based on an order parameter*, Physica D **68** (1993), 326–343.

[29] FRIED E. AND GURTIN M., *Dynamic solid-solid transitions with phase characterized by an order parameter*, Physica D **72**(1994), 287–308.

[30] FLECK N.A. AND HUTCHINSON J.W., *A phenomenological theory for strain gradient effects in plasticity*, J. Mech. Phys. Solids **41** (1993), 1825–1857.

[31] FLECK N.A. AND HUTCHINSON J.W., *Strain gradient plasticity*, Adv. Appl. Mech. **33** (1997), 295–361.

[32] FOREST S., CAILLETAUD G. AND SIEVERT R., *A Cosserat theory for elastoviscoplastic single crystals at finite deformation*, Arch. Mech. **49** (1997), 705–736.

[33] GURTIN M.E., *On the thermodynamics of chemically reacting fluid mixtures*, Arch. Rat. Mech. Anal. **43** (1971), 198–212.

[34] GURTIN M.E., *The nature of configurational forces*, Arch. Rat. Mech. Anal. **131** (1995), 67–100.

[35] GURTIN M.E., *On the plasticity of single crystals: free energy, microforces, plastic-strain gradients*, J. Mech. Phys. Solids **48** (2000), 989–1036.

[36] HILL R. AND RICE J.R., *Constitutive analysis of elastic-plastic crystals at arbitrary strain*, J. Mech. Phys. Solids **20** (1972), 401–413.

[37] HUTCHINSON W., *Elastic-plastic behaviour of polycrystalline metals and composites*, Proc. Roy. Soc. London **319** A (1976), 247–272.

[38] LE K.C. AND STUMPF H., *Non-linear continuum theory of dislocations* Int. J. Eng. Sci. **34** (1996), 339–358.

[39] KOCKS U.F., *Laws for work-hardening and low-temperature creep*, J. Eng. Mat. Techn. **98** (1976), 76–85.

[40] KOCKS U.F., *Constitutive behaviour based on crystal plasticity*, in: "Constitutive equations for creep and plasticity" (Ed. A.K. Miller), Elsevier 1987, 1–88.

[41] KUHLMANN-WILSDORF D., *Theory of plastic deformation: properties of low-energy dislocation structures*, Mat. Sci. Eng. **113** A (1989), 1.

[42] KRÖNER E., *Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen*, Arch. Rat. Mech. Anal. **4** (1960), 273–334.

[43] MAUGIN G., *The method of virtual power in continuum mechanics; application to coupled fields*, Acta Mech. **35** (1980), 1–70.

[44] MAUGIN G., *On internal variables and dissipative structures*, Int. J. Non-Equil. Thermod. **15** (1990), 173–192.

[45] MAUGIN G. AND EPSTEIN M., *Geometrical material structure of elastoplasticity*, Int. J. Plast. **14** (1998), 109–115.

[46] MAUGIN G. AND MUSCHIK W., *Thermodynamics with internal variables. I. General concepts*, Int. J. Non-Equil. Thermod. **19** (1994), 217–249.

[47] MEIXNER J. AND REIK H.G., *Thermodynamik der irreversiblen Prozesse*, in: "Handbuch der Physik III/2", Springer 1959.

[48] MENZEL A. AND STEINMANN P., *On the continuum formulation of higher gradient plasticity for single and polycrystals*, J. Mech. Phys. Solids **48** (2000), 1777–1796.

[49] MURA T., *Micromechanics of defects in solids*, Kluwer Publishers 1987.

[50] MÜLLER I., *A thermodynamic theory of mixtures of fluids*, Arch. Rat. Mech. Anal. **28** (1968), 1–39.

[51] NAGHDI P. AND SRINIVASA A.R., *A dynamical theory of structured solids. I. Basic developments*, Phil. Trans. Roy. Soc. **345** A (1993), 424–458.

[52] NAGHDI P. AND SRINIVASA A.R., *Characterisation of dislocations and their influence on plastic deformation in single crystals*, Int. J. Solids Structs. **7** (1994), 1157–1182.

[53] NOLL W., *Materially uniform simple bodies with inhomogeneities*, Arch. Rat. Mech. Anal. **27** (1967), 1–32.

[54] NYE J.F., *Some geometric relations in dislocated crystals*, Acta Metall. **1** (1953), 153–162.

[55] ORTIZ M. AND REPETTO E.A., *Nonconvex energy minimization and dislocation structures in ductile single crystals*, J. Mech. Phys. Solids **47** (1999), 397–462.

[56] ORTIZ M., REPETTO E.A. AND STAINIER, L., *A theory of dislocation structures*, J. Mech. Phys. Solids **48** (2000), 2077–2114.

[57] SILHAVÝ M., *The mechanics and thermodynamics of continuous media*, Springer Verlag 1997.

[58] SHIZAWA K. AND ZBIB H.M., *A thermodynamical theory of gradient elastoplasticity with dislocation density tensor. I. Fundamentals*, Int. J. Plast. **15** (1999), 899–938.

[59] SHU J.Y. AND FLECK N.A., *Strain gradient crystal plasticity: size-dependent deformation of bicrystals*, J. Mech. Phys. Solids **47** (1999), 297–324.

[60] SHU J.Y., FLECK N.A., VAN DER GIESSEN E. AND NEEDLEMAN A., *Boundary layers in constrained plastic flow: comparison of nonlocal and discrete dislocation plasticity*, J. Mech. Phys. Solids **49**, (2001), 1361–1395.

[61] SLUYS L.J. AND ESTRIN Y., *The analysis of shear banding with a dislocation-based gradient plasticity model*, Int. J. Solids Struct. **37** (2000), 7127–7142.

[62] STEINMANN P., *Views on multiplicative elastoplasticity and the continuum theory of dislocations*, Int. J. Eng. Sci. **34** (1996), 1717–1735.

[63] SVENDSEN B., *A thermodynamic formulation of finite-deformation elastoplasticity with hardening based on the concept of material isomorphism*, Int. J. Plast. **14** (1998), 473–488.

[64] SVENDSEN B., *On the thermodynamics of isotropic thermoelastic materials with scalar internal degrees of freedom*, Cont. Mech. Thermodyn. **11** (1999), 247–262.

[65] SVENDSEN B., *On the formulation of balance relations and configurational fields for materials with microstructure via invariance*, Int. J. Solids Struct. **38** (2001), 700–740.

[66] SVENDSEN B., *On the modeling of anisotropic elastic and inelastic material behaviour at large deformation*, Int. J. Solids Struct. (2000), in press.

[67] SVENDSEN B., *A note on the concepts of material isomorphism and material uniformity for inelastic gradient materials*, in preparation.

[68] SVENDSEN B. AND REESE S., *Continuum thermodynamic modeling and simulation of additional hardening due to deformation incompatibility*; in: "Computational mechanics of solid materials at large strains", Proceedings of the IUTAM Symposium, August 20-24, Stuttgart, Germany, 2001.

[69] TEODOSIU C., *Dislocation modeling of crystalline plasticity*; in: "Large plastic deformation of crystalline aggregates" (Ed. C. Teodosiu), CISM **376**, Springer 1997, 21–80.

[70] TEODOSIU C. AND SIDEROFF F., *A physical theory of finite elasto-viscoplastic behaviour of single crystals*, Int. J. Engrg. Sci. **14** (1976), 165–176.

[71] VALANIS K., *A gradient theory of internal variables*, Acta Mech. **116** (1996), 1–14.

[72] VALANIS K, *A gradient thermodynamic theory of self-organization*, Acta Mech. **127** (1998), 1–23.

[73] VAN DER GIESSEN E. AND NEEDLEMAN A., *Discrete dislocation plasticity: a simple planar model*, Model. Simul. Mater. Sci. Eng. **3** (1995), 689–735.

[74] WANG C.C. AND BLOOM J., *Material uniformity and inhomogeneity in anelastic bodies*, Arch. Rat. Mech. Anal. **53** (1974), 246–276.

AMS Subject Classification: 74A99, 74C20.

Bob SVENDSEN
Department of Mechanical Engineering
University of Dortmund
D-44227 Dortmund, GERMANY
e-mail: bob.svendsen@mech.mb.uni-dortmund.de

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

C. Trimarco

THE STRUCTURE OF MATERIAL FORCES IN ELECTROMAGNETIC MATERIALS

Abstract. Material forces govern the behaviour and the evolution of a defect or of an inhomogeneity in a solid material. In elastic materials these forces are associated with the Eshelby tensor, as is known. In structured or micro-structured materials, an Eshelby–like stress can be assembled by following a simple rule. By appealing to this rule, one is able to propose an expression for the Eshelby tensor in electromagnetism.

A variational procedure is hereby expounded, from which an expression for the classical electromagnetic stress tensor, whose form is otherwise controversial, stems straightforwardly. The electromagnetic Eshelby–like tensor is derived on this base.

1. Introduction

Material forces and configurational forces are customarily understood as two synonymous which label the same notion. In the continuum framework, the configurational forces are usually associated with the energy–stress tensor and they acquire a special importance in structured materials. Most people, who are concerned with materials with an internal structure or with microstructures, are familiar with the notion of energy–stress. Such an energy–stress naturally appears in the theory whenever the material response depends on the gradient of the fields or of the micro-fields of interest. We shall stress out that there are two kinds (at least) of configurational forces and only one of the two is related to the notion of material force. The latter governs the behaviour of material defects or inhomogeneities [1, 2].

The Maxwell electromagnetism can be viewed as one of the first theories of a material endowed with a structure (i.e.the electromagnetic fields), although the Maxwell–Faraday's electromagnetic fields are defined also out of a body of finite extent. As the electromagnetic fields pervade the whole physical space, the mathematical problem for the electromagnetic materials has to be formulated not only in the domain occupied by the body, but also in the exterior domain, accordingly. The electromagnetic fields obey a set of differential equations that are in general coupled with the mechanical equations [3, 4]. Should the Maxwell equations possibly decouple from the mechanical ones, one could think to solve them first and afterward to look for the associated stress tensor, in order to enquire about the mechanical behaviour of the material.

Some people who are interested in liquid crystals share this attitude with those who deal with electromagnetic materials or with other sort of structured materials. However, in most of the cases, the form of the mechanical stress to associate with a structured material may be a controversial matter [5, 6, 7]. This is the case for electromagnetic materials [4]. It is worth to recalling that the quarrel, about the proper form the stress (and the momentum) should have in electromagnetic materials, is still unsettled [8]. As there is not a general agreement on the form of the electromagnetic stress, a challenge for new proposals is open.

Here, we discuss this point basing on a variational approach. In this approach, the Maxwell electromagnetic stress tensor will naturally stem from a Hamilton-like principle for a Lagrangian that we are going also to introduce. Along with the electromagnetic stress, other electromagnetic quantities of interest are derived. These quantities are useful for recovering the final form of the energy–stress tensor which is related to the *material forces* [9, 10]. This energy-stress definitely differs from the Maxwell energy–stress. Maxwell introduced, in his treatise, the electromagnetic stress tensor in order to evaluate the electromagnetic force acting over a body [11]. Thus, the Maxwell tensor is an energy-stress tensor that it is related to the classical notion of force, *not* to the *material forces*, as we will try to show in evidence.

Nonetheless, the procedure suggested by Maxwell in establishing the stress and the force acting on a material body is appealing, as it can be re–proposed in other fields of Continuum Mechanics or Continuum Physics. Eshelby [1] was the first who proposed to apply the Maxwell's procedure to elasticity, in order to evaluate the force acting upon a point-wise defect. In this respect, Eshelby introduced the notion of material force.

2. Maxwell equations in material form

Hereafter, we consider a solid body of infinite extent, which fills the whole physical space. This space is here represented by the Euclidean space E_3. The classical Maxwellian fields **E, D, B, H, P** and **M** (the electric field, the electric displacement, the magnetic induction, the magnetic field, the polarisation and the magnetisation, respectively) are *transformed* in a suitable chosen reference configuration of the deformable body, in the following fashion:

$$\begin{array}{rcl}
\mathfrak{E} & = & \mathbf{F^T}(\mathbf{E}+\mathbf{v}\wedge\mathbf{B}) = \mathbf{F^T}\mathcal{E}; \\
\mathfrak{D} & = & J\mathbf{F}^{-1}\mathbf{D}; \\
\mathfrak{B} & = & J\mathbf{F}^{-1}\mathbf{B}; \\
\mathfrak{H} & = & \mathbf{F^T}\mathcal{H} \equiv \mathbf{F^T}\mathbf{H}+\mathbf{V}\wedge\mathbf{D}; \\
\mathfrak{P} & = & J\mathbf{F}^{-1}\mathbf{P}; \\
\mathfrak{M} & = & \mathbf{F^T}\mathbf{M}
\end{array} \tag{1}$$

The introduction of the following auxiliary fields will be also useful:

$$\begin{array}{rcl}
\mathfrak{E}^* & = & \mathbf{F^T}\mathbf{E} \equiv \mathfrak{E}+\mathbf{V}\wedge\mathfrak{B}; \\
\mathfrak{B}^* & = & J\mathbf{F}^{-1}\mathcal{B} = J\mathbf{F}^{-1}[\mathbf{B}-(1/c^2)\mathbf{v}\wedge\mathbf{E}] \\
 & \equiv & \mathfrak{B}+(1/c^2)\mathbf{C}^{-1}(\mathbf{V}\wedge\varepsilon_0 J\mathbf{C}^{-1}\mathfrak{E}^*); \\
\mathfrak{M}^* & = & \mathbf{F^T}\mathcal{M} \equiv \mathfrak{M}-(\mathbf{V}\wedge\mathfrak{P}).
\end{array} \tag{2}$$

The transformation has to be understood as through the mapping $\chi : (\mathbf{X}, t) \to \mathbf{x}$, which is assumed here to be regular enough for our purposes.

X belongs to the reference configuration and **x** to the actual configuration of a body. $t \in \mathbf{R}$ represents the time. $\mathbf{F} = \nabla_R\chi$, where ∇_R stands for the spatial gradient in the referential frame. $J = det\,\mathbf{F}$. $\mathbf{F^T}$ denotes the transpose of **F**. $\mathbf{v} = \dot{\mathbf{x}}$ and $\mathbf{V} = -\mathbf{F}^{-1}\mathbf{v}$. We also assume, as usual, that $J > 0$.

The fields introduced in (1) satisfy the Maxwell equations in the following form:

$$\begin{array}{rcl}
div_R\mathfrak{D} & = & J\rho_e \\
div_R\mathfrak{B} & = & 0 \\
rot_R\mathfrak{E}+(\partial\mathfrak{B}/\partial t)|_X & = & 0 \\
rot_R\mathfrak{H}-(\partial\mathfrak{D}/\partial t)|_X & = & \mathbf{g}.
\end{array} \tag{3}$$

div_R represents the divergence operator and rot_R the curl operator in the reference configuration; $\mathbf{g}$ is defined as follows:

$$\mathbf{g} = J\mathbf{F}^{-1}\mathbf{j} + J\rho_e\mathbf{V}. \tag{4}$$

ρ_e and $\mathbf{j}$ are the free charge and the free current densities, respectively, per unit volume of the current configuration.

The transformations of the electromagnetic fields, such as given by the relationships (1) and (2), provide the Maxwell equations (3) in the referential frame. These equations are clearly form–invariant.

The reader is referred to [10] for further details on this point.

For future use, we will introduce the following relationships:

$$\mathfrak{P} = \mathfrak{D} - \varepsilon_0 J\mathbf{C}^{-1}\mathfrak{E}^* \tag{5}$$

and

$$\mathfrak{M}^* = \mu_0 J^{-1}\mathbf{C}\mathfrak{B} - \mathfrak{H}. \tag{6}$$

where $\mathbf{C} \equiv \mathbf{F}^{\mathbf{T}}\mathbf{F}$. ϵ_0 and μ_0 are the electric permittivity and the magnetic permeability of a vacuum, respectively.

2.1. The material electromagnetic potentials

The classical electrodynamical potentials, namely the scalar potential Φ and the vector potential $\mathbf{A}$ are also transformed in two analogous fields ϕ and $\mathcal{A}$, respectively, in such a way that they are consistent with the equations (3) [10, 11, 12, 13]. More specifically, one introduces the vector field $\mathcal{A}$, (the vector potential in the material form) as follows:

$$rot_R\mathcal{A} = \mathfrak{B} \tag{7}$$

so that the equation $(3)_2$ is identically satisfied. It is worth to mentioning that $\mathcal{A}$ is uniquely defined, provided that the quantity $div_R\mathcal{A}$ is specified.

Basing on the equations $(3)_3$ and (7), one also introduces the material scalar potential ϕ, so that

$$\mathfrak{E} = -\nabla_R\phi - \dot{\mathcal{A}} \tag{8}$$

The superposed dot on $\mathcal{A}$ denotes the total time derivative of $\mathcal{A}$.

The equations (3) can be now written in terms of ϕ, $\mathcal{A}$, $\mathfrak{P}$ and $\mathfrak{M}^*$, by taking into account the equations (1), (4), (5), (6), (7) and (8). Hereafter, we will be concerned with this form of the Maxwell equations, which is known as the Lorentz form [4, 12].

It is worth to recalling that, had we dealt with bounded domains, the fields $\mathfrak{P}$ and $\mathfrak{M}^*$ would have been identically vanishing out of these domains.

3. A Lagrangian approach

Motivations for introducing the Lagrangian density in the material form, such as written below, will not be reported here as they are illustrated in [10]. Here, we only remark that such a Lagrangian provides the equations (3), in the Lorentz form. This Lagrangian reads:

$$\begin{aligned} L \quad = \quad & \frac{1}{2}\{\varepsilon_0 J\mathfrak{E}^* \cdot \mathbf{C}^{-1}\mathfrak{E}^* - (\mu_0 J)^{-1}\mathfrak{B}\cdot\mathbf{C}\mathfrak{B}\} + \mathfrak{P}\cdot\mathfrak{E} + \mathfrak{M}^*\cdot\mathfrak{B} + \frac{\rho_0 v^2}{2} \\ - \quad & W(\mathbf{F}, \mathbf{F}\mathfrak{P}, J\mathbf{F}^{-1\mathbf{T}}\mathfrak{M}^*, \mathbf{X}). \end{aligned} \tag{9}$$

L is a Lagrangian density per unit volume of the reference configuration and possibly is of the following form:

$$L = \hat{L}(\phi, \dot{\phi}, \nabla_R \phi, \mathcal{A}, \dot{\mathcal{A}}, \nabla_R \mathcal{A}, \mathfrak{P}, \dot{\mathfrak{P}}, \nabla_R \mathfrak{P}, \mathfrak{M}^*, \dot{\mathfrak{M}}^*, \nabla_R \mathfrak{M}^*, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{F}, \mathbf{X}) \ . \tag{10}$$

The corresponding Lagrange equations read:

$$\begin{aligned}
&\frac{d}{dt}\frac{\partial L}{\partial \dot{\phi}} - \frac{\partial L}{\partial \phi} + \operatorname{div}_R \frac{\partial L}{\partial \nabla_R \phi} = 0,\\
&\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathcal{A}}} - \frac{\partial L}{\partial \mathcal{A}} + \operatorname{div}_R \frac{\partial L}{\partial \nabla_R \mathcal{A}} = 0,\\
&\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{x}}} - \frac{\partial L}{\partial \mathbf{x}} + \operatorname{div}_R \frac{\partial L}{\partial \mathbf{F}} = 0,\\
&\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathfrak{P}}} - \frac{\partial L}{\partial \mathfrak{P}} + \operatorname{div}_R \frac{\partial L}{\partial \nabla_R \mathfrak{P}} = 0,\\
&\frac{d}{dt}\frac{\partial L}{\partial \dot{\mathfrak{M}}^*} - \frac{\partial L}{\partial \mathfrak{M}^*} + \operatorname{div}_R \frac{\partial L}{\partial \nabla_R \mathfrak{M}^*} = 0.
\end{aligned} \tag{11}$$

With reference to the expression (9), one notes that:

$$\begin{aligned}
&\frac{\partial L}{\partial \phi} = 0,\\
&\frac{\partial L}{\partial \mathcal{A}} = 0,\\
&\frac{\partial L}{\partial \dot{\phi}} = 0.
\end{aligned} \tag{12}$$

The equations $(11)_1$ and $(11)_2$ simplify accordingly and provide, as a final result, two of the Maxwell equations of interest, in the Lorentz form.

For sake of simplicity, we also assume that

$$\begin{aligned}
\frac{\partial L}{\partial \dot{\mathfrak{P}}} &= 0,\\
\frac{\partial L}{\partial \dot{\mathfrak{M}}^*} &= 0,\\
\frac{\partial L}{\partial \nabla_R \mathfrak{P}} &= 0,\\
\frac{\partial L}{\partial \nabla_R \mathfrak{M}^*} &= 0.
\end{aligned} \tag{13}$$

In accordance with this assumption, the equations $(11)_4$ and $(11)_5$ reduce to the following algebraic equations:

$$\begin{aligned}
&-\frac{\partial W}{\partial \mathfrak{P}} = \mathfrak{E},\\
&\frac{\partial W}{\partial \mathfrak{M}^*} = \mathfrak{B},
\end{aligned} \tag{14}$$

which happen to correspond to the classical constitutive equations. The equation $(11)_3$ has a natural mechanical interpretation, according to which the quantity $\partial L/\partial \dot{\mathbf{x}}$ represents the *momentum*.

4. The electromagnetic stress tensor and momentum

With reference to the expression (9) the momentum density explicitly reads:

$$\frac{\partial L}{\partial \dot{\mathbf{x}}} = \rho_0 \mathbf{v} - (\mathbf{F}^{-1\mathbf{T}})\frac{\partial L}{\partial \mathbf{V}} \equiv \rho_0 \mathbf{v} + J(\mathbf{D}_0 \wedge \mathbf{B}), \tag{15}$$

where $\mathbf{D}_0 \equiv \varepsilon_0 \mathbf{E}$. The electromagnetic stress tensor, in the Piola form, has the following explicit expression

$$\begin{aligned} -\frac{\partial L}{\partial \mathbf{F}} &= \mathbf{E} \otimes \mathfrak{D}_0 + \mu_0^{-1}\mathbf{B} \otimes \mathfrak{B} - \frac{1}{2}J[\varepsilon_0 \mathrm{E}^2 + \mu_0^{-1}\mathrm{B}^2]\mathbf{F}^{-1\mathbf{T}} - J[\mathbf{D}_0 \wedge \mathbf{B} \otimes \mathbf{V}] + \\ &+ \frac{\partial W}{\partial \mathbf{F}} + \frac{\partial W}{\partial(\mathbf{F}\mathfrak{P})} \otimes \mathfrak{P} - J\mathcal{M} \otimes \mathbf{F}^{-1}\left(\frac{\partial W}{\partial J\mathbf{F}^{-1\mathbf{T}}\mathfrak{M}^*}\right) + \\ &+ \left[\frac{\partial W}{\partial J\mathbf{F}^{-1\mathbf{T}}\mathfrak{M}^*} \cdot J\mathbf{F}^{-1\mathbf{T}}\mathfrak{M}^*\right]\mathbf{F}^{-1\mathbf{T}}, \end{aligned} \tag{16}$$

having noted that the dependence of L on $\mathbf{F}$ is through $\mathbf{V} \equiv -\mathbf{F}^{-1}\dot{\mathbf{x}}$ and through W. W, in turn, depends on $\mathbf{F}$ explicitly and through $J\mathfrak{P}$ and $J\mathfrak{M}^*$. The tensor $\partial L/\partial \mathbf{F}$ can be transformed in the *Cauchy–form* and, if we take into account the equation $(11)_4$, $(11)_5$ and (14), we eventually write:

$$\begin{aligned} -J^{-1}\frac{\partial L}{\partial \mathbf{F}}\mathbf{F}^T &= [\varepsilon_0 \mathbf{E} \otimes \mathbf{E} + \mu_0^{-1}\mathbf{B} \otimes \mathbf{B}] - \frac{1}{2}[\varepsilon_0 \mathrm{E}^2 + \mu_0^{-1}\mathrm{B}^2]\mathbf{I} + \\ &- [\varepsilon_0(\mathbf{E} \wedge \mathbf{B}) \otimes \mathbf{v}] + \\ &+ J^{-1}\left(\frac{\partial W}{\partial \mathbf{F}}\right)\mathbf{F}^{\mathbf{T}} + \mathcal{E} \otimes \mathbf{P} - \mathcal{M} \otimes \mathbf{B} + (\mathcal{M} \cdot \mathbf{B})\mathbf{I}. \end{aligned} \tag{17}$$

The expression (17) is consistent with the classical expression of the Maxwell stress tensor in a vacuum, which reads:

$$\mathbf{t}_M = \varepsilon_0 \mathbf{E} \otimes \mathbf{E} + \mu_0^{-1}\mathbf{B} \otimes \mathbf{B} - \frac{1}{2}(\varepsilon_0 \mathrm{E}^2 + \mu_0^{-1}\mathrm{B}^2)\mathbf{I}, \tag{18}$$

having disregarded the velocity $\mathbf{v}$ of the material points.

5. The electromagnetic material tensor

The variational procedure which is based on the Lagrangian density L not only provides the Maxwell equations and the balance of momentum [10, 13]. In fact, along with the *momentum* $\partial L/\partial \dot{\mathbf{x}}$, *two additional canonical momenta*, $\partial L/\partial \dot{\phi}$ and $\partial L/\partial \dot{\mathcal{A}}$, are also introduced.

In the specific case of electromagnetism, one of these momenta vanishes:

$$\frac{\partial L}{\partial \dot{\phi}} \equiv 0, \tag{19}$$

as remarked previously in $(12)_3$.

The following result holds true for the second canonical momentum:

$$\frac{\partial L}{\partial \dot{\mathcal{A}}} = -\mathfrak{D}, \tag{20}$$

taking into account the relationships $(2)_1$, (8), (9) and (10).

Having this remarked, an *additional mechanical quantity*, which is a combination of the two non–vanishing canonical momenta, can be introduced. This mechanical quantity is defined as follows [10]:

$$\mathbf{p}_0 = -\mathbf{F}^{\mathbf{T}}\frac{\partial L}{\partial \dot{\mathbf{x}}} - (\nabla_R \mathcal{A})^T \frac{\partial L}{\partial \dot{\mathcal{A}}}. \tag{21}$$

The expression (21) is a density per unit volume of the reference configuration and leads to the definition of the *material momentum* or *pseudomomentum* [8, 14, 15], which writes as follows:

$$\mathbf{p}_R = \rho_0 \mathbf{CV} + \mathfrak{P} \wedge \mathfrak{B} \equiv \rho_0 \mathbf{CV} + J(\mathbf{P} \wedge \mathbf{B}) \tag{22}$$

or, per unit volume of the current configuration,

$$\mathbf{p} = \rho \mathbf{CV} + \mathbf{P} \wedge \mathbf{B}. \tag{23}$$

This procedure for defining the novel mechanical quantity may not be unfamiliar to people who work on materials with microstructures, from the viewpoint of continuum mechanics. An analogous procedure can be employed for a combination of the quantities $\partial L/\partial \nabla_R \phi$, $\partial L/\partial \nabla_R \mathcal{A}$ and $\partial L/\partial \mathbf{F}$.

This combination defines the *material energy–stress* (an Eshelby–like stress) as follows

$$\mathbf{b} = -L\mathbf{I} + \mathbf{F}^{\mathbf{T}}\frac{\partial L}{\partial \mathbf{F}} + (\nabla_R \phi) \otimes \frac{\partial L}{\partial \nabla_R \phi} + (\nabla_R \mathcal{A})^T \frac{\partial L}{\partial \nabla_R \mathcal{A}}. \tag{24}$$

The expression (24) can be explicitly evaluated by taking into account the equations $(11)_4$, $(11)_5$ and (14). The computations will not reported here as they can be found in [10].

One of the result of interest is the expression of $\mathbf{b}$ that specialises in the following form, for the electrostatics of a dielectric material:

$$\mathbf{b}^{diel} = (W - \mathfrak{P} \cdot \mathfrak{E})\mathbf{I} - \mathbf{F}^{\mathbf{T}}\frac{\partial W}{\partial \mathbf{F}} - \mathfrak{E} \otimes \mathfrak{P}. \tag{25}$$

The corresponding Cauchy–like stress is reported here below for comparison. With reference to the formula (17), it reads:

$$\mathbf{T}^{diel} = -\frac{1}{2}\varepsilon_0 \mathrm{E}^2 \mathbf{I} + \mathbf{E} \otimes \mathbf{D} + J^{-1}\frac{\partial W}{\partial \mathbf{F}}\mathbf{F}^{\mathbf{T}}. \tag{26}$$

where

$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}. \tag{27}$$

6. Comments

By comparing (26) with (25) one can notice the following. First, although the two mentioned expressions are in the form of energy–stress tensors they completely differ from one another. It is not possible to transform one into the other by means of a simple rule, like in pure elasticity.

Second, the Cauchy form of the electromagnetic stress tensor reduces to the Maxwell stress tensor, not only in a vacuum but also in all simple cases that are dealt with in the classical literature. Third, the electrostatic stress tensor survives also out of the domain occupied by the material, whereas the corresponding *electrostatic material stress tensor* $\mathbf{b}^{diel}$ identically vanishes in a vacuum.

References

[1] ESHELBY J.D., *Force on an elastic singularity*, Phil. Tran. Roy. Soc. Lond. **244** A (1951), 87–112.

[2] MAUGIN G.A., *Material inhomogeneities in elasticity*, Applied Mathematics and Mathematical Computation **3**, Chapman and Hall, London 1993.

[3] PENFIELD P. AND HAUS H.A., *Electrodynamics of moving media*, M.I.T. Press, Cambridge, Massachusetts 1967.

[4] NELSON D.F., *Electric, optic and acoustic interactions in dielectrics*, John Wiley, New York 1979.

[5] ERICKSEN J.L., *Remarks concerning forces on line defects*, Zeit. Angew. Math. Phys., (Special issue: Theoretical, experimental and numerical contributions to the mechanics of fluids and solids, dedicated to P.M. Naghdi), **46** S (1995), 247–271.

[6] KRÖNER E., *Configurational and material forces in the theory of defects in ordered structures*, Proceedings CMDS **7** (Eds. K.H. Anthony and H.J. Wagner), Material Science Forum 1993, 447–454.

[7] MAUGIN G.A. AND TRIMARCO C., *On material and physical forces in liquid crystals*, Int. J. Eng. Sci., **33** (1995b), 1663–1678.

[8] NELSON D.F., *Mometum, pseudomomentum and wave momentum : toward resolving the minkowski-abraham controversy*, Phys. Rev. A **44**, 3905–3916.

[9] MAUGIN G.A. AND TRIMARCO C., *Elements of field theory in inhomogeneous and defective materials*, C.I.S.M. Lecture Notes **427**, Springer Verlag, Wien 2000, 55–128.

[10] TRIMARCO C. AND MAUGIN G.A., *Material mechanics of electromagnetic solids*, C.I.S.M. Lecture Notes **427**, Springer Verlag, Wien 2000, 129–171.

[11] MAXWELL J.C., *A treatise on electricity and magnetism*, vol. I and II, Oxford Classic Text in the Physical Sciences, Clarendon Press, Oxford 1891 (1998, reprint).

[12] BECKER R., *Electromagnetic fields and interactions*, Dover, New York 1982 (reprint).

[13] JACKSON J.D., *Classical electrodynamics*, J. Wiley & Sons, New York 1962.

[14] PEIERLS R., *Momentum and pseudomomentum of light and sound*, in: "Highlights of condensed-matter physics" (Ed. M. Tosi), Corso LXXXIX, Soc. Ital. Fisica, Bologna, 237–255.

[15] SCHOELLER H. AND THELLUNG A., *Lagrangian formalism and conservation law for electrodynamics in nonlinear elastic dielectrics*, Annals of Physics **220** 1 (1992), 18–38.

[16] PACK Y.E. AND HERRMANN G., *Conservation laws and the material momentum tensor for the elastic dielectric*, Int. J. Eng. Sci. **24** (1986), 1365–1374.

AMS Subject Classification: 74A10, 74F15.

Carmine TRIMARCO
Dipartimento di Matematica Applicata "U.Dini"
Università di Pisa
Via Bonanno 25/B
56126 Pisa, ITALY
e-mail: trimarco@dma.unipi.it

Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 2 (2000)
Geom., Cont. and Micros., II

R.W. Tucker - C. Wang*

A COSSERAT DETECTOR FOR DYNAMIC GEOMETRY

Abstract. It is proposed to explore the interaction of weak gravitational fields with slender elastic materials in order to assess the viability of achieving enhanced laser interferometric sensitivities for the detection of gravitational waves with frequencies between 10^{-4} and 1 Hz. The aim is the design of novel gravitational antennae in interplanetary orbit. The implementation of these ideas would be complimentary to existing programmes of gravitational wave research but exploiting a current niche in the frequency spectrum.

The dynamics of slender structures, several km in length, are ideally suited to analysis by the simple theory of Cosserat rods. Such a description offers a clean conceptual separation of the vibrations induced by bending, shear, twist and extension and the coupling between eigen-modes due to tidal accelerations can be reliably estimated in terms of the constitutive properties of the structure. The detection of gravitational waves in the 1 Hz region would provide vital information about stochastic backgrounds in the early Universe and the relevance of super-massive black holes to the processes that lead to processes in the centre of galaxies.

1. Introduction

One of the most striking predictions of Einstein's theory of gravitation follows from solutions describing gravitational waves. Such solutions are thought to be produced by astrophysical phenomena ranging from the coalescence of orbiting binaries to violent events in the early Universe. Their detection would herald a new window for the observation of natural phenomena. Great ingenuity is being exercised in attempts to detect such waves in the vicinity of the earth using either laser interferometry or various resonant mass devices following Weber's pioneering efforts with aluminum cylinders. Due to the masking effects of competing influences and the weakness of gravitation compared with the electromagnetic interactions the threshold for the detection of expected gravitationally induced signals remains tantalisingly close to the limits set by currently technology. In order to achieve the signal to noise ratios needed for the unambiguous detection of gravitational waves numerous alternative strategies are also under consideration. These include more sophisticated transducer interfaces, advanced filtering techniques and the use of dedicated arrays of antennae. Earth based gravitational wave detectors require expensive vibration insulation in order to discriminate the required signals from the background. This is one reason why the use of antennae in space offer certain advantages. It is argued here that the gravitationally induced elastodynamic vibrations of slender material structures in space offer other advantages that do not appear to have been considered. Multiple structures of such continua possess attractive properties when used as coincidence detectors of gravitational disturbances with a dominant

*RWT is grateful to BAE-Systems (Warton), the Leverhulme Trust and PPARC for support. Both authors are indebted to valuable conversations with J Hough and M Cruise.

spectral content in the 10^{-4} to 1 Hz region. Furthermore this window can be readily extended to lower frequencies and higher sensitivities by enlarging the size of the structures.

Newtonian elastodynamics [1] is adequate as a first approximation if supplemented by the *tidal stresses* generated by the presence of spacetime curvature that is small in comparison with the detector. The latter are estimated from the accelerations responsible for spacetime geodesic deviations. Since the constituents of material media owe their elasticity to primarily non-gravitational forces their histories are non-geodesic. The geodesic motions of particles offer a reference configuration and the geodesic deviation of neighbours in a geodesic reference frame provide accelerations that are additionally resisted in a material held together by elastic forces. Since in practical situations the re-radiation of gravitational waves is totally negligible the computation of the stresses induced by the tidal tensor of a background incident gravitational wave offers a viable means of exploring the dynamical response of a material domain to a fluctuating gravitational field.

Surprisingly little recent attention seems to have been devoted to problems in gravito-elastodynamics beyond the recognition that the shape, size and density of a material may be tuned in order to expedite the excitation of particular normal modes of vibration by resonance [2, 3, 4, 5]. There appear to be no detailed studies of the dynamic response of interplanetary material structures to gravitational wave phenomena. Current resonant mode detectors are designed to permit reconstruction of the direction and polarisation of gravitational waves that can excite resonances. Clearly such detectors are designed to respond to a narrow spectral window of gravitational radiation and are not particularly good at determining the temporal profile of incident gravitational pulses. A significant advantage of space-based antennae based on slender material structures is that they can be designed to respond to transient gravitational pulses, to polarised uni-directional gravitational waves or omni-directional unpolarised waves.

In 1985 V. Braginsky and K. Thorn proposed [6] an Earth-orbiting gravitational wave detector, called a “skyhook”, which could operate in the 10 to 1000 mHz band. It consisted of two heavy masses, one on each end of a long cable with a spring at its centre. The proposal was refined by R W R Drever who suggested that certain noise pollution could be reduced by increasing the rigidity of the design. These authors explored many of the competing noise perturbations and concluded that such devices offer an attractive, simple instrument with gravity-wave sensitivity in an interesting range where sources might exist. However these conclusions were based on a particular non-resonant radial string configuration in earth orbit and to our knowledge no detailed simulations of the elastic wave excitations in the connecting cable have ever been performed in this or more general scenarios. The proposal here, to use several material structures, differs in a number of important respects not the least of which is the fact that laser technology has advanced enormously since this original proposal. Furthermore the analysis of the original detector ignored the ability of a continuum structure to be tuned to the entire acceleration field of a gravitational wave. Resonant response to such circumferential excitations optimise power absorption from the wave. Such mechanisms deserve a more comprehensive analysis, not only to update the viability of the general skyhook concept but to exploit to advantage the detection of both axial, torsional and flexural elastic wave excitations *of the cable itself* by laser interferometry in much more general dynamical configurations than were originally envisaged.

The general mathematical theory of non-linear Newtonian elasticity is well established. The general theory of one-dimensional Newtonian Cosserat continua derived as limits of three-dimensional continua can be consulted in [1]. The theory is fundamentally formulated in the Lagrangian picture in which material elements are labelled by s. The behaviour of a Cosserat structure at time t may be described in terms of the motion $\mathbf{R}(s, t)$ in space of the line of centroids of its cross-sections and elastic deformations about that line. Such a structure is modelled mathematically by an elastic space-curve with structure. This structure defines the relative orientation of neighbouring cross-sections along the structure. Specifying a unit vector $\mathbf{d}_3$ (which may be identified with the normal to the cross-section) at each point along the structure enables the state of flexure to be related to the angle between this vector and the tangent to the space-curve. Specifying a second vector $\mathbf{d}_1$ orthogonal to the first vector (thereby placing it in the plane of the cross-section) can be used to encode the state of bending and twist along its length. Thus a field of two mutually orthogonal unit vectors along the structure provides three continuous dynamical degrees of freedom that, together with the continuous three degrees of freedom describing a space-curve relative to some arbitrary origin in space, define a simple Cosserat model. It is significant for this proposal that the theory includes thermal variables that can be coupled to the dynamical equations of motion, compatible with the laws of thermodynamics. The theory is completed with equations that relate the deformation strains of the structure to the elastodynamic forces and torques. The simplest constitutive model to consider is based on Kirchoff relations with shear deformation and viscoelasticity. Such a Cosserat model provides a well defined six dimensional quasi-linear hyperbolic system of partial differential equations in two independent variables. It may be applied to the study of gravitational wave interactions by suitably choosing external body forces $\mathbf{f}$ to represent the tidal interaction with each element in the medium. A typical system might consist of at least two material structures orbiting in interplanetary space. Each structure would be composed of several km of hollow segmented pipe. A structure, several km in length , made up of transportable segments, could be conveyed to an orbiting station and the system constructed in space. The lowest quadrupole excitation of a steel circular structure would be about 0.4Hz and vary inversely as the (stress-free) length of the structure. Actuator and feedback instrumentation could be placed inside the pipe to “tune” the system to an optimal reference configuration. A series of laser beams from sources attached to the structure, deflected across its diameters from one side to another and along segments of the circumference of a polygon inscribed within the loop could form the structure of a laser interferometer system. In this manner vibrations induced by a quadrupole deformation of the structure (in which both the variations in length of orthogonal diameters and circumferential elements) contribute to a path difference for laser interference. The precise details of the density and elastic moduli needed to enhance the sensitivity of the receiver would result from an in-depth analytic analysis of the Cosserat equations for free motion. The ability to readily optimise the resonant behaviour for coupled axial, lateral and torsional vibrations by design is a major advantage over other mechanical antennae that have been proposed.

By contrast a broad band detector would consist of an open ended structure coiled into a spiral. For planar spirals with traction free open ends the spectral density of normal transverse and axial linearised modes increases with the density of the spiral winding number. They form an ideal broad band detector with directional characteristics. Such antennae can sustain non-resonant weakly dispersive axial travelling waves excited by incident gravitational pulses. Furthermore by coupling such a spiral at its outer end to a light mass by a short length of high-Q fibre (such as sapphire) one can tune such an extension to internal resonances, thereby amplifying the spiral elastic excitation. Such excitations offer new detection mechanisms based on the enhanced motion of the outer structure of the spiral.

2. Cosserat equations

The dynamical evolution of the structure with mass density, $s \in [0, L_0] \mapsto \rho(s)$, and cross-sectional area, $s \in [0, L_0] \mapsto A(s)$, is governed by Newton's dynamical laws:

$$\rho A \ddot{\mathbf{R}} = \mathbf{n}' + \mathbf{f}$$

$$\partial_t(\rho\,\mathbf{I}(\mathbf{w})) = \mathbf{m}' + \mathbf{R}' \times \mathbf{n} + \mathbf{l}$$

applied to a triad of orthonormal vectors: $s \in [0, L_0] \mapsto \{\mathbf{d_1}(s,t), \mathbf{d_2}(s,t), \mathbf{d_3}(s,t)\}$ over the space-curve: $s \in [0, L_0] \mapsto \mathbf{R}(s,t)$ at time t where $\mathbf{n}' = \partial_s \mathbf{n}$, $\dot{\mathbf{R}} = \partial_t \mathbf{R}$, $\mathbf{f}$ and $\mathbf{l}$ denote external force and torque densities respectively and $s \in [0, L_0] \mapsto \rho\mathbf{I}$ is a structure moment of inertia tensor. In these field equations the *contact forces* $\mathbf{n}$ and *contact torques* $\mathbf{m}$ are related to the *strains* $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ by constitutive relations. The strains are themselves defined in terms of the configuration variables $\mathbf{R}$ and $\mathbf{d}_k$ for $k = 1, 2, 3$ by the relations:

$$\mathbf{R}' = \mathbf{v}$$

$$\mathbf{d}_k' = \mathbf{u} \times \mathbf{d}_k$$

$$\dot{\mathbf{d}}_k = \mathbf{w} \times \mathbf{d}_k.$$

The latter ensures that the triad remains orthonormal under evolution. The last equation identifies

$$\mathbf{w} = \frac{1}{2}\sum_{k=1}^{3} \mathbf{d}_k \times \dot{\mathbf{d}}_k$$

with the local angular velocity vector of the director triad. The general model accommodates continua whose characteristics (density, cross-sectional area, rotary inertia) vary with s. For a system of two coupled continua with different elastic characteristics on $0 \le s < s_0$ and $s_0 < s \le L_0$ respectively one matches the degrees of freedom at $s = s_0$ according to a junction condition describing the coupling.

To close the above equations of motion constitutive relations appropriate to the structure must be specified:

$$\begin{aligned}
\mathbf{n}(s,t) &= \hat{\mathbf{n}}(\mathbf{u}(s,t), \mathbf{v}(s,t), \mathbf{u}_t(s), \mathbf{v}_t(s), \ldots, s)\\
\mathbf{m}(s,t) &= \hat{\mathbf{m}}(\mathbf{u}(s,t), \mathbf{v}(s,t), \mathbf{u}_t(s), \mathbf{v}_t(s), \ldots, s)
\end{aligned}$$

where $\mathbf{u}_t(s)$ etc., denote the history of $\mathbf{u}(s,t)$ up to time t. These relations specify a reference configuration (say at $t = 0$) with strains $\mathbf{U}(s)$, $\mathbf{V}(s)$ in such a way that $\hat{\mathbf{n}}(\mathbf{U}(s), \mathbf{V}(s), \ldots, s)$ and $\hat{\mathbf{m}}(\mathbf{U}(s), \mathbf{V}(s), \ldots, s)$ are specified. A reference configuration free of flexure has $\mathbf{R}_s(s,0) = \mathbf{d}_3(s,0)$, i.e. $\mathbf{V(s)} = \mathbf{d}_3(s,0)$. If a standard configuration is such that $\mathbf{R}(s,0)$ is a space-curve with Frenet curvature κ_0 and torsion τ_0 and the standard directors are oriented so that $\mathbf{d}_1(s,0)$ is the unit normal to the space-curve and $\mathbf{d}_2(s,0)$ the associated unit binormal then $\mathbf{U}(s) = \kappa_0(s)\,\mathbf{d}_2(s,0) + \tau_0(s)\,\mathbf{d}_3(s,0)$.

For a "rod" of density ρ and cross-sectional area A in a weak plane gravitational wave background the simplest model to consider consists of the Newtonian Cosserat equations with a time dependent body force modelled by the tidal interaction $\mathbf{f} = \rho A\, \mathbf{R}_{\dot{C}\xi}\dot{C}$ where $\xi = x\,\frac{\partial}{\partial x} + y\,\frac{\partial}{\partial y} + z\,\frac{\partial}{\partial z}$ is the Newtonian vector locating an element of the structure in a Newtonian frame defined by the gravitational wave and $\mathbf{R}_{X\,Y}$ is the pseudo-Riemannian curvature operator. The plane gravitational wave metric in $\{x, y, z, t\}$ coordinates is expressed as

$$g = -e^0 \otimes e^0 + e^1 \otimes e^1 + e^2 \otimes e^2 + e^3 \otimes e^3$$

where

$$\begin{aligned}
e^0 &= \frac{d\,t + d\,z}{2} + \mathcal{F}(t,x,y,z)\,\frac{d\,(t-z)}{2} + \frac{d\,(t-z)}{2},\\
e^1 &= d\,x,\\
e^2 &= d\,y,\\
e^3 &= \frac{d(t+z)}{2} + \mathcal{F}(t,x,y,z)\,\frac{d\,(t-z)}{2} - \frac{d\,(t-z)}{2}
\end{aligned}$$

and serves to anchor the wave to a Minkowski spacetime when $\mathcal{F} = 0$. An exact plane gravitational wave is given by

$$\mathcal{F} = f_+(t-z)\frac{x^2-y^2}{2} + f_\times(t-z)\frac{xy}{2}$$

for arbitrary profiles f_+ and $f_\times$. The vector $\dot{C}$ is the normalised 4-velocity associated with a time-like observer curve in a geodesic reference frame in the above metric. In the absence of elastic forces each element in the structure would then be governed by the equation of geodesic deviation. Additional stationary Newtonian gravitational fields add terms of the form $\rho A\mathbf{g}$ to $\mathbf{f}$ where $\mathbf{g}$ is the "effective local acceleration due to gravity". Post Newtonian gravitational fields (such as gravitomagnetic and Lens-Thirring effects) can be accommodated with a more refined metric background.

It should be stressed that unlike many current low frequency detectors (e.g. LISA), based on measuring the relative motion of a small number of discrete masses, the loop antennae under discussion provide a response from a vibrating mass continuum where every element of each structure can be made to respond *in an optimal manner* to the acceleration field of a gravitational perturbation. By choosing material with a critical ratio of the shear to Youngs modulus of elasticity, the quadrupole mode of the structure can be induced to absorb maximum power from a plane gravitational wave propagating orthogonal to a circular loop. In such a mode the deformation of each structure element remains along the acceleration vector in the tidal field. This important observation follows by linearising the Cosserat equations about a circular loop of length L_0 with the deformation fields

$$\begin{aligned}
\mathbf{R}(s,t) &= \left[\left(\frac{L_0}{2\pi} + \xi(s,t)\right)\cos\left(\frac{2\pi}{L_0}(s+\lambda(s,t))\right),\right. \\
&\qquad \left.\left(\frac{L_0}{2\pi} + \xi(s,t)\right)\sin\left(\frac{2\pi}{L_0}(s+\lambda(s,t))\right), 0\right] \\
\mathbf{d}_1 &= \left[\cos\left(\frac{2\pi}{L_0}s + \phi(s,t)\right),\ \sin\left(\frac{2\pi}{L_0}s + \phi(s,t)\right), 0\right] \\
\mathbf{d}_2 &= [0,0,1] \\
\mathbf{d}_3 &= \mathbf{d}_1 \times \mathbf{d}_2
\end{aligned}$$

and a tidal perturbation due to a plane gravitational wave in the transverse trace-free gauge. The linearised vibrations correspond to a spectrum of combined flexural and circumferential modes and the quadrupole mode alone can be excited into resonance by the passage of the entire gravitational wave. Such modes have no analogue in detectors composed of discrete masses. A further intriguing property of this system deserves further investigation. Loops can be endowed with a uniform longitudinal speed along their circumference and the damping of the induced resonant modes due to the viscoelasticity of the structure is thereby diminished. More generally by solving for the dynamical evolution of the structure, given $\mathbf{f}$, initial and boundary data and suitable constitutive relations the dynamical behaviour of the structure can be used as a guide to decide how to interface Fabry-Perot devices to the system in order to detect gravitational wave environments by laser interferometry.

3. Anelastic modelling

An important consideration of any modelling of Cosserat continua to low levels of excitation is the estimation of signal to noise ratios induced by anelasticity and temperature. To gain an insight into the former one may attempt to extend the established theory of linear anelasticity to a Cosserat structure. For a slender straight rod with uniform density ρ, static Young's modulus E and area of cross section A, the free damped motion in one dimension is modelled by the equation:

$$\rho A\, \partial_{tt} x(s,t) = n'(s,t)$$

where the axial strain $v(x,t) = \partial_s x(s,t) \equiv x'(s,t)$ and

$$n(s,t) = EA(v(s,t)-1) - EA\int_{\infty}^{t} \phi(t-t')\,\dot{v}(t')dt'$$

for some viscoelastic model ϕ with $0 \le s \le L$. For free motion in the mode:

$$x(s,t) = s + \xi(t)\cos(\pi s/L)$$

the amplitude $\xi(t)$ satisfies

$$\ddot{\xi}(t) + \omega_0^2\,\xi(t) = \omega_0^2\int_{\infty}^{t} \phi(t-t')\dot{\xi}(t')dt'$$

with $\omega_0^2 = \frac{\pi^2 E}{L^2\rho}$ while for a forced harmonic excitation:

$$\ddot{\xi}(t) + \omega_0^2\xi(t) = \omega_0^2\int_{\infty}^{t} \phi(t-t')\dot{\xi}(t')dt' + F_0\exp(-i\Omega t).$$

With $\xi(0) = \dot{\xi}(0) = 0$ the Laplace transformed amplitude of forced axial motion is then given in terms of the Laplace transform *

$$\bar{\phi}(\sigma) = \int_0^{\infty} \phi(t)e^{-\sigma t}d\,t$$

of the anelastic modelling function $\phi(t)$ as:

$$\bar{\xi}(\sigma) = \frac{F_0}{(\sigma - i\Omega)(\sigma^2 - \omega_0^2\sigma\bar{\phi}(\sigma) + \omega_0^2)}.$$

To extend this approach in a simple manner to a 3-D Cosserat model of a slender rod with uniform static moduli E and G, geometric elements A, $K_{\alpha\alpha} = J_{11} + J_{22}$, $J_{\alpha\beta}$, one adopts the following constitutive relations for the local director components of the contact force $\mathbf{n}$ and torque $\mathbf{m}$ in

---

*For a "Hudson" type solid :

$$\bar{E}(\sigma) = k\sigma^{\nu} = E(1 - \sigma\bar{\phi}(\sigma))$$

for some constants k and ν.

terms of the local strain vectors $\mathbf{v}$ and $\mathbf{u}$ and anelastic response functions ϕ_E and ϕ_G:

$$\begin{aligned}
n_3(s,t) &= EA\,(v_3(s,t)-1) - EA\int_\infty^t \phi_E(t-t')\,\dot{v}_3(s,t')\,dt' \\
n_1(s,t) &= GA\,v_1(s,t) - GA\int_\infty^t \phi_G(t-t')\,\dot{v}_1(s,t')\,dt' \\
n_2(s,t) &= GA\,v_2(s,t) - GA\int_\infty^t \phi_G(t-t')\,\dot{v}_2(s,t')\,dt' \\
m_3(s,t) &= K_{\alpha\alpha}G\,u_3(s,t) - K_{\alpha\alpha}G\int_\infty^t \phi_G(t-t')\,\dot{u}_3(s,t')\,dt' \\
m_\alpha(s,t) &= E\sum_{\beta=1}^{2} J_{\alpha\beta}\,u_\beta(s,t) - E\sum_{\beta=1}^{2} J_{\alpha\beta}\int_\infty^t \phi_E(t-t')\,\dot{u}_\beta(s,t')\,dt'
\end{aligned}$$

for $\alpha, \beta = 1, 2$.

4. Estimate of equilibrium thermal noise at resonance

The detailed effects of temperature on low levels of elastic excitation are more difficult to estimate. However order of magnitude estimates may be based on elementary considerations. Let x be the mean thermal R.M.S. displacement of the elastic medium in a thermal equilibrium state at temperature T, for an antenna of mass m resonating with angular frequency ω. Then

$$\frac{kT}{2} \simeq \frac{m\omega^2 x^2}{2}$$

where k is the Boltzman constant. For an antenna of effective length L, mass density ρ and Young's modulus E take

$$\omega \simeq \frac{\pi\sqrt{\frac{E}{\rho}}}{L}$$

and

$$m = \rho L A$$

in terms of the cross-section area A of the structure. If Q is the quality factor of the antenna one may estimate the gravitational signal from a harmonic gravitational wave with amplitude h and frequency ω to be given by $dl = hLQ$. If $S = dl/x$ is the signal to noise ratio:

$$h(T, Q, E, A, L, S) \simeq \frac{S}{Q\pi}\sqrt{\frac{kT}{LEA}}.$$

Choosing $Q = 1E6$, $E = 2.02E11$, $A = (0.01)^2$, $S = 5$ in MKS units and $T = 100K$ one sees that with $L = 1$km one could detect $h = 1E-21$ provided the signal $dl = 1E-12$ is detectable. This corresponds to a resonance at 0.2Hz. Using the above parameters one may estimate the mass and corresponding lowest resonant frequency for such a detector. These are illustrated in Figures 1 and 2.

5. Estimate of thermal fluctuation noise induced by laser measurements

The act of measuring "small" elastic strains can induce thermal fluctuations that contribute to elastodynamic noise. According to Braginsky et al. [7], temperature fluctuations can be induced by laser measurement of strain. Such fluctuations act as a stochastic source for elastic deformations in the structure that compete with the strains induced by gravitational excitations. If one neglects the geometry of the structure and applies the estimates in [7] one finds a temperature dependence for the spectral density of the average induced noise $\chi(T,\omega)^2$ given by:

$$\chi(T,\omega)^2 = 4\frac{\sqrt{2}\alpha(T)^2(1+\sigma)^2 kT^2\tau}{\sqrt{\pi}\rho(T)C(T)r_o(1+\tau^2\omega^2)}$$

where the relaxation time $\tau = r_0^2\rho(T)C(T)/K(T)$, $K(T)$ is the thermal conductivity, σ the Poisson ratio, $\alpha(T)$ the coefficient of linear expansion and $C(T)$ the specific heat of the elastic medium. The radius r_0 is a measure of the spatial dimension of the laser spot used to excite the temperature fluctuations of the structure, taken here to be 0.03m.

The square root $\chi(T,\omega)$ of the spectral density for a structure composed of a Fe-Ni alloy is plotted as a function of temperature for the series of frequencies, 0Hz, 0.001Hz, 0.01Hz, 1Hz in Fig. 3. The noise is limited by the top 0Hz curve. To make a comparison with the thermal noise $x(T)$ above at a resonance frequency Ω, one may integrate the spectral fluctuation noise induced by laser measurement over a band $[\omega_1,\omega_2]$ centered on the resonant frequency:

$$X(T)^2_{[\omega_1,\omega_2]} = \int_{\omega_1}^{\omega_2} \chi(T,\omega)^2\, d\omega.$$

If one takes the window $\omega_1 = 0$ and $\omega_2 = 2\Omega$ for a choice of Ω corresponding to the lowest resonance in structures with lengths of 0.01m, 1, 100m,1km and 10km, then the full curve in Fig. 4 is obtained for $X(T)_{[0,2\Omega]}$. On this scale $X(T)_{[0,2\Omega]}$ is insensitive to the choice of frequency window. By contrast the dotted curves indicate the resonant R.M.S. thermal noise $x(T)$ with the lowest curve corresponding to the shortest length and the others showing noise increasing with length. Clearly the thermal fluctuation noise induced by measurement is several orders of magnitude smaller compared with the thermal R.M.S. noise for a structure of several km in length resonating in the mHz region. The strong temperature dependence around $T = 60$ and $T = 250$ is due to the behaviour of the thermal expansion coefficient in these regions. It offers another means of tuning the antenna by careful selection of material properties. The thermal fluctuation noise may have more significance for the broad band detector configurations mentioned above.

6. Conclusions

Cosserat modelling offers a natural approach to analyse the interaction between gravitational fluctuations and slender elastic structures. Unlike current proposals for low frequency orbiting detectors based on measuring the relative motion of a small number of discrete masses, the antennae discussed above provide a response from an extended vibrating mass continuum where every element can be made to respond *in an optimal manner* to the acceleration field of a gravitational perturbation. Cosserat methods may be generalised to include a more detailed study of the thermo-mechanics of antennae constrained by the Clasius-Duhem inequality and promise a clearer picture of the competing effects of thermal noise on the detection of gravitational waves. If thermal noise is such that cryogenic cooling is not mandatory with current technology they may also provide a cheaper alternative.

Acknowledgement

RWT is grateful to BAE-System (Warton), the Leverhulme Trust and PPARC for support. Both authors are indebted to valuable conversation with J.Hough and M. Cruise.

References

[1] ANTMAN S., *Non-linear problems in elasticity*, Applied Mathematical Sciences **107**, Springer-Verlag 1991.

[2] RAYNER C.B., *Elasticity in general relativity*, Proc. R. Soc. London **272** A (1963), 44–53.

[3] DYSON F.J., *Seismic response of the earth to a gravitational wave in the 1Hz band*, Astrophys. J. **156** (1969), 529–540.

[4] CARTER B. AND QUINTANA H., *Gravitational and acoustic waves in an elastic medium*, Phys. Rev **16** D (1977), 2928–2938.

[5] EHLERS J., *General Relativity*, in: "Relativity, astrophysics, and cosmology" (Ed. W. Israel), Reidel 1973, 1–20.

[6] BRAGINSKY V.B. AND THORN K.S., *Skyhook gravitational-wave detector*, Nature **316** (1985), 610–612.

[7] BRAGINSKY V.B. AND THORN K.S., *Thermodynamical fluctuations and photo-thermal shot noise in gravitational wave antennae*, Phys. Letts **264** A (1985), 1–10.

AMS Subject Classification: 74K10, 83C35.

Robin W. TUCKER, Charles WANG
Department of Physics,
Lancaster University,
Lancaster LA1 4YB, UK
e-mail: `r.tucker@lancaster.ac.uk`
e-mail: `c.wang@lancaster.ac.uk`