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Thermodynamische Materialtheorien

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ABSTRACT. The meeting was focused on research in the broad field of thermodynamic constitutive theories. It provided a contact between physicists, engineers and mathematicians, whose talks led to lively and interesting discussions. The debate concentrated on the physical motivation of the models subjected to mathematical analysis.

Mathematics Subject Classification (2000): 74Axx, 74Bxx, 74Cxx, 74Jxx, 74Nxx, 74Qxx, 74Rxx, 76Rxx, 76Sxx, 76Txx, 76S05, 80xx.

Introduction by the Organisers

The workshop was well-attended with 46 participants of which 9 gave keynote lectures and 25 gave short contributions. After most lectures there were lively discussions to which all attendants contributed.

The overall theme was thermodynamics which, as a universal theory, may be - and was - applied to different types of phenomena and materials, viz.

- plasticity
- visco-plasticity
- creep
- fracture
- fatigue
- phase transitions in solids
- nucleation
- porous materials
- epitaxy
- ferroelectricity
- shape memory alloys
- melting

- surface tension
- liquid crystals
- liquid crystal polymers
- entropic elasticity
- lattice elasticity
- rarefied gases
- shock propagation
- light scattering
- fluid mixtures.

The participants had a varied background: Some were physicists and engineers, others applied mathematicians. The former were mostly interested in modelling of material properties and simulation of observed processes. They generally tended to make their models as simple as possible. The mathematicians took an interest in the properties of the model equations, provided that they offered a challenge to the analyst, or that they permitted the application of their analytical tools.

This dichotomy of the audience was intended by the organizers, of course, and it led to lively discussions. Thus it was hotly debated whether good mathematics should be wasted on bad physics. Or whether it is justifiable to construct mutilated, or arbitrarily extended physical models such that they be amenable for the analytical toolbox. The question arose of what value an existence and uniqueness proof is for non-realistic models.

Another case in point is the regularization of originally hyperbolic equations as they occur in the kinetic theory of gases and in extended thermodynamics. It was debated whether it is worthwhile to smooth out solutions artificially, rather than investigate how nature manages the problem of avoiding jumps.

It could not be expected that such discussions reach an agreeable conclusion but - perhaps - they served to break up questionable ideas in both groups of participants; ideas, that have become all too comfortable and well-accommodated in their minds. The dialogue will be continued in the future between communities that ordinarily do not overlap; this may in fact be an important outcome of the meeting.

There was an evening lecture by Prof. W. Bürger on toys - boomerangs, spinning tops and rattlebacks. Everybody seems to have enjoyed that lecture.

Workshop: Thermodynamische Materialtheorien**Table of Contents**

Sergio Conti	
<i>Relaxation of single-slip crystal plasticity</i>	2977
Martin Brokate (joint with P. Krejčí, H. Schnabel)	
<i>The Gurson model viewed as a quasivariational inequality</i>	2980
Hans-Dieter Alber	
<i>Evolution of phase interfaces by configurational forces:</i>	
<i>A phase field model</i>	2981
Antonio DeSimone (joint with G. Alberti, S. Conti, G. Dolzmann)	
<i>Macroscopic material response arising from microscopic length scales:</i>	
<i>some case studies of multiscale modelling</i>	2984
Klaus Hackl (joint with Sandra Ilić)	
<i>Solution-precipitation creep – continuum mechanical formulation and</i>	
<i>micromechanical modelling</i>	2986
P. Ponte Castañeda	
<i>Nonlinear homogenization and applications to hyperelastic composites</i>	2988
Paolo Cermelli (joint with T. Armano)	
<i>Non-crystallographic motion of a dislocation as a fine mixture of</i>	
<i>rectilinear paths</i>	2989
Gilles A. Francfort	
<i>Energy density and oscillations in the wave equation: the bulk case and</i>	
<i>the thin film case</i>	2990
Alexandre Danescu	
<i>Continuum Models for Molecular Beam Epitaxy</i>	2992
Angelo Morro	
<i>Wave propagation in planarly-stratified media and first integrals</i>	2993
Robin John Knops	
<i>Uniqueness in nonlinear continuum mechanics</i>	2996
R. Kienzler (joint with G. Herrmann, I. Ott)	
<i>On modelling loss of mass and connectivity in bone</i>	2998
Jean-Jacques Marigo	
<i>A variational approach of fatigue</i>	3000
Khanh Chau Le (joint with Victor Berdichevsky)	
<i>Microcrack nucleation in brittle solids</i>	3001

Victor Berdichevsky	
<i>Homogenization in micro-plasticity</i>	3002
Jürgen Sprekels (joint with Pavel Krejčí (WIAS Berlin), Elisabetta Rocca (Pavia), Songmu Zheng (Shanghai))	
<i>On Nonlocal Phase-Field Models</i>	3002
Krzysztof Wilmanski	
<i>Objective relative accelerations in theories of porous materials</i>	3004
Harsimar Sahota	
<i>Hysteresis in ferroelectric materials</i>	3006
Marc Kamlah (joint with Zhenggui Wang, Dayu Zhou, Jörg Büttner)	
<i>Microscopically Motivated Constitutive Model of Ferroelectric Piezoceramics</i>	3007
Tomáš Roubíček	
<i>Incompressible ionized fluid mixtures</i>	3008
Cesare Davini	
<i>A kinematic model for defective crystals</i>	3010
Henning Struchtrup	
<i>Macroscopic models for rarefied gas flows</i>	3014
Tommaso Ruggeri	
<i>Riemann problem in Extended Thermodynamics</i>	3016
Masaru Sugiyama	
<i>Thermodynamics of Elastic Solids up to the Melting Point</i>	3016
Anna Vainchtein (joint with Lev Truskinovsky)	
<i>Kinetics of lattice phase transitions</i>	3017
Alexander Mielke	
<i>Energy Transport in Periodic Lattices</i>	3019
Elvira Barbera	
<i>Boundary conditions in Extended Thermodynamics and Applications</i>	3022
Daniel Reitebuch	
<i>Light scattering in Extended Thermodynamics</i>	3022
Hans Wilhelm Alt	
<i>The entropy principle for fluid interfaces</i>	3023
Britta Nestler	
<i>Modelling and simulation of phase transformation processes</i>	3026
Epifanio G. Virga	
<i>Structural forces in liquid crystals</i>	3027
Yongzhong Huo	
<i>Modeling the light-induced deformation in liquid crystal elastomers</i>	3027

Giuseppe Saccomandi
*On the superposition of generalized plane strain on anti-plane shear
deformations in elastomeric devices*3029

Oliver Kastner
Atomistic simulation of an elastic-plastic body with shape memory.....3030

Abstracts

Relaxation of single-slip crystal plasticity

SERGIO CONTI

Macroscopic plastic deformations of single crystals are typically the result of a complex structure on a microscopic scale. We aim at understanding pattern-formation and relaxation in simple models of crystal plasticity, by means of the tools of nonconvex calculus of variations.

We consider the deformation theory of plasticity, which is appropriate for small time increments and monotonic loading, and which leads to a variational problem for the deformation u of the form [9, 12, 10, 2]

$$(1) \quad \text{minimize } \int_{\Omega} W(\nabla u) dx \quad \text{over deformations } u : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}^n .$$

Crystalline materials flow plastically only along specific directions, which are characterized by a finite set of crystallographically-determined slip systems $\mathcal{S} = \{(s_1, m_1), \dots, (s_N, m_N)\}$ (each pair being composed by two orthonormal vectors). In the single-slip approximation, which corresponds to the limit of large latent hardening, the plastic deformation takes locally the form

$$F_p = \text{Id} + \gamma s_i \otimes m_i$$

where $\gamma \in \mathbb{R}$ and $1 \leq i \leq N$. This nonconvex structure induces the formation of fine-scale oscillations, much as in the elasticity of shape-memory alloys [12, 2]. We exploit this analogy, building upon the mathematical methods which had been developed for the corresponding elasticity problems [8, 11, 4, 3]. We focus on three case studies, based on joint work with M. Ortiz [5] and F. Theil [6].

Firstly, we consider relaxation of single-slip plasticity within a geometrically linear setting. With a quadratic elastic energy and neglecting self-hardening, the energy density in (1) takes the form

$$W(F) = \min_{\gamma \in \mathbb{R}, i \in \{1, \dots, N\}} \frac{1}{2} (C F_e, F_e) + \tau |\gamma| \quad \text{where } F_e = (F - \gamma s_i \otimes m_i)^{\text{sym}} .$$

Here C are the elastic moduli of the crystal, $\gamma \in \mathbb{R}$ the amount of slip, $i \in \{1, \dots, N\}$ the locally active slip system, and $F^{\text{sym}} = (F + F^T)/2$ denotes the symmetric part of a matrix. The relaxation of variational problems of the form (1), which determines the macroscopic material behavior, is characterized by the quasiconvex envelope of the energy density W , which is defined by (see e.g. [11])

$$W^{\text{qc}}(F) = \inf \left\{ \int_{(0,1)^3} W(\nabla u) dx : u \in W^{1,\infty}, u(x) = Fx \text{ on } \partial(0,1)^3 \right\} .$$

This definition corresponds to taking the optimal energy between all those realizable by oscillating gradient fields with prescribed boundary values (hence prescribed average). An application in elasticity was discussed in [7].

We show [5] that if the set of slip systems is sufficiently large (this holds e.g. for fcc and bcc metals), the quasiconvex hull of W equals its convex hull

$$W^{**}(F) = \min_{\gamma \in \mathbb{R}^N} \frac{1}{2} (C F_e, F_e) + \tau \sum_i |\gamma_i| \quad \text{where } F_e = (F - \sum_i \gamma s_i \otimes m_i)^{\text{sym}}$$

Therefore the relaxation of a problem with infinite latent-hardening coincides with a problem with no latent hardening, hence (under the present assumptions) latent hardening does not modify the macroscopic material behavior.

We next address the effect of geometric nonlinearity, which for simplicity is done within rigid elasticity and with only one slip system. Precisely, we consider

$$W_{NL}(F) = \begin{cases} |\gamma| & \text{if } F = Q(\text{Id} + \gamma s \otimes m) \text{ for some } Q \in SO(n) \\ \infty & \text{else.} \end{cases}$$

We show [6] that in two dimensions the relaxation of W_{NL} is given by

$$W_{NL}^{\text{qc}}(F) = \begin{cases} |\lambda_2(F) - \lambda_1(F)| & \text{if } \det F = 1, |Fs| \leq 1 \\ \infty & \text{else.} \end{cases}$$

Here λ_i are the singular values of F . The optimal microstructure is a simple laminate, in qualitative agreement with observation of slip bands in tension experiments. In three dimensions instead the rigidity of the model does not permit any microstructure and leads to the fact that W_{NL} is quasiconvex, i.e. $W_{NL}^{\text{qc}} = W_{NL}$. This is interpreted as a sign that for $n = 3$ this model is oversimplified.

The case of linear self-hardening, i.e.

$$W_{NL-SH}(F) = \begin{cases} |\gamma|^2 & \text{if } F = Q(\text{Id} + \gamma s \otimes m) \text{ for some } Q \in SO(n) \\ \infty & \text{else,} \end{cases}$$

can also be treated with similar methods. The resulting envelope is (again, in two dimensions)

$$(2) \quad W_{NL-SH}^{\text{qc}}(F) = \begin{cases} |Fm|^2 - 1 & \text{if } \det F = 1 \text{ and } |Fs| \leq 1 \\ \infty & \text{else.} \end{cases}$$

The relaxation is obtained with simple laminates, and results in good agreement with the numerical relaxation that was obtained by Bartels, Carstensen, Hackl, and Hoppe [1].

The third case-study focusses a size-dependent problem, where the plastic potentials have been complemented by a singular perturbation representing the line energy of the cores of the geometrically necessary dislocations. This permits to study the behavior of a grain in a polycrystalline material. Precisely we consider, in a simplified antiplane shear geometry, the functional

$$E[u, F_p] = \int_{(0,L)^3} [|\nabla u - F_p|^2 + \tau |F_p| + \sigma |\nabla \times F_p|] dx + \beta \|u - \gamma x_1\|_{H^{1/2}(\partial(0,L)^3)}^2$$

subject to the side conditions $F_{p1} = \pm F_{p2}$ and $F_{p3} = 0$ a.e., which correspond to the restriction to two slip systems. Due to the antiplane shear assumption

here u is a scalar and F_p a vector. The parameter σ represents the line energy of dislocations, L the size of the grain, β the shear modulus of the matrix (i.e. the rest of the polycrystal). We have shown [5] that at varying material parameters different regimes appear, which are characterized by the scaling relation

$$cE_0(\tilde{\sigma}, \beta, \tilde{\tau}) \leq \frac{1}{L^3\gamma^2} \inf E[u, F_p] \leq c'E_0(\tilde{\sigma}, \beta, \tilde{\tau})$$

where c and C are universal constants, $\tilde{\sigma} = \sigma/\gamma L$, $\tilde{\tau} = \tau/\gamma$, and

$$E_0(\tilde{\sigma}, \beta, \tilde{\tau}) = \min\left(1, \beta, \tilde{\tau} + \beta^{1/2}\tilde{\sigma}^{1/2}, \tilde{\tau} + \tilde{\sigma}^{2/3}\right).$$

These four regimes correspond to (i) purely elastic deformation, (ii) decoupling of the grain from the matrix, (iii) laminar microstructure, where the two slip systems are mixed with a one-dimensional pattern, and (iv) branched microstructure, where the oscillations between the two slip systems refine towards the boundary of the sample. In simple tests where the shear is progressively increased we expect a transition from regime (i) to regime (iii), which would give a scaling of the stress with grain size as $L^{-1/2}$, in accordance to the Hall-Petch law.

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The Gurson model viewed as a quasivariational inequality

MARTIN BROKATE

(joint work with P. Krejčí, H. Schnabel)

The Gurson model [1] represents a constitutive model for elastoplasticity which takes into account the evolution of voids within a solid body. Based on considerations on the microscopic scale, it models the void evolution in the macroscopic stress-strain-relation with the aid of a single additional internal variable, namely the volume fraction f of the void. The yield function of the Gurson model is given by

$$(1) \quad \Phi(\sigma, f) = \frac{3}{2} \frac{|\sigma_d|^2}{\sigma_f^2} + 2f \left[\cosh \left(\frac{\text{tr}(\sigma)}{2\sigma_f} \right) - 1 \right] - (1 - f)^2.$$

Here, σ_d denotes the stress deviator and σ_f the yield stress. For any given value of $f \in [0, 1]$, the set of admissible stresses $\Sigma(f)$ and its boundary $\partial\Sigma(f)$, the yield surface, are given by

$$(2) \quad \Sigma(f) = \{\tau : \Phi(\tau, f) \leq 0\}, \quad \partial\Sigma(f) = \{\tau : \Phi(\tau, f) = 0\}.$$

The void volume fraction evolves according to

$$(3) \quad \dot{f} = (1 - f)\text{tr}(\dot{\varepsilon}^p).$$

The principle of maximal dissipation reads

$$(4) \quad \sigma \in \Sigma(f), \quad \langle \dot{\varepsilon}^p, \sigma - \tau \rangle \geq 0, \quad \forall \tau \in \Sigma(f).$$

In the small strain case, we have the decomposition

$$(5) \quad \varepsilon = \varepsilon^p + \varepsilon^e, \quad \sigma = A\varepsilon^e,$$

of the total strain into its elastic and plastic part, A represents the linear elastic law. Thus, the scalar f and the tensor ε^p are the internal variables of the stress-strain-relation (1) – (5). Moreover, suitable initial conditions have to be prescribed.

As an important feature, the Gurson model also describes softening behaviour: When the void volume fraction f increases due to increasing tensile plastic strain, the set of admissible stresses $\Sigma(f)$ shrinks, thus forcing the stress σ to become smaller (in the sense, e.g., of the equivalent v. Mises stress). We also recall that the Gurson model is rate independent.

We pose the question: Given a time-dependent strain evolution $\varepsilon = \varepsilon(t)$, does the model define a unique evolution of the stress $\sigma = \sigma(t)$ and of the internal variables? We refer to this problem as the strain-controlled problem. The problem with the roles of σ and ε reversed is termed the stress-controlled problem.

Because of the dependence of Σ on f in (4), the system (1) – (5) represents an evolution quasivariational inequality. With quasivariational inequalities, the question of uniqueness often is difficult and subtle. However, the authors have recently proved uniqueness for a general class of rate independent evolution quasivariational inequalities [2]. This result is based on the contraction principle and thus requires Lipschitz continuity of the corresponding fixed point mapping, with an overall Lipschitz constant less than 1.

It turns out that, for the strain-controlled problem, the result in [2] can be applied to the Gurson model. We announce some results from [3]. Specifically, existence and uniqueness is guaranteed as long as the stress remains within some domain Σ_* . For sufficiently small values of the hydrostatic pressure part $\text{tr}(\sigma)$, Σ_* includes all deviators admissible for $\Sigma(f)$. For example, for steel StE 460 with the parameters $E = 210$ GPa (Young modulus), $\nu = 0.3$ (Poisson number) and $\sigma_f = 460$ MPa (yield stress at $f = 0$), unique solvability is guaranteed as long as the triaxiality satisfies

$$(6) \quad \frac{|\text{tr}(\sigma)|}{|\sigma_d|} \leq 9.6.$$

For the stress-controlled problem, a simple example shows that uniqueness does not hold. However, if one introduces kinematic hardening into the model, one also obtains uniqueness within a suitable stress domain, with considerations analogous to those in [4].

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Evolution of phase interfaces by configurational forces:

A phase field model

HANS-DIETER ALBER

Changes of the morphology of material structure are often caused by configurational forces. In crystalline materials for example, discontinuous changes of the crystal structure generate configurational forces, which can move the discontinuity surface. A well known sharp interface model for moving surfaces of strain discontinuity has been formulated in [1]. We derive and study a phase field model from it.

To state the sharp interface model, let $\Omega \subset \mathbb{R}^3$ be an open set. It represents the material points of a solid body. The different phases are characterized by the order parameter $S(t, x) \in \mathbb{R}$. A value of $S(t, x)$ equal to zero indicates that the material is in the matrix phase at the point $x \in \Omega$ at time t , a value equal to one indicates that the material is in the second phase. The other unknowns are the displacement $u(t, x) \in \mathbb{R}^3$ of the material point x at time t and the Cauchy stress tensor $T(t, x) \in \mathcal{S}^3$, where \mathcal{S}^3 denotes the set of symmetric 3×3 -matrices. $b(t, x)$ denotes the given volume force, $D : \mathcal{S}^3 \rightarrow \mathcal{S}^3$ is the elasticity tensor and $\bar{\varepsilon} \in \mathcal{S}^3$

the misfit strain. The unknowns must satisfy the quasi-static equations

$$(1) \quad -\operatorname{div}_x T(t, x) = b(t, x),$$

$$(2) \quad T(t, x) = D(\varepsilon(\nabla_x u(t, x)) - \bar{\varepsilon}S(t, x))$$

in $[0, \infty) \times \Omega$, and a condition for the normal speed s of the interface, which must hold at every point (t, x) of the interface $\Gamma \in [0, \infty) \times \Omega$:

$$s(t, x) = c n(t, x) \cdot [C(\nabla_x u(t, x), S(t, x))] n(t, x),$$

with a positive constant c and with the Eshelby tensor

$$C(\nabla_x u(t, x), S(t, x)) = \psi(\varepsilon(\nabla_x u(t, x)), S(t, x))I - (\nabla_x u(t, x))^T T(t, x).$$

Here $(\nabla_x u)^T T$ denotes the matrix product, I is the unit matrix in \mathcal{S}^3 and

$$(3) \quad \psi(\varepsilon, S) = \frac{1}{2}(D(\varepsilon - \bar{\varepsilon}S)) \cdot (\varepsilon - \bar{\varepsilon}S) + \psi_1(S)$$

is the free energy. For the function S defined above only the values of ψ_1 at $S = 0$ and $S = 1$ matter. However, as explained next, we also consider order parameters which vary smoothly between 0 and 1. For $\psi_1 \in C^1(\mathbb{R}, [0, \infty))$ we therefore choose a double well potential with minima at 0 and 1.

In [2, 3] this sharp interface model has been transformed into a phase field model. This transformation runs along the following lines: In [2] it has been observed that the equation for the normal speed of the interface in the sharp interface model can be reformulated as a partial differential equation allowing smooth and distributional solutions. In particular, if $x \mapsto S(t, x) : \Omega \rightarrow \{0, 1\}$ is the characteristic function of the region in Ω , which at time t forms the second phase, and if (u, T, S) solves the equations (1), (2), then (u, T, S) is a distributional solution of this partial differential equation. On the other hand, if (u, T, S) is a smooth solution of the equations (1), (2) and of the distributional partial differential equation, then this partial differential equation simplifies and becomes the Hamilton-Jacobi transport equation

$$(4) \quad S_t = -c\psi_S(\varepsilon(\nabla_x u), S) |\nabla_x S|.$$

The idea suggests itself to approximate the solution of the sharp interface model by smooth solutions (u, T, S) of the system (1), (2), (4). Yet, examples show that in general the function S in such a smooth solution develops a jump after finite time. From that time on the equation (4) can no longer be used to govern the evolution of S . To avoid this problem and to force solutions to stay smooth equation (4) has been replaced by

$$(5) \quad S_t(t, x) = -c\left(\psi_S(\varepsilon(\nabla_x u(t, x)), S(t, x)) - \nu \Delta_x S(t, x)\right) |\nabla_x S(t, x)|$$

with a small positive parameter ν . This yields the model (1), (2), (5) first stated in [3].

To regularize (4) one could also try the equation

$$(6) \quad S_t(t, x) = -c\psi_S(\varepsilon(\nabla_x u), S) |\nabla_x S| + \nu \Delta S.$$

However, in contrast to (1), (2), (6), the system (1), (2), (5) satisfies the second law of thermodynamics with the free energy (3) replaced by

$$(7) \quad \psi^*(\varepsilon, S) = \frac{1}{2}(D(\varepsilon - \bar{\varepsilon}S)) \cdot (\varepsilon - \bar{\varepsilon}S) + \psi_1(S) + \frac{\nu}{2}|\nabla_x S|^2,$$

cf. [3]. One expects that this is an advantage, which is confirmed by our mathematical investigations. They indicate that the system (1), (2), (5) has better mathematical properties than the system (1), (2), (6), though (5) is seemingly more singular than (6).

To verify that (1), (2), (5) is indeed a phase field model regularizing the sharp interface model in [1], it must be shown that an initial-boundary value problem to the equations (1), (2), (5) with positive ν has solutions which exist globally in time, and that these solutions tend to solutions of the sharp interface model for $\nu \rightarrow 0$. This program has been carried out only to a small extent; namely in [4] it has been shown that in one space dimension the initial-boundary value problem has solutions. Whether solutions in three space dimensions exist and whether these solutions converge to a solution of the sharp interface model when ν tends to 0 is an open problem.

However, in [3] we also investigated the initial-boundary value problem to the system, which consists of the (1), (2) and of the distributional partial differential equation mentioned above. This is a problem more general than the sharp interface model: Solutions of the sharp interface model are also solutions to this initial-boundary value problem. We showed that in one space dimension this problem with hyperbolic character has distributional solutions. The proof uses new mathematical techniques related to methods used in the theory of hyperbolic conservation laws.

The dynamics determined by the evolution equation (5) for the order parameter is non-conserving. Comparison of this equation to the Cahn-Allen and Cahn-Hilliard models suggests to formulate an analogous evolution equation with conserving dynamics. This leads to a hierarchy of models:

$$\begin{aligned} S_t &= -c(\psi_S - \mu \Delta_x S), && \text{Cahn-Allen equation, } S \text{ is not conserved,} \\ S_t &= c \operatorname{div}_x \nabla_x(\psi_S - \mu \Delta_x S), && \text{Cahn-Hilliard equation, } S \text{ is conserved,} \\ S_t &= -c(\psi_S - \mu \Delta_x S)|\nabla_x S|, && \text{configurational forces, } S \text{ is not conserved,} \\ S_t &= c \operatorname{div}_x \left(\nabla_x(\psi_S - \mu \Delta_x S) |\nabla_x S| \right), && \text{configurational forces, } S \text{ is conserved.} \end{aligned}$$

The first two equations model processes, for which the evolution of the interface is predominantly driven by diffusion, the third equation models a process, where the evolution is driven by configurational forces. We surmise that the fourth equation also models a process with evolution predominantly driven by configurational forces. This, however, is an open problem which remains to be investigated.

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Macroscopic material response arising from microscopic length scales: some case studies of multiscale modelling

ANTONIO DESIMONE

(joint work with G. Alberti, S. Conti, G. Dolzmann)

The theme of this lecture is the study of macroscopic physical properties arising from microscopic phenomena, and the derivation of coarse-grained models as macroscopic limits of those holding at the microscopic scale.

Whenever the property of interest can be described through the global minimization of a free-energy functional, the derivation of a coarse-grained model consists, essentially, in evaluating the minimal energy in the class of all microscopic realizations of the state variables compatible with a given macroscopic average. Two case studies are chosen for the illustration of this procedure: soft elasticity in nematic elastomers, and super-hydrophobic properties of rough water-repellent surfaces. These two systems challenge our intuitive perception of the boundaries between solid and liquid response (sheets of an ideally soft nematic elastomer can be stretched by infinitesimal forces, as if they were freely flowing; liquid drops roll and bounce on a superhydrophobic surface as if they were solid beads). On the other hand, they put into a proper perspective some of the recent progress we want to report. Many interesting properties exhibited by these two systems cannot be captured by only coarse-graining the energetics, but rather require careful consideration of dissipation, kinetics and dynamics.

The analysis of nematic elastomers [1] is based on joint work with S. Conti (Duisburg–Essen) and G. Dolzmann (Maryland) [2]–[6]. We model the soft elastic response of these materials through minimization of a non-convex stored energy density W , obtained as a small perturbation of the neo-hookean expression of rubber elasticity. The coarse-grained model is obtained from the explicit computation of the quasi-convex hull W^{qc} of W

$$W^{\text{qc}}(\mathbf{F}) = \inf_{\mathbf{y} \in W^{1,\infty}} \left\{ \frac{1}{|\Omega|} \int_{\Omega} W(\nabla \mathbf{y}(\mathbf{x})) d\mathbf{x} : \mathbf{y}(\mathbf{x}) = \mathbf{F}\mathbf{x} \text{ on } \partial\Omega, \det \nabla \mathbf{y}(\mathbf{x}) = 1 \right\},$$

where Ω is a representative volume element. The calculation of W^{qc} provides a phase diagram for the mesoscopic response of the system, and answers to the following questions:

- What is the smallest energy cost of imposing the affine deformation $\mathbf{y}(\mathbf{x}) = \mathbf{F}\mathbf{x}$ at the boundary $\partial\Omega$ of a representative volume element?

- Which are the energetically optimal microstructures which develop in the interior of a representative volume element, when this is energetically advantageous?

This information can be used to set up numerical simulations of the elastic response of stretched sheets of nematic elastomers which resolve, at the same time, the macroscopic length scales (e.g., the deformed shape of the sample) and the microscopic ones (i.e., the microscopic domain patterns and their evolution which is the microscopic origin of the soft elastic response of these materials.) The simulations help us to understand many qualitative features of the experimentally observed behavior.

The analysis of wetting properties of rough surfaces [7] is based on joint work with G. Alberti (Pisa) [8]. The equilibrium shape of a drop of water L , of prescribed volume, on a substrate S , and in the presence of a vapor phase V can be obtained by minimizing the total interfacial energy

$$\sigma_{SL}|\Sigma_{SL}| + \sigma_{SV}|\Sigma_{SV}| + \sigma_{LV}|\Sigma_{LV}|,$$

where Σ_{AB} is the interface between phases A and B, $|\Sigma_{AB}|$ is its area, and σ_{AB} is the corresponding surface energy density. Equivalently, we can minimize

$$E = |\cos\theta||\Sigma_{SL}| + |\Sigma_{LV}|, \quad \cos\theta = \frac{\sigma_{SV} - \sigma_{SL}}{\sigma_{LV}}.$$

We consider the case of a solid with periodic asperities, obtained by ϵ -rescaling of a one-periodic surface. By taking the limit $\epsilon \rightarrow 0$, we show that the limit problem is that of minimizing

$$E^{hom} = |\cos\theta^{hom}||\Sigma_{SL}| + |\Sigma_{LV}|,$$

where $|\cos\theta^{hom}|$ is the minimal energy of a transition layer from phase S to phase L in the periodicity cell, allowing for the presence of phase V in between. It turns out that $|\cos\theta^{hom}| > |\cos\theta^{hom}|$ if $\theta > \pi/2$, so that the macroscopic contact angle θ^{hom} of a drop of water on a rough hydrophobic surface is amplified with respect to the flat case.

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Solution-precipitation creep – continuum mechanical formulation and micromechanical modelling

KLAUS HACKL

(joint work with Sandra Ilić)

Solution-precipitation creep is considered to be one of the major deformation mechanisms of polycrystalline solid-liquid aggregates. Normal pressure on the crystallite-interfaces was first identified as driving force in [1] and models built on that observation have been treated extensively in the literature [2, 8, 7]. Still there are some continuum-mechanical problems associated with those models, for example an unrealistic continuity of normal stresses at the intersection of interfaces. We are going to present a micromechanical model which might be able to resolve some of those issues.

Let a representative volume element consist of disjoint crystallites Ω_i . The deformation of every crystallite is decomposed into an elastic and an inelastic part:

$$(1) \quad \phi_i = \phi_i^E \circ \phi_i^I$$

leading to a corresponding multiplicative decomposition of the deformation gradients

$$(2) \quad \mathbf{F}_i = \mathbf{F}_i^E \mathbf{F}_i^I.$$

Note that inelastic deformation is compatible within crystallites but incompatible at crystallite-interfaces.

The material formulation is now based on a common assumption in continuum mechanics, namely minimization of energy locally in time. To be more specific let us suppose, that the entire elastic energy which can be released by elastic deformation, i.e. by change of ϕ_i^E , will be invested into inelastic deformation. The latter on the other hand will be restricted by dissipation of energy, hence there will be a thermodynamical force opposed to elastic stress as driving force. Or otherwise stated, the inelastic deformation will be as fast as possible while still in agreement with the first and second law of thermodynamics. In mathematical terms this concept can be expressed as minimization the sum of total elastic power and dissipation, i.e. we consider a Lagrangian

$$(3) \quad L = \dot{E} + \Delta,$$

where the total stored elastic energy is given by

$$(4) \quad E = \sum_i \int_{\Omega_i} \psi(\mathbf{F}(\mathbf{F}_i^I)^{-1}) J_i^I dV,$$

and the dissipation by

$$(5) \quad \Delta = \sum_i \int_{\partial\Omega_i} \left[\frac{\gamma}{2} \mathbf{Q}_i^2 + \frac{\kappa}{2} (v_i^n)^2 \right] J_i^I |(\mathbf{F}_i^I)^T \mathbf{N}| dS.$$

Here $\psi(\mathbf{F}^E)$ denotes the Helmholtz free-energy,

$$(6) \quad J_i^I = \det \mathbf{F}_i^I$$

the Jacobian, \mathbf{N} the unit-normal to the crystallite surface in the undeformed configuration, \mathbf{Q}_i the velocity of material transport within the crystallite-interfaces and

$$(7) \quad v_i^n = \frac{d}{dt} \phi_i^I \cdot \bar{\mathbf{n}}$$

the normal velocity of precipitation, where $\bar{\mathbf{n}}$ is the unit-normal to the crystallite surface in the inelastically deformed configuration. We have material constants γ and κ related to specific dissipation. We assume that $\kappa/\gamma \ll d^2$, where d corresponds to a characteristic dimension of a crystallite, i.e. the main cause of dissipation is material transport.

Taking into account the relation

$$(8) \quad v_i^n = \nabla \cdot \mathbf{Q}_i$$

using Lagrange-parameters α_i variation with respect to the variables ϕ_i^I, \mathbf{Q}_i yields the following set of equations:

$$(9) \quad \kappa v_i^n + \alpha_i = \beta_i,$$

$$(10) \quad \gamma \mathbf{Q}_i = -\nabla \alpha_i.$$

where β_i denotes the normal component of the Eshelby-tensor, [3, 6],

$$(11) \quad \beta_i = -\frac{1}{J_i^I} \bar{\mathbf{n}} \cdot \frac{\partial}{\partial \mathbf{F}_i^I} (J_i^I \psi)(\mathbf{F}_i^I)^T \bar{\mathbf{n}}.$$

Substitution of (8) and (10) in (9) now gives

$$(12) \quad -\frac{\kappa}{\gamma} \Delta \alpha_i + \alpha_i = \beta_i.$$

The material model obtained in this way allows some interesting insights. Equation (11) identifies the normal component of the Eshelby-tensor as the driving thermodynamical force for solution-precipitation creep. This is consistent with the observation made in continuum mechanics, that the Eshelby-tensor is generally responsible for configurational changes in materials, [3, 6].

Equation (9) now introduces a modification of the point of view stated above. Not β_i is the actual driving force but $\beta_i - \alpha_i$. Whereas β_i is discontinuous at corners and bifurcation-points of the crystallite-interfaces, equation (12) defines α_i as a smooth approximation of β_i . Moreover we obtain

$$(13) \quad v_i^n = -\frac{1}{\gamma} \Delta \alpha_i.$$

This explains some observations made in [5]. Especially one finds that constant stress applied to one single crystal does not induce creep, since $\Delta \alpha_i = 0$ in this case, with the exception of a boundary layer at the outer edge of the loaded surface as observed in [5] and predicted by equation (12).

Furthermore one should notice that in the case of negligible elastic strains and steady deformation processes, the model presented here reduces to that one developed in [4].

We will give precise arguments for all the statements made above. Moreover we will report on a micromechanical model of Taylor-type, which can be generated from the model introduced above and allows to perform numerical simulations of texture-evolution in the polycrystal.

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Nonlinear homogenization and applications to hyperelastic composites

P. PONTE CASTAÑEDA

This work presents the application of a recently proposed "second-order" homogenization methods [4, 5] to generate estimates for effective behavior and loss of ellipticity in hyperelastic porous and fiber-reinforced elastomers with *random* microstructures that are subjected to *finite* deformations. The main concept behind the method is the introduction of an optimally selected "linear thermoelastic comparison composite," which can then be used to convert available linear homogenization estimates into new estimates for the nonlinear hyperelastic composite [6, 2, 3]. In these works, explicit results are provided for the case where the matrix is taken to be isotropic and strongly elliptic. In spite of the strong ellipticity of the matrix phase, the homogenized "second-order" estimates for the overall behavior are found to lose ellipticity at sufficiently large compressive deformations corresponding to the possible development of shear band-type instabilities [1]. The reasons for this result have been linked to the evolution of the microstructure, which, under appropriate loading conditions, can induce geometric softening leading to overall loss of ellipticity. Furthermore, the improved "second-order" homogenization method [5] has the merit that it recovers the exact incompressibility constraint for the rigidly reinforced elastomers, as well as the exact evolution of

the porosity for the porous elastomers, in the limit of incompressible behavior for the matrix.

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Non-crystallographic motion of a dislocation as a fine mixture of rectilinear paths

PAOLO CERPELLI

(joint work with T. Armano)

In this work we discuss the convergence of an approximation scheme for the solution, near an attractor, of a discontinuous dynamical system arising in the theory of dislocations in crystalline solids. It is well known that dislocations can only move along a finite number of crystallographic directions: in two dimensions, the resulting trajectories are piecewise rectilinear paths. However, in special situations such as near an attractor, dislocations are forced to move along curved paths: we characterize this class of motions as fine mixtures of crystallographic motions, using the notion of generalized curves due to L. C. Young, and explicitly compute the parametrized measure associated to a sequence of polygonals. The result is then used to motivate a simple numerical scheme, and show that it is physically consistent. Numerical simulations based on this scheme are also presented and discussed.

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Energy density and oscillations in the wave equation: the bulk case and the thin film case

GILLES A. FRANCFORT

Since the 1970's, there has been a tremendous push towards the computation of the overall behavior of mixtures under the label of "homogenization". Most of the attention has however focussed on the macroscopic constitutive laws that can be derived from the knowledge of the microstructural characteristics of the mixture. This is fine as long as statics are investigated, but it gives no clue as to the proper thermodynamic limit. In other words, the knowledge of the macroscopic (overall) constitutive law does not say anything about the allocation of the energy, part of which may have dissipated through the homogenization process.

The goal of this talk is to quantify such a mechanism in a very simple setting, that of the wave equation with smooth, but non-constant coefficients, which in the film case depend only on the in-plane variables denoted by x_α . Fast oscillations are created by rapidly oscillating initial conditions, as well as, in the case of thin films, the vanishing thickness of the film, which we will assume to be of the order of the wavelength of the oscillations. The computation of the limit behavior (the macroscopic acoustics) is straightforward, in both bulk and film settings. In the bulk setting, it is simply the wave equation with, as initial conditions, the average of the oscillations in the initial conditions; in the film setting, it is the two-dimensional wave equation with, as initial conditions, the average in the film thickness of the average of the oscillations in the initial conditions.

In both cases, we propose to compute the limit of the energy density as the wavelength ε of the oscillations goes to 0. By linearity, we are at liberty to factor out the effect of averaging (the macroscopic limit constitutive behavior), and thus to consider that all oscillations average to 0. Then, whatever energy remains at the macroscopic level is the part that is dissipated through the homogenization process. It is that energy that we propose to compute.

Specifically, we consider

$$(1) \quad \begin{cases} \rho(x) \frac{\partial^2 u^\varepsilon}{\partial t^2} = \operatorname{div}(k(x) \nabla u^\varepsilon) & \text{in } \mathbb{R}^N \\ u^\varepsilon(0) = u_0^\varepsilon, \quad \frac{\partial u^\varepsilon}{\partial t} = v_0^\varepsilon, \end{cases}$$

with

$$(2) \quad \begin{cases} u_0^\varepsilon \xrightarrow{H^1(\mathbb{R}^N)} 0 \\ v_0^\varepsilon \xrightarrow{L^2(\mathbb{R}^N)} 0. \end{cases}$$

We further assume the initial conditions to be uniformly compactly supported. In the film case, after a dilation of the transverse direction that permits to formulate the problem on a fixed domain, the x_3 -derivatives are rescaled by a factor $1/\varepsilon$, so

that (1) becomes

$$(3) \quad \begin{cases} \rho(x_\alpha) \frac{\partial^2 u^\varepsilon}{\partial t^2} = \operatorname{div}_\alpha(k(x_\alpha) \nabla_\alpha u^\varepsilon) + 1/\varepsilon^2 \frac{\partial}{\partial x_3} (k(x) \frac{\partial u^\varepsilon}{\partial x_3}) & \text{in } \mathbb{R}^N \\ u^\varepsilon(0) = u_0^\varepsilon, \quad \frac{\partial u^\varepsilon}{\partial t} = v_0^\varepsilon, \end{cases}$$

while (2) becomes

$$(4) \quad \begin{cases} u_0^\varepsilon \xrightarrow{H^1(\mathbb{R}^N)} 0 & \text{with } 1/\varepsilon \frac{\partial u_0^\varepsilon}{\partial x_3} \text{ bounded in } L^2(\mathbb{R}^N) \\ v_0^\varepsilon \xrightarrow{L^2(\mathbb{R}^N)} v_0^0 & \text{with } \int_0^1 v_0^0 dx_3 = 0. \end{cases}$$

The quantity we wish to investigate is the (measure) limit e_b^0 of

$$e_b^\varepsilon(t) := 1/2 \left\{ \rho(x) \left(\frac{\partial u^\varepsilon}{\partial t} \right)^2 + k(x) |\nabla u^\varepsilon|^2 \right\},$$

or, in the film case, the (measure) limit e_f^0 of

$$e_f^\varepsilon(t) := 1/2 \left\{ \rho(x_\alpha) \left(\frac{\partial u^\varepsilon}{\partial t} \right)^2 + k(x_\alpha) |\nabla_\alpha u^\varepsilon|^2 + 1/\varepsilon^2 k(x_\alpha) \left(\frac{\partial u^\varepsilon}{\partial x_3} \right)^2 \right\}.$$

The computation of the (measure) limits of these quantities is not obvious; the adequate tools are microlocal measures (in phase space) that compute limits of quadratic products of weakly converging quantities: in the bulk case, those are H-measures introduced by L. TARTAR [5], also introduced by P. GÉRARD [3], and, in the film case, those are both H-measures and semi-classical measures introduced by P. GÉRARD [4].

The results are as follows, upon denoting the acoustic wave speed $\sqrt{\frac{k(x)}{\rho(x)}}$ by $c(x)$. In the bulk case [2],

$$e_b^0(t, x) = \int_{\{\eta \in \mathbb{R}^3: c(x)|\eta|=1\}} \{ \nu^+(t, x, d\eta) + \nu^-(t, x, d\eta) \},$$

where ν^\pm are the push-forward in time of some measures ν_0^\pm (solely determined by the initial conditions) along the geodesic flow associated to the metrics $dx^2/c^2(x)$.

In the film case [1],

$$e_f^0(t, x) = \sum_{n=0}^{\infty} e_f^{0,n},$$

with $e_f^{0,0}$ computed as for the bulk case (but in a two-dimensional setting) and $e_f^{0,n}$, $n \neq 0$, given as

$$e_f^{0,n}(t, x) = \int_{\eta \in \mathbb{R}^2} \left(1 + \frac{|\eta|^2}{|\eta|^2 + n^2 \pi^2} \cos 2n\pi x_3 \right) \{ \mu^+(t, x_\alpha, d\eta) + \mu^-(t, x_\alpha, d\eta) \}.$$

There, μ_n^\pm are the push-forward in time of some measures $\mu_{n,0}^\pm$ (solely determined by the initial conditions) along the $n\pi$ -homothetics of the $\mathbb{R}^2 \times \mathbb{R}^2$ -projection of the (three-dimensional) geodesic flow associated to the metrics $dx^2/c^2(x_\alpha)$.

Let me illustrate the result in the bulk case. Say the initial conditions on u^ε both oscillate at the speed ε in one direction η_0 and concentrate at speed $\sqrt{\varepsilon}$ around x_0 (with the appropriate scalings). Then, the initial H-measures are Dirac masses in both space and frequency, and the limit energy density $e_b^0(0, x)$ at time 0 is a Dirac mass at x_0 . The result is that, at time t , the dissipated energy $e_b^0(t, x)$ is still concentrated at $x(t)$, where $x(t)$ is the image at t of x_0 by the geodesic flow with initial speed $c(x_0)\eta_0$. If however the initial condition on u^ε merely concentrates around x_0 , then the initial H-measures are Dirac masses at x_0 in x but they are equi-distributed in frequency. Then, each frequency direction generates its own geodesic and, thus, for each positive time, the support of $e_b^0(t, x)$ has a non denumerable set of points. In effect it looks very much like a diffusion process, although it is not clear how to macroscopically quantify that diffusion.

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Continuum Models for Molecular Beam Epitaxy

ALEXANDRE DANESCU

The molecular beam epitaxy is a recent technique for crystal growth of coherent thin films. The temperatures of various evaporation sources is responsible for the concentration of different components of the film and the growth process takes place in ultra-vacuum conditions, i.e. at $\sim 10^{-10}$ torrs. Experimental evidence shows that after a coherent 2D growth, at a critical thickness h_{cr} , a transition between a layer-by-layer mode to a roughening of the free surface takes place. This is commonly called the Asaro-Tiller-Grinfeld instability and a straightforward computation based on available numerical data shows that at the scale of the problem the bulk energy induced by the misfit between the film and the substrate and the surface energy are of the same order of magnitude.

A direct variational argument shows that both in the framework of linear elasticity and in finite strains elasticity a flat free-boundary of a homogeneous deformed material is unstable with respect to variations of the free-boundary at constant volume. In order to obtain a quantitative estimate a first order elastic problem in the bulk and an approximation of the surface energy provide together an estimate

for the critical thickness as $h_{\text{cr.}} = \mu\psi/\sigma_0^2$, where σ_0 is the misfit stress, μ is the shear modulus and ψ is the surface energy [1].

From a variational point of view, a model problem was analysed in [2] in a 1D situation and we discuss several open problems related to this setting. In a time-dependent setting, the problem can be regarded as a free-boundary problem where the sharp interface (the free-surface of the thin film) is driven by the temperature gradient, bulk stress and surface energy. In the framework of thermoelasticity the simplest theory for evolution of an immaterial interface that includes bulk elasticity effects as sources of instability is the theory of structured interfaces proposed in [3]. We discuss some specific features of this formulation.

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Wave propagation in planarly-stratified media and first integrals

ANGELO MORRO

The subject of this talk is existence and uniqueness of the time-harmonic solution to the reflection-transmission (RT) problem originated by an unbounded layer. The layer is planarly stratified in that the material properties vary only in one direction, say z , and occupies the region $z \in (0, L)$. The dependence of the functions involved on the time t is through the common factor $\exp(i\omega t)$, $\omega \in \mathbb{R}$. Two models are considered and a research in progress is outlined.

- The unknown function $u(x, y, z, t)$ satisfies the Helmholtz equation

$$(\Delta + k^2 n^2(z))u = 0,$$

which is the case for linear acoustics ($u = p/\sqrt{\rho}$), isotropic dielectrics ($u = E_y, \mathbf{E} \cdot \nabla \epsilon = 0$), isotropic elasticity ($u = U\sqrt{\mu}$). For oblique incidence, the solution is sought in the form

$$u(x, y, z, t) = \exp[i(k_x x + \omega t)]f(z), \quad k_x \in \mathbb{R},$$

and hence f satisfies the differential equation

$$f'' + h(z)f = 0$$

where h is real valued and related to n^2 while a prime $'$ means differentiation with respect to z . The solution f is subject to the first integral

$$\mathcal{F} := \Im(f^* f') = \text{constant}.$$

Letting $h_-(h_+)$ be the constant value of h as $z < 0$ ($z > L$), we assume $h_- > 0$ and represent the solution f as

$$f(z) = \begin{cases} f^i \exp(-i\sigma_- z) + f^r \exp(i\sigma_- z), & z < 0, \\ \tilde{f}(z), & z \in (0, L), \\ f^t \exp[-i\sigma_+(z - L)], & z > L, \end{cases}$$

where $\sigma = \sqrt{k^2 n^2 - k_x^2}$; if $h_+ < 0$ then $i\sigma_+$ is replaced with $\sqrt{|h_+|}$, as $z > L$. The RT problem reads: given f^i find f^r , f^t and \tilde{f} . Preliminarily we show that $f = 0$, as $z < 0$, if and only if $f^i, f^r = 0$. Hence, by means of the first integral \mathcal{F} and the jump conditions at possible discontinuity planes, we can show that ([1, 2])

$$h_+ > 0: \quad f = 0 \text{ in } \mathbb{R} \iff f^t = 0,$$

$$h_+ \leq 0: \quad |f^r| = |f^i|.$$

Irrespective of the value of h_+ ,

$$f^i \neq 0 \implies f \neq 0 \text{ in } \mathbb{R}.$$

In addition, if \mathcal{F} is continuous (and hence constant) across discontinuities, and $h_+ > 0$, we obtain the energy conservation law

$$\sigma_- (|f^i|^2 - |f^r|^2) = \sigma_+ |f^t|^2.$$

As a comment, however is h in the layer (possibly $h < 0$), wave propagation is not precluded in any zone (interval) of \mathbb{R} .

- An abstract scheme for wave propagation is given as follows.

The pertinent variables are taken as $\mathbf{w}(z, \omega) \exp(i\omega t)$, $\mathbf{w} \in \mathbb{C}^{2m}$, and the governing equations are written as a first-order system

$$\mathbf{w}' = \mathbf{A}(z, \omega) \mathbf{w}, \quad \mathbf{A} \in \mathbb{C}^{2m \times 2m},$$

where ω is a real-valued parameter. There is a function

$$\mathcal{F} = \mathbf{w}^\dagger \mathbf{I} \mathbf{w},$$

where \mathbf{I} is Hermitian, $\mathbf{I}^\dagger = \mathbf{I}$, and m eigenvalues of \mathbf{I} are positive, m are negative. The function \mathcal{F} is the energy flux and, as such, characterizes the direction of a wave; if $\mathcal{F} > 0$ the wave propagates in the positive z -direction. Also \mathcal{F} satisfies the condition

$$\mathcal{F}' \leq 0.$$

The eigenvectors $\mathbf{p}_1, \dots, \mathbf{p}_{2m}$ of \mathbf{A} are linearly independent. Let

$$\mathbf{P} = [\mathbf{p}_1, \dots, \mathbf{p}_{2m}], \quad \mathbf{\Phi} = \mathbf{P}^\dagger \mathbf{I} \mathbf{P}.$$

The diagonal $m \times m$ blocks $\mathbf{\Phi}^f$ and $\mathbf{\Phi}^b$ of $\mathbf{\Phi}$ are positive and negative definite. If these conditions hold then the solution to the RT problem exists and is unique ([3, 4]).

The scheme is shown to hold for oblique incidence in anisotropic elasticity and normal incidence in isotropic viscoelasticity.

• The application of the scheme to linear thermoelasticity is given as follows. With a view to materials with memory, the governing equations are taken in the form

$$\mathbf{T} = \Sigma \nabla \mathbf{u} - \beta \vartheta, \quad \dot{\epsilon} = \gamma \cdot \nabla \dot{\mathbf{u}} + c \dot{\vartheta}, \quad \mathbf{q} = -\kappa \nabla \vartheta$$

where $\vartheta = \theta - \theta_0$ is the difference temperature relative to a uniform configuration, \mathbf{T} is the Cauchy stress tensor, ϵ is the internal energy, \mathbf{q} is the heat flux and a superposed dot means time differentiation. Of course, $\Sigma, \beta, \gamma, c, \kappa$ are complex valued. The first-order form $\mathbf{w}' = \mathbf{A} \mathbf{w}$ is found to hold. In classical thermoelasticity, β and γ are related by $\rho \gamma = \theta^0 \beta$, ρ being the mass density. The thermodynamic analysis shows that the constraint

$$\rho \gamma = \theta^0 \beta^*$$

has to be considered, where $*$ means complex conjugate; along with others, this constraint is sufficient for the validity of the second law. Hence we find that

$$\mathcal{F} = -\omega \Im(\mathbf{t} \cdot \mathbf{u}^*) + \frac{1}{\theta^0} \Re(\vartheta q_z^*)$$

where \mathbf{t} is the traction at the planes $z = \text{constant}$. In addition,

$$\mathcal{F}' = -\omega \Im(\nabla \mathbf{u}^* \cdot \Sigma \nabla \mathbf{u}) - \frac{\rho}{\theta^0} \omega \Im c^* |\vartheta|^2 + \frac{1}{\theta^0} \Re(\nabla \vartheta \cdot \mathbf{q}^*)$$

and the right-hand side proves to be non-positive because of the thermodynamic restrictions. The analysis of Φ is decisively more involved and is now under investigation.

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Uniqueness in nonlinear continuum mechanics

ROBIN JOHN KNOPS

1. NOTATION AND OTHER PRELIMINARIES

We report on work in progress. Let a nonlinear homogeneous compressible elastic material in its reference configuration occupy the bounded region $\Omega \subset \mathbb{R}^3$ and let it be set in motion by specified initial deformation and velocity, and subject to given displacement of the smooth surface $\partial\Omega$. Zero body-force is assumed. For a given Cartesian coordinate system, let the point in Ω whose vector position is X be deformed into a point whose vector position is $x = x(X, t)$ at time t . Here, and subsequently, a direct notation is employed in which, for example, the tensor gradient operator with respect to the variable X is denoted by $Grad$ so that the components of the deformation gradient F are given by $(Grad x)_{ij} = \partial x_i / \partial X_j$ where $X_i, x_i, i = 1, 2, 3$ are the cartesian components of the vectors X, x respectively. The corresponding divergence operator is given by Div , while the tensor product of vectors a, b is indicated by $a \otimes b$, transposition by superscript T , and the unit tensor by I . The set of deformation gradients having positive determinant is denoted by M^+ .

The elastic material possesses a strain energy function $W \in C^1(M^+, \mathbb{R})$ per unit volume of Ω , in terms of which the Piola-Kirchhoff stress tensor is represented by $T = \partial W / \partial F$.

The initial displacement boundary value problem considered here assumes that sufficiently smooth deformations exist locally on some finite time interval which by an appropriate rescaled time variable may be taken as $[0, 1]$. The governing equations of motion are:

$$(1) \quad Div T = \rho \ddot{x}, \quad (X, t) \in \Omega \times [0, 1],$$

where $\rho (> 0)$ is the uniform material density in the reference configuration, and a superposed dot indicates time differentiation. The initial and boundary conditions are

$$(2) \quad x(X, 0) = u(X), \quad \dot{x}(X, 0) = v(X), \quad X \in \Omega,$$

and

$$(3) \quad x(X, t) = g(X, t), \quad (X, t) \in \partial\Omega \times [0, 1],$$

where u, v, g are specified functions.

Equations (1)–(3) lead to balance of energy in the form:

$$(4) \quad \int_{\Omega(t)} [W(F) + \frac{1}{2} \rho \dot{x} \dot{x}] dX = \int_0^t \oint_{\partial\Omega(\eta)} tr T N \otimes \dot{x} dX d\eta + \int_{\Omega(0)} [W(Grad u) + \frac{1}{2} \rho v v] dX,$$

where $\Omega(t)$ denotes that the integrand is evaluated at time t . The equations also show that the energy-momentum (Eshelby) tensor, given by

$$(5) \quad \mathbb{B} = (F)^T T - (W - \frac{1}{2} \rho \dot{x} \dot{x}) I,$$

satisfies the relation

$$(6) \quad \text{Div} \mathbb{B} = \rho \frac{d}{dt} [(F)^T \dot{x}], \quad (X, t) \in \Omega \times [0, 1].$$

Multiplication of the last equation by X and slight rearrangement yields

$$(7) \quad \text{Div}(X\mathbb{B}) - \text{tr} \mathbb{B} = \rho X \frac{d}{dt} [(F)^T \dot{x}], \quad (X, t) \in \Omega \times [0, 1].$$

A weak formulation of the problem is possible using, for example, the variational calculus.

We seek sufficient conditions for uniqueness of locally smooth solutions to (1)–(3), complementary to those derived in [1],[2], and [3].

2. UNIQUENESS OF SMOOTH SOLUTIONS

The affine initial displacement boundary value is considered first and then a generalisation is briefly discussed.

Proposition 1. *Let Ω be star-shaped with respect to an interior point, and let the initial and boundary data (2) and (3) be given by*

$$(8) \quad u(X) = AX + a, \quad X \in \Omega,$$

$$(9) \quad v(X) = BX + b, \quad X \in \Omega,$$

$$(10) \quad g(X, t) = (AX + a) + t(BX + b), \quad (X, t) \in \Omega \times [0, 1],$$

where $A, B \in M^+$, $a, b \in \mathbb{R}^3$ are constants. Let W be quasi-convex at $A + tB, t \in [0, 1]$ and rank-one convex. Then the affine solution

$$(11) \quad y(X, t) = (AX + a) + t(BX + b), \quad (X, t) \in \Omega \times [0, 1],$$

is the unique solution to (1)–(3) in the class of functions f satisfying the constraints:

$$(12) \quad \sup_{[0,1]} \int_{\Omega(t)} \left(\text{tr} G^T G + \text{tr}(\dot{G})^T \dot{G} \right) dX \leq N^2,$$

and

$$(13) \quad \sup_{[0,1]} \int_{\Omega(t)} \text{tr} T^T(G) T(G) dX \leq M^2,$$

for prescribed constants N, M , and where $G = \text{Grad } f$.

We sketch the proof. The expression (11) obviously is a solution to the stated initial boundary value problem. Suppose a second smooth solution $x(X, t)$ exists such that the common interval of existence contains $[0, 1]$ after suitable scaling. Set $w = x - y (\neq 0)$ and define the function $H(t)$ to be

$$(14) \quad H(t) = \int_0^t \int_{\Omega(\eta)} \rho w w dX d\eta + \beta(t + t_0)^2, \quad t \in [0, 1],$$

where β and t_0 are positive constants to be chosen. Equations (1),(4), (7), the conditions of the Proposition, and standard inequalities may then be combined to show that for constant $\alpha > 1$ the function $H(t)$ satisfies the differential inequality: (15)

$$H(t)\ddot{H}(t) + (\alpha - 1)\dot{H}^2(t) \leq H(t) \left[2\beta(2\alpha - 1) + 2\dot{H}(t)^{\frac{1}{2}}Q_1 + Q_2 \right], \quad t \in [0, 1],$$

where $Q_1(N, R, \lambda)$ and $Q_2(M, a, b, B, \alpha)$ are computable positive constants, λ is the least eigenvalue for the corresponding fixed membrane problem, and $R^2 = \sup_{\Omega} XX$. Appropriate choice of β and t_0 and of subsequently introduced similar disposable constants leads after reduction and integration of (15) to a contradiction on a sufficiently small time interval, and consequently to uniqueness of the affine solution (11). Iteration extends the result to $[0, 1]$.

The assumptions of star-shapedness and generalised convexity of the strain energy function are not essential and uniqueness may be established provided the smooth solutions belong to the class of functions that besides (12) and (13) additionally satisfy certain boundedness conditions, including ones on second and third order derivatives. This form of the uniqueness result not only aligns with that for linear elastodynamics, but is similar to theorems for the stabilisation of ill-posed problems. Moreover, the proof appears applicable, in particular, to the moving elastic dielectric.

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On modelling loss of mass and connectivity in bone

R. KIENZLER

(joint work with G. Herrmann, I. Ott)

Osteoporosis is defined as a systemic skeletal disease characterized by loss of mass and deterioration of the microarchitecture (i.e., connectivity). Patients affected by osteoporosis often suffer fracture with the additional difficulty of fracture fixation in osteoporotic bone. In order to assist physicians in the diagnosis, therapy and in the prediction of the development of the disease it seems to be worthwhile to establish a mechanical/numerical model for osteoporotical bone.

In this paper, and as a start, a very simple model is proposed. A long bone is represented as a one-dimensional bar. From the elementary theory of strength-of-materials we know that the elongation of such a bar due to a longitudinal force

is given by

$$\Delta l = \frac{Fl}{EA} .$$

The length of the bar is l , E is the material-dependent modulus of elasticity and A is the cross-sectional area. Loss of mass is modelled by the reduction of the cross-sectional area $A = A_0(1 - \omega)$ and loss of connectivity, i.e., decrease in strength, by $E = E_0(1 - \eta)$. The constant initial values are A_0 and E_0 and the internal, time-dependent variables which describe the deterioration of the material are thus ω and η . Due to the progression of damage in the bone the total energy Π of the bar (bone) is changed; it is reduced to

$$\Pi = \Pi(\tilde{\epsilon}, \omega, \eta) = \frac{1}{2} A_0 E_0 l \tilde{\epsilon}^2 (1 - \omega)(1 - \eta) ,$$

with the effective stress $\tilde{\sigma}$ and the effective strain $\tilde{\epsilon}$ given, respectively, by

$$\tilde{\sigma} = \frac{F}{A} = \frac{F}{A_0(1 - \omega)} = \frac{\sigma_0}{1 - \omega}, \quad \tilde{\epsilon} = \frac{\tilde{\sigma}}{E} = \frac{\sigma_0}{E_0(1 - \omega)(1 - \eta)} = \frac{\epsilon_0}{(1 - \omega)(1 - \eta)} .$$

Differentiation of the specific Helmholtz free energy f , i.e., the total energy divided by the bar volume $A_0 l$, with respect to the internal variables ω and η leads to the affinities A_ω and A_η , respectively, which can be understood as material or driving forces of the damage process

$$A_\omega := -\frac{\partial f}{\partial \omega} = \frac{1}{2} E_0 \tilde{\epsilon}^2 (1 - \eta) ,$$

$$A_\eta := -\frac{\partial f}{\partial \eta} = \frac{1}{2} E_0 \tilde{\epsilon}^2 (1 - \omega) .$$

In the local-state approximation of thermodynamics, a first guess for the time-rate of change of the internal variables $\dot{\omega}$ and $\dot{\eta}$ is that they are proportional to the affinities A_ω and A_η :

$$\dot{\omega} = k_{\omega\omega} A_\omega + k_{\omega\eta} A_\eta ,$$

$$\dot{\eta} = k_{\eta\omega} A_\omega + k_{\eta\eta} A_\eta .$$

Based on the implications of the first and second laws of thermodynamics, the evolution equations for ω and η are integrated, from which time-dependent stress, strain and stiffness of osteoporotic bone are calculated. The model involves three parameters that have to be determined experimentally. In [1] the change of mass, structure and mechanical properties of trabecular bone are reported for ovariectomized sheep during and after glucocorticoid treatment. Subject to an adjustment of the model parameters the qualitative agreement between measured and calculated results appears to be quite satisfactory. Details of the analysis and the results are discussed in a forthcoming paper [2].

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A variational approach of fatigue

JEAN-JACQUES MARIGO

Francfort and Marigo [1] propose a variational approach of brittle fracture in which the cracks appear and grow in an elastic brittle body in such a manner that the total energy of the body is minimal at each step of the loading history. In that work, the authors conserve Griffith's hypothesis by assuming that the surface energy is proportional to the surface area of the crack independently of the value of the displacement jump discontinuity. But, with this choice, it is impossible to render account for fatigue phenomenon. We propose in the present work to extend this approach in order to model the propagation of cracks in bodies submitted to cyclic loadings. The idea is to conserve the principle of least energy, but to replace the Griffith-type surface energy by an energy depending on the displacement jump through the crack (as in [2]) and to introduce an irreversibility condition. The ingredients and the method are developed in the case of the fatigue debonding of a thin layer.

Specifically, in this particular context, the energy functional at step i , \mathcal{E}_i , is defined on the set of admissible displacement fields \mathcal{V}_i ,

$$(1) \quad \mathcal{V}_i = \{v \in W^{1,2}(0, L) : v(0) = 0, v \geq 0, v(L) = V_i\},$$

by

$$(2) \quad \mathcal{E}_i(v) = \frac{N}{2} \int_0^L v'(s)^2 ds + \int_0^L \phi(\delta_{i-1}(s) + \langle v(s) - v_{i-1}(s) \rangle) ds.$$

In (1)–(2), L denotes the length of the film, V_i is the prescribed opening at the end L , v is the opening displacement field, N is the prescribed tension of the film, δ is the accumulated opening displacement field and the brackets $\langle \cdot \rangle$ denote the positive part. The field δ is then the memory variable introduced to take into account the irreversibility of the debonding. The function ϕ is the surface energy density. It can be chosen either as Griffith surface energy density ($\phi(0) = 0$, $\phi(\delta) = G_c$ when $\delta > 0$), or as a Barenblatt surface energy density, that is a continuous increasing function starting from 0, for $\delta = 0$, and tending to G_c when δ goes to infinity.

The minimization incremental problem reads as For $i \in \mathbb{N}$, find v_i and δ_i such that

$$(3) \quad \mathcal{E}_i(v_i) = \min_{v \in \mathcal{V}_i} \mathcal{E}_i(v), \quad \delta_i = \delta_{i-1} + \langle \delta_{i-1} - v_{i-1} \rangle.$$

with the initial condition $v_0 = \delta_0 = 0$.

The main results are the following:

(i) We first prove that this incremental problem admits a unique solution and that the solution is independent of the discretization. Consequently, when the film is submitted to a cyclic loading $t \mapsto V(t)$ such that $V_{max} = V_m$ and $V_{min} = 0$ each loading or unloading part of a cycle can be treated in one step. That allows us to consider from now that the index i refers to the ends of a half-cycle. Moreover the debonding does not evolve during the unloading loading steps and the layer returns to its initial displacement configuration at the end of an unloading step, $v_{2i} = 0$ and $\delta_{2i} = \delta_{2i-1}$.

(ii) When ϕ is the Griffith surface energy density, then the debonding only evolves during the first half-cycle : $\delta_{2i+1} = \delta_1$. There is no fatigue effect.

(iii) When ϕ is a Barenblatt surface energy density, then the debonding evolves at each cycle and the film tends asymptotically to be completely debonded, $\lim_{i \rightarrow \infty} \delta_{2i+1}(s) = +\infty$, for $s \in (0, L)$. There is fatigue effects.

Moreover, for Barenblatt surface energy density, the evolution of the debonding depends on the ratio ϵ between the characteristic length appearing in ϕ and the overall length L of the film. An asymptotic study is made when ϵ goes to 0. We obtain that

(iv) The evolution of the debonding during the first cycle is approximately given by Griffith law.

(v) The fatigue phenomenon is a second order effect, that is the growth of the debonding length is of the order of ϵ at each cycle after the first one.

(vi) After rescaling the number of cycles, that is by considering number of cycles N of the order of $1/\epsilon$, then the evolution of the debonding follows approximately a Paris law

$$(4) \quad \frac{d\ell}{dN} = f(G)$$

where $\ell(N)$ denotes the effective debonding length after N cycles, G is the energy release rate as it is usually defined in Griffith theory and f is the effective fatigue function which depends in particular on the surface energy density ϕ . For small values of G , $f(G)$ is approximately given by $k G^{3/2}$ where only the constant k depends on ϕ .

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Microcrack nucleation in brittle solids

KHANH CHAU LE

(joint work with Victor Berdichevsky)

The microcrack nucleation in brittle solids is studied within the probabilistic approach, according to which the crack radius is regarded as a random continuous

Markovian process. Its probability density function obeys the Fokker-Planck equation. It is natural to assume that, at large time, the probability density function approaches the Gibbsian distribution asymptotically. This assumption, together with the reflecting boundary condition, determines the drift uniquely. Thus, the model has two entries, the energy and the diffusion coefficient.

In this talk I present some arguments in favor of a specific choice of the energy and of the diffusion coefficient. Our model contains two material characteristics additional to the Griffith's toughness [1]. One of them, the ultimate strain, can easily be extracted from the tensile test of crack-free fibres at the liquid helium temperature (see [2]). The other parameter which determines the diffusion coefficient is identified by the maximum speed of crack propagation at room temperature. We apply the model to predict the nucleation of internal and edge microcracks in defect free silica glass fibres. It provides a reasonably good coincidence with the experimental data in the interval of temperatures (0,600°K).

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Homogenization in micro-plasticity

VICTOR BERDICHEVSKY

Homogenized description of plasticity on micro-scale and macro-scale are principally different. A key distinction is that the energy of micron-size specimens, in contrast to that of macro-specimens, is not a functional of integral characteristics of the dislocation nets. Thus, energy must be considered as an independent characteristic of the body which is additional to all other characteristics. In this talk, a homogenized description of dislocation motion on micro-scale is proposed. The theory is considered for the case of anti-plane constrained shear where all the propositions can be evaluated analytically.

On Nonlocal Phase-Field Models

JÜRGEN SPREKELS

(joint work with Pavel Krejčí (WIAS Berlin), Elisabetta Rocca (Pavia), Songmu Zheng (Shanghai))

We consider nonlocal phase-field systems that model non-isothermal phase transitions characterized by a nonconserved order parameter χ . Typically, χ denotes the fraction of the high temperature phase (say, the liquid fraction in a solid–liquid transition) and thus has to attain values in $[0, 1]$.

The total free energy F that governs the evolution of χ and θ typically has the form

$$(1) \quad F[\theta, \chi] = \int_{\Omega} \left[c_V \theta(x) (1 - \ln(\theta(x))) + \theta(x) \sigma(\chi(x)) + \lambda(\chi(x)) \right. \\ \left. + (\beta + \theta(x)) \varphi(\chi(x)) + \int_{\Omega} K(\theta(x) + \theta(y), x, y) G(\chi(x) - \chi(y)) dy \right] dx,$$

where $c_V > 0$ is the specific heat, σ, λ are smooth functions, φ is a proper, convex and l.s.c. function forcing χ to attain values in $[0, 1]$ (typically, the indicator function of $[0, 1]$ or the configurational entropy $\chi \ln(\chi) + (1 - \chi) \ln(1 - \chi)$). The symmetric kernel K accounts for long-range interactions (which may depend on θ), and G is smooth and even.

Assuming that the evolution runs in the direction where total entropy is maximized under constant total internal energy, one obtains the thermodynamically consistent phase-field system

$$(2) \quad c_V \theta_t(x) - \kappa \Delta \theta(x) - 2\theta(x) \int_{\Omega} K_{\tau\tau}(\tau, x, y)|_{\tau=\theta(x)+\theta(y)} (\theta_t(x) + \theta_t(y)) \\ \times G(\chi(x) - \chi(y)) dy \\ = -(\lambda(\chi(x)) + \beta \varphi(\chi(x)))_t - 2\chi_t(x) \int_{\Omega} K(\theta(x) + \theta(y), x, y) \\ \times G'(\chi(x) - \chi(y)) dy \\ + 2\theta(x) \int_{\Omega} K_{\tau}(\tau, x, y)|_{\tau=\theta(x)+\theta(y)} G'(\chi(x) - \chi(y)) (\chi_t(x) - \chi_t(y)) dy,$$

$$(3) \quad \mu(\theta(x)) \chi_t(x) + \theta(x) \sigma'(\chi(x)) + \lambda'(\chi(x)) \\ + 2 \int_{\Omega} K(\theta(x) + \theta(y), x, y) G'(\chi(x) - \chi(y)) dy \in -(\beta + \theta(x)) \partial \varphi(\chi(x)),$$

where we always have suppressed the argument t . The system (2), (3) is complemented by appropriate initial and boundary conditions.

For the resulting system (2), (3) of integro-differential equations/inclusions, an existence result has been established (cf. [1]). This result extends earlier existence, uniqueness and regularity results established in [2], [3] for special cases for the system (2), (3).

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Objective relative accelerations in theories of porous materials

KRZYSZTOF WILMANSKI

1. INTRODUCTION

It is known from the theory of suspensions (e.g. [1]) that relative inertia influence the dynamics of multicomponent systems. A linear theory of poroelastic materials with such an influence was constructed by M. Biot [2]. Since this work, a lot of attention is given to this contribution both from theoretical and experimental points of view. It is claimed (e.g. [3]) that the relative inertia arise due to the tortuosity of porous materials and that this contribution is essential for an explanation of experimental results.

From the formal point of view of continuum mechanics, such a contribution is non-objective (see [4]). Simultaneously, its influence on the behavior of acoustic waves does not seem to correspond with a physical expectation. Namely, it leads to a reduced attenuation of waves by growing tortuosity ([5]).

In this lecture we present a construction of an objective relative acceleration for two-component poroelastic materials. It is shown that an objective form is necessarily nonlinear and that there exist infinitely many objective relative accelerations. In this sense Biot's model may be considered as a linear (nonobjective) approximation of a full objective nonlinear model.

2. MATERIAL OBJECTIVITY

In continuum mechanics and thermodynamics it is required that constitutive relations are invariant with respect to Euclidean transformation in the space of motion. This transformation follows from the assumption on isometry of the space of motion and it has the form

$$(1) \quad \mathbf{x}^* = \mathbf{O}(t) \mathbf{x} + \mathbf{c}(t), \quad \mathbf{O}^T(t) = \mathbf{O}^{-1}(t),$$

i.e. it consists of a time dependent rotation described by the orthogonal matrix $\mathbf{O}(t)$, and a time dependent translation $\mathbf{c}(t)$.

If we use a Lagrangian description of motion of the two-component porous material (e.g. [6]) that the motion of skeleton is described by the following diffeomorphism

$$(2) \quad \mathbf{x} = \mathbf{f}^S(\mathbf{X}, t), \quad \mathbf{X} \in \mathbf{B}_0, \quad t \in \mathbb{T},$$

where \mathbf{B}_0 is the reference configuration of the body, and \mathbb{T} is the time interval. Then the velocity of the skeleton, its acceleration and the deformation gradient are given by the relations

$$(3) \quad \dot{\mathbf{x}}^S = \frac{\partial \mathbf{f}^S}{\partial t}, \quad \ddot{\mathbf{x}}^S = \frac{\partial \dot{\mathbf{x}}^S}{\partial t}, \quad \mathbf{F}^S = \text{Grad } \mathbf{f}^S.$$

Simultaneously, the velocity of the fluid which is usually introduced in the Eulerian description can be transformed to the reference configuration of the skeleton. After

easy calculations, we obtain also the relation for the acceleration of the fluid

$$(4) \quad \dot{\mathbf{x}}^F = \dot{\mathbf{x}}^F(\mathbf{X}, t), \quad \ddot{\mathbf{x}}^F = \frac{\partial \dot{\mathbf{x}}^F}{\partial t} + (\text{Grad } \dot{\mathbf{x}}^F) \dot{\mathbf{X}}^F, \quad \dot{\mathbf{X}}^F = \mathbf{F}^{S-T} (\dot{\mathbf{x}}^F - \dot{\mathbf{x}}^S),$$

where $\dot{\mathbf{X}}^F$ is the so-called Lagrangian relative velocity.

The above quantities behave in the following way under Euclidean transformation

$$(5) \quad \begin{aligned} \dot{\mathbf{x}}^{S*} &= \mathbf{O}\dot{\mathbf{x}}^S + \dot{\mathbf{O}}\mathbf{x} + \dot{\mathbf{c}}, & \dot{\mathbf{x}}^{F*} &= \mathbf{O}\dot{\mathbf{x}}^F + \dot{\mathbf{O}}\mathbf{x} + \dot{\mathbf{c}}, & \mathbf{F}^{S*} &= \mathbf{O}\mathbf{F}^S, & \dot{\mathbf{X}}^{F*} &= \dot{\mathbf{X}}^F, \\ \ddot{\mathbf{x}}^{S*} &= \mathbf{O}\ddot{\mathbf{x}}^S + 2\dot{\mathbf{O}}\dot{\mathbf{x}}^S + \ddot{\mathbf{O}}\mathbf{x} + \ddot{\mathbf{c}}, & \ddot{\mathbf{x}}^{F*} &= \mathbf{O}\ddot{\mathbf{x}}^F + 2\dot{\mathbf{O}}\dot{\mathbf{x}}^F + \ddot{\mathbf{O}}\mathbf{x} + \ddot{\mathbf{c}}, \\ \text{Grad } \dot{\mathbf{x}}^{S*} &= \mathbf{O} \text{Grad } \dot{\mathbf{x}}^S + \dot{\mathbf{O}}\mathbf{F}^S, & \text{Grad } \dot{\mathbf{x}}^{F*} &= \mathbf{O} \text{Grad } \dot{\mathbf{x}}^F + \dot{\mathbf{O}}\mathbf{F}^S. \end{aligned}$$

These relations indicate rules of transformation for balance equations provided we assume the following transformation rules for the partial Piola-Kirchhoff stress tensors, $\mathbf{P}^S, \mathbf{P}^F$, and for the momentum source, $\hat{\mathbf{p}}$, (a diffusive force).

$$(6) \quad \mathbf{P}^{S*} = \mathbf{O}\mathbf{P}^S, \quad \mathbf{P}^{F*} = \mathbf{O}\mathbf{P}^F, \quad \hat{\mathbf{p}}^* = \mathbf{O}\hat{\mathbf{p}}.$$

Material objectivity for poroelastic materials means that the following relations must hold

$$(7) \quad \mathbf{P}^{S*} = \mathbf{P}^S(\rho^F, \mathbf{F}^{S*}, \dot{\mathbf{X}}^F, n, \text{Grad } n), \quad \hat{\mathbf{p}}^* = \hat{\mathbf{p}}(\rho^F, \mathbf{F}^{S*}, \dot{\mathbf{X}}^F, n, \text{Grad } n),$$

where $\rho^F = \rho_t^F J^S$, ρ_t^F is the current mass density of the fluid, $J^S = \det \mathbf{F}^S$, n – porosity. The essential part of this assumption is that constitutive functions on the right-hand side of these relations are the same for the initial and transformed frames of reference.

Biot's model contains a linear contribution to $\hat{\mathbf{p}}$ of the relative accelerations with a material coefficient ρ_{12} – the so-called added mass coefficient. Inspection of the above relations shows easily that such a contribution violates the rule (7).

3. OBJECTIVE RELATIVE ACCELERATIONS

Making use of the last two relations (5), the transformation rule for relative accelerations can be easily written in the following form

$$(8) \quad \begin{aligned} \ddot{\mathbf{x}}^{F*} - \ddot{\mathbf{x}}^{S*} &= \mathbf{O}(\ddot{\mathbf{x}}^F - \ddot{\mathbf{x}}^S) + 2\dot{\mathbf{O}}(\dot{\mathbf{x}}^F - \dot{\mathbf{x}}^S) = \\ &= \mathbf{O}(\ddot{\mathbf{x}}^F - \ddot{\mathbf{x}}^S) + (2 - \mathfrak{z}) \text{Grad}(\dot{\mathbf{x}}^{F*} - \mathbf{O}\dot{\mathbf{x}}^F) \dot{\mathbf{X}}^F + \mathfrak{z} \text{Grad}(\dot{\mathbf{x}}^{S*} - \mathbf{O}\dot{\mathbf{x}}^S) \dot{\mathbf{X}}^F, \end{aligned}$$

where \mathfrak{z} is an arbitrary scalar. Consequently, we can introduce the quantity

$$(9) \quad \mathbf{a}_r = \frac{\partial}{\partial t}(\dot{\mathbf{x}}^F - \dot{\mathbf{x}}^S) - (1 - \mathfrak{z}) \dot{\mathbf{X}}^F \cdot \text{Grad } \dot{\mathbf{x}}^F - \mathfrak{z} \dot{\mathbf{X}}^F \cdot \text{Grad } \dot{\mathbf{x}}^S,$$

which is objective

$$(10) \quad \mathbf{a}_r^* = \mathbf{O}\mathbf{a}_r.$$

Hence it can be used as an additional constitutive variable in (7) and, in the linear case, the model reduces to this proposed by Biot.

This extension of the model can be made thermodynamically admissible [5]. Among other properties, it can be shown that partial stresses must be at least quadratic functions of relative velocities. Consequently free energies contain as well quadratic contributions of relative velocities, i.e. a sort of kinetic energy of diffusion. Such a contribution was expected to arise from fluctuations of microscopic kinetic energies of components.

4. EULERIAN DESCRIPTION

In the case of Eulerian description of motion the above derived relative acceleration has the form

$$(11) \quad \begin{aligned} \mathbf{a}_r &= \frac{\partial}{\partial t} (\mathbf{v}^F - \mathbf{v}^S) + (\mathbf{L}^F - \mathbf{L}^S) \mathbf{v}^S - \\ &\quad - (2 - \mathfrak{J}) \mathbf{L}^F (\mathbf{v}^F - \mathbf{v}^S) - \mathfrak{J} \mathbf{L}^S (\mathbf{v}^F - \mathbf{v}^S), \\ \mathbf{L}^S &= \text{grad } \mathbf{v}^S, \quad \mathbf{L}^F = \text{grad } \mathbf{v}^F. \end{aligned}$$

It is clear that one can use as well a relative acceleration with an additional contribution $\alpha^S \mathbf{D}^S (\mathbf{v}^F - \mathbf{v}^S) + \alpha^F \mathbf{D}^F (\mathbf{v}^F - \mathbf{v}^S)$, where α^S, α^F are arbitrary scalars and $\mathbf{D}^S, \mathbf{D}^F$ are symmetric parts of the velocity gradients, $\mathbf{L}^S, \mathbf{L}^F$. Situation is similar to this appearing in the definition of objective time derivatives of the classical continuum mechanics.

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Hysteresis in ferroelectric materials

HARSIMAR SAHOTA

Ferroelectric materials exhibit a complex behaviour upon electric and mechanical loading. Their change of polarization and length is accompanied by hysteresis. Remarkable is the so-called butterfly loop characterizing the strain due to an applied electric field. As these materials are technically used as sensors and actuators, it seems important to be able to simulate these hysteretic phenomena. Here a one-dimensional model is proposed, capable of describing the qualitative behaviour of widely used perovskite-type ferroelectric materials.

Microscopically Motivated Constitutive Model of Ferroelectric Piezoceramics

MARC KAMLAH

(joint work with Zhenggui Wang, Dayu Zhou, Jörg Büttner)

In most cases, piezoelectric coupling is utilized by means of ferroelectric ceramics. Besides linear electromechanical coupling, these materials exhibit a variety of strong non-linear electromechanical coupling phenomena and hysteresis effects. The microscopic origin for this behavior lies in the specific symmetry properties of the unit cell and the capability to switch the orientation of domains of unit cells under strong electromechanical loads.

In literature, a commonly accepted framework for the macroscopic constitutive modeling of piezoceramic materials has been established, which relies on the additive decomposition of strains and polarization into reversible and irreversible parts. In the current model, the orientation state of domains is represented by stepwise approximated orientation distribution functions (ODF). Assuming a polar tetragonal unit cell, the macroscopic strain and polarization states are derived from these ODF by integration. In this way, the parameters representing the approximate ODF become physically motivated internal variables of the constitutive model [1].

The ordinary differential equations (ODE) of the rate dependent formulation of the model turn out to be stiff. In an investigation of the numerical integration of the system of ODE, the performance of the explicit Dormand-Prince scheme and the implicit Radau IIa scheme were compared, both with a convergence order of 5. An automatic step size control based on a local error was employed. The average step size of the implicit code turned to be almost 50 times larger than that of the explicit code [2].

The von Mises-type switching criterion used in the present and other models fails to describe that the critical compressive stress for the onset of switching is almost identical for poled and unpoled specimens. In a recent investigation, the onset of switching was investigated for proportional loading paths in the plane of electric field and coaxial compressive stress. By means of an offset method the starting of switching was detected from the strain measurements. A preliminary analysis revealed that the resulting switching points are represented rather by a Tresca/Drucker-Prager-type yield condition than by the von Mises criterion [3].

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Incompressible ionized fluid mixtures

TOMÁŠ ROUBÍČEK

A model of a fluid mixture of L incompressible chemically reacting charged constituents in Prigogine's description (i.e. balancing barycentric impulse but not impulses of particular constituents) was presented. Under the volume-additivity hypothesis and some other simplifying assumptions, the model combines the Navier-Stokes equation (1a) for the barycentric velocity v and the pressure p with the Nernst-Planck equation with advection (1b) for the concentrations c_ℓ of the particular mutually reacting constituents, the Poisson equation (1d) for self-induced quasistatic electric field ϕ , and the heat equation (1c) for temperature θ :

$$(1a) \quad \varrho \frac{\partial v}{\partial t} + \varrho(v \cdot \nabla)v - \nu \Delta v + \nabla p = \sum_{\ell=1}^L c_\ell f_\ell, \quad \operatorname{div} v = 0,$$

$$(1b) \quad \frac{\partial c_\ell}{\partial t} + \operatorname{div}(j_\ell + c_\ell v) = r_\ell(c_1, \dots, c_L, \theta), \quad \ell = 1, \dots, L,$$

$$(1c) \quad \varepsilon \Delta \phi = -q, \quad q = \sum_{\ell=1}^L e_\ell c_\ell,$$

$$(1d) \quad c_v \frac{\partial \theta}{\partial t} - \operatorname{div}(\kappa \nabla \theta + c_v v \theta) = \nu |\nabla v|^2 + \sum_{\ell=1}^L (f_\ell \cdot j_\ell - h_\ell(\theta) r_\ell(c_1, \dots, c_L, \theta))$$

where the Lorenz force and the phenomenological diffusive fluxes are considered as

$$(2) \quad f_\ell = -e_\ell \nabla \phi, \quad j_\ell = -d \nabla c_\ell - m c_\ell (e_\ell - q) \nabla \phi,$$

and where $\varrho > 0$ is the mass density both of the mixture and of the particular constituents, $\nu > 0$ is viscosity, e_ℓ valence (i.e. electric charge) of the ℓ -constituent, $\varepsilon > 0$ permittivity, $r_\ell(c_1, \dots, c_L, \theta)$ production rate of the ℓ -constituent by chemical reactions, $h_\ell(\theta)$ the enthalpy contained in the ℓ th constituent, $d > 0$ a diffusion coefficient, $m > 0$ a mobility coefficients, $c_v > 0$ a specific heat, and $\kappa > 0$ a heat conductivity coefficient.

Thermodynamics of this model is based on the energy balance, which sounds essentially as

$$(3) \quad \frac{d}{dt} \left(\int_{\Omega} \left(\underbrace{\frac{\varrho}{2} |v|^2}_{\text{kinetic energy}} + \underbrace{\frac{\varepsilon}{2} |\nabla \phi|^2}_{\text{electrostatic energy}} + \underbrace{c_v \theta}_{\text{internal energy}} \right) dx \right) - \int_{\Omega} \underbrace{\sum_{\ell=1}^L h_\ell(\theta) r_\ell(c, \theta)}_{\text{heat production via chemical reactions}} dx = 0$$

in an isolated system on a fixed domain Ω , i.e. no contribution from (here nonspecified) boundary conditions on $\partial\Omega$ is counted. The heat sources on the right-hand side of (1d), i.e.

$$(4) \quad \nu |\nabla v|^2 + d \nabla q \cdot \nabla \phi + \sum_{\ell=1}^L m c_\ell e_\ell^2 |\nabla \phi|^2 - m q^2 |\nabla \phi|^2 - \sum_{\ell=1}^L h_\ell r_\ell,$$

includes respectively the heat production due to viscosity, the power of the electric current arising by due to the diffusion flux which may have a local Peltier-type cooling effects although globally it cannot cool because of

$$(5) \quad \int_{\Omega} d\nabla q \cdot \nabla \phi \, dx = \varepsilon \int_{\Omega} -d\nabla(\Delta\phi) \cdot \nabla \phi \, dx \varepsilon \int_{\Omega} d|\Delta\phi|^2 \, dx \geq 0,$$

the further term in (4) is Joule's heat produced by the electric currents which always dominates the 4th term (i.e. the rate of cooling by a "reaction force" which balances the volume-additivity constraint $\sum_{\ell=1}^L c_{\ell} = 1$), while the 5th term is the heat produced or consumed by chemical reactions. The entropy balance based on Helmholtz' free energy $\frac{\varepsilon}{2}|\nabla\phi|^2 - c_v\theta\ln(\theta)$ can formally be established for spatially isothermal processes or electroneutral processes; the violation of Claussius-Duhem inequality for such an entropy may be due to incompressible simplification or due to certain inconsistency of Prigogine concept with electrostatics.

Existence of a weak solution to an initial-boundary-value problem for (1)–(2) can be shown in two special cases: the Stokes' one (i.e. the convective term $\varrho(v \cdot \nabla)v$ in (1a) neglected) or the isothermal one (i.e. the heat equation (1d) neglected). A Kakutani fixed-point argument can be used for both cases [1]. The Galerkin approach has been used for the latter case in [2]. In both cases, fine design of the scheme is necessary, using a certain correcting retract of concentrations from the linear manifold $\sum_{\ell=1}^L c_{\ell} = 1$ to its subset of non-negative c_{ℓ} 's, which eventually may be forgotten in the fixed point or in the limit, respectively. The a-priori L^{∞} -bound of retracted concentrations facilitates the whole procedure. In the isothermal case, a (very) weak solution has then the quality: $c_{\ell} \in L^{\infty}((0, T) \times \Omega) \cap L^2([0, T]; W^{1,2}(\Omega))$ with $\frac{\partial}{\partial t}c_{\ell} \in L^{4/3}([0, T]; W^{1,2}(\Omega)^*)$, and $v \in L^2([0, T]; W^{1,2}(\Omega; \mathbb{R}^3)) \cap L^{\infty}([0, T]; L^2(\Omega; \mathbb{R}^3))$ with the acceleration $\frac{\partial}{\partial t}v \in L^{4/3}([0, T]; W_{0,\text{DIV}}^{1,2}(\Omega; \mathbb{R}^3)^*)$ where the notation $W_{0,\text{DIV}}^{1,2}$ indicates divergence-free functions, and eventually $\phi \in L^{\infty}([0, T]; W^{1,2}(\Omega))$. In case the Stokes the convective term in (1a) is neglected, a regularity for the Poisson and the Stokes equations yields additionally $\phi \in L^{\infty}([0, T]; W^{2,2}(\Omega))$ and $v \in L^6([0, T]; W^{2,6}(\Omega; \mathbb{R}^3))$, and then $\theta \in L^2([0, T]; W^{1,2}(\Omega)) \cap L^{\infty}([0, T]; L^2(\Omega))$ with $\frac{\partial}{\partial t}\theta \in L^2([0, T]; W^{1,2}(\Omega)^*)$.

The application of the model is limited to situations where the magnetic field can be neglected and where all constituents are incompressible and have equal mechanical response (i.e. have the same mobility d and diffusivity m as well as the "reaction force" $q\nabla\phi$ in (2) which balances the volume-additivity constraint $\sum_{\ell=1}^L c_{\ell} = 1$ influence them equally). *Acknowledgement:* The work was supported also by

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A kinematic model for defective crystals

CESARE DAVINI

The interest for the theory of crystalline defects in mechanics moves from the common believe that defects and their evolution under loads play a central role in the inelastic behaviour of materials, so that a good model of defects can be the basis for a satisfactory macroscopic theory of plasticity.

The subject started being studied in the 50's and had most relevant contributors such as Kondo, Bilby, Eshelby and Köner, who were the founders of the so called *continuum theory of defects in solids*. The continuum theory of defects became then very popular in the 60 and 70's, especially under the effect of an influential paper by Noll [6], which had the merit of reformulating the problem in terms of modern concepts of Continuum Mechanics and the defect, on the other end, of strengthening a trend towards abstraction that proved to be rather sterile.

The object of this seminar is a continuum model for defective crystals I proposed in [1] and successively elaborated together with G. P. Parry in a series of articles [2, 3, 4]. We introduced on a systematic basis old and new tensor densities of defects and provided a finite list of them which was shown to be exhaustive in a well precise sense. A distinctive feature of the approach is that the changes of states which preserve these densities, when they are kinematically possible, turn out to be slips in certain surfaces associated with crystal geometry. So the basic mechanism of plasticity emerges naturally from abstract ideas which neither anticipate, nor involve the kinematics of particular types of crystal defects. In spite of these encouraging results, a mechanical theory of the model has not been fully elaborated yet. Hereafter my purpose is to present the main ideas underneath and to sketch some of the difficulties that obstruct the construction of a mechanics for the model.

A crystal body is described by means of three lattice vectors \mathbf{d}_a and mass density ρ , regarded as the primitive quantities of the model. Its *state* Σ is then specified by the assignment of these quantities throughout the region \mathcal{B} macroscopically occupied by the body at the present time: $\Sigma = \{\mathbf{d}_a(\cdot), \rho(\cdot), \mathcal{B}\}$.

The lattice vectors are imagined to characterize the behaviour of the crystal at macroscopic scale and are envisaged as averages, on a mesoscale, of vectors representing interatomic positions. They are supposed to vary smoothly on macroscopic scale, as is also the density function. So, even if defects occur at the atomistic scale and there is no recognizable lattice of atoms, it is assumed that these averages are observable at a coarser (mesoscopic) level. The evolution of defects is then supposed to account for the observed discrepancy between the macroscopic deformation and the behavior of the \mathbf{d}_a .

A central premise of the model is that the material particles which comprise the crystal are indistinguishable, and that the knowledge of the lattice vector and density fields is all we need in order to determined the mechanical response of the material. Accordingly, a Eulerian point of view is adopted and no special role is attached to the notion of a reference configuration and to the macroscopic deformation gradient. A stand point that is unusual in solid mechanics, but that

seems to me quite natural in describing the mechanics of a system of identical particles interacting with one another.

This view carries over a major difficulty in the analysis because, since all fields are assumed to be smooth, there is no natural notion of defectiveness in the model. In fact, there is a way to introduce such a notion rather neatly on the basis of the following requirements: *a)* that it be compatible with “Taylor’s conjecture” that the evolution of defects reflects into discrepancy of mesoscopic and macroscopic behavior; *b)* that it mimic the atomistic notion that defects can be counted and add up over the union of regions in physical space.

Let $\Sigma \rightarrow \Sigma^*$, with

$$\chi : \mathbf{x} \rightarrow \mathbf{x}^* \quad \text{and} \quad \Sigma^* = \{\mathbf{d}_a^*(\cdot), \rho^*(\cdot), \mathcal{B}^* = \chi(\mathcal{B})\},$$

be a change of state. A priori there is no reason for assuming a connection between the new fields and the old ones under the macroscopic transplacement $\chi(\cdot)$, because lattice vectors and transplacements reflect observations at different scales. On the other hand, we may adopt Taylor’s view and assume that defectiveness stay unchanged under the class of state changes defined by

$$\mathbf{d}_a^*(\mathbf{x}^*) = \mathbf{F}(\mathbf{x}) \mathbf{d}_a(\mathbf{x}) \quad \text{with} \quad \mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{x}^*}{\partial \mathbf{x}}.$$

These state changes are called *elastic deformations*.

It is natural to look for features of the fields \mathbf{d}_a and ρ that are left unchanged under elastic deformations and to regard them as descriptive of defectiveness. Furthermore, accepting the prejudice that defectiveness is to be additive over subregions of \mathcal{B} , we are lead to search for integral forms, defined over the parts of \mathcal{B} , which are left invariant under the elastic deformations. That is, we search for integrals of the form

$$(1) \quad \oint_c \mathbf{g} \cdot d\mathbf{x}, \quad \int_S \mathbf{g} \cdot \mathbf{n} dS, \quad \int_V g dV,$$

with c , S , V circuits, surfaces and volumes in \mathcal{B} respectively, such that

$$\oint_{c^*} \mathbf{g}^* \cdot d\mathbf{x}^* = \oint_c \mathbf{g} \cdot d\mathbf{x} \quad \forall c \subset \mathcal{B}, \quad \text{with } c^* = \chi(c),$$

etc..

These integrals are called *elastic invariants*.

With an eye towards a constitutive theory of local type, here the integrands are assumed of the form

$$g = g(\mathbf{d}_a(\mathbf{x}), \nabla \mathbf{d}_a(\mathbf{x}), \nabla^2 \mathbf{d}_a(\mathbf{x}), \dots, \rho(\mathbf{x}), \nabla \rho(\mathbf{x}), \nabla^2 \rho(\mathbf{x}), \dots),$$

and we intend that

$$g^* = g(\mathbf{d}_a^*(\mathbf{x}^*), \nabla^* \mathbf{d}_a^*(\mathbf{x}^*), \nabla^{*2} \mathbf{d}_a^*(\mathbf{x}^*), \dots, \rho^*(\mathbf{x}^*), \nabla^* \rho^*(\mathbf{x}^*), \nabla^{*2} \rho^*(\mathbf{x}^*), \dots).$$

It is possible to characterize the invariants in a rather systematic way. In fact to construct an infinite list of them. Disregarding the density field, for simplicity,

and proceeding towards invariants involving gradients of increasing order, among the first few invariants we find

$$\oint_c \mathbf{d}^a \cdot d\mathbf{x}, \quad \int_S \mathbf{d}^a \times \mathbf{d}^b \cdot \mathbf{n} dS, \quad \int_{\mathcal{V}} \mathbf{d}^1 \cdot \mathbf{d}^2 \times \mathbf{d}^3 dV,$$

and

$$\int_{\mathcal{V}} \beta^{ab} dV, \quad \text{with } \beta^{ab} = \nabla \times \mathbf{d}^a \cdot \mathbf{d}^b,$$

where the \mathbf{d}^a are the dual lattice vectors defined by

$$\mathbf{d}^a \cdot \mathbf{d}_b = \delta_b^a \quad (\delta_b^a \text{ Kronecker symbol}).$$

The interpretation of these invariants is suggestive: the first two respectively measure the unbalance of lattice step and lattice faces of type a and ab , respectively, when going around c and \mathcal{S} ; the third one counts the total number of lattice cells contained in \mathcal{V} . The invariants $\oint_c \mathbf{d}^a \cdot d\mathbf{x}$ are the well known Burgers integrals of the continuum theory of dislocations; the other two, on the contrary, are new. The β^{ab} are the lattice components of Nie's dislocation density tensor.

Applying Stokes or Gauss theorem, one finds *defect densities* associated with these integrals. For instance, some of them are: $b^a = \nabla \times \mathbf{d}^a$, $n = \mathbf{d}^1 \cdot \mathbf{d}^2 \times \mathbf{d}^3$ and β^{ab} , with β^{ab} naturally distinguished into symmetric and skew symmetric parts. One of the most important results of the analysis is that, although an infinite list of integral invariants and related defect densities can be constructed, the following (finite) list

$$(2) \quad b^a, \beta^{ab}, n, \nabla(\beta^{ab}/n) \times \mathbf{d}^c, \nabla(\nabla(\beta^{ab}/n) \cdot \mathbf{d}_c) \times \mathbf{d}^d$$

is a functional basis for the elastic invariants of the class described by (1). This means that for two states (defined over the same \mathcal{B} , for brevity) that share the previous defect density fields all the invariants of the form (1) match.

It is reasonable to ask whether the invariants really capture the essence of defectiveness as we perceive that notion on a more intuitive basis. To answer that question one has to understand whether there are non elastic deformations that also leave the integral invariant unchanged and how they look like. Such deformations were called *neutral*. We showed that neutral deformations may occur, but only for very special states, where a certain uniformity along planes or lines in \mathcal{B} takes place. In those cases, neutral deformations correspond to slips and rearrangements within those subsets, so evoking familiar mechanisms of crystal plasticity. More specifically, it turns out that

Theorem 1. *Let Σ and Σ' be two neutrally related states defined over the same \mathcal{B} (for brevity). Then, at each $\mathbf{x} \in \mathcal{B}$, there are neighborhoods $\mathcal{N}(\mathbf{x})$ and $\mathcal{N}'(\mathbf{x})$ and an elastic deformation χ_{el} that maps $\Sigma|_{\mathcal{N}}$ onto $\Sigma'|_{\mathcal{N}'}$.*

Since the character of locality is a rather primitive requisite of defectiveness, it would be difficult to think that defectiveness around any point \mathbf{x} in the two states be different, according to any more intuitive notion of defectiveness. It also follows from the previous theorem that

Theorem 2 (Completeness of the densities). *If the densities of list (2) match in two states Σ and Σ' over the same \mathcal{B} (for brevity), then all invariants of the form (1) match.*

The previous results follow from a detailed analysis of the uniqueness of solution of a (overdetermined) system of partial differential equations, see [2, 3, 4]. With different words, the studied problem is analogous to one considered by Cartan in his work on the “moving frames”, and it would be possible to derive the main results above from a theorem of Fröbenius, see [7].

In spite of a kinematic framework that seems fairly well settled, a satisfactory mechanical theory has not been developed so far. The most severe obstruction comes from the renounce to using the Cauchy-Born hypothesis in order to connect micro and macro deformations. This, which is a founding assumption of the model and that is in my opinion the natural way to describe, though at macroscopic level, the behavior of a discrete system of particles, is a quite unusual point of view in solid mechanics. And the way how to manage the consequences of this assumption in mechanics has not been clarified. Some attempts to study mechanical problems in simple instances have been done by Fonseca and Parry [5], who considered the equilibrium under loading of a crystal body without defects, but able to undergo rearrangements. They studied it in a variational context and imagined to penalize rearrangements in order to prevent their occurrence. Unfortunately, their analysis shows that no penalization avoids that the crystal can stand only hydrostatic stresses at equilibrium. A disappointing result that is not new to researchers in the field, but that indicates that more understanding of the model is to be provided.

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Macroscopic models for rarefied gas flows

HENNING STRUCHTRUP

This talk presents an overview on classical and recent methods to derive macroscopic transport equations to model rarefied gas flows, and a critical examination of the resulting models.

It is well known that the Navier-Stokes-Fourier equations cannot describe rarefaction effects in gases, which appear in processes with Knudsen numbers $Kn > 0.05$ (say). A variety of extended models can be derived from the Boltzmann equation—the basic equation to accurately describe rarefied gases—which aim at describing rarefied gas flows at least approximately. The best known among these are the Burnett and super-Burnett equations, derived by means of the Chapman-Enskog method [1], and Grad's 13 moment equations, which follow from Grad's moment method [2, 3].

Burnett and super-Burnett equations suffer from instabilities in transient processes [4], and several modifications have been suggested to stabilize the equations, including the augmented Burnett equations [5], and the regularized Burnett equations [6]. Both sets of equations improve the Burnett equations only partly, and are difficult to justify from the Boltzmann equation.

Grad's moment equations [2, 3] exhibit unphysical sub-shocks in shock structures at large Mach numbers [7, 8], and so far could not be related to the rarefaction of the gas, i.e. to the Knudsen number. Since the equations can be derived for an arbitrary number of variables, a criterion that relates the number of moments to the Knudsen number was missing.

A technique for the regularization of Grad's 13 moment equations was presented recently, producing the regularized 13 moment equations (R13) which guarantee smooth shock structures [9, 10]. However, this method can be used for any number of moments, and thus leaves the question of how many moments need to be considered unanswered.

A recent approach within the framework of extended thermodynamics, termed as "consistently ordered extended thermodynamics" (COET), gave a first answer to this question [11]. However, COET yields certain sets of Grad-type equations, and thus does not remove the problem of discontinuous shocks. Moreover, the method was only applied to simple molecular interaction models—Maxwell molecules or the BGK model—and it is not clear how the method should be generalized to more realistic interaction models.

Elements of the COET method were blended with some new ideas to design a method for deriving transport equations for rarefied gases from the Boltzmann equation within higher orders of the Knudsen number [12, 13]. The method focuses on the order of magnitude of the moments of the phase density, and the order of accuracy of the transport equations, both measured in powers of the Knudsen number. This "order of magnitude method" was developed up to the third order for the special case of Maxwell molecules [12], and it yields the Euler equations at zeroth order, the Navier-Stokes-Fourier equations at second order, Grad's 13

moment equations (with omission of a non-linear term) at second order, and the regularization of these (R13) at third order.

The order of magnitude method was also used to derive a set of 13 moment equations for arbitrary molecular interaction potentials [13]. It was shown that the new set of equations is accurate to second order, while Grad's original 13 moment equations are of second order accuracy only for Maxwell molecules and BGK models.

An important feature of the order of magnitude method is that the equations of any order are stable, other than in the Chapman-Enskog method, where the second and third order approximations—Burnett and super-Burnett equations—are unstable. The latter can be extracted from the derived equations by means of the Chapman-Enskog method. It follows that the new method includes Burnett type and Grad type equations and the regularization of the latter, and thus forms a common umbrella for all known theories for macroscopic transport equations in rarefied gases.

A difficult issue in the theory of macroscopic transport equations is the problem to ascribe boundary conditions for higher moments, which are not controlled in experiments [14]. For better understanding of this issue, the Couette flow problem was split into two sub-problems, which concern the solution in the bulk and Knudsen boundary layers.

The bulk solution requires only jump and slip boundary conditions for temperature and velocity, which are well-known, and thus the bulk solution can be obtained readily.

The ability of macroscopic equations to provide Knudsen layer solutions was discussed in Refs. [9, 15], where it was also shown that additional boundary conditions are required. Alternatively, one can fit the amplitudes of the Knudsen layer solutions to accurate numerical solutions of the Boltzmann equation. Superpositions of the bulk solutions with fitted Knudsen layer solutions can then be compared to the Boltzmann solutions. The results presented here indicate that only the R13 equations can quantitatively describe Knudsen boundary layers, while the Burnett and super-Burnett equations fail.

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Riemann problem in Extended Thermodynamics

TOMMASO RUGGERI

The Riemann problem for a system of balance laws is still an often question. We study the problem with particular attention to the asymptotic behaviour. Moreover we study also the solutions when the initial data are a "perturbation" of the Riemann data proving results similar to the one of T. P. Liu obtained in the case of conservation laws. Applications are presented in the core of Extended Thermodynamics for rarefied gases and in the case of a binary mixture of Euler fluids.

Thermodynamics of Elastic Solids up to the Melting Point

MASARU SUGIYAMA

Thermodynamic quantities of linear isotropic elastic solids, that is, elastic constants, specific heats, coefficients of thermal expansion and Grüneisen parameters are estimated and discussed on the basis of the linearized macroscopic basic equations proposed recently by the author's group [1-4]. The equations were derived from a nonequilibrium statistical-mechanical model for crystalline lattices with a continuum approximation. The equations take microscopic thermal vibration of constituent atoms into account explicitly, and they are valid in a wide temperature range including the melting point as a limiting case. Some new coefficients relating thermal vibrations of constituent atoms to temperature variation and strain are also studied in detail in both isothermal and adiabatic processes. Peculiar temperature dependences of these quantities near the melting point are found. With these analytical results, Helmholtz free energy for elastic solids is formulated explicitly up to the melting point. The present model can be applied to many nonequilibrium phenomena in solids near the melting point, for an example, wave propagation phenomena [3,5].

The present analysis also reveals that we can analyze mechanical phenomena in solids separately from the thermal effect within the linear theory. This fact has, of course, long been taken granted implicitly in the usual theory of elasticity. However this is, in general, no longer true in a nonlinear model such as the one proposed by the author's group.

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Kinetics of lattice phase transitions

ANNA VAINCHTEIN

(joint work with Lev Truskinovsky)

A characteristic feature of martensitic phase transitions in active materials is the energy dissipation leading to experimentally observed hysteresis. The dissipation is due to propagating phase boundaries which can be represented at the continuum level as surfaces of discontinuity. Classical elastodynamics admits nonzero dissipation on moving discontinuities but provides no information about its origin and kinetics. The arbitrariness of the rate of dissipation is known to be the cause of nonuniqueness in problems involving subsonic phase boundaries. The ambiguity at the macroscale reflects the failure of the continuum theory to describe phenomena inside the narrow transition fronts where the dissipation actually takes place.

To illustrate this fundamental problem, it suffices to consider longitudinal deformation of a homogeneous elastic bar with a unit cross-section and initial density ρ . Let $u(x, t)$ be the displacement of a reference point x at time t , and let $\phi(u_x)$ denote the elastic energy density of the bar. The balances of linear momentum is

$$(1) \quad \rho u_{tt} = (\sigma(u_x))_x,$$

where $\sigma(u_x) \equiv \phi'(u_x)$ is the stress-strain relation. Although in classical elastodynamics equation (1) is hyperbolic, the hyperbolicity condition $\sigma'(u_x) > 0$ is violated for martensitic materials with non-monotone stress-strain curve $\sigma(u_x)$

[3]. This makes the initial-value problem associated with the mixed-type equation (1) ill-posed. In particular, it leads to the appearance of non-evolutionary or undercompressed discontinuities (kinks, or subsonic phase boundaries). The parameters of these discontinuities satisfy both the classical Rankine-Hugoniot jump conditions and the entropy inequality $\mathcal{R} = GV \geq 0$, where V is the velocity of the discontinuity and $G = \llbracket \phi \rrbracket - \{\sigma\} \llbracket u_x \rrbracket$ is the configurational (driving) force. Here $\llbracket \cdot \rrbracket$ denotes the jump across the kink and $\{\sigma\} \equiv (\sigma_+ + \sigma_-)/2$. However, the kinks fail to satisfy the Lax condition $c_+ < V < c_-$, where c_{\pm} are the sound velocities in front of and behind the moving kink. One way to remedy the resulting instability is to supplement the Rankine-Hugoniot jump conditions by a *kinetic relation* $G = G(V)$ specifying the dependence of the configurational force on the velocity of the phase boundary [1, 5].

We obtain the closing kinetic relation by replacing the continuum model with its natural discrete prototype. The procedure can be viewed as either regularization by discretization or as a physically motivated account of underlying discrete (atomic or mesoscopic) microstructure. We consider fully inertial dynamics of a one-dimensional lattice with bi-stable nearest-neighbor interactions. Our work complements previous analyses of the local discrete problem by including an arbitrary number of harmonic long-range interactions. Following some previous work in plasticity [2] and fracture [4], we assume piecewise linear interactions between nearest neighbors (NN), which allows us to construct an explicit traveling wave solution describing an isolated phase boundary.

Although the model is Hamiltonian at the microscale, it generates a nontrivial macroscopic kinetic relation. The dissipation at the macrolevel is due to the nonlinearity-induced radiation of lattice waves carrying energy away from the propagating front. We demonstrate the degeneracy of the local NN model and analyze in detail the nonlocal model accounting for next-to-nearest neighbor (NNN) interactions. We show that nonlocality affects the size of lattice trapping: as NNN bonds become stronger, the trapping region reduces in size in terms of stresses. However, it increases in terms of driving forces, which emphasizes an important difference between the real and configurational forces. In addition to enlarging the domain of existence of steady state regimes with high-frequency radiation in both directions, sufficiently strong coupling significantly alters the mobility curves near the sonic speeds. Contrary to the simplest local theory, strongly nonlocal model produces multivalued kinetic relations with several admissible branches and rich variety of configurations of emitted lattice waves. Although we have not studied stability of the constructed traveling waves, the fact that the dissipation potential associated with these dynamic regimes is locally convex suggests that they may be infinitesimally stable. The details of this analysis are described in [6, 7].

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Energy Transport in Periodic Lattices

ALEXANDER MIELKE

This work concerns the problem of deriving macroscopic, continuum models from microscopic, discrete systems. More precisely, we start from the atomistic model of a crystal which consists of periodically spaced mass points whose motion is governed by linear interaction forces. The aim is to provide exact mathematical links between this microscopic system and its macroscopic limits arising when the atomic distance ε tends to 0. In fact, we will obtain one equation which describes the evolution of the macroscopic displacement and another equation which allows to calculate the transport of energy in the crystal.

The analysis of discrete systems attracted a lot of attention over the last decades. However, most work is restricted to the one-dimensional oscillator chain

$$(1) \quad \ddot{x}_\gamma = \sum_{\alpha=1}^M \left(V'_\alpha(x_{\gamma+\alpha} - x_\gamma) - V'_\alpha(x_\gamma - x_{\gamma-\alpha}) \right) - W'(x_\gamma), \quad \gamma \in \mathbb{Z},$$

where V_α is the interaction potential with the neighbors at distance α and W the on-site potential which couples the atoms to a background. Rigorous justifications of macroscopic PDEs for the oscillator chain are provided in [3, 10] where the Korteweg–de Vries equation is obtained as the macroscopic model for describing the evolution of long-wave interactions. In [4, 2] the nonlinear Schrödinger equation or the quasilinear Whitham equation is derived to describe macroscopic evolution of pulses which modulate a periodic pattern on the microscopic scale.

The purpose of this work aims in a similar direction, however it is different in the methodology. We restrict ourselves completely to the linear setting and thus are free to generalize in many other directions. First we are able to study very general lattices in any dimension. Second we are able to investigate the dynamics of solutions for much more general initial data. Finally our results will be more detailed. In a certain sense our work is closer to the statistical approaches for harmonic lattices, see e.g. [9]. In particular, the latter work also derives a energy transport equation. However, we stay fully in the deterministic setting.

To be more specific, consider a d -dimensional Bravais lattice $\Gamma \subset \mathbb{R}^d$ and the infinite set of coupled ODEs

$$(2) \quad M\ddot{x}_\gamma = - \sum_{\beta \in \Gamma} A_{\beta\gamma} x_{\gamma+\beta} \quad \text{for } \gamma \in \Gamma,$$

which will be our basic microscopic system. Here the vector $x_\gamma \in \mathbb{R}^m$ may contain the displacement of several atoms in the cell associated with the lattice point γ . The mass matrix $M \in \mathbb{R}^{m \times m}$ is symmetric and positive definite and the interaction matrices satisfy $A_\beta = A_{-\beta}^\top$ and $\|A_\beta\| \leq Ce^{-b|\beta|}$.

An essential feature of such harmonic lattices is the presence of many traveling wave solutions in the form

$$(3) \quad x_\gamma(t) = e^{i(\theta \cdot \gamma + \omega t)} \Phi \quad \text{where } \theta \in \mathbb{R}_*^d \text{ and } (\mathbb{A}(\theta) - \omega^2 M)\Phi = 0,$$

where the symbol matrix $\mathbb{A}(\theta)$ reads $\mathbb{A}(\theta) = \sum_{\beta \in \Gamma} e^{i\theta \cdot \beta} A_\beta \in \mathbb{C}^{m \times m}$. We always impose the basic assumption of stability in the form $\mathbb{A}(\theta) \geq 0$ for all $\theta \in \mathbb{R}_*^d$.

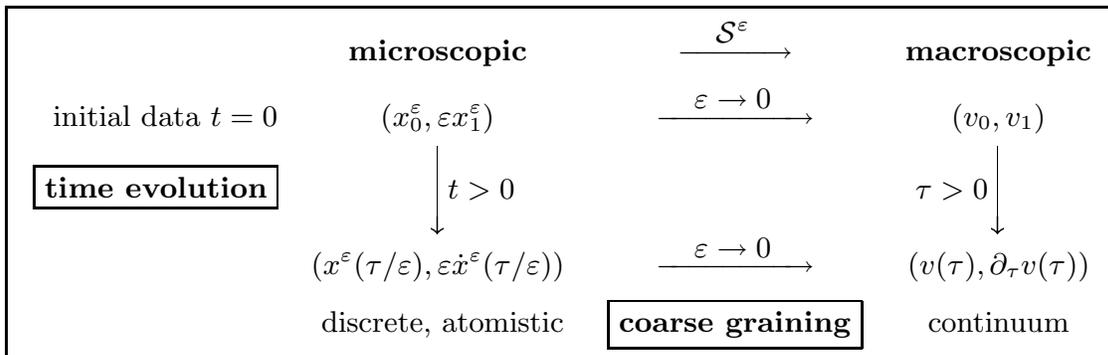
First we derive a continuum-limit equation for the displacements in the case of the atomic distance ε tending to 0. Denoting by $V \subset \mathbb{R}^m$ the kernel of $\mathbb{A}(0)$ we construct the polynomial $\mathbb{Q} : V \rightarrow \mathbb{R}$ which is homogeneous of degree 2 and satisfies

$$\langle \mathbb{Q}(\eta)v, v \rangle = \inf \left\{ \liminf_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^2} \langle \mathbb{A}(\varepsilon\eta)w_\varepsilon, w_\varepsilon \rangle \mid \lim_{\varepsilon \rightarrow 0} w_\varepsilon = v \right\}.$$

Then, \mathbb{Q} defines the second order differential operator $\mathcal{A}_0 = \mathbb{Q}(i\nabla_y)$. We obtain the partial differential equation

$$(4) \quad M_V \frac{\partial^2}{\partial \tau^2} v + \mathcal{A}_0 v = 0 \quad \text{for } (\tau, y) \in \mathbb{R} \times \mathbb{R}^d,$$

where M_V is the restriction of M to V . Eqn. (4) includes the equations of linear elastodynamics and is a macroscopic limit equation for (2) in an exact mathematical sense: the limit $\varepsilon \rightarrow 0$ commutes with the time evolution, i.e., the following abstract diagram commutes.



Second, we study the transport of energy which does along the group velocity of the microscopic wave pattern. The classical WKB method (cf. [1]) shows that macroscopically modulated pulses of the harmonic traveling waves (3) propagate with the group velocity $c_{\text{group}} = \nabla_\theta \omega(\theta)$. For studying macroscopic energy transport we have to know how much energy is located at which point, in which wave length and in which energy band, i.e., in which of the m eigenpairs (ω, Φ) associated with θ .

For this purpose it is convenient to reformulate the Fourier transformed version of (2) as a first order system in diagonal form:

$$(5) \quad \frac{\partial}{\partial \tau} \widehat{U}(\tau, \eta) = \frac{i}{\varepsilon} \widehat{\Omega}(\varepsilon\eta) \widehat{U}(\tau, \eta), \quad \text{with } \widehat{\Omega}(\theta) = \text{diag}(\omega_1(\theta), \dots, \omega_{2m}(\theta)),$$

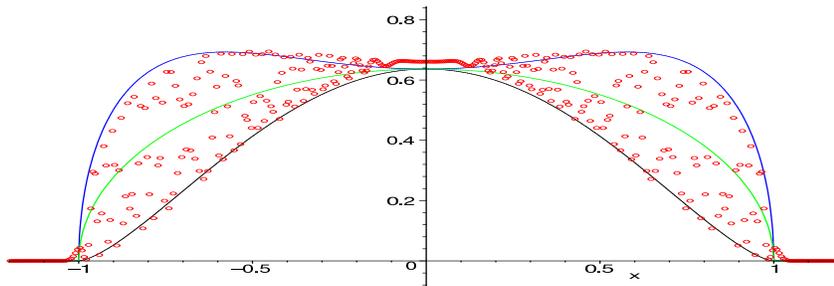
where $\omega_{j+m} = -\omega_j$ for $j = 1, \dots, m$. The relevant tools for studying the macroscopic spatial distribution of microscopic oscillations is the Wigner transform W^ε and its limit, the matrix-valued Wigner measure μ , see [8, 5, 6]. We derive the energy transport equation for the diagonal entries μ_{jj} , $j = 1, \dots, 2m$ of the Wigner measure:

$$(6) \quad \partial_\tau \mu_{jj}(\tau, y, \theta) = \widetilde{\nabla}_\theta \omega_j(\theta) \partial_y \mu(\tau, y, \theta) \quad \text{for } (\tau, y, \theta) \in \mathbb{R} \times \mathbb{R}^d \times \widetilde{\mathbb{T}}.$$

The energy density $e(\tau, y)$ at a macroscopic point y at time τ is then recovered via

$$e(\tau, y) = \int_{\widetilde{\mathbb{T}}} \sum_{j=1}^{2m} \mu_{jj}(\tau, y, d\theta).$$

The tilde \sim indicates that a certain continuous continuation of $\nabla_\theta \omega_j(\theta)$ has to be chosen, since in general the functions are only Lipschitz continuous but not differentiable. In fact, in the point $\theta = 0$ one always has such a singularity, since $\omega_1(\theta)$ behaves like $|\theta|$. Thus, we are able to maintain certain features of the H-measure, see [11].



Discrete energy distribution in the linear oscillator chain and its continuum limit

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Boundary conditions in Extended Thermodynamics and Applications

ELVIRA BARBERA

The problem of the boundary conditions has been discussed in the context of Extended Thermodynamics [1]. In all the versions of Extended Thermodynamics and in particular in Consistently Ordered Extended Thermodynamics [2] one needs more boundary values than one can assign and control.

In the talk a new proposal [3] for the determination of the remaining boundary values has been presented. It is based on the idea that the gas is subject to thermal fluctuations and so are the fields including their boundary values. The fluctuations are very rapid, so that the gas may not adjust to their fluctuating boundary values. Therefore one may assume that the gas adjusts the not controllable boundary values to the mean values of the fluctuating boundary data.

The mean values may be calculated by employing the Boltzmann formula $S = k \ln W$. This proposal has been applied to a simple problem of stationary heat conduction in a gas at rest [3], to the study of the stationary plane Couette flow [4] and to a problem of heat conduction in cylindrical symmetry [5].

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Light scattering in Extended Thermodynamics

DANIEL REITEBUCH

Ordinary thermodynamics works very well for most engineering problems. Only in some extreme cases it fails, especially if steep gradients or rapidly changing fields play a role. In such a case, a better theory is needed, for instance extended

thermodynamics. In the consistently ordered version of extended thermodynamics (COET), the moments are ordered in terms of the steepness of gradients. The light scattering experiment is a very good test for the theories of extended thermodynamics. This test is applied to the COET as well as to the previously existing extended thermodynamics. Both theories converge in the sense that they describe the light scattering spectrum perfectly if the number of variables considered is high enough. But in order to obtain a result with a given accuracy, the COET needs less variables than the theories of the previously existing extended thermodynamics. Therefore we may say that the new theory is more efficient, albeit only slightly.

The entropy principle for fluid interfaces

HANS WILHELM ALT

We present a systematic theory for interfaces of fluids based on the entropy principle of rational thermodynamics. It differs substantially from existing presentations of interface problems and provides several new aspects. We focus on viscous fluids, whereas [4, 5, 7, 9] deal with solids, and [6] concentrates on gases.

First of all, balance laws including interfaces are formulated as distributional equations. In this version they attain the simplest and also their natural form. Moreover, the covariant structure of these basic laws always is present. The traditional presentation (for example, in the books [3, 4, 5, 6, 7, 8]) uses the formulation with test volumes instead of test functions. For our distributional formulation only one additional notation is needed:

If Γ is an evolving d -dimensional surface (that is $\Gamma_t := \{x; (t, x) \in \Gamma\}$ has dimension d , $0 \leq d \leq n$, $n = 3$ the physical space dimension), let μ_Γ be the measure $L^1 \otimes H^d$ restricted on Γ , as distribution

$$\langle \zeta, \mu_\Gamma \rangle := \int_{\mathbb{R}} \int_{\Gamma_t} \zeta(t, x) dH^d(x) dL^1(t).$$

Let Ω^1 and Ω^2 be two time-space domains Ω^1 and Ω^2 occupied by two fluids (or bulk materials) separated by an evolving interface Γ . We consider the following distributional balance laws for mass, momentum, and (total) energy:

$$\partial_t(\rho^m \mu_{\Omega^m}) + \operatorname{div}(\rho^m v^m \mu_{\Omega^m}) = \tau^m \mu_\Gamma \quad \text{for } m = 1, 2,$$

$$\begin{aligned} & \partial_t(\sum_m \rho^m v^m \mu_{\Omega^m}) \\ & + \operatorname{div}(\sum_m (\rho^m v^m \otimes v^m + \Pi^m) \mu_{\Omega^m} + \Pi^s \mu_\Gamma) \\ & = \sum_m \mathbf{f}^m \mu_{\Omega^m} + \mathbf{f}^s \mu_\Gamma, \end{aligned}$$

$$\begin{aligned} & \partial_t(\sum_m e^m \mu_{\Omega^m} + e^s \mu_\Gamma) \\ & + \operatorname{div}(\sum_m (e^m v^m + \Pi^{mT} v^m + q^m) \mu_{\Omega^m} + \Phi^s \mu_\Gamma) \\ & = \sum_m v^m \bullet \mathbf{f}^m \mu_{\Omega^m} + g^s \mu_\Gamma, \end{aligned}$$

with $\tau^1 + \tau^2 = 0$. Here Π^m are the fluid pressure tensors and Π^s is the surface pressure tensor.

Secondly, we apply the entropy principle in the strict sense of rational thermodynamics (as in [6]). This means, that the entropy production is not prescribed, its structure is a result of the exploitation of the principle. For interface problems the entropy principle has to be understood in distributional sense. It postulates, that for a given class of physical processes there exists a (distributional) entropy H and a (distributional) entropy flux Ψ satisfying

$$\partial_t H + \operatorname{div} \Psi \geq 0$$

in distributional sense. Moreover, as a postulate, this equation transforms between observers as a scalar equation. This implies (in classical continuum physics), that H is a distributional objective scalar. In isothermal descriptions, the entropy inequality reduces to a free energy inequality. In either case such an inequality is the basic ingredient for mathematical theories. For the above system the entropy identity is of the form

$$\begin{aligned} & \partial_t (\sum_m \eta^m \mu_{\Omega^m} + \eta^s \mu_{\Gamma}) \\ & + \operatorname{div} (\sum_m (\eta^m v^m + \frac{1}{\theta^m} q^m) \mu_{\Omega^m} + \Psi^s \mu_{\Gamma}) \\ & = \sum_m h^m \mu_{\Omega^m} + h^s \mu_{\Gamma}, \end{aligned}$$

and the entropy principle is equivalent to $h^m \geq 0$ in Ω^m and $h^s \geq 0$ on Γ .

Thirdly, the principle of objectivity (principle of frame indifference) is used systematically. It is used not only for constitutive functions, but also for balance laws. We give a formulation of this principle for distributional balance laws, therefore it applies to interface systems of the above form. This distributional formulation implies important structural properties of interfacial terms. For the momentum equation the conclusion simply is, that Π^s is an objective tensor and \mathbf{f}^s an objective vector.

We apply the entropy principle, under constitutive assumptions, for interface systems and study its consequences. We are mainly interested in constitutive restrictions for surface tension. For the exploitation of the entropy principle the local version of the balance laws are used, which consists of differential equations in Ω^m and Γ , as well as constraints for the surface flux terms. For the momentum equation this constraint is $\Pi^s \nu = 0$. The standard constitutive relation for Π^s is $\Pi^s = \hat{\Pi}^s(a, \nu)$, where a consists of objective scalars not depending on ν . If Π^s is symmetric, objectivity implies

$$\Pi^s = -\sigma(\operatorname{Id} - \nu \otimes \nu), \quad \sigma = \hat{\sigma}(a),$$

where σ is surface tension.

Consequences of the entropy principle depend on the particular physical situation. We treat several well known classes of processes like slip boundary conditions, mean curvature flow, liquid drops, Marangoni convection, and diffusion on a fluid interface. In the talk we explained the following cases (\mathbf{v}_{Γ} and κ_{Γ} denote the velocity and the curvature vector of Γ):

Mean curvature flow. Ω^1 and Ω^2 are two phases of an isothermal rigid body with a phase transition rate τ^1 depending on ν_1 and κ_Γ . Then the free energy inequality leads to

$$\mathbf{v}_\Gamma \bullet \nu_1 = \hat{\tau}^1(\kappa_\Gamma \bullet \nu_1) \quad \text{with } \sigma \hat{\tau}^1(s) \cdot s \geq 0.$$

Within a concept for fluids the unisotropic case is not treated.

Surfactant on a fluid interface. Ω^1 is an isothermal fluid, Ω^2 treated as vacuum, and γ the density of a diffusive surfactant on Γ with mass conservation

$$\partial_t(\gamma \mu_\Gamma) + \text{div}((\gamma v^1 + q^s) \mu_\Gamma) = 0.$$

Let the constitutive relations be $q^s = \hat{q}^s(\gamma, \rho^1, v^1, \nabla^\Gamma \gamma)$, $\Pi^s = \hat{\Pi}^s(\gamma, \rho^1, v^1, \mathbf{v}_\Gamma, \nu_1)$, and $f^s = \hat{f}^s(\gamma, \rho^1, v^1)$ for the surface free energy. Objectivity reduces this to

$$\begin{aligned} q^s &= -a \nabla^\Gamma \gamma, & a &= \hat{a}(\gamma, \rho^1, |\nabla^\Gamma \gamma|), \\ \sigma &= \hat{\sigma}(\gamma, \rho), & f^s &= \hat{f}^s(\gamma, \rho). \end{aligned}$$

Then the free energy inequality implies, that f^s and σ are independent of ρ^1 . Moreover, a “surface Gibbs relation”

$$\sigma = f^s - \gamma f'_{\gamma}$$

has to be satisfied and (for $a > 0$) the inequality $f'_{\gamma\gamma} \geq 0$. This implies, that σ is decreasing in γ .

Marangoni convection. Ω^1 and Ω^2 are two fluids We consider the above system with $\tau^1 = 0$ and $\mathbf{f}^s = 0$, assuming that absolute temperature and velocity are continuous at Γ . We allow additional constitutive dependence on θ and compute the surface entropy production h^s . For fluxes $\Phi^s = e^s v + \Pi^{sT} v$, $\Psi^s = \eta^s v$, and vanishing surface energy production g^s this is

$$\begin{aligned} h^s &= (\partial_t + v \bullet \nabla) \eta^s - \frac{1}{\theta} (\partial_t + v \bullet \nabla) e^s \\ &\quad + \left(\eta^s - \frac{1}{\theta} e^s + \frac{1}{\theta} \sigma \right) \text{div}^\Gamma v, \end{aligned}$$

where σ , e^s , η^s depend on (ρ^1, ρ^2, θ) . Then the entropy principle implies independence on ρ^1, ρ^2 , and

$$\sigma = e^s - \theta \eta^s, \quad \sigma_{,\theta} = -\eta^s.$$

As a result, surface tension may depend on intrinsic quantities on the interface. Moreover, generically it always depends on temperature, but it is independent of other fluid quantities.

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Modelling and simulation of phase transformation processes

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A general class of non-isothermal phase-field models for crystal growth and solidification in complex alloy systems is presented. The new model is capable to simultaneously describe the diffusion processes of multiple components, the phase transitions between multiple phases and the development of the temperature field. Both, surface energy and kinetic anisotropy is incorporated in the new phase-field model. We introduce our 3D parallel simulator that is based on a finite difference discretization including effective adaptive strategies and multigrid methods to reduce computation time and memory usage. In particular, the three types of partial differential equations for the concentrations, the phase fields and the temperature are solved on three different numerical meshes with a different grid fineness and with different time discretizations. Taking advantage of the multi-obstacle potential, the phase-field equations are only solved in regions of the phase boundaries. The parallelization is realized for distributed as well as shared memory computer architectures using MPI libraries and OpenMP concepts. Applying the new computer model, we show a variety of simulated crystal structures in 3D for different types of crystalline and smooth anisotropies. Simulation results are presented showing the motion of multiple interfaces (phase and grain boundaries) in complex alloy systems. In particular, phenomena such as anisotropic curvature flow, grain growth and coarsening are described. Another special emphasis of the computations is modelling of phase transformations and solidification processes in multi-component alloys. The specific phase diagrams of the alloys are incorporated in the diffuse interface model via the free energies. Within this context, complex ternary eutectic structures are simulated in 2D and 3D. The effect of anisotropy on eutectic structures, such as the growth of tilted eutectic lamellae, and the formation of eutectic grains at different length scales: the grain structure on a larger scale and the eutectic substructure on a smaller scale are investigated. The stability of ternary eutectic growth fronts for different recombination of the three solid phases and the characteristic spacings depending on process conditions are analyzed by iterative computations. The numerical results are supported by a generalized Jackson-Hunt theory for ternary eutectics. Finally, we apply the phase-field simulations to model complex multiscale growth of eutectic colonies resulting from small amounts of ternary impurities.

Structural forces in liquid crystals

EPIFANIO G. VIRGA

Nematic liquid crystals are complex anisotropic fluids with variable molecular ordering. When rigid particles are submerged in these fluids, the molecular ordering is affected by the interactions of the molecules with the particles boundaries. In turn, the change in ordering can result in an elastic distortion that induces a displacement or a rotation of the particle to relax the excess of energy associated with the distorting interactions. This essentially explains the ability of nematic liquid crystals to exert forces and torques on submerged particles. Actually, when the submerged particles prescribe the nematic molecules to be aligned in the direction orthogonal to their boundaries (homeotropic anchoring), the intervening liquid crystal mediates an interaction between the particles that prompts them to acquire regular equilibrium patterns. Despite the significance of these interactions, only few direct measurements have so far become available. Theoretically, when the particles size becomes comparable to the length scale over which the molecular ordering is organized, typically between a few and ten nanometers, the conventional description of the molecular organization in terms of the nematic director \mathbf{n} becomes insufficient, and both forces and torques exerted on a submerged particle must be evaluated within the Landau-de Gennes theory, which employs a full second-rank tensor \mathbf{Q} to describe the local molecular ordering. This lecture concerns forces and torques exerted on bodies submerged in a nematic liquid crystal and forces and torques transmitted through the liquid crystal from one body to another. Particular emphasis will be laid on the effect of structural ordering changes onto the behaviour of these elementary mechanical actions.

Modeling the light-induced deformation in liquid crystal elastomers

YONGZHONG HUO

Liquid crystal elastomers (LCE) are polymeric materials with mesogenic liquid crystalline moieties. The cross-linked polymer network exhibits an entropy-induced elastic behavior. The liquid crystalline moieties show an order-disorder phase transition upon cooling-heating processes. At a higher temperature, the moieties are randomly oriented so the elastomer is in the disordered phase, called the isotropic phase. Upon cooling to a critical temperature, the liquid crystalline moieties align themselves to certain preferred orientations so to transform to the liquid crystal (LC) phase. The most commonly observed liquid crystal phase is the nematic phase with the moieties aligned to a direction \mathbf{n} . Then, the critical temperature is called the nematic-isotropic (NI) transition temperature T_{NI} . The phase transition is reversible upon heating.

As a typical soft matter, the orientations of the liquid crystalline molecules of LCEs can be changed rather easily by small external and internal disturbances such as temperatures, stresses, electric fields and impurities. Experiments have shown that even a very small amount of the molecules in a LCE sample are photochromic,

the orientations of the whole liquid crystalline molecules can be modulated by light[1]. In particular, if the photochromic molecules can change their shape from a LC phase stabilizing rod-like to a destabilizing bended shape upon light irradiation, the nematic-isotropic transition temperature T_{ni} can be raised by light.

For cross-linked LC polymers, the orientation change of the LC molecules can induce a macroscopic shape change at the NI transition through the interaction of the LC molecules with the backbone. Thus, they can be used as an active materials in various application fields such as artificial muscle technology [2]. Especially, large deformations up to 20% can be induced by light for LCEs with photochromic molecules as first discovered in [3]. The mechanism of such a light-induced deformation consists of the following steps,

- (1) UV-induced trans-cis isomerization of azo(N=N) bonds such that the photosensitive mesogenic molecules change from a rod-like shape to a bended shape. This process can be modeled by a rate equation as

$$\frac{dN_{cis}}{dt} = p^{t \rightarrow c}(T)N_{trans} - p^{c \rightarrow t}(T)N_{cis} + \alpha N_{trans}I(t)$$

- (2) The kinked mesogenic molecules act as impurities so to reduce the NI transition temperature through

$$T_{ni} = T_{ni}^{\circ}(1 - N_{cis}/N_{meso}^{\circ})^{\epsilon}$$

- (3) The lowered T_{ni} will result in a reduction of the order parameter Q of the nematic phase since

$$Q = A(T_{ni} - T)^{\xi}$$

- (4) The stress free length of a LCE sample is a decrease function of the order parameter Q as

$$\lambda_{\circ} = \left(\frac{l_{\perp}^{\circ}(Q_{\circ})}{l_{\parallel}^{\circ}(Q_{\circ})} \frac{l_{\parallel}(Q)}{l_{\perp}(Q)} \right)^{1/3}$$

From a thermodynamical point of view, it is desired to know how the above light irradiation changes the internal energy, the entropy and the stress-strain relations of LCEs. The total Helmholtz free energy should consist of the following terms

$$F_{total} = F_{\circ}(T) + F_{nl}(Q, T) + F_{el}(\lambda, Q_{\circ}, Q, T) + F_{is}(N_{cis}, T)$$

where F_{\circ} is the free energy of the undistorted stress-free isropic phase. F_{nl} is the nematic free energy that can be taken as the Landau-de Gennes expansion of the order parameter Q . F_{el} is the entropic-induced elastic free energy and F_{is} is the free energy change due to the trans-cis isomerization. The internal energy, the entropy and the stress-strain relations of LCEs can be then calculated from above free energy function. The temperature equation can be deduced from the energy balance by considering the radiation energy flux due to light as

$$C_p \frac{dT}{dt} = -c(T - T_e) + \sigma_{ij} \frac{\partial v_i}{\partial x_j} + \Delta H_{ni} \frac{dQ}{dt} + \left[-\frac{dN_{cis}}{dt} + \alpha N_{trans}I(t) \right] \Delta U_{tc}$$

Consider a LCE sample with photochromic molecules under constant UV light for an extensive time, all the rate terms approach zero. Thus, we would have the final temperature at the end state as

$$T_{\infty} = T_e + \alpha N_{trans}^{\infty} I_o \Delta U_{tc} / c \approx T_e + p^{c \rightarrow t}(T_{\infty}) N_{cis}^{\infty} \Delta U_{tc} / c$$

and the total fraction of the cis isomers

$$x_{cis}^{\infty} = \frac{N_{cis}^{\infty}}{N_{azo}} = \frac{p^{t \rightarrow c}(T_{\infty}) + \alpha I_o}{p^{c \rightarrow t}(T_{\infty}) + p^{t \rightarrow c}(T_{\infty}) + \alpha I_o}$$

Therefore, the sample should be hotter than its environment due to the energy of light irradiation even there is little directly heating of the UV light. Rather the sample is heated by the relaxation of the higher energy cis isomer back to the trans form. Such a self-heating effect has been indeed observed in experiment [4].

The above thermodynamical considerations can serve as the basis for a more systematical thermodynamical model of the light active behavior in certain LCEs.

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On the superposition of generalized plane strain on anti-plane shear deformations in elastomeric devices

GIUSEPPE SACCOMANDI

In this talk we investigate the basic issues that arise when generalized plane strain deformations are superimposed on anti-plane shear deformations in isotropic incompressible hyperelastic materials. This problem arise from the observation of what happens in some technical devices made of elastomeric materials like bush mounting or bump stoppers. First of all attention is devoted to a subclass of such materials for which the strain-energy density depends only on the first invariant of the strain tensor. The governing equations of equilibrium are a coupled system of three nonlinear partial differential equations for three displacement fields. It is shown that, for general plane domains, this system decouples the plane and anti-plane displacements only for the case of a neo-Hookean material. Even in this case, the stress field involves coupling of both deformations. For generalized neo-Hookean materials, universal relations may be used in some situations to uncouple the governing equations. Then we discuss why some of the results are also valid for inhomogeneous materials, in dynamical setting and more general constitutive settings as quasistatic viscoelasticity. These results explains why in many

elastomeric devices failure is more complex than we use to idealize using idealized pictures of the deformations where, for example, axial shear is assumed uncoupled from rotational shear. For this reason qualitative estimates of the magnitude of in-plane deformations is an important aspect for a careful mechanical design of such devices.

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Atomistic simulation of an elastic-plastic body with shape memory

OLIVER KASTNER

In a previous work a two-dimensional, molecular dynamic model was presented, which is capable to represent the characteristics of austenite \leftrightarrow martensite lattice transitions in metallic solids, see [1], [2]. These transitions appear under the influence of load/strain and/or temperature control, as it was explained by use of numerical experiments concerning small crystallites: Quadratic lattices are stable at high temperature and in absence of a load, while sheared, rhombic-shaped lattices are stable at low temperature, or upon loading. Due to the obvious similarities to shape memory alloys, the quadratic phase is called the austenite, and the sheared phases are called variants of martensite. By use of thermodynamic arguments, the phase stability of such small crystallites was investigated. It turned out, that even 41-atomic crystallites exhibit temperature-dependent, non-monotonic stress-strain relations and thus non-convex free energy functions.

The work presented on the meeting in 2004 uses this numerical model in order to simulate phase transitions in larger bodies upon loading at different temperatures. Therefore I refer to an idea used by I. Mueller & P. Villaggio [3] for modelling elastic-plastic bodies. The authors made use of bistable snapsprings, which exhibit two distinguished states, representing — in a way — two generic phases of the material points in a solid body. Mueller & Villaggio then derived the stress-strain relation of an elastic-plastic body by the superposition of the stress-strain curves of many snapsprings, which are exerted to the same load P . In detail this procedure is explained for 11 snapsprings.

In the present work the snapsprings are replaced by 2-dimensional crystallites consisting of 41 particles. 11 of these crystallites are placed in a chain, where two neighbored bodies are connected via corner atoms, shared by both respective bodies. Each individual crystallite may belong to three phases possible, austenite and two martensitic variants. Their phase stability is dependent on load AND temperature, and thus — in contrast to a body created by snapsprings — the

stress-strain relation of the entire chain is temperature-dependent too. In my talk I have presented numerical tensile tests on the crystallite chain at different temperature. Upon loading, phase transitions of the individual crystallites occur giving rise to the state of the overall chain: At low temperature the chain exerts quasiplastic stress-strain behaviour, while at high temperature the stress-strain behaviour is pseudoelastic.

The work presented is still in progress. It is aimed on the theoretical understanding of solid-solid phase transitions in atomic clusters and crystallites.

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